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Common assessment framework for HRA and ERA higher tier assessments including fish and drinking water and multi-species ERA via SSD, population-level ERA via IBM and food web vulnerability ERA

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Dissemination Level		
PU	Public	
PP	Restricted to other programme participants (including EC)	
RE	Restricted to a group specified by the consortium (including EC)	X
CO	Confidential, only for members of the consortium (including EC)	

I. Summary

We present an advanced framework for the assessment of ecotoxicological and human health risks from combined exposures to multiple chemicals in European surface waters. The framework presents several innovations: It implements a systematic tiering scheme that removes the uncertainties associated with widely used mixture risk assessment methods derived from concentration addition. We developed quantitative criteria that allow us to identify chemicals with high impacts on projected mixture risks, so-called drivers. For the first time, we delimit when the alternative concept of independent action can be introduced without stalling the assessment.

The framework was evaluated in a case study of measured water concentrations for ca. 300 pollutants in the Danube. It was highly effective in isolating sub-sets of chemicals for which the required toxicity data were available and for which mixture risks could be established with relative certainty.

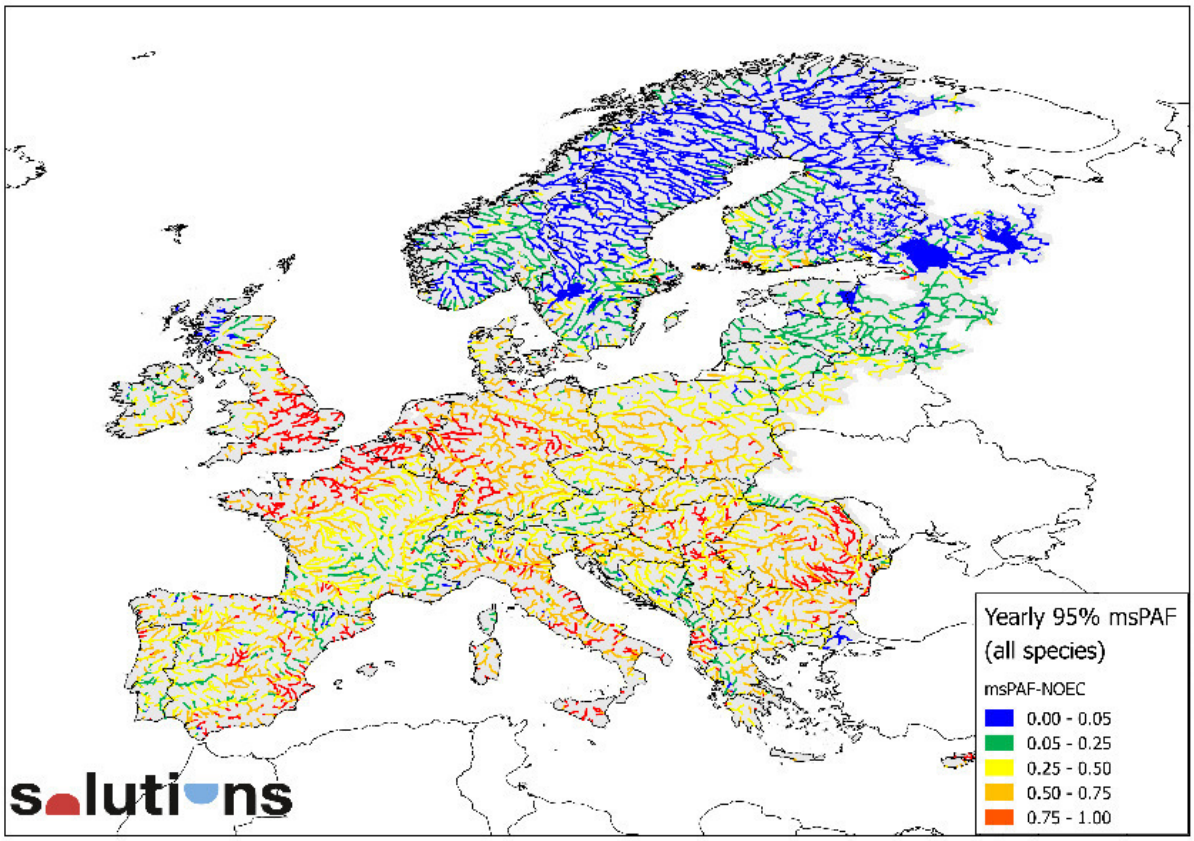
Taxa-specific tiered ecological and human mixture risk assessments for modelled concentrations of 1811 substances were carried out for the Danube, Rhine and Spanish river basins (SCARCE) on the basis of modelled water concentrations, as described in D 14.2. Across all river basins, the mixture risk assessments suggest that many river segments are insufficiently protected from chronic impacts on algal and daphnid communities. Many chemicals not currently regulated under the Water Framework Directive (WFD) were projected to drive the associated mixture risks. For almost the entire Rhine catchment, and Western and Southern parts of the Danube basin, the analysis did not identify concerns for chronic impacts on fish, at least not for the chemicals for which relevant chronic toxicity data were available. However, indications for impacts on fish are anticipated in Spanish basins, and in the Central parts of the Danube basin. In many river segments there were indications for concerns for the water quality when used directly as a resource for drinking water. The modelled mixture exposures that result from human consumption of fish caught in rivers exceeded levels judged to be safe.

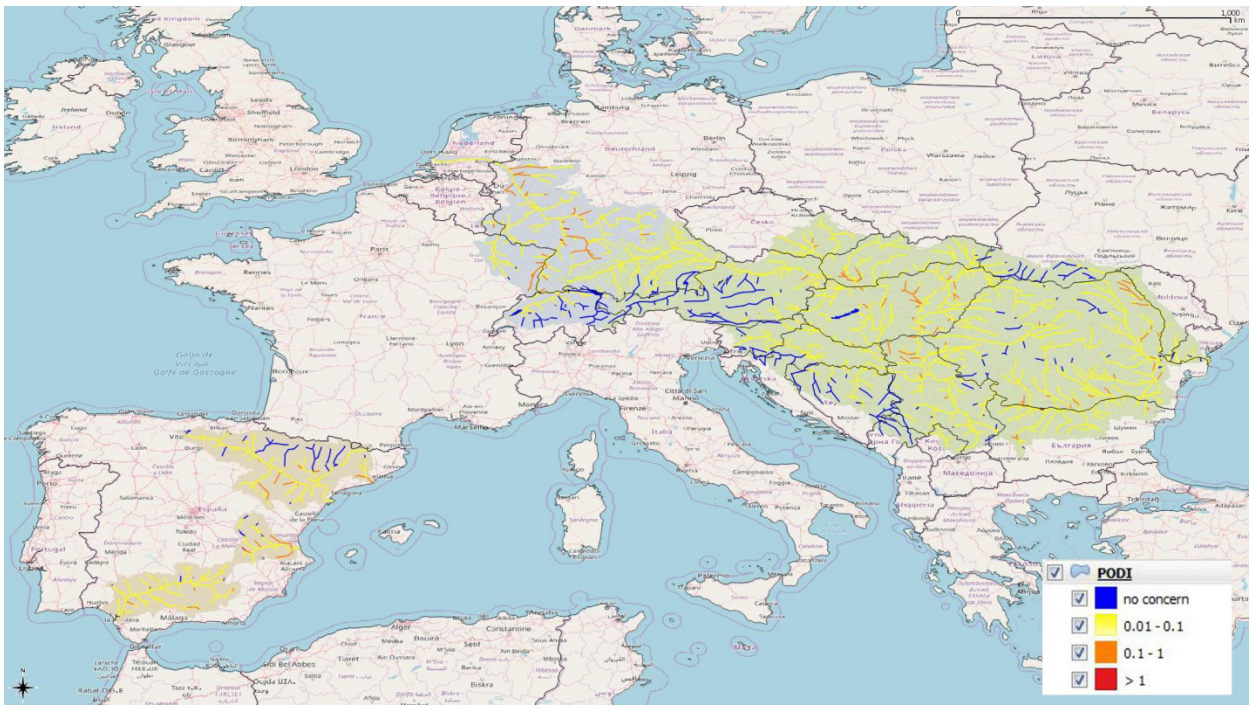
These assessments express mixture risks in terms of exceedances of combined exposure standards. Possible impacts in terms of effect magnitudes are not directly accessible through these analyses, but can be inferred indirectly. To better specify ecological consequences, we also conducted individual-based modelling which allows analyses of combined chemical impacts on life history parameters such as viability metrics. We also predicted impacts in terms of population development of selected sentinel species and effects on species assemblages by utilizing an extension of the Species Sensitivity Distribution concept to mixture risk analysis.

We demonstrated the utility of these approaches for water quality assessments at the European scale, where we considered 1,760 chemicals. The role of chemical pollution in compromising aquatic ecosystems could be specified, both in relation to the regulatory concept of sufficient protection (WFD and REACH) and to anticipated species loss (WFD ecological status classification).

Our results suggest that WFD protection goals cannot currently be realized for combined exposures to chemicals projected to occur in European water bodies.

II. Graphical summary





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V. Abbreviations and symbols

AbwV	Abwasserverordnung (German waste water ordinance)
ADI	acceptable daily intake
AF	assessment factor
AhR	aryl hydrocarbon receptor
AL	acceptable level
BEQ	bioanalytical equivalent concentration
BMD	benchmark dose
BP	biocidal products
BPR	Biocidal Product Regulation
BQE	biological quality element
c	concentration
CA	concentration addition
CAG	common assessment group
CBA	component-based approach
CEU	Council of the European Union
CLP	classification, labelling and packaging of substances and mixtures (Regulation (EC) 1272/2008)
CMR	carcinogenic, mutagenic, or toxic for reproduction
COMMPS	combined monitoring-based and modelling-based priority setting scheme (as established by Decision No 2455/2001/EC)
CRC	concentration response curve
CYP	cytochrom P450
D	deliverable
d	dose
DA	dose addition
DNEL	derived no effect level
DOW	description of work
DRC	dose response curve
E	effect
EBM	effect-based monitoring
EBMT	effect-based monitoring tool[1]
EBTV	effect-based trigger value[1]
EC	European Commission
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECHA	European Chemicals Agency
ECx	effect concentration for the effect x (e.g. EC50)
ED	endocrine disrupter
EDA	effect-directed analysis

[1] Other SOLUTIONS documents use the abbreviation *EBT* for '*effect-based tools*' (for monitoring), but in the literature cited in this report, the same abbreviation is also used for '*effect-based trigger value*'. For clarification and for avoiding any confusion, throughout this report the longer abbreviations EBMT and EBTV are used for *effect-based monitoring tools* and *effect-based trigger values*, respectively.

EDx	effect dose for the effect x (e.g. ED50)
EFSA	European Food Safety Authority
EFSA	European Food Safety Authority
EIFAC	European Inland Fisheries Advisory Commission (of the FAO)
EL	exposure level
Eq.	equation
EQS	environmental quality standard (as defined under the WFD)
ERA	environmental risk assessment
EU	European Union
F	concentration response function
F^{-1}	inverse concentration response function
FAO	Food and Agriculture Organization (of the UN)
FRAM	Center for future chemical risk assessment and management strategies at Gothenburg University (https://fram.gu.se/)
HBGV	health based guidance value
HC5	hazardous concentration for 5% of the species
HI	hazard index
HQ	hazard quotient
HRA	human health risk assessment
IA	independent action
ICPS	International Programme on Chemical Safety
ID	internal deliverable
JRC	Joint Research Centre of the European Commission
LOEL	lowest observed effect level
MAF	mixture assessment factor
MCR	maximum cumulative ratio (MCR) (as defined by Price et al. 2012)
MCS	multi-constituent substance (as defined under REACH)
MEC	measured environmental concentration
mix	mixture
MM	mixed model
MoA	mode of action
MRA	mixture risk assessment
MS	Member States (of the EU)
msPAF	multisubstance potentially affected fraction
NEC	no effect concentration
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NORMAN	Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances (http://www.norman-network.net/)
OECD	Organisation for Economic Co-operation and Development
p	proportion
PAH	polycyclic aromatic hydrocarbon
PBDE	poly-brominated diphenyl ether
PBT	persistent, bioaccumulative, and toxic
PEC	predicted environmental concentration
PICT	pollution induced community tolerance

PNEC	predicted no effect concentration
POD	point of departure (LOEL, NOAEL, or NOEC)
PODI	point of departure index
PPP	plant protection products
PPPR	plant protection products Regulation (Regulation (EC) No 1107/2009)
QO	quality objective
QS	quality standard
$QS_{biota, hh food}$	quality standards (concentration levels) for pollutants in fish which should not be exceeded in order to protect human health (as derived according to rules laid down in the Technical Guidance for Deriving Environmental Quality Standards (Common Implementation Strategy for the Water Framework Directive (2000/60/EC), Guidance Document No. 27, European Communities 2011)
QSAR	quantitative structure activity relationship
RBSP	river-basin specific pollutants (as defined under the WFD)
REACH	registration, evaluation, authorisation and restriction of chemicals (Regulation (EC) No 1907/2006)
REP	relative effect potency
RQ	risk quotient
RV	regulatory or reference value
SCCS	Scientific Committee on Consumer Safety (of the EC)
SCENIHR	Scientific Committee on Emerging and Newly Identified Health Risks (of the EC)
SCHER	Scientific Committee on Health and Environmental Risks (of the EC)
SSD	species sensitivity distribution
SSG	single species group
STE	spatial, temporal and extent of PNEC exceedances approach (as proposed in Carvalho et al. 2016).
TEF	toxic equivalency factor
TEQ	toxic equivalent (dose or concentration)
TER	toxicity exposure ratio (as defined under the PPPR)
TG	technical guidance
TGD	technical guidance document
TTC	thresholds of Toxicological Concern
TU	toxic unit
TUS	toxic unit summation
UN	United Nations
US EPA	Unites States Environmental Protection Agency
UVCBs	materials of unknown or variable composition, complex reaction products or biological materials (as defined under REACH)
WEA	whole effluent assessment
WFD	Water Framework Directive (Dir 2000/60/EC)
WG	working group
WHO	World Health Organization
WMA	whole mixture approach
WMT	whole mixture testing
WP	work package

1 Introduction

1.1 Aims and scope

This deliverable describes progress with developing concepts for ecotoxicological and human/mammalian mixture risk assessment, applicable to prospective and retrospective assessments in the context of management regarding chemical pollution. It operationalizes these concepts as building blocks for an integrated modelling framework, which can then be used for the prioritisation of emerging pollutants (chemical safety assessment context) and for the assessment of abatement options (environmental management context). The underpinning work was structured into two main tasks.

First, we developed a common tiered framework for human and ecological mixture risk assessment (MRA). This integration was achieved by basing the assessments on so-called risk quotients (RQ) familiar from single chemical risk assessment. RQ express the degree to which exposure levels deemed to be acceptable are exceeded and are available for both human and ecotoxicological assessments. However, estimations of the strength of an effect, or the probability with which an adverse effect may materialise, are not accessible through RQ. Such estimates require dose-response information for each of the chemical in the mixture, data not normally available for human health effects (except in epidemiological studies).

However, probabilistic assessments are achievable for ecological MRA. In the second task we therefore advanced ecological MRA, with the specific aim of increasing our predictive modelling capacity with respect to the characterisation of the magnitude of ecological risks of emerging compounds and the associated effects on species and species assemblages. The work has focused in particular on the Biological Quality Elements as distinguished in the WFD, and on sensitive species and ecosystem functioning.

1.2 The structure of this Deliverable report

Accordingly, this report is structured as follows, with some sections elaborating principles (Sections 2 and 3) and others with case studies to illustrate the use of concepts (Sections 4 – 7):

- We present the common ecotoxicological/human MRA framework (Section 2)
- We elaborate the details of defining parameters for fish accumulation modelling in the context of model-based identification of potential human health risks from fish consumption (Section 3)
- The utility of the framework is assessed in a case study of monitored pollutant water concentrations at a monitoring site in the Danube (JDS 3) (Section 4)
- Based on modelled water concentrations for the Danube, Rhine, Ebro, Guadalquivir, and Llobregat, we utilize the framework to anticipate mixture risks for the three taxa algae, daphnids and fish, and for human health via the exposure routes drinking water and fish consumption (Section5)
- We approach the quantification of expected impacts of combined exposures on aquatic species and species assemblages, by using individual-based modelling and species sensitivity distributions (Section 6)

- We illustrate toxic pressures on species assemblages for Europe-wide MRA on species assemblages (Section 7).

1.3 Key terms

'*Pollutants*' and the similar term '*contaminants*', '*mixtures*' and the related terms '*co-occurrence*', and '*co-exposure*' are key terms of this deliverable report. For the sake of clarity and to avoid any possible ambiguities, the understanding of these terms is explicitly defined in Deliverable D 2.1. Here, we adopt these definitions, as follows:

'*Pollutants*' vs '*contaminants*'

In the title of this deliverable (as it was contractually fixed in the DOW), the terms '*contaminants*' and '*contaminant mixtures*' are used in the general meaning of potentially harmful anthropogenic chemicals. Unfortunately, however, the terms could be misunderstood by readers familiar with the terminology of the European chemicals legislation. '*Contaminant*' is no term used in the WFD, but it has a specific legal meaning under EU food law[2] which was not intended to be the focal point here. To avoid such confusion, the term '*contaminant*' is replaced by '*pollutant*' throughout the text of this report. The term '*pollutant*' is used within the meaning of Article 2 of the WFD to denote substances introduced, "*as a result of human activity, (…) into the air, water or land which may be harmful to human health or the quality of aquatic ecosystems or terrestrial ecosystems directly depending on aquatic ecosystems (…)*[3]*.*" Most pollutants may also become food contaminants, but the considerations in this report are not limited to such pollutants which actually meet both definitions.

'*Mixtures*', '*co-occurrence*', and '*co-exposure*'

The term '*mixtures*' is used in this deliverable report to denote any '*co-occurrence*' of pollutants in environmental media, such as air, water, sediments, soil, or in biota, including the human body. Such '*co-occurrence*' may result from

(i) releases of chemicals that are legally registered as single substances on the EU market, but which are mixtures in themselves, so-called *multi-constituent substances* (MCS) and *materials of unknown or variable composition, complex reaction products or biological materials* (UVCBs) as defined under REACH[4],

(ii) releases of intentionally prepared mixtures that are placed on the EU market as chemical products (formerly denoted as *preparations*[5]),

[2] Under Council Regulation (EEC) No 315/93, '*contaminant*' "*means any substance not intentionally added to food which is present in such food as a result of the production (…), manufacture, processing, preparation, treatment, packing, packaging, transport or holding of such food, or as a result of environmental contamination*" (Article 1).

[3] In addition to human health and environmental safety, the WFD includes other protection goals such as damage to material property, or impairment of amenities and other legitimate uses of the environment, which are out of the scope of this deliverable report.

[4] Regulation (EC) No 1907/2006

[5] From 1 June 2015, Directive 1999/45/EC on dangerous preparations was repealed by Regulation (EC) 1272/2008 on classification, labelling and packaging of substances and mixtures (CLP) which entered into force in 2009. In the

(iii) joint releases of chemicals from a single source, such as a production, transportation, consumption, recycling, or waste (water) treatment process, or the

(iv) coincidental mixing of chemicals released from various sources and reaching environmental media, environmental organisms, and humans through multiple routes of exposure.

Type (i) and type (ii) mixtures, and partly also type (iii) mixtures are subject to regulations under different pieces of EU law (Kortenkamp, Backhaus, Faust 2009; EC 2012; Kienzler at al. 2014). Type (iv) mixtures represent the main focus of regulatory concern. In 2012, the Commission concluded that "*within the framework of EU legislation, there is no mechanism for a systematic, comprehensive and integrated assessment of mixture effects taking into account different routes of exposure and different product types"* (EC 2012). This continues to apply.

'*Co-exposure*' of organisms may result from the co-occurrence of pollutants in the same environmental medium, such as water or sediments, or from the simultaneous or sequential uptake of pollutants via different routes, such as food and water, resulting in a mixture of pollutants co-occurring in an environmental organism or in a human body. Considerations on resulting mixture risks in this paper are not confined to any of these specific phases of co-occurrence of pollutants but include them all.

In a very narrow sense, the assessment of the co-occurrence of substances in water, sediment, or biota may refer to a specific point in time only. In a somewhat wider sense, it may be understood to include all substances to which an organism may be exposed over a certain period of time simultaneously or sequentially. From a toxicological perspective, the very narrow understanding is inappropriate. Both simultaneous and sequential exposure must be taken into consideration, unless there is sufficient time between independent exposure events ensuring a full recovery of an individual or a population. The development of detailed rules for a regulatory distinction between simultaneous, sequential, and independent exposure events remains subject to future work. As a pragmatic and precautionary default assumption, sequential exposures during a certain time window may be assessed like simultaneous exposures. The definition of appropriate time windows may strongly depend on the generation time of a species and needs further research work.

Another key term is *risk*. In chemical safety assessment, risk assessments are made prospectively in a format that evaluates whether expected exposures under anticipated usage patterns of a chemical will exceed a well-defined exposure standard. On the basis of such standards regulatory decisions are made, e.g. about the chemical status of waters in the context of the WFD. A well-known example are PEC/PNEC-ratios (Predicted Environmental Concentration / Predicted No Effect Concentration), where values <1 suggest sufficient protection against adverse effects on human health and the environment. In environmental quality assessments, the same principle can be used, using the concept of sufficient protection, which in the WFD is implemented as the ratio of measured concentration over the EQS (Environmental Quality Standard), with values <1 again signalling sufficient protection. In addition, risk commonly pertains not only to the absence or presence of an exposure that exceeds an exposure standard, but may also relate to the exceedance of a certain effect magnitude (so that higher risk is interpreted as higher probability or magnitude of effects).

new legislation, the term "*preparation*" was replaced by "*mixture*". However, in other pieces of EU legislation, such as the PPPR, the term "*preparation*" continues to be used.

In this report, risk is understood as both, exceedance of exposure standards and exceedance of certain effect magnitudes. This is in alignment with the WFD and its daughter regulations where *risk* is understood as:

- the likelihood of failing the objective of the WFD (Annex II)
- exceedance of an EQS (that is: a “presence/absence of risk” metric in the sense of compliance testing)
- quantitative expression of likelihood and magnitude of expected impacts (that is: a “probability * magnitude” metric)

Accordingly, mixture risk assessment refers to all three aspects of the risk concept. The reader should be aware of these aspects.

2 An advanced framework for human and ecological mixture risk assessment – presentation of the concept

2.1 Introduction

Although humans and wildlife are exposed to large numbers of chemicals, risks from chemical mixtures were until recently regarded as negligible, as long as exposure to all individual chemicals stays below the levels judged to be acceptable for each chemical alone. However, evidence is accumulating that regulatory values for single chemicals do not protect against mixture risks (Kortenkamp and Faust 2018). This increases pressure on risk assessors to broaden the scope of their activities to include scenarios where chemicals in combination might pose risks to humans and wildlife.

Situations where humans and wildlife are exposed to mixtures of chemicals through a common environmental medium, such as water, present particular challenges to mixture risk assessment (MRA). Here, all receptors need to be protected from direct and indirect toxicity of chemical substances, as laid down in the European Water Framework Directive (WFD, EC 2000). Relevant exposure pathways include consumption of water as drinking water, consumption of fish caught in rivers or lakes and direct uptake of pollutants from the water column, feed or sediments by aquatic organisms. Although risk assessment approaches for single chemicals that deal with all these receptors are available (EC 2011), a coherent framework for conducting MRA which can successfully implement such overarching protection goals is missing.

Several approaches for conducting MRA have been developed in recent years, with an emphasis on either human MRA (e.g. Meek et al 2011, Moretto et al. 2017) or ecotoxicological MRA (Backhaus and Faust 2012). The only scheme with application to both human and ecotoxicological MRA has been presented by the European Scientific Committees on Consumer Safety, Health and Environmental Risks, and Emerging Risks (SCHER et al. 2012) and was further developed by Price et al. (2012). However, the details of how a common framework should deal with the differing protection goals in human and ecotoxicological risk assessment (emphasis on protection of the individual, and of functional integrity of ecosystems, respectively) and its implications for the choice of toxicity endpoints and assessment factors (AF) have yet to be worked out. Is there scope for integration that goes beyond common and consistent assessment principles, or are specific methods for human and ecotoxicological MRA more appropriate?

Common to all MRA frameworks is a component-based approach in which the expected combined toxicity is estimated on the basis of the toxicity of the mixture constituents and relevant exposure data. Methods derived from the mixture assessment concept of concentration (dose) addition (CA) are usually applied as a default. Implicit in these methods is a comparison between combined exposures and exposure standards deemed as signalling no or little concern. These methods allow good approximations of the combined toxicity of chemicals with similar modes of action (Kortenkamp et al. 2009), but may introduce errors when predicting the effects of combinations that produce common toxicity through a variety of mechanisms (Thrupp et al. 2017). Accordingly, the schemes developed by the European Scientific Committees (SCHER et al. 2012) and by Price et al. (2012) contain a decision point for the application of independent action (IA) which is the concept of choice for dissimilarly acting mixtures. Unlike CA however, the use of IA requires well-defined dose-response relationships for all mixture components (EFSA PPR Panel 2013b), a condition not normally met in regulatory practice. This

renders MRA based on IA impractical in most but the rarest of cases (but see Sections 6 and 7 for the quantitative approach developed for species assemblages, where this issue is approached from a different angle). How this constraint can be overcome without stalling the MRA has not been addressed.

All MRA frameworks also adopt the principle of a tiered analysis, where the assessment begins with often simplified worst case assumptions concerning exposures and hazards of chemicals in the mixture. Only if there are indications of risks (in the sense that combined exposures exceed certain standards) at lower tiers does the assessment continue with step-wise refinements at subsequent tiers. A significant strength of the available frameworks and decision trees (Meek et al. 2011, Price et al. 2012, Moretto et al. 2017) lies in their capability of identifying mixtures that do *not* pose concerns. However, for many situations, they may lead into prolonged scientific refinement loops that lose sight of the needs of regulatory decision making. To a large degree, this is due to a lack of generally agreed tiering rules and principles, which are often left open to accommodate a variety of problem formulations and assessment situations. As a result, there is no general agreement when to stop refinement and begin considering risk mitigation.

Price et al. (2012) introduced an innovation by proposing a classification scheme that differentiates types of mixtures according to various risk management approaches. Before addressing risks from exposure to the entire mixture, they suggested to focus risk management measures on those chemicals that pose concerns already individually. Similarly, Moretto et al. (2017) advocated a “gatekeeper” step in which commencement of an MRA is delayed until risks from chemicals that already present concerns singly are addressed. However, this ignores that the remainder of mixture components, although individually compliant with regulatory values (RV), may sum up to unacceptable levels, with the consequence that protection from mixture risks may not be achieved even when successful risk mitigation is achieved for single non-compliant substances. The idea of a “gatekeeper step” also ignores the fact that RV have not been defined for the vast majority of chemicals.

The substances that make up a multi-component mixture will usually not contribute in equal measure to the overall mixture risk. In many cases, only a few chemicals, so-called drivers, explain most of the mixture toxicity, although spatio-temporal variability in mixture composition may be high, and the dominant set of chemicals not necessarily constant (Vallotton and Price 2016). Applied to MRA, especially when dealing with large numbers of chemicals, the driver concept can potentially afford parsimonious use of resources and effective problem resolution as it allows focusing efforts on those chemicals in a mixture that matter most. However, its application requires quantitative criteria which have not yet been elaborated.

In this Deliverable, we present a new MRA framework and decision tree which introduces several conceptual innovations to overcome these difficulties. For the first time, we elaborate detailed tiering principles for the hazard assessment arm of the MRA. Application of CA requires the use of compound-specific toxicity data for identical endpoints and the same effect magnitudes. In regulatory practice however, these stringent data requirements can rarely be met. To deal with this difficulty while still enabling MRA, simplifications of CA were introduced, such as the Hazard Index (HI, Teuschler and Hertzberg 1995), the Point of Departure Index (PODI, Wilkinson et al. 2000) and the sum of PEC/PNEC ratios (Calamari and Vighi 1992). However, with these MRA methods, data from several toxicity endpoints and species are lumped together. Furthermore, the RVs that are used in the HI method or during the summation of PEC/PNEC ratios are often based on assessment factors (AF) of widely varying magnitude, from chemical to chemical. When used for assessing mixture risks, these simplifications may significantly distort the outcome. To improve the reliability of the assessment and its interpretation, we

introduce a tiering scheme that removes these distortions in a step-wise manner, with the aim of approximating the data requirements necessary to meet the scientific principles of CA as much as is possible, and another aim of providing a clear interpretation context. For the first time, we also define situations when the assessment concept of IA can be utilised without leading to paralysis of the MRA process due to irreconcilably high data demands. Finally, we develop decision rules that define situations where further refinement is unnecessary and when risk mitigation should be considered. We adopt the principle that MRA should neither be more, but also not less stringent that single chemical assessments.

Our ambition was to develop a framework that can cope with large numbers of chemicals (several hundred) and is sufficiently generic and flexible to accommodate data used in ecotoxicological as well as human risk assessment. As a relevant test case for the utility of our framework we chose exposure scenarios that relate to the final goal of protection of both human health and ecosystems functionality from the toxicity of water-borne chemicals, as enshrined in the European WFD. With large numbers of chemicals found in surface waters, the issue of missing data on toxicity or exposure levels for single chemicals is of concern. Omission of analytical non-detects or chemicals with unknown toxicity might bias the analysis towards the null, but the utility of methods for bridging these gaps in MRA (e.g. the concept of Thresholds of Toxicological Concern, TTC, read-across, QSAR, adopting limits of detection, LOD, for analytical non-detects in monitoring data) has not been explored. Additionally, for the ecotoxicological assessment, we also show how the MRAs can be further refined to express expected magnitudes of impacts (Sections 6 and 7).

Here, we elaborate the principles of the framework and explain its rationale and decision rules.

2.2 Problem formulation

The problem formulation step in MRA should analyse whether co-exposure to multiple chemicals is likely to occur within a relevant time frame and whether the chemicals that make up the mixture exposure scenario of interest are likely to exhibit common toxicities to the relevant receptors. If both these questions can be answered in the affirmative, an MRA should commence, regardless of whether one or a few chemicals in the combination exceed their regulatory values already on their own. Thus, our scheme does not contain a “gatekeeper” step as suggested by Solomon et al. (2016) and Moretto et al. (2017). Furthermore, there is no consideration of modes of actions at the problem formulation stage; this is reserved for higher tiers of the analysis.

2.3 Use of Concentration Addition (CA) as a default

In our framework, we adopt the mixture assessment concept of CA as a pragmatic and precautious default assumption. This is justified by a combination of four arguments (EFSA 2013b):

- Data requirements for a proper application of CA are much easier to fulfil than for IA or MM.
- Usually, the assumption of CA provides a more conservative estimate of mixture toxicity than the alternative assumption of IA.
- Synergistic effects that significantly exceed the CA expectation are exceptions and are rare with multi-component mixtures (Boobis et al. 2011, Cedergreen 2014).
- The CA assumption is conservative, but not vastly over-protective. Typically, the “prediction window” between CA and IA is not very wide. For realistic assessment situations it will rarely exceed an order of magnitude on the concentration axis. Typically, it is much smaller. Even with

mixtures composed of up to 100 chemicals, predicted effect concentrations of the mixture derived from CA and IA may usually differ by a factor of less than 5 only (Kortenkamp et al. 2012, Chapter 13.4). Considering that RVs such as EQS are just order-of-magnitude-estimates, overestimations by less than a factor of 5 may be acceptable for regulatory purposes.

At higher tiers of our framework we define conditions for the use of alternative concepts such as independent action or hybrid models of CA and IA.

2.4 The scientific principles of CA and the distorting influence of pragmatic simplifications of CA used in regulatory practice

The use of CA for calculations of the expected toxicity of combinations of chemicals requires that toxicity data for all single components are available. Ideally, the toxicity has to be determined for the same toxicity endpoint and effect magnitude, in the same test under identical experimental conditions. To achieve reliable predictions of mixture effects, well characterised dose-response relationships should be available for all mixture components.

Although these stringent data requirements can be realised in experimental studies, they are practically never met in regulatory practice. Simplifications of the scientific CA concept are intended to overcome this problem, such as the Point-of-Departure-Index (PODI, Wilkinson et al. 2000), the Hazard Index (HI, Teuschler and Hertzberg 1995) and for ecotoxicological assessments, the summation of PEC/PNEC ratios (Calamari and Vighi 1992) (**Table 2.1**). These approaches make use of the CA formula as a calculation rule, but they use input which does not fully comply with the strict requirements of the original concept but which may be easier available for regulators. This includes the use of values which (i) may have been derived by using different AFs, (ii) merge data for different endpoints or species, or (iii) are estimates of not exactly defined effect levels such as LOEL or NOAEL, as further detailed in the following.

Table 2.1: Regulatory approaches to mixture risk assessments derived from the concept of concentration addition

Approach	Assessment term	Notes
CA (DA) *Concentration (Dose) Addition*	$E(c_{mix}) \leq x$ if $\sum_{i=1}^{n} \frac{c_i}{ECx_i} \leq 1$	Procedure termed Toxic Unit Summation (TUS) $\frac{c_i}{ECx_i} = TU_i = ToxicUnit$
PODI *Point of Departure Index*	No significant effect if $\sum_{i=1}^{n} \frac{EL_i}{POD_i} \leq 1$	EL = Exposure Level POD = LOEL, NOAEL, NOEC
HI *Hazard Index*	No reason for concern if $\sum_{i=1}^{n} \frac{EL_i}{AL_i} \leq 1$	EL = Exposure Level AL = Acceptable Level = ADI, DNEL, …
PEC/PNEC Summation	No unacceptable risk if $\sum_{i=1}^{n} \frac{PEC_i}{PNEC_i} \leq 1$	PEC = Predicted Environmental Concentration PNEC = Predicted NEC

Instead of effect doses associated with the same effect magnitude, the PODI can also be based on estimates of so-called points of departure (PODs) as inputs, including no-observed-effect-concentrations (NOEC), no-observed-adverse effect-levels (NOAEL) or lowest observed effect levels (LOEL). The simplifying pragmatic assumption is that all these PODs refer to the same (low) effect magnitude, when in fact most NOAELs or NOECs correspond to effects of between 10 and 30% (Moore and Caux 1997). To blur matters further, PODs may refer to different toxicity endpoints determined in different test species from the same species group. Thus, in comparison to the use of CA in experimental studies, the PODI introduces two sources of uncertainty for the prediction of mixture risks: it mixes inexactly defined effect sizes and different toxicity endpoints as well as species (although from similar species groups).

By using regulatory values or reference values such as ADI or DNEL as input, the HI introduces a further source of uncertainty. These reference values are derived from PODs by using assessment factors (AFs) intended to accommodate various extrapolations steps and to compensate for differences in data quality. Since AFs can vary from 10 to 10,000, chemicals with regulatory values of the same magnitude may not always have comparable potency. The size of regulatory values may simply reflect vastly differing uncertainties inherent in their derivation.

Finally, the sum of PEC/PNEC ratios is the equivalent of the human-oriented HI, but is applied to ecotoxicological assessments. Conceptually, PNECs are intended to protect all species in the aquatic environment and accordingly, are based on toxicity data from algae, daphnia and fish, and different considerations such as direct impacts or effects via secondary poisoning, which introduces an even wider range of uncertainties than ADI (EC 2011). Thus, in mixing toxicity values for different species and exposure pathways and endpoints, PNECs introduce a further dimension of uncertainty, when used in MRA. Accordingly, exceedances of sums of PEC/PNEC ratios can signal non-compliance with legal

protection goals, but are of limited toxicological significance, unless one invokes chimeric species such as a photosynthesing fish with invertebrate body parts.

2.5 Tiering rules: Improving the reliability of MRA by step-wise removal of the distortions introduced by simplifications of CA

To improve the reliability of mixture risk assessment, our tiering scheme removes the distortions introduced by the use of HI, PODI or PEC/PNEC ratios in a step-wise manner, with the aim of realising the scientific principles of CA as much as is possible. Moreover, increasingly sophisticated assumptions about modes of action are introduced at higher tiers.

Accordingly, our decision tree is divided into 3 main tiers.

In **Tier 1**, regulatory or reference values (RV) such as ADI, TDI and EQS (or their equivalents such as PNECs) are used together with modelled or measured data about exposures. Expected mixture risks are calculated by using the HI approach.

In **Tier 2**, the distorting influence of assessment factors of differing magnitude is removed. For ecotoxicological MRA, this necessitates a new focus on taxa-specific PODs. As much as possible, the blurring influence of mixing of toxicity values for different species that is inherent in applying PNECs is also removed and PODs for common toxicities and adverse outcomes relevant for risk assessment are introduced. The mixture risk assessment method of choice for these input data is the PODI.

In **Tier 3**, we institute sub-groups of mixture components that affect a common endpoint through a similar mode of action. We introduce a hybrid approach (so-called mixed models) that allows us to aggregate mixture effects for a common endpoint resulting from sub-groups with similar modes of action. This aggregation is achieved by using IA.

Tiers 2 and 3 are further divided into **sub-tiers** designed to evaluate whether definitive conclusions about expected mixture risks can be reached without meeting all the data requirements defined for the respective main tiers 2 and 3. An overview of this tiering system, together with its assumptions and improvements of preceding tiers is shown in **Table 2.2**. Detailed explanations are given below.

In accordance with the DOW, the proposed tiered scheme was confined to MRAs for humans and fish. However, it can easily be expanded to include MRAs for any other single species groups such as algae or daphnids. For a detailed explanation of the mathematical formulation of the concepts of CA, IA, and MM and their use for the calculation of predictions mixture toxicity and assessments of mixture risks, the reader is referred to SOLUTIONS Deliverable 2.1.

Table 2.2: Conceptual outline of the WP 18 tiered MRA for humans and fish

Tier	Assessment concept		Input data	Method	Advantage over preceding tiers	Assessment rule	Decision logic
	Assumption	**Specification**					
Premise: mixture of concern defined in terms of components i and exposure levels EL_i for humans ($EL_{i,HUMAN}$) and for fish ($EL_{i,FISH}$)							
1	**DA (or CA)** for all mixture components	Worst case risk estimations following from conservative input data not exactly meeting model requirements	**RVs**	HI		No significant risk if HI ≤ 1	Assessment moved to the next tier if a significant risk cannot be ruled out by a reasonable worst case estimate (of the maximum expectable risk)
2A			**Species(-group) specific (lowest) PODs**	PODI	No distortion by varying AFs. No merging of incomparable species	No significant risk if (PODI x AF) ≤ 1	
2B			Species(-group) specific (lowest) **BMDs or low ECs**	BMD- or low-EC-based PODI	No distortion by ill-defined effect levels	No significant risk if (BMD- or ECx-based PODI x AF) ≤ 1	
2C		Exact modelling of maximum expectable risks	**Endpoint-specific** BMDs or low ECs	TUS (for low-effect levels *x*)	No aggregation of toxicity data across different endpoints	No significant risk if (∑TUx x AF) ≤ 1	
3A	**Mixed Model (MM)**, i.e. DA (or CA) for groups of similarly acting mixture components, IA between groups	Limit value calculations of minimum expectable risks following from incomplete specifications of IA model parameters and/or insufficient knowledge on MoAs		Assumption of No Addition of single substance toxic units (TUx_i) as a (lower) limit value for IA-based predictions	Expansion of the one-sided conservative MRA to a two-sided "Prediction Window" between minimum and maximum expectable risk	Significant risk if $TUx_i > 1/AF$	Assessment stopped if a significant risk is demonstrated for a reasonable best case scenario (of the minimum expectable risk)
3B			Endpoint-specific BMDs or low ECs **+ MoA information**	TUS within MoA group *j* for endpoint *k* and assumption of No Addition between groups, as a (lower) limit value for MM-based predictions	Available knowledge on MoAs taken into account	Significant risk if $\sum TUx_{j,k} > 1/AF$	
3C			**Dose (or concentration) response functions** (for common endpoints)	Assumption of completely independent MoAs for all mixture components as an extreme case of MM	All parameters of the IA model specified; IA-based predictions of BMD_{mix}^{IA} and/or $EC10_{mix}^{IA}$ calculated (where available data allow to do so)	▪ Significant risk if $BMD_{mix}^{IA} < (\sum EL_{i,HUMAN}) \times AF$, and/or $EC10_{mix}^{IA} < (\sum EL_{i,FISH}) \times AF$ ▪ Inconclusive evidence if available information on slope of DRCs or CRCs is insufficient but Tier 2C assessments give a reason for concern	As before. Assessment also stopped in case of serious data gaps on slope of DRCs (or CRCs)
3D		Best possible mixture risk modelling	Dose (or concentration) response functions **+ MoA information**	State-of-the-art MM-based calculation of low-effect doses or concentrations of the mixture (BMD_{mix}^{MM}, $EC10_{mix}^{MM}$); MRA derived by means of an AF	Prediction Window narrowed down to a precise mixture toxicity prediction and definite MRA derived (where available knowledge and data allow to do so)	▪ Significant risk if $BMD_{mix}^{MM} < (\sum EL_{i,HUMAN}) \times AF$, and/or $EC10_{mix}^{MM} < (\sum EL_{i,FISH}) \times AF$; ▪ No significant risk otherwise, provided MM is applicable; ▪ Inconclusive evidence if MM is inapplicable but Tier 2C assessments give a reason for concern	Component-based MRA completed

2.6 Assessment rules for the main Tiers

If the use of regulatory values in conjunction with the HI in Tier 1 yields indices < 1, no significant mixture risks are expected and the analysis can be stopped. The assessment is moved to Tier 2 only in cases where a significant risk cannot be ruled out under reasonable worst-case assumptions (regarding both exposures and toxicity), i.e. when the HI > 1. If there is pre-existing information about significant mixture risks and if the necessary input data are readily available, Tier 1 may be skipped. At any time, the analysis can begin at appropriate higher tiers.

The PODI to be used in Tier 2 assessments is normally applied in connection with margin-of-exposure (MoE) considerations. For example, a PODI of 0.1 indicates that the components in the mixture jointly reach concentrations (doses) 10-fold below PODs, with a margin-of-exposure (MoE) of 10. The assessment requires decisions about acceptable MoEs. Following the principle that MRA should neither be more, nor less stringent than single chemical risk assessments, a default MoE of 100 suggests itself for human MRA. Accordingly, a PODI of smaller than 0.01 (or a PODI x 100 < 1) signals that combined exposures of concern are not to be expected and that the analysis can be discontinued. In all other cases, the assessment is moved to Tier 3.

For ecotoxicological assessments of single chemicals AFs are made dependent on the availability of chronic toxicity data for the three taxa algae, daphnids and fish and range from 1000 to 10, in some cases even smaller. For the evaluation of the ecotoxicological safety of pesticides, a MoE of 10 is normally required in connection with chronic toxicity data (EFSA PPR Panel 2013a). Accordingly, for ecotoxicological MRAs, a PODI below 0.01 would indicate minimal mixture risks. PODIs between 0.01 and 0.1 signify a grey area where the decision to move the analysis forward to the next higher tier can be subject to case-by-case considerations, while PODIs exceeding 0.1 clearly require continuation of the analysis in the next higher tier.

In Tier 3, the refined CA-based worst-case estimates from the previous Tier are complemented by IA-based best-case estimates. This extends the conservative, CA-based MRA to the minimum risk of the "prediction window" delimited by predictions derived from IA. The assessment is stopped, if a significant risk is detected on the basis of a reasonable best-case estimate of the lowest expectable risk and if this cannot to be ruled out by any further refinement (Tier 3A). This is the case when the ratio of exposure to POD of one single component in the mixture exceeds its permissible value (0.01 for human MRA, 0.1 for ecotoxicological MRA) for a reasonable best-case scenario. This is analogous to the "gatekeeper step" proposed by Moretto et al. 2017 as a filtering step at the beginning of the assessment.

If an exceedance of exposure standards for a single component is not apparent, the above exercise is repeated for groups of mixture components that contribute to a common adverse outcome through similar modes of action, by calculating PODIs for these sub-groups (Tier 3B). If any of these PODIs exceed the critical value under reasonable best-case assumptions, we conclude that the mixture exposure exceeds the standard and stop the assessment.

In the remaining cases, Tier 3 considers scenarios where the maximum expectable risk may be of concern, while the minimum expectable risk is not. Only these cases are taken forward to the final sub-tier (Tier 3C), which means a full application of mixed-modelling approaches. Where the high data demands and the conceptual premises of this approach can be met, a definite final assessment of the

significance or insignificance of the mixture risks can be derived. Otherwise the evidence remains inconclusive, because CA-based concerns cannot be ruled out by advanced modelling due to missing data or knowledge.

2.7 Drivers of mixture effects

The identification of drivers of mixture effects is central to our framework, and directly helps to inform risk management to focus on compounds that apparently matter most. It will allow us to simplify the analysis by avoiding to carry those chemicals forward into higher tiers that clearly make only a marginal contribution to mixture effects. To identify such drivers of mixture risk, quantitative criteria are needed. Price et al. (2012) proposed to define drivers as chemicals that contribute at least 50% to the overall mixture exposure, i.e. when the ratio $\sum RQ/RQ_{max} > 2$. However, this criterion might be too restrictive when dealing with scenarios where several chemicals contribute to mixture toxicity.

An alternative would be to define drivers as those mixture components that do not fit the case where all components contribute equally to the combined effect. In such artificial "balanced" mixtures, the hazard quotients of all components are equal to the quantity $\sum RQ/n$, where n is the number of components. Drivers can then be defined as those mixture components whose RQ is larger than the average RQ, i.e. $RQ_i > 1/n \sum RQ$.

However, especially with large $\sum RQ$ and highly skewed RQ distributions, this approach may underestimate the number of drivers: Consider the case of $\sum RQ = 2$. To achieve acceptable mixture exposures, assume that the $\sum RQ$ has to reduce to 1 or smaller. This can be realised by a 50% decrease of $\sum RQ$. If mixture components are ranked according to the numerical value of their RQ, from large to small, drivers would be those chemicals whose RQ together make up 50% of $\sum RQ$. With $\sum RQ = 10$, this expands to 90%, with $\sum RQ = 100$ to 99%, and so on (**Fig 2.1**). According to this approach, a driver belongs to the group of chemicals whose RQs cumulatively exceed acceptable mixture exposures, i.e. $\sum RQ_{drivers} = \sum RQ_{mixture} - \sum RQ_{acceptable}$. To capture those chemicals that contribute the largest RQs, it is additionally required that $\sum RQ_{drivers}$ is a rank order of individual RQs from largest to smallest.

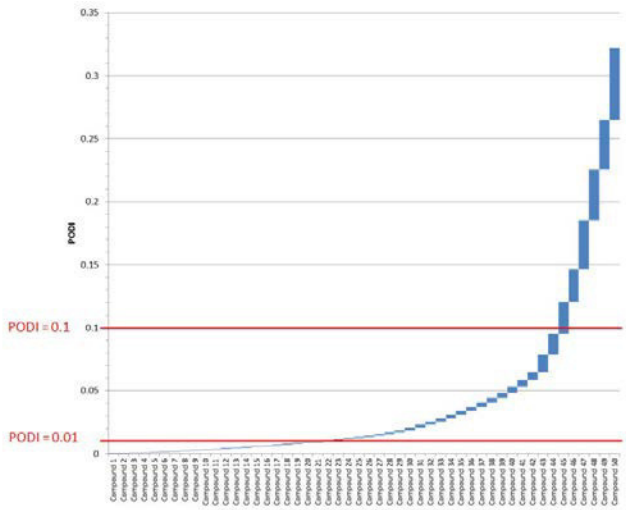

Figure 2.1: The principle of driver identification. Chemicals 1 – 50 are arrayed in ascending order according to the size of their RQ (here demonstrated for the Point of Departure Index, PODI, where RQ = exposure/POD). If PODI = 0.01 is used as the limit of acceptable exposures, chemicals 1 – 22 comply with this standard, but jointly, chemicals 23 – 50 exceed it and will be identified as drivers of a PODI. Accordingly, if PODI = 0.1 is deemed acceptable, the group of drivers reduces to chemicals 45 - 50.

2.8 Dealing with missing toxicity data and implications for the identification of drivers

As a minimum requirement for starting the MRA in Tier 1, regulatory maximum acceptable doses or protective concentrations, so-called regulatory or reference values (RV) must be available for all mixture components, and for all receptors. This will include ADI, TDI, EQS, PNEC and others, as appropriate. In Tier 2 of the analysis, this will be replaced by POD (NOECs, NOAELs, BMD and equivalent). The required data may not be available for all chemicals that make up mixture exposure scenarios of interest. In principle, there are two options for dealing with such data gaps: (a) chemicals without RV shall be excluded from analysis – this will lead to underestimations of risks associated with combined exposures; (b) missing RV will be bridged by using methods that estimate RV by various methods, but this may imply overestimations of risks. To avoid a bias towards the null, we propose to follow option b.

Mixture components whose potency had to be estimated due to missing toxicity data may in some cases make a disproportionately large contribution to the overall mixture risk. These chemicals cannot be said to drive a mixture risk, but instead signal a high priority for further testing with the aim of filling the respective toxicity data gaps. It is suggested to identify these chemicals and to collect them in a list termed “Pool I” (**Fig 2.2**). If the remainder of the chemicals exceeds acceptable mixture exposures, the analysis moves to the next Tier, but chemicals with unknown toxicity are omitted from further consideration. This filtering step ensures that the analysis is not stalled by insurmountable data gaps. However, it should be noted that only a sub-set of chemicals is taken forward into the next Tiers of the assessment. The advantage is that the analysis is put on a secure footing in that it allows assessments of partial risks on the basis on sound data. The mixture risk associated with the entire ensemble of chemicals originally entered into the analysis cannot be smaller than the risk identified for a sub-sets for which toxicity data are available.

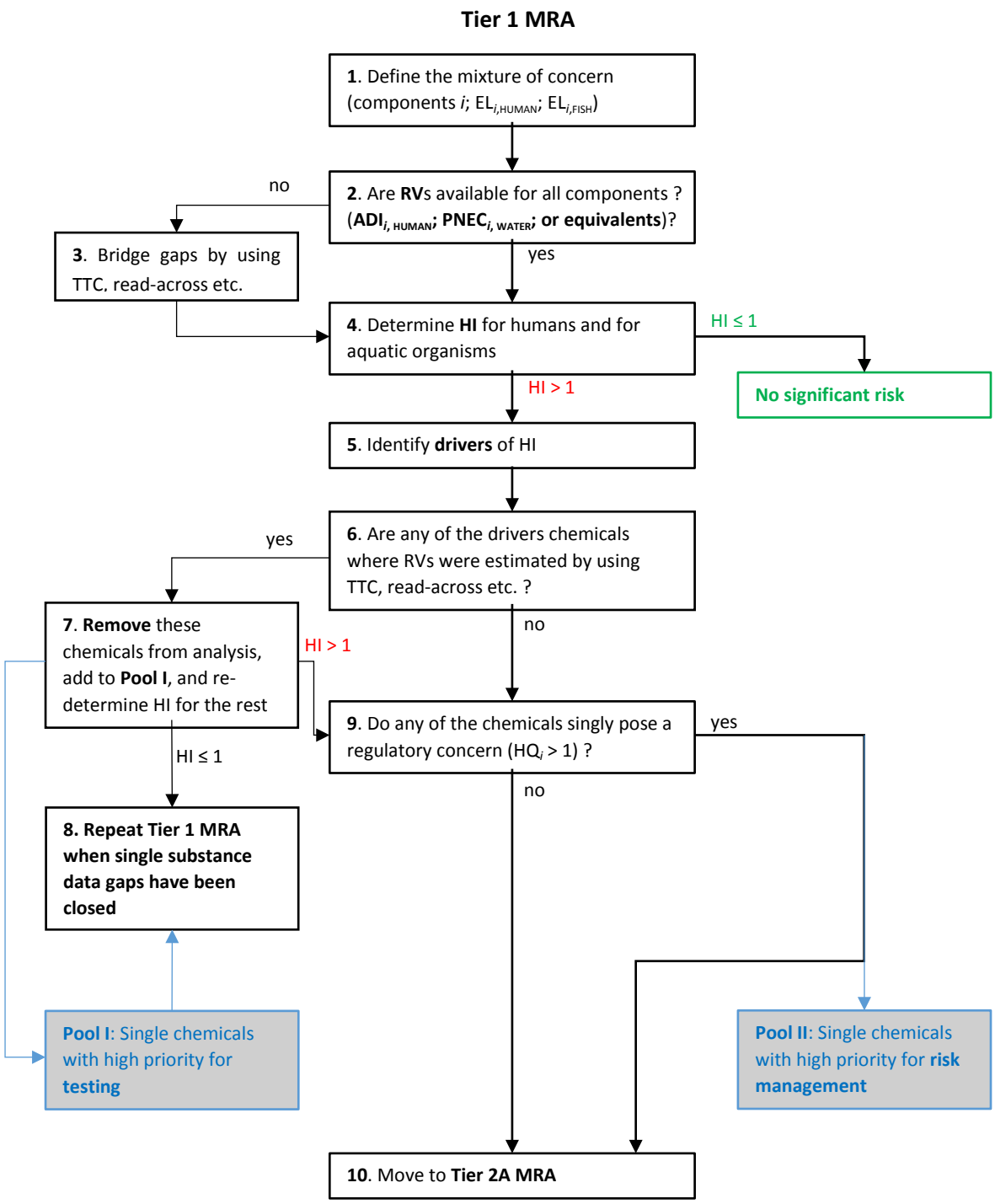

Figure 2.2: Decision tree and workflow scheme for MRA for humans and fish – Tier 1

2.9 Application to measured and modelled exposure data: Tiering in the exposure assessment arm of the framework

MRA also requires data about co-exposures to all chemicals that make up the exposure scenario of interest. Exposure information can be based on monitoring data (e.g. water concentrations, levels of substances in food, air or soil) or on exposure estimates established by modelling, and our proposed

framework can be used in connection with both these sources of exposure information. In the same way as refinements of hazard data are implemented as the analysis moves to higher tiers, exposure data can also be refined. As suggested by Meek et al. (2011), the necessary refinements of exposure data can be implemented independently of the tiering in the hazard assessment arm of the assessment framework. Accordingly, we suggest that each Tier should begin with worst-case exposure assumptions. With monitored exposure data, this requires decisions regarding the handling of chemical analytical non-detects. We propose to begin by setting non-detects to their LOD (worst case) and only to relax this in higher tiers of the analysis, e.g. by assuming 50% LOD as substitute concentrations for non-detects. However, uncritical implementation of this procedure may lead to the paradox that mixture risks increase as growing numbers of substances are measured, but without reaching analytical detection limits. This can be addressed by uncertainty analyses.

For many environmental pollutants the measured (total) concentrations in water are a poor reflection of the bioavailable fraction, due to adsorption phenomena and speciations (relevant for transition metal complexes). In some cases, RQ calculated on the basis of total measured concentration will need to be adjusted downwards to reflect bioavailable concentrations. To avoid overlooking drivers of mixture risk, we propose to address these issues only for those chemicals that have been identified as drivers at higher tiers of the analysis.

2.10 Decision tree and work flow scheme of the integrated framework

An overview of the conceptual outline of the proposed tiered human and ecotoxicological MRA is given in **Table 2.2**. For Tiers 1, 2 and 3, the corresponding decision tree and work flow scheme is detailed in **Fig 2.2, 2.3 a-c** and **2.4 a, b**, respectively.

For modelled exposure scenarios, the scheme starts with defining the mixture of concern in Step 1 of Tier 1 (**Fig 2.2**), which is assumed to be fixed and not subject to further refinements; only the hazard assessment aspect of the MRA is refined in a stepwise fashion.

For exposure scenarios derived from monitored (measured) values, it is necessary to also refine the exposure assessment arm by dealing with analytical non-detects and by making adjustments for bioavailability. We propose to deal with these issues in higher Tiers of the analysis, after identification of drivers of mixture risks.

The scheme is divided into three major tiers, with tiers 2 and 3 each being sub-structured into a number of sub-tiers (2A-C and 3A-D):

- Tier 1 MRA, assuming CA and using the HI method with RV (or equivalents)
- Tier 2 MRA, assuming CA and using
    - (A) the PODI method based on species group specific NOAELs or NOECs, for different toxicity endpoints
    - (B) the PODI method based on endpoint specific species group NOAELs or NOECs; if available, NOAELs or NOECs can be replaced by BMD or EC10
    - (C) the TUS approach based on endpoint-specific and species-specific NOAELs or NOECs (or BMD or EC10 if available),

thereby removing distorting factors of the CA calculation in a stepwise fashion.

- Tier 3 MRA, taking a Mixed Model (MM) approach, i.e. assuming DA for groups of similarly acting mixture components, and IA between the groups, structured into

  (A-C) limit value calculations, defining a "prediction window" between minimum and maximum expectable risk on the basis of incomplete specifications of IA model parameters and/or insufficient knowledge of MoAs, and finally

  (D) exact MM-based MRA, based on knowledge of DRCs and MoAs for all (relevant) mixture components.

At every tier and sub-tier, similar tasks are performed, including:

- compilation of the necessary input data
- bridging of data gaps
- assessment of the mixture risk
- identification of drivers of the overall risk
- identification of single chemicals with a high priority for testing, i.e. suspected drivers with missing test data (Pool I)
- identification of single chemicals with a high priority for risk management, i.e. confirmed drivers that exceed their permissible exposure levels (Pool II)

As pointed out earlier, it is not necessary to take all analyses through every proposed step; if there are indications of unacceptable mixture risks on the basis of simple worst case assumptions, the MRA can commence at a higher tier.

Where the core task of assessing the mixture risks reveals indications of absence or presence of a significant risk, this is highlighted in the schemes (**Fig 2.2, 2.3** and **2.4**) by green and red colouring, respectively. Assignments to Pools I and II are highlighted in **blue**.

As the MRA becomes more certain in higher Tiers, so does the identification of drivers. This means that driver identification in higher tiers overrules lower tiers and consequently the substances assigned to Pool II may be sub-grouped accordingly.

The scheme is designed to provide clear decisions about the absence or presence of exceedances of combined exposures, wherever possible. In Tiers 1 and 2, CA-based worst case estimates are generated and refined step by step. The assessment is discontinued, if there is no indication for a significant risk. Otherwise it is moved forward to the next Tier.

Tier 3 MRA is based on the conceptual assumptions of a hybrid CA/IA model, or Mixed Model (MM). The data and knowledge requirements for correct application of the MM approach are hard to fulfil and the conceptual premises may not be exactly met. To deal with these issues, the proposed scheme includes three pre-evaluation steps (Tier 3A –C), which provide best-case estimates of minimum expectable risks that can be calculated with limited data.

In Tier 3A the RQ of individual mixture components are assessed. The mixture toxicity predicted by the MM can never be lower than the toxicity of the most toxic mixture component alone (at the dose or concentration present in the mixture). Where a risk is estimated for one or more individual mixture components for an endpoint relevant in fish, the evaluation is stopped. Performing an MM-based assessment is not worth the considerable effort this will entail: significant risks from single substances cannot be ruled out by assuming IA for dissimilarly acting (groups of) mixture components.

Tier 3B is an assessment of the sums of RQ for sub-groups of similarly acting mixture components, where the available knowledge allows to identify such groups. The mixture toxicity predicted by the MM can never be lower than the joint toxicity of the chemicals in the most toxic sub-group, as calculated by assuming DA within the groups. Where a significant risk can be demonstrated for one or more sub-groups of similarly acting mixture components for one or more endpoints relevant in fish, the evaluation stops. The conclusion is essentially the same as in Tier 3A: performing an MM-based assessment is not worth the considerable necessary effort. Significant risks from a common-MoA-group cannot be ruled out by assuming IA for dissimilarly acting (groups of) mixture components.

Tier 3C assumes completely independent action for all mixture components as an extreme case for the MM approach. In Tiers 1 and 2 we assumed completely similar action as the other extreme. If this extreme assumption of IA in Tier 3C indicates a significant risk, the conclusion is essentially the same as in Tiers 3A and 3B: completing the MM-based assessment by introducing MoA-based grouping of mixture components is not worth the effort. Significant risks from a completely independent action of all mixture components cannot be ruled out by assuming DA (or CA) for similarly acting groups of mixture components.

Finally, in Tier 3D we apply the MM approach as the final step in our proposed scheme. It is conducted in situations where the maximum expectable risk is significant (as calculated in Tier 2C on the basis of the CA assumption), while the best case estimate of the minimum expectable risks is not (as calculated in Tier 3C on the basis of the IA assumption). Where all data requirements and conceptual assumptions can be met, Tier 3D will provide a definite assessments in terms of combined risks. Otherwise, the assessment will end with the finding that all available data and information provide “inconclusive evidence”. In cases where Tier 3D assessments provide “inconclusive evidence” for unacceptable mixture risks, the logic of the proposed decision tree means that the problem cannot simply be solved by additional standard testing of single substances, but only by further research of MoAs and/or by experimental testing of the whole mixture. Alternatively, precautionary risk reduction measures may be taken into consideration.

Where the procedure finally results in the indication of a significant risk, validation of predictions by experiments or field observations may be taken into consideration. Alternatively, options for risk reduction should be explored. Where the procedures provide inconclusive evidence, dedicated follow-up studies on MoAs or experimental mixture toxicity testing may provide the missing evidence. Alternatively, precautionary risk reduction measures may be considered.

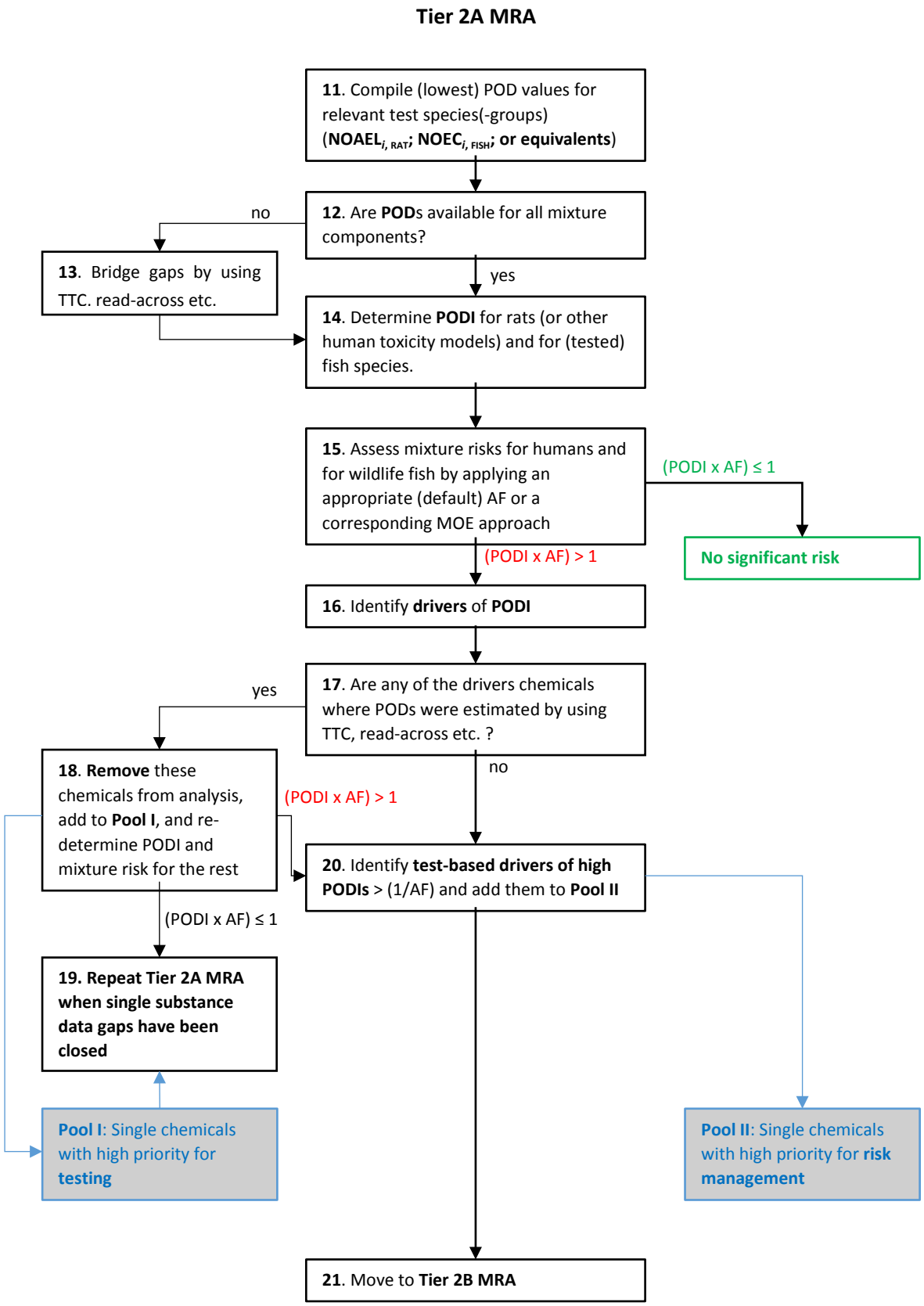

Figure 2.3 a: WP 18 decision tree and workflow scheme for MRA for humans and fish – Tier 2A

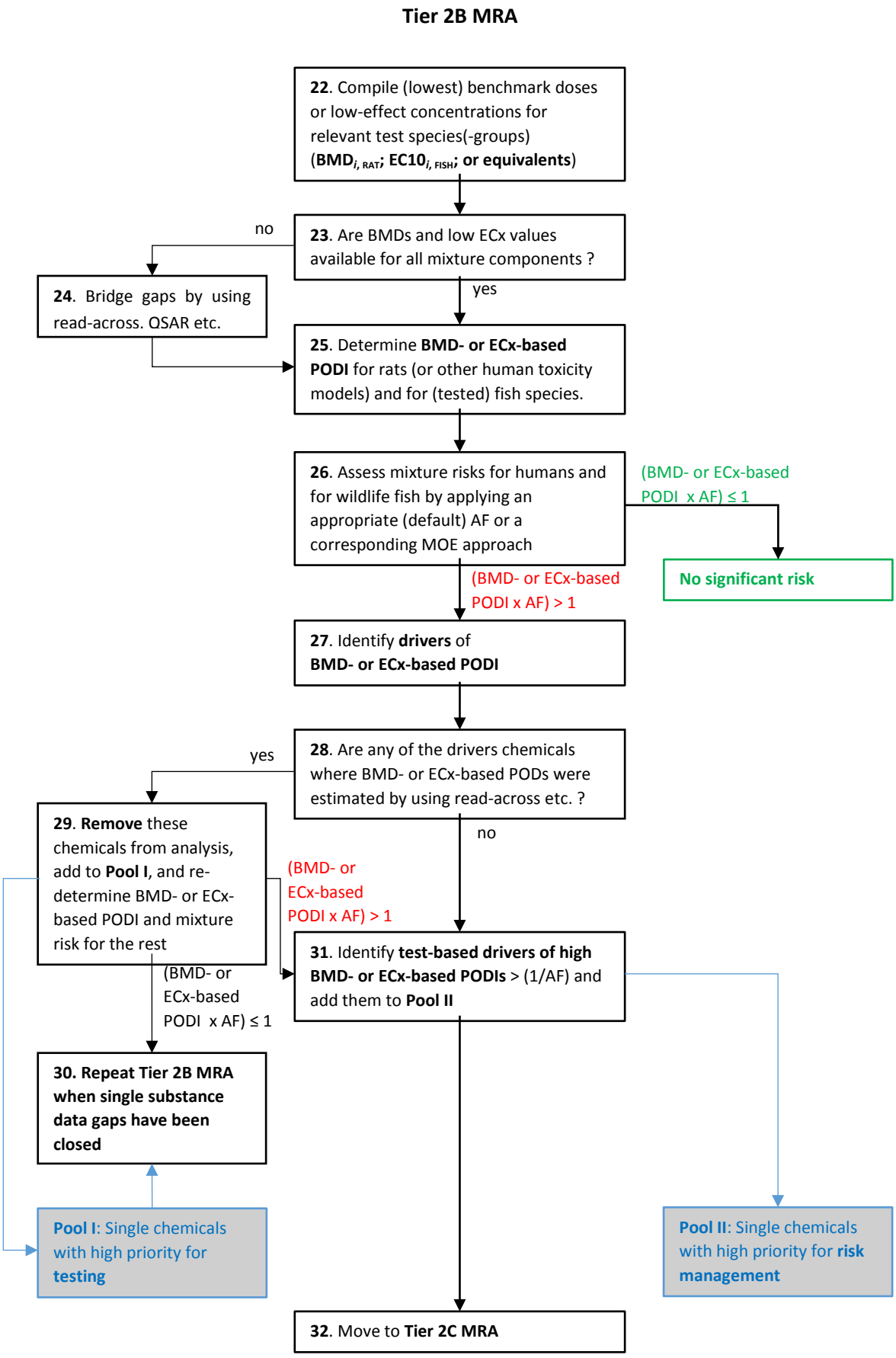

Figure 2.3 b: Decision tree and workflow scheme for MRA for humans and fish – Tier 2B

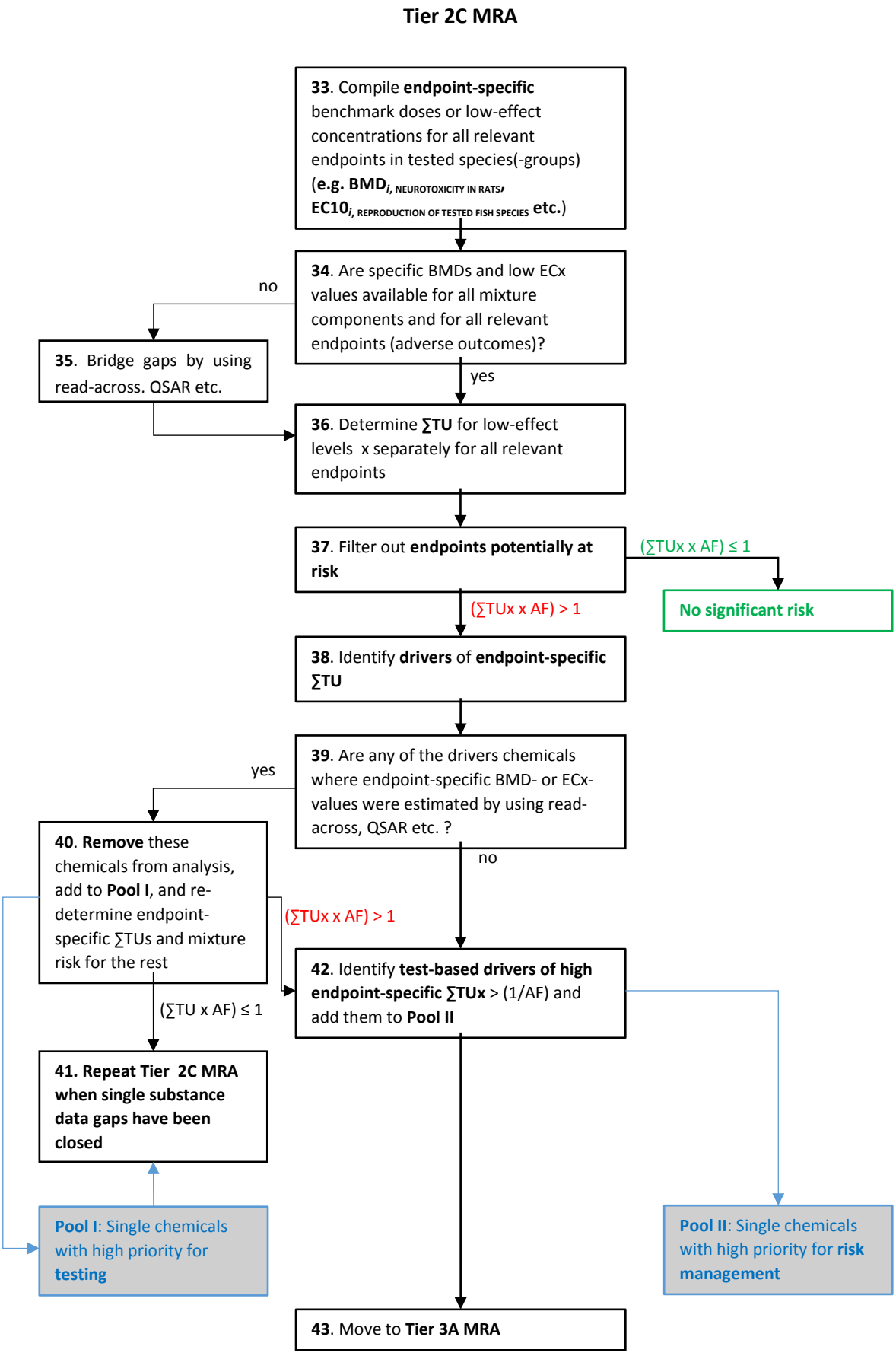

Figure 2.3 c: Decision tree and workflow scheme for MRA for humans and fish – Tier 2C

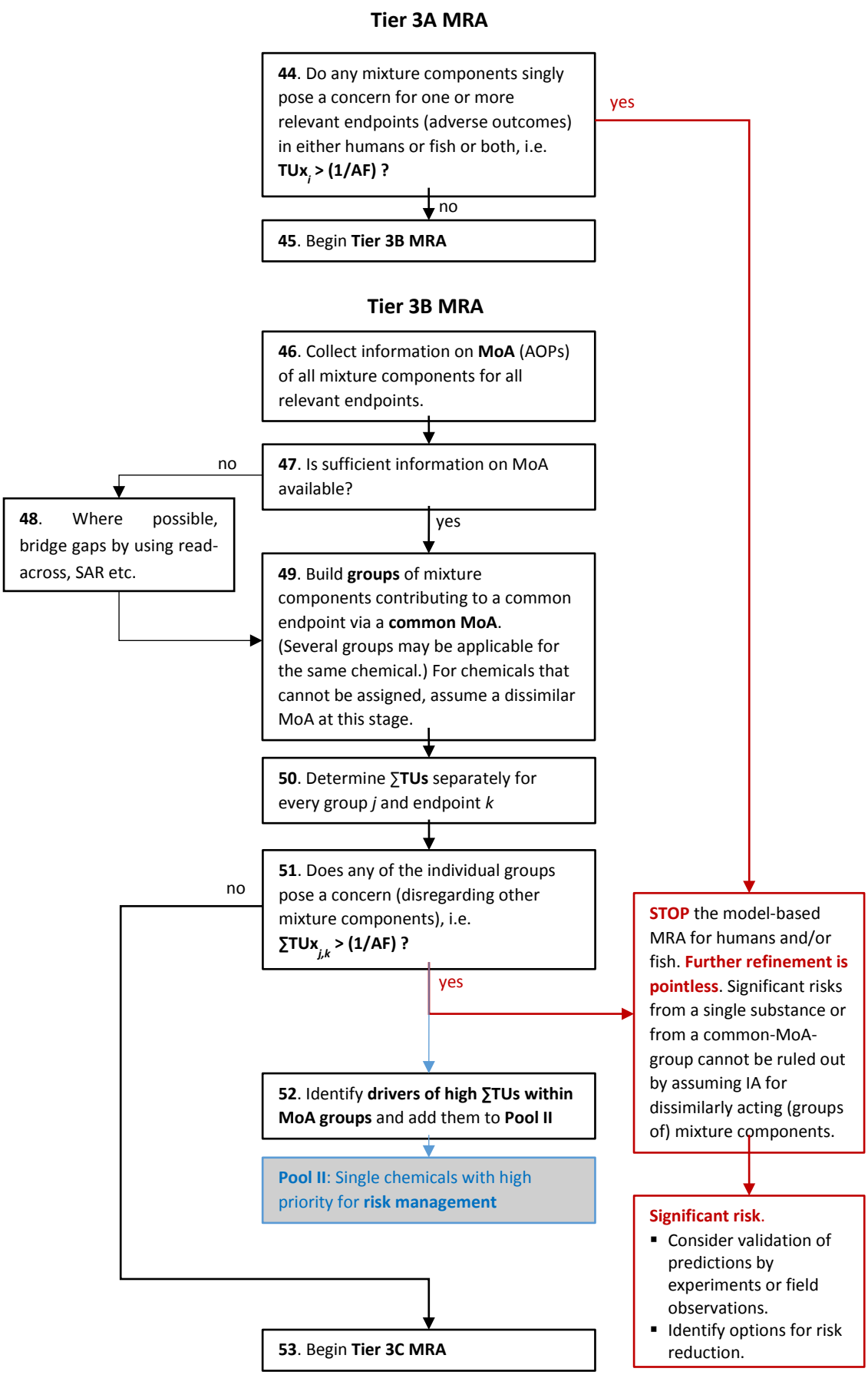

Figure 2.4 a: Decision tree and workflow scheme for MRA for humans and fish – Tier 3A, 3B

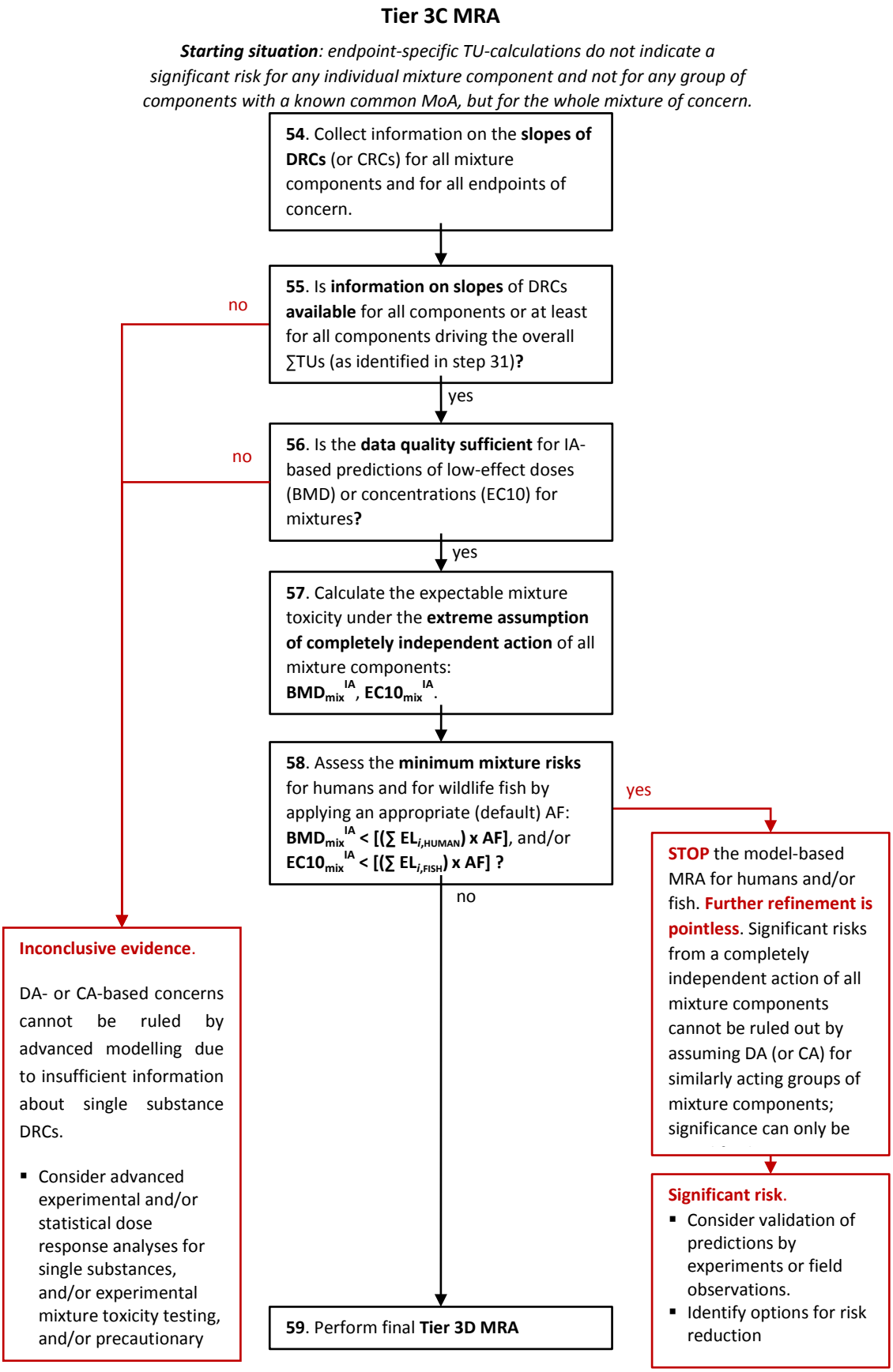

Figure 2.4 b: Decision tree and workflow for MRA in humans and fish: Tier 3C

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3 Bioaccumulation and biomagnification modelling for the identification of potential human health risks from exposure to aquatic pollutants via fish food consumption

3.1 Aim and scope

In SOLUTIONS WP18, measured or modelled concentrations of pollutants in European freshwaters provided the starting point for the model-based identification of potential human health risks from exposure to a mixture of aquatic pollutants via fish food consumption. These water concentrations apply to specific sites or regions where samples were taken for chemical analyses or for which exposure modelling was performed, respectively.

The question to be answered is:

- **Is the fish caught from a given freshwater site safe for human consumption?** Or may the pollutants accumulated in the fish pose a health risk?

To derive an initial model-based answer, we assumed a scenario where the fish food consumed by a local population mainly originates from a given freshwater site for which pollutant concentrations were modelled. The examination of more complex scenarios of a mixed fish food diet, including fish from various sites and both freshwater and marine species, was beyond the scope of the case study presented in section 4.

For performing initial human health risk assessments for local exposure scenarios by means of a component-based MRA procedure, two main preparatory steps were necessary:

(i) Conversion of measured or modelled water concentrations of pollutants into expectable concentrations in fish tissues by means of bioaccumulation modelling.

(ii) Conversion of estimated internal concentrations in fish into potentially resulting intake values for humans eating such fish. These intake values could then be fed into a component-based mixture risk assessment procedure.

For step two, the same standard rules and assumptions were applied as those which have been laid down in the Technical Guidance (TG) for Deriving Environmental Quality Standards (EQS) for the purpose of deriving Quality Standards in aquatic biota from regulatory acceptable levels for human health protection, such as ADI, TDI, or an oral NOAEL divided by an appropriate assessment factor (EC 2011, section 4.5)[6]. For step one, however, no such regulatory standard rules or assumptions apply. Where needed, they had to be developed. This is the subject of this section 3.

[6] Established rules for deriving concentration levels of pollutants in fish which should not be exceeded in order to protect human health ($QS_{biota, hh food}$) include the assumptions of a body weight of 70 kg and an average consumption rate of 115 g fish per day, as well as the rule that exposure via fish food alone should not exceed 10 % of the total acceptable dietary exposure level. "*The $QS_{biota, hh food}$ is intended to protect all humans against adverse health effects from consuming contaminated fishery products*" (EC 2011, section 4.5). The assumed consumption of 115 g/day, however, is an average rate. Thus, as explicitly said in the TG, "*the approach does not specifically consider (…) subpopulations that consume more fish food than the European average*", but it is argued that "*the assumption that fishery products make up no more than 10% of the threshold level (…) provides a margin of safety*". The average value of 115 g/day applies to all fish, not distinguishing between fresh and sea water fish.

The methodology applied in WP18 for food web fish bioaccumulation modelling of organic chemicals is based on established approaches, summarized in the following section 3.2, full details are given in Annex 1. For the application of the method, three types of input data are required:

(i) descriptors of environmental conditions, such as temperature,

(ii) properties of the chemical, such as hydrophobicity, and

(iii) characteristics of the fish, as detailed below.

Values for the physico-chemical descriptors of environmental conditions and chemical properties (*I* and *ii*) were the same as those used for the entire SOLUTIONS exposure modelling train. For biological parameters characterizing the fish (iii), however, appropriate values needed to be defined in WP18 additionally, to serve the specific purpose of deriving human health risk assessments. Their derivation by definition of a set of prototype freshwater fish species is explained in section 3.3.

3.2 Definition of bioaccumulation and biomagnification modelling approach

3.2.1 Introduction

The bioaccumulation and biomagnification modelling follows the approach of Arnot and Gobas (2004) and Armitage et al. (2013) and extends and adapts it in several ways. Firstly, the use of concentration time-series as input was enabled, calculating dynamic body concentrations instead of equilibrium concentrations. Secondly, the food web perspective was integrated with applicability of the model to ionisable organic compounds, combining the advantages of the models of Arnot and Gobas (2004) and Armitage et al. (2013) with each other. The resulting model accounts for fish at different positions in the food web, where different fish types consume different food items, hence accounting for biomagnification of chemicals along the food chain. Internal concentrations are calculated for all components in a food web, including plant material-eating (phytovorous), zooplankton-eating (planktivorous) and predatory (piscivorous) fish (**Figure 3.1**). Concentrations of organic compounds per fish group are described in general by a one-compartment model:

$$\frac{dC_b}{dt} = k_w C_w + k_d C_d - k_e C_b$$

where C_b is the concentration in biota (mg kg^{-1}), t denotes time (days), k_w is the uptake rate constant for uptake from water (L kg^{-1} day^{-1}), C_w is the concentration (freely dissolved and available for uptake) in water (mg L^{-1}), k_d is the uptake rate constant for uptake from food (diet, kg kg^{-1} day^{-1}), C_d denotes the concentration of the compound in the diet (mg kg^{-1}), and k_e denotes the overall elimination rate constant (day^{-1}).

When using that value for assessing concentrations in fish from a contaminated freshwater site, this means to assume that on average 115 g fish are consumed per day which originate from that site. This assumption should be protective for the scenario of a local population which mainly consumes fish from the site of concern. For populations with a mixed mixed fish food diet, including fish from various sites and both freshwater and marine species, such a local scenario may over-estimate risks from pollutants which dominate the contamination at the investigated site. On the other hand, a scenario of a mixed fish food diet may include a broader spectrum of pollutants. Fish from different sites may be polluted by different chemicals. As a consequence, where there are indications for significant mixture risks, regulatory decision making may require refined examinations of fish consumption patterns. Performing such examinations was beyond the scope of WP18 work.

3.2.2 Bioaccumulation model

The bioconcentration model described by Armitage et al. (2013) is an extension of the bioaccumulation model for organic compounds described by Arnot and Gobas (2004), extending the applicability of the latter to ionisable organic compounds. The Armitage et al. (2013) model enables the calculation of rate constants for uptake from water and total elimination through gill ventilation, faecal egestion, metabolism and growth dilution. Equations for the estimation of respective chemical-specific rate constants per are given in detail in **Annex 1**. The mathematical description of uptake of organic compounds through consumption of food items was added to the model equations for the SOLUTIONS bioaccumulation model.

Metabolism

The rate constant for elimination through metabolism (day^{-1}) is a critical parameter for the bioaccumulation modeling, and depends on the chemical and on the species of fish. Since it is difficult to measure experimentally, it is typically estimated through QSAR-techniques. The rates used in the SOLUTIONS modelling were provided by SOLUTIONS partner UFZ and estimated using a method published by Arnot et al. (2008a).

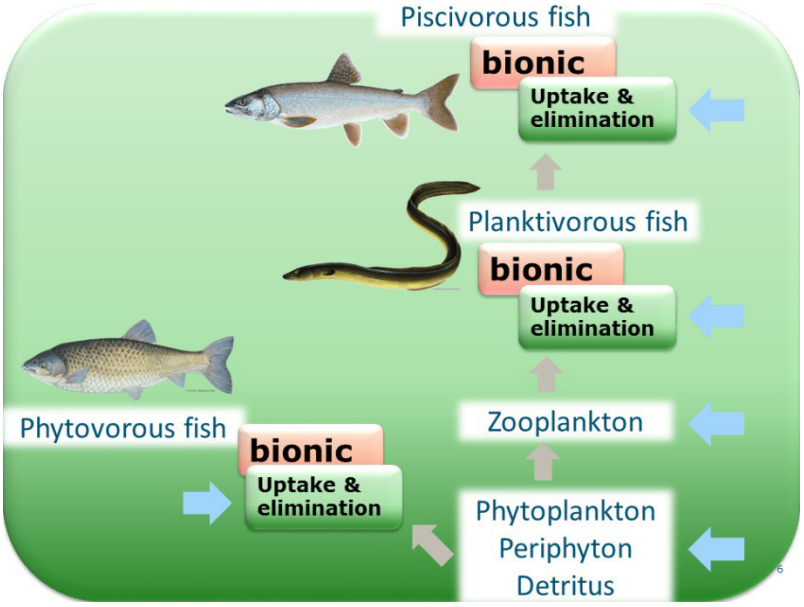

Figure 3.1: The food-web with 3 prototype fish components Phytovorous fish feeding on living or dead plant material, planktivorous fish feeding on zooplankton and piscivorous fish being predators feeding on other fish.

Arnot et al. (2008b) investigated the results of this estimation method of transformation rates in fish and concluded that correlations between predicted and experimental transformation rates for fish were modest. If no data on metabolism are available, it can also be assumed zero, i.e. it is assumed that elimination through metabolism is negligible.

Estimation of concentration in the fish food chain

The concentration of an organic chemical in consumed biota was estimated using the concept of the Trophic Magnification Factor (*TMF*). The *TMF* describes the biomagnification potential of a chemical over a range of trophic levels (Jonker, 2012) and simply describes by which factor the (lipid normalised) concentration in biota increases when going up in the food web by one trophic level.

The method assumes that phytoplankton is in immediate equilibrium with the surrounding water. The ratio between concentrations of a substance in phytoplankton and water is given by the bioconcentration factor of the compound in phytoplankton BCF_{phyto}. From the concentration in phytoplankton, the concentrations in higher trophic levels can be estimated using the Trophic Magnification Factor (*TMF*). In general, the predicted concentration of a substance in a species is:

$$C_{species} = \frac{F_{lipid,species}}{F_{lipid,phyto}} TMF^{\Delta \mathrm{TL}} BCF_{phyto} C_w$$

where ΔTL is trophic levels up from phytoplankton, $F_{lipid,species}$ is the lipid content (fraction) in the species and the lipid content (fraction) in the phytoplankton is given by $F_{lipid,phyto}$.

This equation enables the prediction of concentrations of a substance in any species at any trophic level. It is used in the SOLUTIONS biomagnification modelling to predict concentrations in the food items of fish food-web components. For the fish themselves, the Armitage et al. (2013) bioconcentration modelling approach is used, where the concentrations in the food of the 'Armitage fish' are calculated from weighted average concentrations in the various food items.

Standard estimation methods for the bioconcentration factor of organic chemicals in phytoplankton (*BCFphyto*) and for the TMF of organic chemicals can be used in more or less 'standard' food web systems. For both quantities estimation methods use readily available physico-chemical properties of a compound, in particular the logarithm of its octanol-water partition coefficient, log K_{ow}. Concerning equations are given in the **Annex 1**.

The food-web context

Fish used for human consumption belong to different species and age/size-classes, with different positions in the aquatic food-web. Trophic level index (*TL*) defines the position, at least its 'vertical' dimension: primary producers are the first level, primary consumers the second, etc (**Figure 3.1)**. Trophic levels for the prototype species considered in the SOLUTIONS modelling are defined explicitly (see section 3.3), and in addition the assumption is made that TL increases one unit when going from phytoplankton to zooplankton.

Model output

The bioaccumulation and biomagnification model can be used with time-series of concentrations, e.g. with daily values for one year as generated by the fate models in the SOLUTIONS modelling train, or be based on an measured concentration values. In the first case, time-series of daily body concentrations constitute the output. These time-series are summarized in monthly and annual maximum and mean (geometric and arithmetic) values, for use in the human health risk assessment. In the second case, the

model is run for one year for a constant water concentration and the 'equilibrium' concentrations reached at the end of the simulation are reported per food-web component.

3.3 Definition of prototype freshwater fish species

3.3.1 The task

The food web fish bioaccumulation modelling requires a characterization of the receiving fish in terms of three input parameters:

(i) trophic level (TL),

(ii) lipid content (LC), and

(iii) weight (W).

In addition, the lipid content (ii) must be split into estimates for the polar fraction (membrane lipids) and the neutral fraction (storage fat).

The predicted bioaccumulation factor increases with the trophic level and with the lipid content of the fish. It decreases with increasing weight. These relationships are non-linear.

Values for the three parameters TL, LC, and W differ widely, from species to species and from individual to individual, depending on genetic factors, environmental conditions, age and developmental stage, seasons and the availability of feed. In addition, the real composition of fish communities is unknown or not exactly known for most of thousands of sites all over Europe for which SOLUTIONS generated measured or modelled concentration data. Furthermore, not only wild fish have a relevance for human health risk assessment but also fish cultivated in cages in natural freshwaters as well as fish farmed in ponds and reservoirs that receive water from the river in which pollutant concentrations have been measured or modelled.

Given these sources of variability and inexactness, calculations of pollutant bioaccumulation in fish and potentially resulting human intake values were not performed for any specific real scenario of fish species composition at a given site. Instead, we aimed to model bioaccumulation for "prototype fish".

Such prototype fish are

- defined in terms of the three biological model input parameters (TL, LC, and W) and are
- intended to represent realistic worst and best case situations, in terms of high or low potentials for pollutant accumulation.

The aim is to facilitate a "traffic-light type" assessment, distinguishing between three situations:

- indications for potential risks seen even under best case (lowest) bioaccumulation assumptions (red),
- indications for significant potential risks seen under worst case assumptions for fish bioaccumulation potentials only (yellow), and
- no indications for significant risks seen under any realistic assumptions for bioaccumulation potentials of relevant fish species (green).

Thus, **the task was to define parameter values for trophic level (TL), lipid content (LC), and weight (W) of prototype fish, representing realistic scenarios for high and low bioaccumulation potentials in European freshwater fish species which are or may be eaten by humans**

3.3.2 Relevant fish species

Data on the occurrence of fish species in European freshwaters as well as information on human use of freshwater species were compiled from *FishBase for Europe*, a regional section of the global *FishBase* database (www.fishbase.org). The database was accessed on 30 June 2017 and all following data analyses refer to that state.

In *FishBase*, a total of 1097 species is reported to occur in European freshwaters, including both native and introduced species. The information on freshwater occurrence was compared to habitat classifications for fish species given in Romanuk et al. (2011), the primary information source on TL values (see below). For ten species, the information was found to be inconsistent. A check showed that these are species which usually occur in marine coastal waters or brackish waters and which only occasionally have been reported to be also present in freshwater zones of estuaries. These ten species were omitted from the further data analyses. This did not have an effect on the distribution of TL values reported below: extreme values remained unchanged and mean values did not change by more than 0.01 units.

The remaining figure of 1087 different European freshwater species includes both fish which stay in freshwaters over the whole life cycle as well as diadromous species which migrate between fresh and salt waters.

In *FishBase*, the occurrence of species is reported on the level of countries. This means that data for Turkey and Russia include both species occurring in their European parts and in their Asian parts. Hence it is not surprising that omitting Turkey and Russia from the database results in a significant reduction of the number of species for consideration. It drops by about 50 % to 570 relevant freshwater species (Tab. 1). Further confining the analysis to EU Member States results in a minor additional reduction of the figure by about 12 % to 503 remaining species.

FishBase provides information on the use of species by humans in terms of two categories: *commercial use* and *game fishing*. The information on commercial use is not complete for all European countries. Commercial use includes subsistence fisheries. Commercially caught freshwater fish is usually edible but may also be traded for other purposes such as pet food or ornamental fish.

Including Turkey and Russia, 155 out of the total of 1087 species (14 %) is reported to be used by humans. Excluding Turkey and Russia, the absolute figure drops to 125 species used by humans, which is 22 % of the freshwater species occurring in these European countries. Further confining the analysis to EU Member States results in only a very minor additional reduction of the absolute figure by just one species, while the relative importance increases further. Almost 25 % of the 503 freshwater species in EU Member States are reported to be used by humans (124 species).

These **124 species with human use were considered to be of primary relevance for the examination of relevant values for trophic level (TL), lipid content (LC), and weight (W)** in the context of bioaccumulation modelling for human health risk assessments.

3.3.3 Trophic level

Based on information included in *FishBase*, Romanuk et al. (2011) prepared a compilation of all available TL values for fish. It is documented in Appendix S1 of the Supplementary Information to their article. That information was used for this work. The analysis yielded the information on the distribution of TL data for European freshwater fish given in **Table 3.1**. By definition, a TL value of 1.0 denotes phytoplankton and higher aquatic plants, 2.0 denotes primary consumers, 3.0 primary carnivores, 4.0 secondary carnivores, and so on. In reality, many fish species feed on a mixed diet and the feed may change with seasons and life stages. Therefore, TL values are means and often not whole numbers.

Including Turkey and Russia, TL values are available for 256 of the total of 1087 species occurring in freshwaters (24 %). Excluding Turkey and Russia, the absolute figure drops to 178 species, which is 31 % of all freshwater species in the remaining European countries. Further confining the analysis to EU Member States results in only a very minor additional reduction of the absolute figure by just four species. TL values are available for 174 of the 503 species occurring in freshwaters in EU Member States.

Table 3.1: Distribution of trophic level (TL) data for European freshwater fish species

		All species			**Species used by humans**[3] (commercial or game fishing)		
		Europe	Europe excl. Turkey & Russia	EU	Europe	Europe excl. Turkey & Russia	EU
Number of species[1]	all	1087	570	503	155	125	124
	TL data available	256	178	174	110	86	86
Trophic Level (TL)[2]	min	2.00	2.00	2.00	2.00	2.00	2.00
	5% quantile	2.00	2.00	2.00	2.06	2.20	2.20
	geometric mean	3.23	3.20	3.19	3.33	3.30	3.30
	median	3.26	3.23	3.22	3.33	3.33	3.33
	arithmetic mean	3.29	3.25	3.24	3.39	3.36	3.36
	95% quantile	4.31	4.30	4.24	4.39	4.39	4.39
	max	4.60	4.50	4.50	4.50	4.50	4.50

Confining the analysis to species used by humans, further reduces the absolute figures, but the relative fraction of species for which data are available increases considerably. Including Turkey and Russia, TL values are available for 110 of 155 species used by humans (71 %). Excluding Turkey and Russia, the figure decreases to 86 of 125 species (69 %). Finally confining the analysis to EU Member States,

basically does not change the picture further: TL values are available for 86 of 124 species used by humans.

The TL values for these 86 species span a range from 2.0 (primary consumers) to 4.5 (secondary and tertiary carnivores). Values for the 5 % and the 95 % quantiles are 2.2 and about 4.4 respectively. The median value is 3.3 (omnivores and primary carnivores). Geometric mean, median, and arithmetic mean are almost the same with differences of less than 0.1 units. All this indicates that the data are almost normally distributed with no significant outliers.

This distribution remains almost unchanged if the analysis is no longer confined to the values available for 86 species with human use in EU Member States, but if it is expanded to include all available TL data for all European countries and for all European freshwater species.

Based on these distribution analyses, it is concluded that **values of 2.0 and 4.5 provide realistic assumptions for the minimal and maximal trophic level of European freshwater fish consumed by humans.**

3.3.4 Lipid content (LC)

The lipid content of individual fish may change considerably with the developmental stage, seasons, and environmental conditions, in particular the availability of feed. Considerable decreases of lipid content may occur during migration or other periods of starvation. Farmed fish may be fatter than wild fish, depending on diet, feeding rate and farming conditions. For the purpose of human health risk assessments, the lipid content of adult fish in a healthy condition was of primary interest (while juvenile or ill fish may be relevant for assessing risks for predatory birds and mammals). For diadromous species, only data for freshwater live stages were relevant for the questions addressed in WP18.

Unfortunately, no database and no recent review was found to be available on the lipid content of fish that would cover a considerable fraction of European freshwater species, at least a considerable part of those 124 species which are reported to be used by humans in EU Member States.

However, for the purpose of this examination it was neither possible nor necessary to perform a comprehensive review of the issue. Instead, targeted information searches were performed with the aims of getting reliable indications for

(i) minimal and maximal LC values for all European freshwater fish that may be eaten by humans, and

(ii) minimal and maximal LC values for edible low and high trophic level species, respectively, as explained in section 2.2.2 below.

Lipid content (LC) of all edible European freshwater fish

As a primary source of information on lipid contents of relevant freshwater species, nutritional reference values were compiled which have been established by competent national and international bodies. To limit the effort, the search was confined to databases provided by

(i) the Food and Agriculture Organization of the United Nations (FAO 2016),

(ii) the German Society for Nutrition (Souci et al 2016), and

(iii) the United States Department of Agriculture (USDA 2016).

Reference values for fish LC established by these organisations

- provide means of representative sets of samples,
- refer to the edible portions of fish, and
- apply to fish in the developmental stage in which it is typically caught for human consumption at relevant sites and seasons.

These are the advantages. The disadvantage is that reference values for lipid content are available for 25 different European freshwater species only, including species which only occur in Russia and Turkey, and including values which are not specific for a single species but for groups of species from the same genus. Nevertheless, this limited set of species apparently provides a good indication for the relevant span of data, with mean values ranging from 0.7 % wet weight (ww) for pike-perch to 25.3 % for the European eel (Tab. 2).

For the purpose of defining prototype species, we rounded these values to full numbers and concluded that **1 % and 25 % (ww) provide reasonable estimates for the lower and upper end of mean lipid contents of European freshwater fish eaten by humans**.

Lipid content (LC) of edible low and high trophic level species

As already mentioned in the Section above, the bioaccumulation is expected to increase with both trophic level and lipid content. Theoretically, the best case situation with the lowest bioaccumulation potentials would therefore be represented by species with both low lipid content and low trophic level. Conversely, the worst case situation with the highest bioaccumulation would be expectable for a species with both high lipid content and high trophic level.

This raises the question, whether such best and worst case coincidences of low and high TL and LC values occur in relevant real species, or whether this would only be theoretical constructs, which lead to unrealistically low or high estimates of bioaccumulation factors.

To clarify the question, the compilation of nutritional reference values was complemented by targeted searches for relevant research papers. The searches were performed in Google and Google Scholar. As search strings, relevant species names were combined with the search terms “fat content” or “lipid content”.

The searches were performed for all relevant species on the lowest possible trophic level (TL 2.0) and all relevant species at the upper end of the trophic ladder with TL values from 4.0 to 4.5, provided that no nutritional reference values were already available.

Literature from the last 10 years was checked first. Older papers were only examined if the more recent literature did not provide sufficient information. Only data for raw fish were taken into consideration, data for processed fish food was disregarded. The same applies to data for laboratory fish used for toxicity testing or other research purposes. For diadromous species, only data for catch from freshwaters were considered.

Table 3.2: Nutritional reference values for lipid contents of edible European freshwater fish species (by order of increasing mean lipid content)

Species	FishBase name	Lipid Content RANGE [% ww]	Lipid Content MEAN [% ww]	Reference (for LC)	Occurrence in Europe (incl. Turkey and Russia)
Sander lucioperca	Pike-perch	0.3-1.97	**0.7**	Souci et al 2016	native
Lepomis gibbosus	Pumpkinseed		**0.7**	USDA 2016	introduced
Esox lucius	Northern pike		**0.8**	FAO 2016	native
Lota lota	Burbot	0.7-3.7	**0.8**	USDA 2016	native
Eleginus spp.	Navaga (different species)		**1.3**	USDA 2016	native
Osmerus eperlanus	European smelt	1.0-2.4	**1.7**	Souci et al 2016	native
Lateolabrax japonicus	Japanese seabass		**2.0**	USDA 2016	native
Morone saxatilis	Striped bass		**2.3**	USDA 2016	introduced
Ictalurus punctatus	Channel catfish	1.3-3.6	**2.8**	USDA 2016	introduced
Stenodus leucichthys	Sheefish		**2.8**	USDA 2016	native
Oncorhynchus keta	Chum salmon		**3.8**	USDA 2016	native
Mugil cephalus	Flathead grey mullet	0.9-11.8	**3.8**	USDA 2016	native
Clarias gariepinus	North African catfish		**3.8**	FAO 2016	native
Oncorhynchus nerka	Sockeye salmon	3.9-5.6	**4.7**	USDA 2016	native
Cyprinus carpio	Common carp	0.9-19.0	**5.2**	Souci et al 2016	native
Oncorhynchus mykiss	Rainbow trout		**5.2**	FAO 2016	native
Coregonus spp.	Whitefish (different species)		**5.9**	USDA 2016	native
Oncorhynchus kisutch	Coho salmon		**5.9**	USDA 2016	native

Silurus glanis	Wels catfish	3.4-19.9	**7.4**	Souci et al 2016	native
Salmo trutta	Sea trout	1.7-10.2	**7.6**	Souci et al 2016	native
Acipenser spp.	Sturgeon (different species	1.9-9.2	**8.5**	Souci et al 2016	native
Oncorhynchus tshawytscha	Chinook salmon	3.3-19.6	**10.4**	USDA 2016	native
Salmo salar	Atlantic salmon	3.8-18.1	**11.5**	Souci et al 2016	native
Alosa sapidissima	American shad		**13.8**	USDA 2016	introduced
Anguilla anguilla	European eel	7.1-32.5	**25.3**	Souci et al 2016	native

Where searches provided several data for the same species, selections were made according to the following rules:

- data from Europe were preferred over data from North America or other continents,
- data for wild fish were preferred over data for farmed fish and data for natural populations were preferred over domesticated strains that have undergone selective breeding,
- data with an indication of the range of measured values were preferred over single means,
- where different means for different samples were available from the same or from different studies, the highest mean was chosen.

As a result, the nutritional reference values were complemented by data for another seven relevant species at the higher and the lower end of the trophic web (**Table 3.3**).

Examination of the data shows:

- Edible species with both a low trophic level of 2.0 and a low lipid content in the range of 1 % (ww) indeed exists. Examples are the common nase and the grass carp.
- Edible species with both a high trophic level value of 4.0 or larger and an upper-end mean lipid content of about 25 %, however, do not exist in European freshwaters.
- For edible high trophic level fish species, the maximal reported mean lipid contents are in a range of about 15 %. Examples are the sea lamprey (13.4 % LC), the lake trout (15.2 % LC), and the river lamprey (16.1 % LC).
- In contrast, the edible species with the highest mean lipid content of about 25 %, the European eel, is an omnivorous species with a trophic level of only 3.5.

Given these findings, **the necessity resulted to define two different types of possible worst case situations for bioaccumulation modelling:**

(i) a maximal trophic level of 4.5 in combination with a mean lipid content of about 15 %, and

(ii) a maximal lipid content of about 25 % in combination with a moderate trophic level of about 3.5.

Polar lipids fraction

It is well known that almost all fish, crustaceans, and molluscs contain phospholipids at a level of approximately 0.7 to 1.0 % (ww) to maintain cellular integrity (Gooch et al. 1987, Hendriks et al. 2005). For the purpose of defining prototype species for fish bioaccumulation modelling, we chose a default estimate of 0.8 %. The remainder of the total lipid content is assumed to be neutral storage fat.

Weight (WL)

Stadnicka et al (2012) have performed sensitivity analyses of toxico-kinetic model predictions for bioconcentration in rainbow trout and fathead minnow. The results showed that

(i) the fish weight has a much smaller impact on predicted internal concentrations than the fish lipid content, and

(ii) a significant decrease of bioconcentration with increasing fish weight is only seen for small fish. In rainbow trout no more significant decrease was seen when the fish weight reached values of about 2 kg and beyond (Fig. S3 in the Supporting Information to Stadnicka et al 2012).

We assumed that the same may apply to predictions generated by means of the food-web bioaccumulation model used in SOLUTIONS. As a consequence, 2 kg fish fresh weight was considered to provide a reasonable estimate for a best case situation in which predicted bioaccumulation rates get minimal.

For the opposite situation we assumed a minimal weight of 20 g. The reasons for this assumption are the following:

- eating of very small fish below 20 g is a usual habit for some marine species such as anchovies, but usually not for freshwater species,
- adult stages of relevant freshwater species are usually larger than 20g, and catching of juvenile fish does not comply with the principles of sustainable fisheries which is assumed to be respected by the actors involved.

3.3.5 Summary of suggested scenarios

In summary of the considerations detailed in the preceding sections, three different prototype fish were defined for the purpose of bioaccumulation modelling in WP18, representing two different worst case scenarios and a single best case scenario. In **Table 3.4**, the properties of these three prototype fish are defined in terms of the three biological model input parameters TL, LC, and W. Illustrative examples for real fish species representing these parameter constellations are included in the Table.

Table 3.3: Lipid content of edible high and low trophic level freshwater fish species
(by order of increasing mean lipid content)

Species	FishBase name	TL	Lipids proximate mean [% ww]	Matrix	Reference (for LC)	Occurrence in Europe (incl. Turkey and Russia)
High Trophic Level (TL 4.0 - 4.5)						
Sander lucioperca	Pike-perch	3.99	0.7	edible portion	Souci et al 2016	native
Esox lucius	Northern pike	4.40	0.8	edible portion	FAO 2016	native
Lota lota	Burbot	4.03	0.8	edible portion	USDA 2016	native
Perca fluviatilis	European perch	4.35	0.9	muscles	Luczynska et al 2008	native
Morone saxatilis	Striped bass	4.50	2.3	edible portion	USDA 2016	introduced
Stenodus leucichthys	Sheefish	4.15	2.8	edible portion	USDA 2016	native
Sander volgensis	Volga pikeperch	4.13	4.2	whole fish	Szabo et al 2009	native
Oncorhynchus gorbuscha	Pink salmon	4.19	4.4	edible portion	Souci et al 2016	native
Oncorhynchus mykiss	Rainbow trout	4.42	5.2	edible portion	FAO 2016	native
Oncorhynchus kisutch	Coho salmon	4.22	5.9	edible portion	USDA 2016	native
Silurus glanis	Wels catfish	4.37	7.4	edible portion	Souci et al 2016	native
Salmo salar	Atlantic salmon	4.43	11.5	edible portion	Souci et al 2016	native

Petromyzon marinus	Sea lamprey	4.37	13.4	edible portion	Arajo et al 2013	native
Salvelinus namaycush	Lake trout	4.29	15.2	whole fish	Hoffman et al 1999	introduced
Lampetra fluviatilis	River lamprey	**4.50**	**16.1**	edible portion	Merivirta 2007	native
Low Trophic Level (TL 2.0)						
Chondrostoma nasus	Common nase	2.00	1.3	edible portion	Aggelousis et al 1991	native
Ctenopharyngodon idella	Grass carp	2.00	0.5 - 1.4	edible portion	Shimma and Shimma 1969	introduced
Hypophthalmichthys molitrix	Silver carp	2,00	5,5	fillet	Romvari et al. 2002	introduced

Table 3.4: Summary of suggested definitions of prototype fish for the modelling of best and worst case bioaccumulation scenarios

Scenario	Weight	Trophic Level (TL)	Lipid Content (LC) [% wet weight]			Representative Species (for TL and LC)
			Polar	Neutral	Total	
Worst Case I: max TL	20 g	4.5	0.8 %	14.2 %	15.0 %	Lake trout River lamprey Sea lamprey
Worst Case II: max LC	20 g	3.5	0.8 %	24.2 %	25.0 %	Eel
Best Case	2,000 g	2.0	0.8 %	0.2 %	1.0 %	Grass carp Common nase

3.3.6 Adjustments for meeting model requirements

The food-web bioaccumulation model used in WP18 requires integers as input values for TL; it is not able to deal with decimal digits. As a consequence, for practical model runs TL values for worst cases I and II, were adjusted to 4.0 and 3.0, respectively.

3.4 References

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4 Case study of chronic mixture risks to fish and humans: Evaluation of the utility of the decision tree on the basis of monitored water concentrations

In the following section we assess the value of the framework by way of a case study of MRA for 293 chemicals monitored at the confluence of the rivers Arges and Danube in Romania (Joint Danube Survey, JDS 3, site 58, Liska et al. 2015). We estimate chronic mixture risks to fish and possible human health risks that might arise from consumption of fish and drinking water at this site. We examine the extent to which our framework can realise the scientific principles of CA in a step-wise fashion with the toxicity data normally available in regulatory practice and investigate the degree of bias introduced by omitting chemicals from the analysis due to missing toxicity data and explore ways of bridging toxicity data gaps. Finally, we assess whether our proposed decision criteria are helpful in excluding or substantiating possible mixture risks on the basis of available exposure and toxicity data and whether this provides clear guidance for risk assessment practitioners as to when risk management measures should be considered.

Following the ideas expressed by Solomon et al. (2016) and Moretto et al. (2017), our case study begins with a problem formulation step.

4.1 Problem formulation

Europe-wide water monitoring programmes have revealed the presence of hundreds of chemicals in European riverine waters (Busch et al. 2016). Many of these chemicals have the potential to exhibit common toxicities to aquatic organisms and humans. An assessment of potential combined toxicities is therefore warranted. Our aim was to assess whether fish are protected from direct toxicity of multiple pollutants in the water column. We also investigated whether drinking water quality goals are met when taking account of combined exposures, and whether fish caught from riverine sites are fit for human consumption.

Possible mixture risks to algae and macroinvertebrates were excluded from this case study; these topics will be addressed in the subsequent section on the basis of modelled concentrations of pollutants in European surface waters.

To realise our goals, we selected a monitoring site of the Joint Danube Survey 3 (JDS 3) at the confluence of the rivers Arges and Danube in Romania. At this site (JDS 3, site 58) the concentrations of 293 chemicals were measured. The site is representative of the pollution patterns seen in the Danube, with pollutant water concentrations in the mid-range; we could have selected a multitude of sites with similar patterns.

4.2 Materials and Methods

4.2.1 Features of the JDS monitoring data

During the JDS 3 monitoring exercise, a wide range of pesticides, pharmaceuticals, and industrial chemicals was measured at 68 monitoring stations). Common cations such as sodium, potassium, magnesium, and calcium and anions such as chloride, sulfate, or phosphate are excluded from the

analysis as they do not normally present direct toxic hazards. The monitoring data are shown in **Annex 2** to this Deliverable.

4.2.2 Features of the monitoring site

Monitoring site 58 of JDS 3 is situated at the confluence of the rivers Arges and Danube in Romania and Bulgaria, southeast of Bucharest, near the towns of Tutrakan (Bulgaria) and Oltenita (Romania). The site is in an agricultural area; there are no obvious industrial emissions (**Figure 4.1**).

Figure 4.1: Location of monitoring site 58 at the confluence of Arges and Danube. **Google maps**

4.2.3 Assumptions for exposure assessment in human MRA

To determine the exposure to contaminants via drinking water or consumption of contaminated fishery products for human MRA, regulatory values (RV) or their equivalents were converted to express tolerable concentrations in drinking water or fish. In these conversions we used the following assumptions (as outlined in EC 2011): human body weight of 70 kg, daily water consumption of 2 L and 0.115 kg fish consumption. We allocated 10% of the permissible total exposure to uptake via drinking water and 10% to fish consumption. Further, it was assumed that surface water is consumed untreated.

4.2.4 Provenance of regulatory values and toxicity data

At Tier 1 fish ecotoxicological MRA, quality standards (QS) for the pelagic community were used, which were available for 25 chemicals. For the remaining chemicals, we retrieved chronic toxicity values (NOECs and equivalent) and applied the decision rules for the deterministic approach of the WFD guidance document No 27 (EC 2011), as follows: a QS for protection of the pelagic community was derived using the lowest chronic toxicity value from the three taxa (algae, daphnids and fish) in combination with an assessment factor (AF) which depended on the availability of data. If only one long-term result for either fish or daphnia was available, an AF of 100 was applied. For two long-term results from two trophic levels (fish and/or daphnids and/or algae) the AF was 50. Finally, if long-term data for

all three taxa were available an AF of 10 was used. Data from species sensitivity distributions (SSD), from field experiments or short-term studies were not used.

At Tier 2 of the fish MRA, the lowest available NOEC from long-term toxicity data for fish were identified for 66 chemicals. At TIER 2A, the lowest NOEC, irrespective of toxic endpoint was applied. After driver identification, the lowest NOEC for reproductive toxicity was used for Tier 2B.

Human chronic toxicity data were located for 198 chemicals: In Tier 1, QS for drinking water or consumption of fish were used. 25 QS were available for WFD priority substances (PS), for all other compounds the equivalent provisional guideline values (pGLV) for drinking water and consumption of fish were derived in accordance with WFD GD27. For WFD PS with default QS, such as pesticides (0.1 µg/l), this was replaced by a health based guideline value derived from available toxicity data. (p)GLVs for Tier 1 were based on acceptable daily intake (ADI) or tolerable daily intake (TDI) where available. For substances where a ADI or TDI was not available, these were derived from the lowest available NOAEL by combination with a default assessment factor of 100. For pharmaceuticals for which no toxicity data was available, equivalent values were derived using the derived daily dose (DDD) divided by bodyweight (70 kg), as previously described (Schriks et al. 2010, Houtman et al. 2014). The pGLVs for drinking water (DW) and fish consumption (food) were calculated using the equations below, respectively.

$$pGLV_{DW} = \frac{0.1 \times ADI \times bw}{uptake_{DW}}$$

$$pGLV_{food} = \frac{0.1 \times ADI \times bw}{uptake_{food}}$$

A bodyweight (bw) of 70 kg, drinking water consumption ($uptake_{DW}$) of 2 L/day and fish consumption of 0.115 kg/day ($uptake_{food}$) were assumed. Both equations contain an allocation factor of 10% to account for the fraction of the toxicity value allocated to drinking water or fish consumption.

In Tier 2, the AF were removed and the ADI values in the equations above were replaced by NOAELs, including the NOAELs for pharmaceuticals which were used to derive DDD.

Toxicity data for fish and human MRA can be found in **Annex 3**.

4.2.5 Dealing with missing toxicity data

The large number of chemicals for which toxicity data could not be retrieved made it necessary to bridge these data gaps.

For ecotoxicological data, values were available for 79 and 67 chemicals in Tier 1 and 2, respectively. Thus, data gaps had to be bridged for 214 and 226 compounds in Tier 1 and 2. For human toxicity, data were available for 198 chemicals, for the remaining 95 chemicals, the gaps had to be bridged.

For the fish toxicity MRA we adopted the equivalent of the human TTC concept by constructing frequency distributions of taxa-specific chronic NOECs for algae, daphnids and fish similar to previously suggested approaches (Belanger et al. 2015). To derive the distributions we used all available chronic toxicity data for the three taxa and derived the 5th percentile values. In addition, we also determined the 50th percentiles. In Tier 1, the lowest value of the three taxa was used in combination with an assessment factor (100). The 5th and 50th percentile values for fish toxicity were used in Tier 2.

Data gaps in the human MRA were bridged using the TTC approach in line with the recent review by EFSA and WHO (2016). First, the Cramer class for each compound without toxicity data was determined, as well as structural alerts for genotoxicity, using Toxtree 2.6.13 (Patlewicz et al. 2008). TTC values for the Cramer structural classes III, II and I used were or 30, 9 and 1.5 µg/kg bw /day, for organophosphates or carbamates a TTC of 0.3 µg/kg bw/day and for compounds with genotoxic structural alerts a value of 0.0025 µg/kg bw/day was used (Kroes et al. 2004, EFSA and WHO, 2016). Specific TTCs for drinking water values have previously been proposed (Mons et al. 2013, Baken et al. 2018). However, to use consistent values for assessment of exposures via drinking water and fish consumption, we decided to use the above values in conjunction with equations x and y to derive pGLV both exposure routes in Tier 1. In Tier 2, the AF of 100, which is contained within the TTC was removed and the pGLV were derived as before.

4.2.6 Fish accumulation modelling

The internal levels of water pollutants in fish were modelled with monitored concentrations as input. It is well established that the degree to which fish can accumulate pollutants dissolved in the water column depend on three major factors: Trophic level, size of the fish and fat content of the fish. Rather than conducting the modelling for specific species of fish, we defined three prototypes. The details of the fish accumulation modelling are described in the preceding Section 3.

4.3 Ecotoxicological MRA for chronic toxicity to fish

4.3.1 Tier 1 MRA for pelagic organisms and fish

Tier 1 MRA (**Fig 2.2**) uses the Hazard Index method (HI) to generate an initial worst case mixture risk estimate. The procedure starts in Step 1 with the definition of the mixture of concern in terms of components (*i*) and exposure levels for pelagic organisms including fish ($EL_{i,FISH}$). The analysis continues with the compilation of regulatory reference values (RV) for all mixture components as the necessary input data (Step 2). These RV are intended to protect all pelagic water organisms from direct toxicity and are derived from toxicity data for algae, daphnia and fish (**Annex 2)**. Since RVs were not available for all monitored chemicals, we derived equivalent values by applying established decision rules and AF (EC 2011, see Materials and Methods).

For mixture components of unknown toxicity, Step 3 introduces a loop for bridging data gaps. We employed an approach similar to the proposed eco-TTC (Belanger et al. 2015), by constructing taxa-specific frequency distributions of NOECs for a variety of toxicity endpoints based on 1200 chemicals. For algae, this distribution had a median of 600 µg/L and a 5th percentile of 1 µg/L. The corresponding values for daphnia were 100 µg/L and 0.04 µg/L and for fish 87 µg/L and 0.039 µg/L. We then derived estimated Quality Standards for the protection of pelagic organisms from direct toxicity of water pollutants by applying the decision rules defined in WFD guidance document 27. Accordingly, we combined the lowest of these taxa-specific estimates with an AF of 100. The lowest estimates were from the frequency distributions for toxicity to fish. Accordingly, the 5th percentile (0.039 µg/L) yielded an estimated RV of 0.00039 µg/L (here referred to as “ecoTTC”) and the median of this distribution (87 µg/L) produced an estimated RV of 0.87 µg/L. These values were used for chemicals with unknown toxicity.

The resulting HI were calculated In Step 4 of Tier 1 MRA. Application of the conservative eco-TTC approach produced an HI of 67650, far in excess of 1. When the toxicity data gaps were bridged by estimating RV on the basis of the 50th percentile, the HI reduced to 167.6.

As both scenarios produced HI in excess of 1, we proceeded by identifying drivers in Step 5 of the analysis. We compared the results obtained on the basis of three operational definitions: First, we used the approach by Price et al. (2012) and defined as driver a chemical that contributes >50% to the HI. There was no chemical that fulfilled this criterion. Next, we identified drivers in terms of RQ that exceed the average RQ. With the conservative "eco-TTC" approach for bridging toxicity data gaps, every chemical whose unknown toxicity had to be estimated turned out to be a driver (25 of the 293 chemicals). With the less conservative estimate based on the median of the potency distribution in fish, 24 of the 293 monitored substances were identified as drivers. Of these, 10 substances were of unknown toxicity. Finally, we defined as drivers those chemicals whose RQ collectively exceeded the acceptable HI of 1. With the eco-TTC approach for bridging toxicity data gaps, this returned 241 of the 293 monitored chemicals as drivers. Almost all the untested chemicals with an estimated NOEC at the 5th percentile were drivers. Under the assumption of median potency for substances with unknown toxicity, 98 chemicals were identified as drivers. Of these, 55 were of unknown toxicity. We therefore abandoned the use of the eco-TTC approach for estimating the toxicity of untested substances. It would appear that the large number of drivers returned under these assumptions makes the driver concept unworkable.

Step 6 introduces an assessment loop to capture chemicals with missing toxicity data that were identified as drivers. In Step 7, these chemicals are added to Pool I, the chemicals with high testing priority. Furthermore, all chemicals with unknown toxicity are removed from the analysis and the HI determined again. This filtering step reduced the HI from 167.6 to 137. Had the HI no longer exceeded 1 after this step, the Tier 1 evaluation would have been suspended until toxicity data gaps had been closed. However, in our case, the analysis proceeds to Tier 2.

4.3.2 Tier 2 MRA for fish

Conceptual considerations and deviations from the scheme proposed in Section 2

The basic feature that distinguishes Tier 2 MRA from the effort in Tier 1 is in the avoidance of the use of single substance data that already include AFs, thereby removing the distorting effect that varying AFs may have on the mixture toxicity calculations. The method of choice that is adequate for this approach is the PODI. The assessment progresses in a step-wise fashion to approximate the scientific principles of the CA concept, from Tier 2A to Tier 2C. A margin of exposure of between 10 and 100 should be applied, equivalent to a PODI of between 0.01 and 0.1. Thus, the MRA can be discontinued if the PODI is below 0.01.

For Tier 2A assessments, the lowest POD values for the relevant test species-groups were used as input data, i.e. $NOEC_{i,\ FISH}$ for fish risk assessment. In addition to removing possible distortions introduced by differing AFs, Tier 2A also eliminates distortions that had to be introduced in Tier 1 through the merging of toxicity data from physiologically not comparable species, such as algae, daphnids and fish.

For Tier 2B assessments, the NOAELs and NOECs used in Tier 2A for different toxicities should have been replaced by statistics that describe effect concentrations associated with the same effect magnitude, e.g. EC10 or benchmark concentrations. However, we found that these statistics were rarely measured with the consequence that relevant data could not be located for the majority of chemicals. We therefore based the analysis in Tier 2B on chronic NOECs for reproductive toxicity to fish. In this way, the assessment was moved towards effects with clearly defined adversity, without mixing of different toxicity endpoints. However, data from different fish species were used.

Finally, in Tier 2C assessments, the TUS approach should have been employed, with endpoint specific benchmark doses or low-effect concentrations for reproductive toxicity in the same fish species as input data. In this way, distortions of mixture toxicity calculations are removed that may result from aggregations of toxicity data across different fish species. As shown below, this was only partly achieved.

Tier 2A MRA for fish

As before, the Tier 2A analysis begins with a compilation of relevant toxicity input values for all 293 chemicals monitored at site 58 JDS (**Annex 2**), in this case the lowest chronic NOECs observed in different species of fish for any toxicity endpoint.

As in Tier 1, gaps from missing chronic toxicity data were bridged by assigning the 5th and 50th percentile of the frequency distribution for NOECs in fish; here 0.039 and 87 µg/L, respectively, followed by a determination of the PODI. With the assumption that the toxicity of untested substances is at the 5th percentile of the NOEC frequency distribution for fish, the PODI was determined as 743; under the assumption of a NOEC at the 50th percentile of the distribution, the PODI reduced to 6.29.

As both calculations returned PODIs far in excess of acceptable levels (i.e. > 0.1), we proceeded to identifying drivers. Since only substances identified as drivers in Tier 2A will be taken forward to subsequent Tiers, it is essential that the most inclusive operational criterion for driver identification is used at this stage. The analysis in Tier 1 has shown that driver identification in terms of the group of chemicals whose PODI collectively exceeds 0.01 when ranked according to size, from smallest to largest, meets these requirements. We therefore applied this method.

With the assumption that the NOECs for chemicals with unknown chronic toxicity to fish is equivalent to the 5th percentile of the frequency distribution, we identified 247 of the 293 monitored chemicals as drivers. Of these, 224 were substances not tested in fish. With the less conservative estimate of NOECs at the 50th percentile, the number of drivers reduced to 94 of the 293 monitored chemicals, of which 63 were of unknown toxicity to fish.

When we removed all drivers with missing fish chronic toxicity data from consideration, 31 chemicals were left. With these, the PODI reduced to 5.89, well above the trigger level of 0.1. Accordingly, the analysis proceeded to Tier 2B.

Tier 2B MRA for fish

In Tier 2B, the assessment becomes endpoint-specific with a focus on reproductive toxicity which is regarded as critical for risk assessments in fish. Thus, we abandoned the mixing of different chronic toxicity endpoints in fish and increased the comparability of RQ by admitting only NOECs for chronic

reproductive toxicity in fish as toxicity input values. At this stage, it was not deemed necessary to repeat all assessment steps of the decision tree with the full set of the 293 monitored chemicals. Instead, only the 31 chemicals identified as drivers in Tier 2A were taken forward to Tier 2B. This shortcut assumes that the set of 31 Tier 2A drivers encompasses all Tier 2B drivers. This is only possible if the Tier 2A analysis is strictly based on the lowest chronic NOECs for any endpoint, leading to correspondingly higher mixture toxicity estimates. Thus, substitution for reproductive toxicity-specific NOECs should yield the same, or lower mixture risk estimates than in Tier 2A.

Table 4.1: Tier 2B MRA for fish for JDS 3 site 58

Drivers Tier 2B fish							
non-detects set to LOD							
Reproduction							
PODI = 2.43							
bold: analytical non-detects							
11 out of 293 chemicals							
CAS	**Chemical**	**POD (NOEC) ug/L**	**Species**	**Toxicity endpoint**	**Source**	**concentration ug/L**	**conc/POD site 58**
50-28-2	**17-beta Estradiol**	0.0005	Oncorhynchus mykiss	semen quality, semen fertility	Lahnsteiner 2005	0.001	2
1912-24-9	Atrazine	0.50	Pimephales promelas	repro egg prod	Tillitt 2010	0.07	0.14
298-46-4	Carbamazepine	**0.50**	Danio rerio	embryo production	Galus 2013	0.068	0.136
525-66-6	Propranolol	0.50	Oryzias latipes	repro number of eggs, hatchabilit	Huggett 2002	0.06	0.12
120068-37-3	Fipronil	0.85	Cyprinodon variegatus	repro	US EPA OPP data	0.02	0.023529
333-41-5	Diazinone	0.9160	Pimephales promelas	repro	US EPA OPP data	0.007	0.007642
104-40-5	Nonylphenol (4-Nonyl	5.00	?	repro, survival	Lei et al 2012	0.012	0.0024
60207-90-1	**Propiconazole**	5.00	Pimephales promelas	egg production	Skolness 2013	0.003	0.0006
80-05-7	**Bisphenol A**	10	Danio rerio	repro, egg prod	Keiter 2012	0.0056	0.00056
15307-79-6	Diclofenac	1000.00	Oryzias latipes	repro egg hatchability	Lee 2011	0.25	0.00025
1071-83-6	**Glyphosate**	500.00	Jenynsia multidentata	repro	Hued 2012	0.015	0.00003
122-34-9	Simazine	no data				0.0013	0
88-85-7	**Dinoseb**	no data				0.004	0
37350-58-6	Metoprolol	no data				0.82	0
41859-67-0	**Bezafibrate**	no data				0.005	0
117-81-7	Di(2-ethylhexyl)phthal	no data				0.48	0
330-55-2	Linuron	no data				0.0057	0
886-50-0	Terbutryn	no data				0.0029	0
124495-18-7	**Quinoxyfen**	no data				0.004	0

We made adjustments for the bioavailability of metals and PAHs on the exposure assessment arm of the MRA. The monitoring data for these chemicals represent the total levels including the fraction adsorbed to particulate matter or present as metal complexes. The fraction that is bioavailable to fish from the water column can be regarded as negligible, due to speciations (metals) or adsorption to particulate matter (relevant for substances with high log Kow as e.g. PAHs). For this reason, all metals and PAHs among the 31 Tier 2A drivers were omitted from further consideration. This left 19 chemicals. In the Tier 2A analysis, this would have reduced the PODI from 5.89 to 5.62.

We replaced the NOECs used in Tier 2A with NOECs for endpoints relevant to chronic reproductive toxicity, including semen quality, egg production and egg hatchability. For 11 of the 19 chemicals, relevant chronic NOECs could be retrieved. The PODI for these substances was 2.43 (**Table 4.1**). Assuming that the reproductive toxicity of the remaining 8 chemicals for which relevant data could not

be identified is in the same range as the NOECs for Tier 2A toxicity endpoints, 0.35 would have to be added, increasing the PODI estimate to 2.78.

Four of the chemicals, 17 beta-estradiol, atrazine, carbamazepine and propranolol, had concentration/POD ratios above the trigger level of 0.1. We judged that these chemicals require risk management measures and returned them to Pool II.

Tier 2C MRA for fish: chronic reproductive toxicity in the same species of fish

The Tier 2C assessment becomes endpoint- and species-specific. Hence, we took the 11 chemicals from Tier 2B and arranged their RQs according to NOECs from the same species. This produced three groups of substances with reproductive NOECs for 2 or more species: (i) atrazine, diazinone and proprioconazole for the fathead minnow (*Pimephales promelas)* with a PODI of 0.148; (ii) carbamazepine and bisphenol A for the zebrafish (*Danio rerio*) with a PODI of 0.136 and (iii) propranolol and diclofenac for the medaka (*Oryzias latipes*) with a PODI of 0.12. In each of these groups, only one chemical contributed the lion's share of the PODI (atrazine, carbamazepine and propranolol, respectively). The impact of the other substances on the PODI was negligible. As the PODI's in each of these groups was above 0.1, the analysis moved to Tier 3A.

4.3.3 Tier 3 MRA for fish

Tier 3A MRA for fish

In Tier 3A we evaluated whether a significant risk can be estimated for one or more individual mixture components for chronic reproductive toxicity in fish. As shown in **Table 4.1**, 17 beta-estradiol, atrazine, carbamazepine, and propranolol exhibited concentration/POD ratios above 0.1. Of these, 17 beta-estradiol was an analytical non-detect and we assumed the LOD as the effective concentration for this substance. If we relax this conservative assumption and replace the LOD with 0.5 LOD, the concentration/POD ratio for 17 beta-estradiol changes to 1, still above the critical level of 0.1.

Thus, under the assumption of IA, the combined acceptable mixture exposure cannot be smaller than that of 17 beta-estradiol alone. Since this exposure is above levels estimated to be acceptable, there is no incentive to further substantiate mixture risks. Accordingly, we discontinued the evaluation and concluded that significant risks from single substances cannot be ruled out by assuming IA for dissimilarly acting (groups of) mixture components.

4.4 Human MRA for drinking water intake

4.4.1 Tier 1 MRA for human drinking water intake

Tier 1 is essentially a scoping assessment to gather whether there might be potential human health risk from utilizing water drawn at JDS 3 site 58 as drinking water without further treatment. As before, the analysis began by collecting relevant RV, in this case drinking water Quality Standards (**Annex 3**). 25 of the compounds were WFD-PS, for which QS values were available. Additional drinking water standards were available from the WHO, the US and Australia. As recommended in risk assessment guidance (EC 2011), we allocated 10% of the RV to drinking water consumption of 2 L per day and assumed a body weight of 70 kg. For 95 of the 293 monitored chemicals, human relevant toxicity data were not

available. We bridged these data gaps by adopting the TTC approach. This produced an HI of 367. We identified 20 substances as drivers, by arraying their HQ from largest to smallest and determining the rank associated with an HI – 1 = 366. Among these drivers, there were 16 chemicals for which we had to assign toxicity estimates according to the TTC approach. After omission of these 16 substances from further consideration, the HI reduced to 3.9, still larger than the acceptable level of 1. Accordingly, we continued with a Tier 2A analysis.

4.4.2 Tier 2A MRA for human drinking water intake

The assessment factors used to derive the RV in the Tier 1 analysis ranged from 1 to 3000. To avoid the possible distorting effect this may have on the MRA, we used toxicity values without AF. As before, toxicity data gaps were bridged by using the TTC approach.

Table 4.2: Tier 2A MRA for human drinking water

Tier 2A			
PODI minus unknowns		**PODI**	**1.410952**
Sorted on conc/POD xAF			
Chemicals	**JDS58 conc/POD**	**AF**	**Conc/POD x AF**
Arsenic (As) - dissolved	0.892857	1	0.892857
Lead (Pb) - dissolved	0.245714	1	0.245714
Atropine	0.001867	100	0.186667
Nickel (Ni) - dissolved	0.000857	100	0.085714
PODI			**1.410952**

The use of the PODI requires considerations of appropriate margins of exposure. In line with accepted practice for single chemical risk assessment we used a margin of exposure of 100 for toxicity data from animal experiments, equivalent to an AF of 100. The RV for some chemicals (e.g. arsenic, lead, cadmium) were based on human observations. For such substances we assumed an AF of 1.

Since the calculation of the PODI was based on an AF of 100 for the majority of the chemicals entered into this analysis, its value (365) did not differ much from the HI of 367 estimated in Tier 1 of this analysis. We identified 19 of these chemicals as drivers, 15 of which were assigned TTC values.

Removal of chemicals with insufficient toxicity data to establish acceptable human exposures left 4 substances which together gave a PODI of 1.41, larger than the acceptable value of 1. This would have mandated continuation of the analysis in Tier 2B. However, for the 4 chemicals returned by this analysis (arsenic, lead, atropine and nickel) a common toxicity could not be identified. Furthermore, none of these substances exceeded their critical RQ. For these reasons, continuation of the assessment was not possible (**Table 4.2**).

4.5 Human MRA for fish consumption

4.5.1 Tier 1 MRA for human fish consumption

In line with established risk assessment practice (EC 2011) we assumed a daily fish consumption of 112 g, and a human body weight of 70 kg. As with the drinking water MRA, we allocated 10% of RV to fish

consumption (EC 2011). The internal concentrations in fish that result from the monitored levels were calculated for piscivorous fish (**Annex 3**). The analysis followed the same steps as outlined above for the drinking water analysis. We estimated an HI of 4944, and identified 25 of the 293 chemicals entered into this analysis as drivers, of which 13 were of unknown toxicity, bridged by using the TTC concept.

After removal of substances with unknown toxicity from the analysis, the HI reduced to 120, mandating a continuation in Tier 2A.

4.5.2 Tier 2A MRA for human fish consumption

By making the same assumptions about margins of exposure and AF as in the Tier 2A MRA for drinking water, we calculated a PODI of 4943, essentially the same value as returned by the HI approach. We identified 23 chemicals as drivers, with 13 chemicals among them for which the toxicity was estimated by using the TTC approach.

Table 4.3: Tier 2A MRA for human fish consumption

Tier 2A drivers minus unknowns minus PAHs						
PODI	108.5					
Chemicals in order	**intake/POD**	**AF**	**intake/POD xAF**	**POD mg/k**	**intake from fish site 58, mg/kg**	**Toxicity endpoint**
Telmisartan	1.025438	100	102.5438	34.8	35.6	Blood pressure lowering, angiotensin II inh
Digitoxin	0.044515	100	4.45154	0.087	0.003871	cardiovascular, cardiac arrhythmia
Fipronil	0.012828	100	1.282763	1.217	0.015616	neurotoxicity
Flupentixol	0.002232	100	0.223188	5.17	0.011645	nervous system, antidepressant
PODI			**108.5013**			

Omitting the 13 chemicals for which acceptable exposures were estimated by TTC reduced the PODI to 119. Among the 10 remaining chemicals were 5 PAHs and the phthalate DEHP. However, the modelled fish concentrations for these chemicals are likely to be overestimated, as total concentrations, and not their bioavailable fractions were used as input values. It can be assumed that the fraction bioavailable to fish is negligible, and accordingly the resulting internal concentrations in fish can be predicted to be very low. We therefore removed these chemicals from further consideration and were left with 4 substances, telmisartan, digitoxin, fipronil and flupentixol which together gave a PODI of 108 (**Table 4.3**). The lion's share of this was contributed by the blood pressure lowering drug telmisartan. The values for digitoxin and fipronil also exceeded the acceptable limit of 1.

As with the drinking water MRA, this outcome would mandate continuation of the analysis in Tier 2B. However, the 4 chemicals returned by this analysis show toxicities that are hard to aggregate in terms of common adverse outcomes. Furthermore, 3 of these chemicals, telmisartan, digitoxin and fipronil, exceed their individual acceptable exposures.

4.6 Discussion

Our new framework implements a tiering scheme that systematically removes the uncertainties associated with widely used CA-based methods (HI, PODI, PEC/PNEC ratios) by realising the data

requirements of the scientific principles of CA. Combined with quantitative criteria for the identification of drivers, this tiering scheme proved to be effective in isolating sub-sets of chemicals for which the required toxicity data were available and for which mixture risks could be established with relative certainty. This may deliver useful information to water quality managers who want to assess the likelihood that mixture exposures may prohibit reaching the WFD and public health targets. For the first time, we delimit when the alternative concept of IA can meaningfully be introduced into the scheme without stalling the assessment. This enabled us to establish the lower limits of estimated mixture risks that are to be expected from IA-based best case estimates.

4.6.1 The MRA for fish

Of the three investigated scenarios (chronic risks to fish, human health risks from drinking water consumption and intake of fish caught at the study site), the predicted mixture risks to fish reproduction were the most pronounced. With the data available from toxicity databases, it was possible to extend the more conservative CA-based MRA to the lower margin of the "prediction window" that is delimited by IA-based predictions. The analysis was stopped at Tier 3A; further refinements would have been pointless since the modelled risks attributed to 17-beta estradiol alone, the substance projected to make the largest contribution to the overall mixture risk, exceeded acceptable concentrations. The smallest expected mixture effect derived from IA cannot be smaller than the effect already produced by 17-beta estradiol. However, as is often the case with hormonally active substances of great potency, the monitored levels of 17-beta estradiol stayed below the LOD of the chosen analytical method. We therefore used the LOD as the estimated concentration, but alternative concentration estimates, such as 0.5 LOD would still have yielded an RQ 10-fold above acceptable levels, in the range of concentrations that induced reproductive toxicity in experimental studies (Lahnsteiner et al. 2006). The proximity of the monitoring site to the towns of Tutrakan and Oltenita southeast of Bucharest makes it likely that 17 beta-estradiol is present at biologically active levels. The issue could be resolved by effect-based testing with suitable bioassays.

A more definitive estimate of the lower limit of the IA-based mixture risk could have been derived by including atrazine, carbamazepine and propranolol, which also exceeded their acceptable concentrations individually. However, this would have necessitated forming sub-groupings of 17-beta estradiol, atrazine, carbamazepine and propranolol according to similar modes of action involved in fish reproductive toxicity, but this information is not currently available. Furthermore, the estimation of IA-derived mixture risks of 17-beta estradiol, atrazine, carbamazepine and propranolol by aggregation of mode of action subgroups would have required dose-response information in the range of small effects, data that are also not available. By steering clear of a decision step that screens for modes of action at the early stages of the MRA, and by relegating such considerations to the higher tiers of our framework, we avoided stalling the analysis without conclusive results.

The most definitive CA-derived estimate for fish reproductive toxicity (Tier 2B) was based on 11 chemicals and returned a PODI of 2.43. This reduces to 1.43 if we substitute the 17-beta estradiol LOD with 0.5 LOD, still 14-fold above trigger levels, and indicating that the goals of the WFD are not met. Together, atrazine, carbamazepine and propranolol contributed 0.39 to the PODI. The remaining 7 chemicals made a relatively marginal contribution of 0.035. Among the drivers identified in Tier 2A, and taken forward to Tier 2B, there were another 8 chemicals for which we could not locate data on fish

reproductive toxicity. Inclusion of these substances under the assumption that their (unknown) reproductive toxicity is similar in potency to the endpoints considered in Tier 2A, would add 0.35, raising the PODI to 2.78 (or 1.78 with 0.5 LOD for 17-beta estradiol). This value can be considered as the upper limit of a realistic CA-based MRA outcome.

4.6.2 Data gaps in the fish MRA and impact on assessment outcome

Of potential concern are the 63 chemicals among the Tier 2A drivers for which we could not locate chronic fish toxicity data. With a toxicity estimate (for the most sensitive endpoints) at the median of the potency distribution for fish, inclusion of these chemicals would have added 0.34 to the PODI. Of these, the iodinated contrast agent iopamidol showed the largest RQ (0.13), followed by saccharin (0.02). We could not find suitable toxicity data for iopamidol. According to Selderslaghs et al. (2012), saccharin produced malformations in zebrafish embryos with an EC50 around 25 mM which would suggest that the contribution of saccharin to chronic fish toxicity is negligible.

It was not possible to eliminate the distorting influence on PODI calculations that is introduced through the poorly defined effect magnitudes associated with NOECs. As is well established, NOECs are poor indicators of low toxicities, and are associated with 10 – 30% of a maximally possible effect (Moore and Caux, 1997). Despite the long-standing criticism directed against the practice of hypothesis testing that underpins NOEC estimations, fish toxicity testing continues to report NOECs, instead of effect concentrations associated with defined magnitudes, such as EC10. It is difficult to make an estimate of the uncertainties that these data problems contributed to our MRA.

Similarly, we could not remove the uncertainties associated with the mixing of reproductive toxicity data from different fish species. Since all of the species routinely used in guideline tests (i.e. fathead minnow, zebrafish and medaka), are not native to Europe, there is a species-species extrapolation issue that equally applies to single chemical risk assessment.

It was beyond the scope of this study to quality-check the experimental studies used to derive the Tier 3A estimates, but it is noteworthy that the study by Lahnsteiner et al. (2006) forms the basis of the provisional 17-beta estradiol EQS set by the European Commission.

In summary, our MRA has uncovered mixture risks that would have gone unnoticed in single chemical analyses. Targeting of 17-beta estradiol alone by risk reduction measures would not reduce the PODI to acceptable levels, mainly due to the presence of atrazine, carbamazepine and propranolol. With the fish toxicity data accessible through databases it was possible to arrive at estimates that delineated the lower and upper boundaries of margins of exposure for mixtures associated with chronic reproductive toxicity, despite the data gaps we highlighted.

4.6.3 The human MRA

The application of our MRA framework to human exposure scenarios uncovered several new issues. Because of difficulties associated with retrieving potency data about common toxicities, it was generally not possible to advance the analysis much beyond Tier 2A where PODs from different toxicity endpoint are jumbled together. In the case of the drinking water MRA, four substances, arsenic, lead, atropine and nickel summed up to a PODI of 1.4, slightly higher than the acceptable level of 1, a relatively

conservative CA-based estimate. None of the four chemicals individually exceeded acceptable levels which means that the lower limits of an IA-based best case estimate will signal little of concern.

Similarly, the estimates for intake via fish consumption could not advance beyond Tier 2A which returned a PODI of 108 from 4 substances, telmisartan, digitoxin, fipronil and flupentixol; with a RQ of 102.5, the blood pressure lowering pharmaceutical telmisartan contributed the lion's share. It would appear that fish are capable of accumulating telmisartan to such levels that consumption of one meal of fish (112 g) reaches intakes in the range of therapeutically active doses. If confirmed by analytical determinations, this situation would require risk mitigation. The RQs for digitoxin and fipronil also exceeded acceptable limits, with a margin of exposure smaller than the desirable level of 100. But again, it proved difficult to gather data that would have allowed us to pinpoint common adverse outcomes of these 4 chemicals.

4.6.4 Data gaps in the human MRA and impact on assessment outcomes

There were 15 chemicals among the Tier 2A drivers of the drinking water MRA, for which we could not retrieve data helpful in estimating acceptable exposures; in the fish consumption MRA 13 chemicals fell into this category. Accordingly, these data gaps were bridged by assuming a TTC. In the drinking water MRA, the chemicals that returned the largest RQ under these assumptions were n-acetyl-4-aminoantipyrine and n-formyl-4-aminoantipyrine, both drug metabolites. In the fish consumption MRA this was JWH-073 (2-methylnaphthyl analog), a cannabinoid break-down product predicted to be present in fish. Substances also yielding large RQs in the fish MRA were some chlorinated alkyl phosphate esters used as flame retardants. These chemicals should be subjected to toxicity testing. In the case of the substances with large RQs in the fish consumption MRA, analyses confirming their presence in fish should be conducted to substantiate the fish accumulation modelling.

In both the drinking water and fish consumption MRA, omission of these substances from the MRA could lead to substantial underestimations of risk, but this assessment has to be balanced against the fact that substitution of the TTC values with median potency estimates would have produced RQs in the acceptable range. Unfortunately, this renders the drinking water MRA inconclusive, because possible concerns about combined exposures could not be fully ruled out. This is a consequence of data availability and the data gaps we had to bridge, but does not invalidate the practicability of our scheme. In contrast, the degree of certainty we can attach to the fish consumption MRA is somewhat higher, due to the RQ of telmisartan which, if the levels modelled to accumulate in fish can be confirmed analytically, far exceeds acceptable levels.

4.6.5 Bridging of toxicity data gaps

In our analysis, we used frequency distributions of chronic toxicity data for large numbers of chemicals for the bridging of toxicity data gaps, such as the well-established TTC concept for human MRA and its equivalent for the fish MRA. Alternative methods would have included acute-chronic extrapolations, estimates based on QSARs or read-across methods. In principle, any of these methods could also have been used; our choice in favour of probabilistic approaches was borne out of convenience and because the use of TTC in human toxicology is broadly accepted. It would be timely to conduct a comparative analysis of the impact of alternative choices on the outcome of our MRA, but this was considered beyond the scope of this Deliverable.

4.6.6 Identification of drivers of mixture risks

One of the innovative features of our MRA framework is the integration of driver identification into our new tiering scheme. This required a quantitative criterion for identifying drivers. This criterion had to be sufficiently discriminative to ensure that only a fraction of mixture components turned out as drivers. Too inclusive a criterion would have led the driver concept *ad absurdum*. On the other hand, too restrictive a criterion could have led to overlooking drivers. The solution we finally adopted, defining as drivers those mixture components whose RQs collectively exceeded acceptable exposures, when arrayed from largest to smallest, allowed us to filter out those chemicals that make only a marginal contribution to mixture risks. Only when used in tandem with the driver concept can a tiered MRA realise its potential of being economical with resources; tiering as such does not necessarily achieve this.

It is remarkable how few chemicals, out of the large number entered into this analysis, made significant contributions to the sum of RQs. The reason for this can be found in the nature of the size distributions of the RQs. Both in the fish MRA and the human MRAs these distributions were highly skewed. They appear to follow power laws, similar to the Pareto distribution, and they have been found more frequently on the basis of substantial bodies of measured compounds and sites (Vallotton and Price 2017). This allows for cost-effective interventions, by targeting drivers with risk mitigation or by generating priority lists for toxicological testing. The specific rank order of chemicals identified as drivers depends on the toxicity endpoint chosen for analysis, and on the specifics of the exposure scenario. It will be interesting to uncover the generalities of the power laws behind RQ distributions and to assess whether there are general features applicable to many exposure scenarios and groups of chemicals. We will analyse the implications of the driver concept for approaches to prioritising chemicals for risk mitigation in a separate publication.

With less skewed RQ distributions, more chemicals are identified as drivers. We experienced this to our detriment when we adopted the “eco-TTC” approach for bridging toxicity data gaps in the fish MRA. The introduction of a conservative toxicity estimate drove up the numerical value of the resulting RQs, which were now more strongly driven by the analytically determined concentrations. As a result, almost every chemical of undefined toxicity to fish was identified as a driver, rendering the driver concept unmanageable when used in conjunction with the eco-TTC concept.

In principle, “drivers” can be identified at any tier of the decision tree, however, the meaning and significance of the term cannot be separated from the uncertainties associated with each tier of the MRA and the possible distortions introduced by simplifications of CA. For example, use of the HI method may wrongly identify drivers when AF of widely differing magnitudes were used for establishing reference doses. The same applies to PNECs where they were derived from toxicity data for test species from different taxonomic groups, such as algae, daphnids and fish. Thus, “drivers” identified in Tier 1 of an ecotoxicological MRA on the basis of a ranking of PEC/PNEC ratios cannot be said to drive a mixture risk. Instead, they could perhaps be considered to drive a regulatory concern, or better, drive further attention, to look whether the numerical value relates to ignorance or to (eco)toxicological impact. As the comparability of RQs increases in the higher tiers, with better approximation of the scientific principles of CA, this increasingly removes distortions and ignorance, so that it is possible to identify chemicals that are drivers of mixture risks in the narrow sense of the term.

4.6.7 The scope for a common tiered MRA approach in human and ecotoxicological risk assessment

As our case study showed, our framework is sufficiently flexible to deal with human and ecotoxicological MRA on the basis of common and consistent assessment principles. The tiering principles and decision rules were essentially the same in both cases; the fundamental differences in protection goals that govern human and ecotoxicological risk assessment (focus on the individual and on populations and/or species assemblages, respectively) can be accommodated by the use of AF and the choice of toxicity endpoints. Specific methods for human MRA may come into play at the level of toxicity endpoints and mode-of-action considerations which are correspondingly more diverse than the endpoints relevant in ecotoxicology (mainly centring on reproduction).

4.7 Concluding remarks

Our framework proved to be effective in handling very large numbers of chemicals entered into an MRA. The combination of rigorous tiering principles with an operationalisation of the driver concept enabled us to develop a resource-effective scheme with transparent decision rules. Utilizing the scheme finally informs the water quality assessor with information on the likelihood that the goals of the WFD are possibly not met due mixture exposures, so that water quality management plans can be drafted to counteract mixture impacts. This eventually enables reaching the goals of the WFD, being good water quality by 2027, via both good chemical and ecological quality metrics.

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5 Taxa-specific tiered ecological and human MRA for the Danube, Rhine and SCARCE river basins on the basis of modelled concentrations of up to 1811 pollutants in the water column

In this section we elaborate the results of ecotoxicological and human MRAs conducted on the basis of modelled concentrations for up to 1811 pollutants in the water column of the Danube, Rhine and Spanish river basins (the modelling is described in Deliverables D 14.1 and D 14.2). In this analysis we adopt the tiered common framework that we developed in Section 2 and assessed by way of the case study of monitored water concentrations elaborated in Section 4. The analysis was largely CA-based, but in assessing the number of chemicals predicted to exceed an RQ of 1, we also gained an impression of the minimum boundaries of risk that can be expected in an IA-based MRA.

5.1 Problem formulation

We extended the problem formulation step of the Section 4 case study to include all receptors relevant to pelagic aquatic communities (algae, daphnids and fish). Exposure pathways important to human health, consumption of drinking water and fish caught in river basins were also assessed, as detailed in the case study. Our aim was to investigate whether impacts from direct toxicity of up to 1811 chemicals in combination on algal communities, macro-invertebrates and fish are to be expected, and if so, where such impacts would be most pronounced and which chemicals are main contributors. For human health risks, we investigated whether water taken from river segments in the Danube, Rhine and SCARCE basins would be suitable for drinking water production without purification and whether fish caught from riverine sites are fit for human consumption.

5.2 Materials and methods

5.2.1 Features of the modelled water concentrations

Emission data for 1811 substances were used to model water concentrations for river basin segments by projection onto the E-HYPE hydrology model (Donnelly and others 2013) with further refinements. The basic assumptions and the technical detail of this modelling exercise are described in Deliverables 14.1 and 14.2. For the MRA presented here, we used these data as input values for the tiered MRA described in Sections 2 and 4. Common cations such as sodium, potassium, magnesium, and calcium and anions including chloride, sulphate, or phosphate were excluded from the analysis. The modelling exercise also did not encompass metals or persistent organic pollutants such as PCBs, PCDDs, PCDFs, PBDEs or PAHs.

To make the ecotoxicological MRAs (algae, daphnids, fish) comparable with the MRAs based on species sensitivity distributions (and expressed as msPAF to quantify the magnitude of impact in terms of fraction of species affected) presented in Sections 6 and 7, we utilised the 95th percentile of modelled annual concentrations. For the human MRAs (drinking water, fish consumption) median annual concentrations were used.

5.2.2 Assumptions for exposure assessment in human MRA

We adopted the assumptions for exposure assessment in human MRA, as described in Section 4. Briefly, we converted RVs or equivalents to express tolerable concentrations in drinking water or fish. We assumed a human body weight of 70 kg, a daily water consumption of 2 L and 0.115 kg fish consumption. We allocated 10% of the permissible total exposure to uptake via drinking water or fish consumption. Further, it was assumed that surface water is consumed untreated.

5.2.3 Provenance of regulatory values and toxicity data

In view of the Tier 1 analysis conducted in the Section 4 case study, which indicated combined exposures far in excess of regulatory benchmarks, we skipped Tier 1 and began the MRA in Tier 2, for all receptors: algae, daphnids, fish and humans.

Accordingly, the ecotoxicological MRA was based on chronic toxicity values (NOECs and equivalent) from the three taxa groups (algae, daphnids and fish). The POD determination for a single substance was conducted according to the decision rules for the deterministic approach as outlined by the WFD guidance document No 27, i.e. for each taxa group we used the lowest available chronic toxicity value. Similarly, for the human MRA, the toxicity inputs for drinking water or consumption of fish were based on the lowest reported (sub)chronic oral toxicity values (NOAELS and equivalent) for each single substance.

Ecotoxicity data were collected from the data base created and curated by RIVM and Mermayde, as explained in detail in Section 7. Where a chronic EC50 was the lowest reported value, it was converted into a NOEC equivalent by using an extrapolation factor of 3.

The starting point for the collection of human toxicity data was the OpenFoodTox data base by EFSA which provided (sub)chronic toxicity values for ca. 7% of all substances. Data for the remaining compounds were obtained from a variety of sources, including REACH registry data, ECHA Draft Assessment Reports, OECD reports (SIAP-SIDS and ITAP-SIDS via the INCHEM Portal), JMP reports, UK ACP, Toxnet, Pesticide Manual, IRIS data portal (US EPA), IUPAC-PPDB portal, and APVMA Australia. Oral toxicity values from (sub)chronic animal studies were selected and, if available, from the most recent assessment report. A NOAEL (LOAEL) was prioritized over a NOEL (LOEL), and NOAELs (or equivalent) from studies on humans were given preference over toxicity values from mammalian studies. Differences between systemic and targeted toxicity were ignored, and route to route extrapolations or other predictive approaches (e.g. QSAR) avoided. Extrapolation factors such as from sub-acute (28-day) study to lifetime or chronic exposure (for which a default AF of 6 is often recommended) and from a sub-chronic (i.e. 90-day) to chronic exposure (with AF=2 recommended) were ignored, i.e. toxicity data from all non-acute studies were treated equally. Similar to the data treatment of ecotoxicity values, if a LO(A)EL was reported as lowest value it was converted into a NO(A)EL equivalent by using an extrapolation factor of 3 (ECETOC recommendation, 2014).

A POD derived from human studies does not require assessment factors for interspecies and intraspecies extrapolation, and to achieve a better comparability to PODs at higher Tiers that could be established only from toxicity data of animal studies, a human-based POD was “back-converted” to an animal-based POD by multiplying a factor of 100 (equalling the product of the standard AFs for both extrapolations). This pragmatic step was accordingly recorded at the driver identification. For the

majority of pharmaceuticals (sub)chronic oral toxicity values are not available, and in that case we derived a NO(A)EL equivalent from defined daily doses (DDD) as reported in the WHO ATC/DDD index 2018 (https://www.whocc.no/atc_ddd_index/).

A compilation of all toxicity data for the 1812 chemicals that are the subject of this analysis can be found in **Annex 3.**

5.2.4 Dealing with missing toxicity data

The 1811 chemicals for which water concentrations were modelled included a large number of substances for which chronic toxicity data could not be retrieved. This made it necessary to bridge these data gaps.

Data gaps in the ecotoxicological MRA were filled according to the principles of the human TTC concept by constructing frequency distributions of taxa-specific chronic NOECs for algae, daphnids and fish (Belanger et al. 2015), and on basis of all available chronic toxicity data 5th percentile values were derived for each taxa group (daphnids: 0.03 ug/l, algae: 1ug/l, fish: 0.039 ug/l). These worst-case values were used as default NOEC for missing chronic toxicity values (see Section 4).

Data gaps in the human MRA were bridged using the TTC approach in line with the recent review by EFSA and WHO (2016). First, the Cramer class for each compound was estimated together with a possible structural alert for genotoxicity, using the software Toxtree 2.6.13 (http://toxtree.sourceforge.net/). Next, TTC values were allocated to the Cramer structural classes III, II and I used as 3, 0.91 and 0.15 mg/kg bw /day, and for compounds with genotoxic structural alerts a value of 0.00025 mg/kg bw/day was assumed (Kroes et al. 2004, EFSA and WHO, 2016). The latter value was preferred over the Cramer class value.

5.2.5 Fish accumulation modelling

The internal levels of water pollutants in fish were modelled with monitored concentrations as input, as described in Sections 3 and 4.

5.2.6 Driver identification

We identified drivers of mixture toxicity according to the quantitative criteria described in Section 4.

5.2.7 Assessment rules

We applied the assessment rules that were developed for the common ecotoxicological/human MRA framework, as described in Section 2. Briefly, combined exposures not exceeding a PODI of 0.1 were judged as being at a level unlikely to violate the standards of the WFD for the protection of pelagic organisms. For human MRA, a PODI of < 0.01, equivalent to a margin of exposure of 100, was deemed acceptable.

5.2.8 Visualisation of the outcome of MRAs as river basin maps

We visualized the outcome of the ecotoxicological, taxa-specific MRAs by creating maps of river basin segments that depict exceedances of combined exposures, as follows: A PODI of < 1 was represented in blue and interpreted as signaling a low likelihood that the taxa considered would be affected by chronic

toxicity. A PODI of between 1 and 10 (equivalent to an up to 10-fold exceedances of levels of low concern) was shown as yellow segments and interpreted as signaling first indications of potential chronic effects. PODIs of between 10 and 50 (orange) were regarded as indicating chronic risks to the investigated taxa. Finally, a PODI exceeding 50 (red) was taken to indicate strong chronic effects.

The outcome of the human MRAs (based on annual median modelled concentrations) were visualized as follows: PODIs of < 0.01 were taken as signaling no concern for human health mixture risks under life-long consumption (blue). PODIs of between 0.01 and 0.1 indicate that the margin of exposure of 100 normally required in human risk assessment is not maintained and therefore signal some concern (yellow). The range of PODIs between 0.1 and 1 (orange) suggests that margins of exposure are nearly exhausted and signals concern. PODIs exceeding 1 (red) indicate concern.

5.3 Results

The ecotoxicological MRAs for algae and daphnids proceeded to Tier 2C, in which species-specific RQ for chronic reproductive toxicity were aggregated by using the PODI method (see Section 2). This ensured high comparability of the RQs. There was no lumping together of different toxicity endpoints as is practiced at lower Tiers of the MRA. As discussed in Section 4, a species-specific MRA could not be realized for reproductive toxicity in fish, as too few chemicals were tested in the same species. A focus on one fish species would have reduced the number of chemicals considered in the MRA even further.

The analysis focused on drivers of mixture toxicity, as defined in Section 2 and rehearsed in the case study in Section 4. At this relatively high Tier of the MRA, chemicals with only marginal contributions to the PODI were removed from the analysis, as were chemicals for which toxicity values had to be estimated by using the TTC approach or equivalents. The inevitable bias towards underestimating mixture risks is compensated by increasing the certainty of the analysis. The outcome of our MRA therefore represents the lower boundaries of risks that can be assumed with a correspondingly higher degree of certainty. We also examined the number of chemicals that exceeded a RQ of 1, which demarcates the minimum risk to be expected in an IA-based analysis in Tier 3A of the MRA.

The human MRAs for the exposure routes drinking water and fish consumption proceeded to Tier 2A. Similar to the situation with the JDS 3 case study (Section 4), it was not possible to advance to Tier 2B, due to difficulties in locating potency values for common toxicity endpoints, but the identification of substances that exceed an RQ of 0.01 (equivalent to a margin of safety of 100) enabled us to define the lower boundaries of a Tier 3A IA-based MRA.

Table 5.1 shows the numbers of chemicals that could be entered into the ecotoxicological and human MRAs, for each of the river basins considered, due to the availability of relevant toxicity data.

Table 5.1: Number of chemicals entered into taxa-specific ecotoxicological MRAs and human MRAs

			Number of compounds entered into the MRA due to availability of relevant toxicity data			
	Number of subcatchments ("sites")	**Number of compounds**	algae	daphnids (chronic, reproduction)	fish (chronic & reproduction)	human (NOEL or DDD)
Scarce	696	1811	1693	159	69	633
Rhine	813	1795	1677	159	69	633
Danube	3477	1788	1670	159	69	632

5.3.1 Ecotoxicological MRA for algae

As shown in **Table 5.1**, chronic toxicity data for algal reproduction could be retrieved for up to 1693 substances, the majority of the chemicals for which modelled water concentrations were available. The Tier 2C MRA which we present in the Figures below is therefore by far the most comprehensive of all the taxa-specific ecotoxicological MRAs, and a correspondingly higher degree of certainty can be attached to this analysis. **Figure 5.1** shows the resulting PODIs for the Danube, Rhine and SCARCE river basins. The analysis suggests that many river segments are insufficiently protected from impacts on algal communities. Only for certain streams in upland areas in the Pyrenees and the Alps (Switzerland) is the modelled mixture exposure lower than the protection level aimed at. First indications of chronic effects on algal reproduction are to be expected in most river segments, with chronic toxicity predicted in many other segments.

We analysed the number of chemicals that contributed significantly to the modelled chronic mixture risks to algal communities. For the majority of river segments in all basins, between 20 and 50 chemicals are projected to drive the combined reproductive toxicity (**Figure 5.2**). In many cases, the RQ of single chemicals were predicted to exceed 1. As shown in **Figure 5.3**, this was projected to occur with between 1 and 5 chemicals in the majority of sites and it demarcates the minimum boundaries of mixture risks expected according to an IA-based MRA. In large stretches of upland rivers and in the Guadalquivir in Spain, all modelled chemicals showed RQs < 1. Even so, in many segments where no chemical was anticipated to exceed a RQ of 1, there were indications of combined toxicity to algae according to a CA-based assessment (compare **Figure 5.1 and 5.3**).

Across all river basins, we identified approximately 40 chemicals projected to make a substantial contribution to combined risks to algal communities (**Table 5.2**). Many of these chemicals are currently not regulated in the WFD.

Figure 5.1: Projected chronic combined toxicity to algal reproduction in the Danube, Rhine and SCARCE river basins. Shown is the outcome of a Tier 2C analysis based on the 95th percentiles of modelled annual water concentrations, expressed as PODI. For interpretation of colour codes see Material and Methods.

Figure 5.2: Number of chemicals ("drivers") contributing significantly to modelled chronic reproductive mixture risks to algal communities

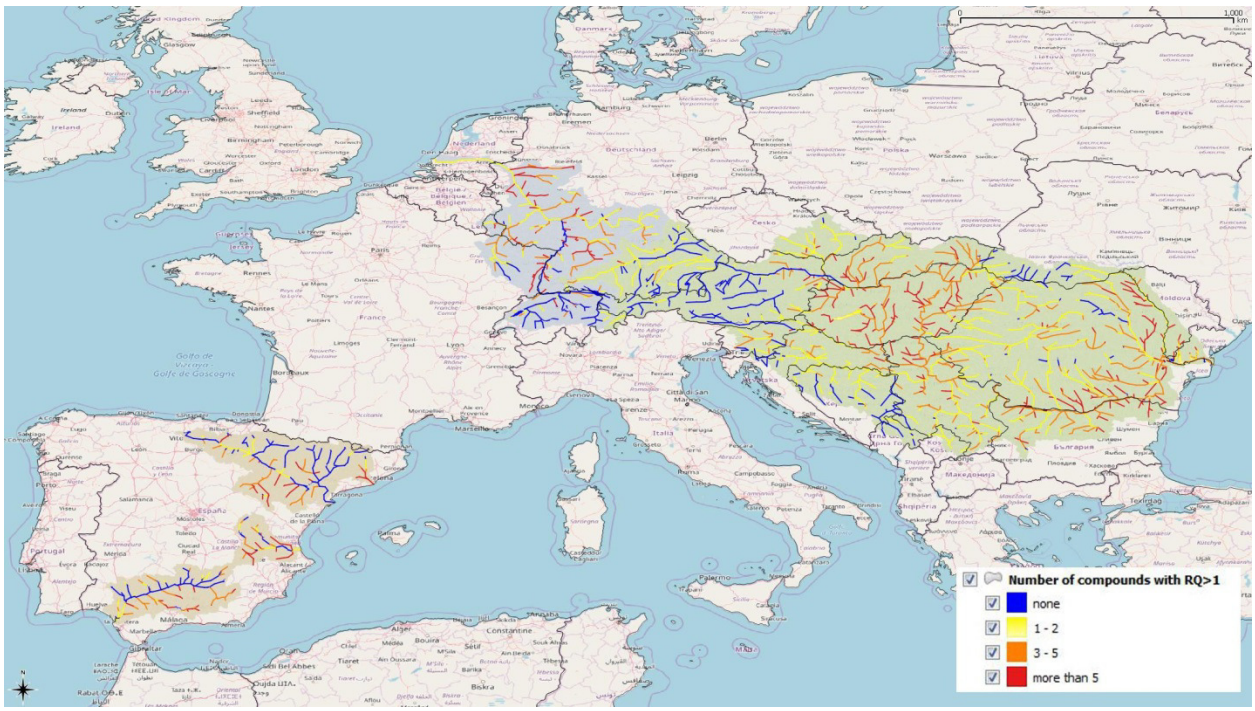

Figure 5.3: Number of chemicals predicted to exceed an RQ of 1. Segments coloured yellow, orange and red signify locations signaling the lower boundary of mixture risks of concern in IA-based MRAs (Tier 3A).

Table 5.2: The 40 Chemicals projected to contribute substantially to modelled mixture risks to algal communities, across all modelled river basins

CAS_NR	Compound
106478	4-chloroaniline
1897456	Chlorothalonil
872059	dec-1-ene
34256821	Acetochlor
79118	chloroacetic acid
103902	paracetamol
7287196	Prometryn
106503	p-phenylenediamine
87392129	S-Metolachlor
15972608	Alachlor
5915413	Terbuthylazine
112754	dimethyl(tetradecyl)amine
83164334	Diflufenican
4685147	Paraquat
80057	4,4'-isopropylidenediphenol
123319	hydroquinone
122394	diphenylamine
34123596	Isoproturon
108930	cyclohexanol
886500	Terbutryn
98828	cumene
300765	Naled
112414	dodec-1-ene
1912249	atrazine
108952	phenol
122349	Simazine
120127	anthracene
87674688	Dimethenamid
330552	Linuron
2439352	2-(dimethylamino)ethyl acrylate
793248	N-1,3-dimethylbutyl-N'-phenyl-p-pher
2312358	propargite
1746812	Monolinuron
80159	Cumene hydroperoxide
2243621	1,5-naphthylenediamine
556672	octamethylcyclotetrasiloxane
84852153	Phenol, 4-nonyl-, branched
112538	dodecan-1-ol
60207901	Propiconazole
142459583	Flufenacet

5.3.2 Ecotoxicological MRA for daphnids

For 159 of the modelled chemicals we retrieved toxicological data for chronic reproductive risks to daphnids that could be entered into Tier 2C of the MRA. **Figure 5.4** shows the resulting PODIs for the Danube, Rhine and SCARCE basins. As with algal communities, the analysis suggests that many river segments are insufficiently protected from impacts on macroinvertebrates, with the exception of streams in upland regions in the Pyrenees and the Alps (Switzerland, Austria) where there are no indications of concern of not maintaining the WFD goals on water quality. For the majority of river segments in all basins, between 20 and 50 chemicals are projected to drive the combined reproductive toxicity to daphnids (**Figure 5.5**).

Again, a number of chemicals were predicted to exceed RQs of 1. As shown in **Figure 5.6**, this was predicted to occur for between 1 and 5 chemicals for the majority of sites. In large stretches of upland rivers, in parts of Austria, the Eastern tributaries of the Danube and in the Guadalquivir in Spain all modelled chemicals stayed below RQs of 1.

As with the analysis for algae, in many stretches where no chemical was anticipated to exceed an RQ of 1, there were indications of CA-based combined toxicity to daphnids (compare **Figure 5.4 and 5.6**).

Across all river basins, we identified 19 chemicals predicted to make a substantial contribution to combined risks to daphnids (**Table 5.3**). Many of these chemicals are currently not regulated in the WFD.

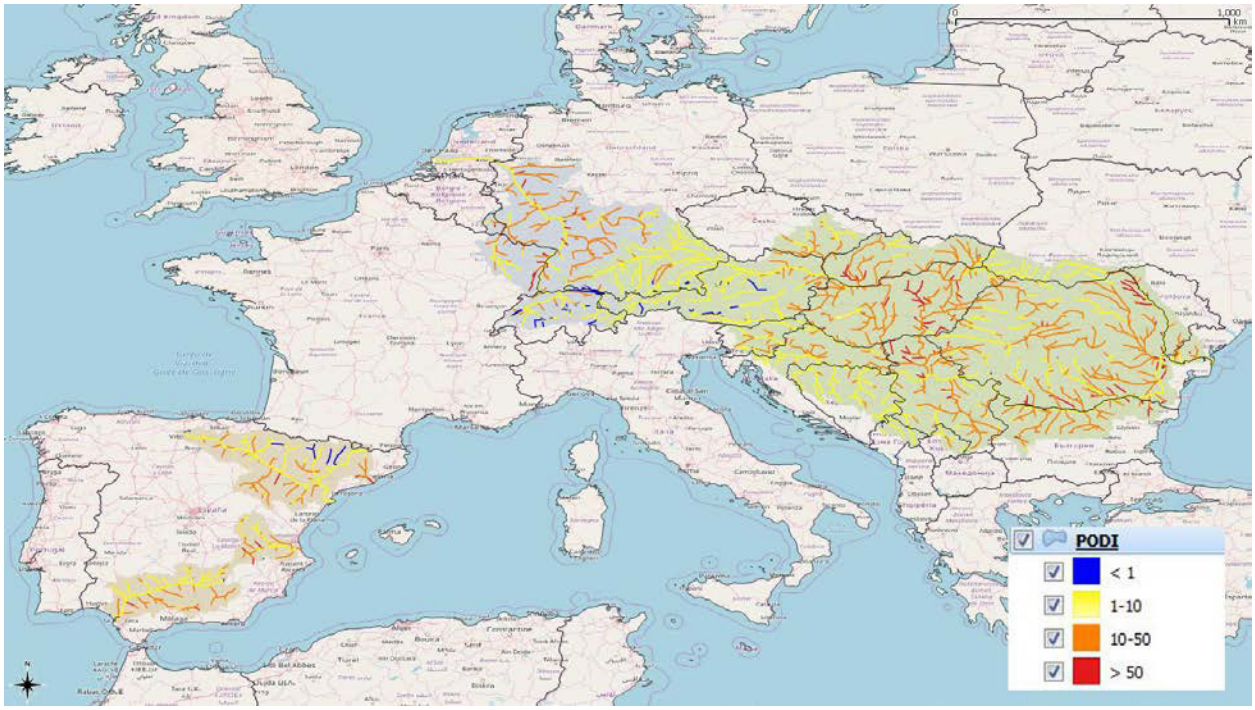

Figure 5.4: Projected chronic combined toxicity to daphnids in the Danube, Rhine and SCARCE river basins, expressed as PODI. Shown is the outcome of a Tier 2C analysis based on the 95th percentiles of modelled annual water concentrations. For interpretation of colour codes see Material and Methods.

Figure 5.5: Number of chemicals ("drivers") contributing significantly to modelled chronic reproductive mixture risks in daphnids

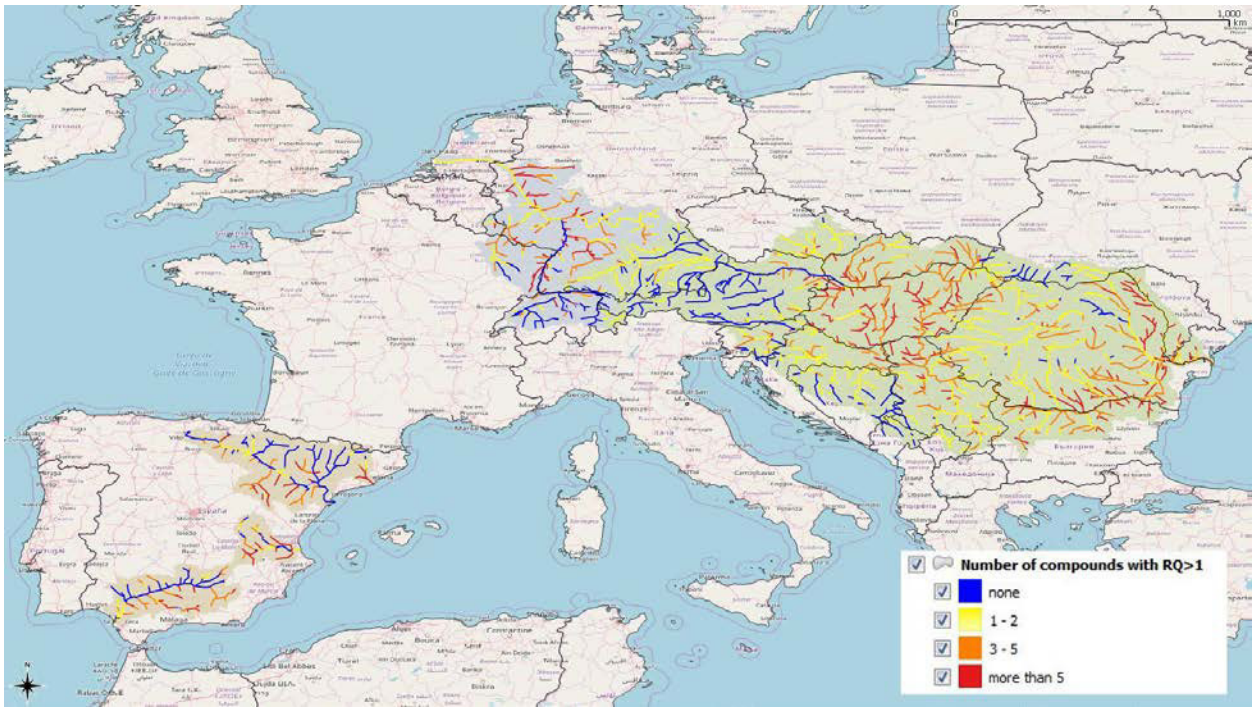

Figure 5.6: Number of chemicals predicted to exceed RQs of 1 for chronic reproductive toxicity in daphnids. Segments coloured yellow, orange and red signify locations signaling the lower boundary of mixture risks of concern in IA-based MRAs in Tier 3A.

Table 5.3: The 17 Chemicals projected to contribute substantially to modelled mixture risks to daphnids, across all modelled river basins

CAS_NR	Compound
62533	aniline
80057	4,4'-isopropylidenediphenol
56382	Parathion
72490018	Fenoxycarb
106478	4-chloroaniline
556672	octamethylcyclotetrasiloxane
2921882	Chlorpyrifos
57636	Etinylestradiol
24017478	Triazophos
298464	Carbamazepine
95512	2-chloroaniline
15307865	diclofenac
298044	Disulfoton
300765	Naled
108952	phenol
55389	Fenthion
86500	Azinphos-methyl

5.3.3 Ecotoxicological MRA for fish

For 69 of the modelled chemicals we retrieved toxicological data for chronic reproductive risks to fish that could be entered into Tier 2B of the MRA. **Figure 5.7** shows the resulting PODIs for the Danube, Rhine and SCARCE basins. The MRA suggests that almost the entire Rhine catchment does not pose concerns for chronic impacts on fish for the chemicals for which effect data were available (which is a small fraction of the number of modelled chemicals). This is also true for large swathes of the Western and Southern parts of the Danube basin and for upland river stretches in the Ebro basin. Indications for impacts on fish are seen in the Llobregat and Guadalquivir basins, and in central areas of the Danube basin.

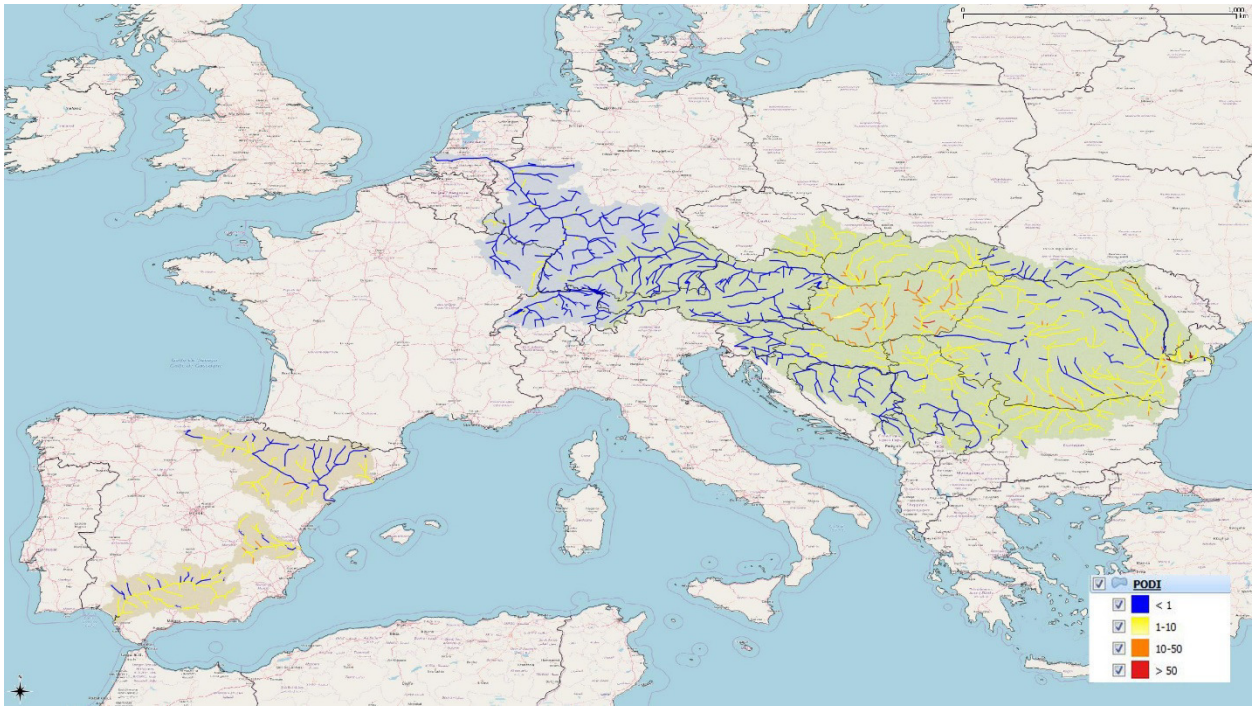

Figure 5.7: Predicted chronic combined toxicity to fish in the Danube, Rhine and SCARCE river basins, expressed as PODI. Shown is the outcome of a Tier 2B analysis based on the 95th percentiles of modelled annual water concentrations. For interpretation of colour codes see Material and Methods.

For the majority of river segments in all basins, fewer than 20 chemicals were predicted to contribute significantly to the PODI (**Figure 5.8**).

Relatively few chemicals were anticipated to exceed RQs of 1. In the Central and Eastern area of the Daube basin, and in parts of the Spanish river basins, this was modelled to be the case with 1 – 2 chemicals. In all other river segments, we did not identify exceedances of RQ = 1 for any of the modelled chemicals.

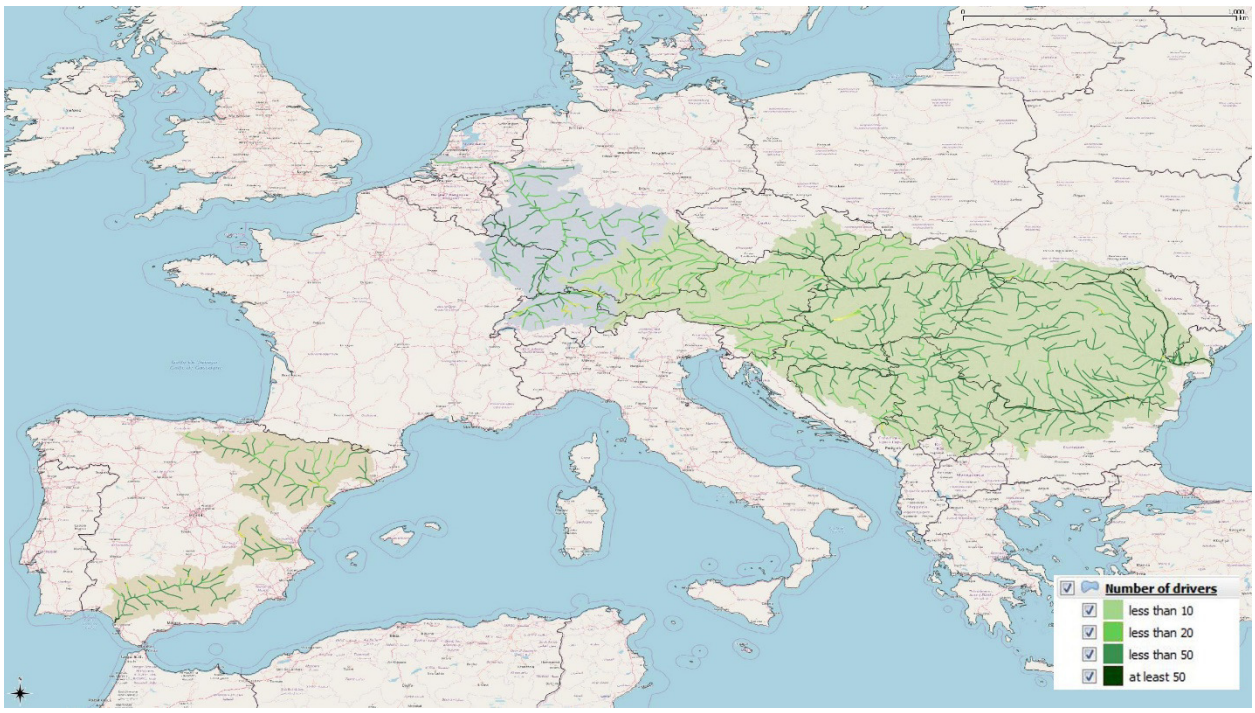

Figure 5.8: Number of chemicals ("drivers") contributing significantly to the PODI in fish

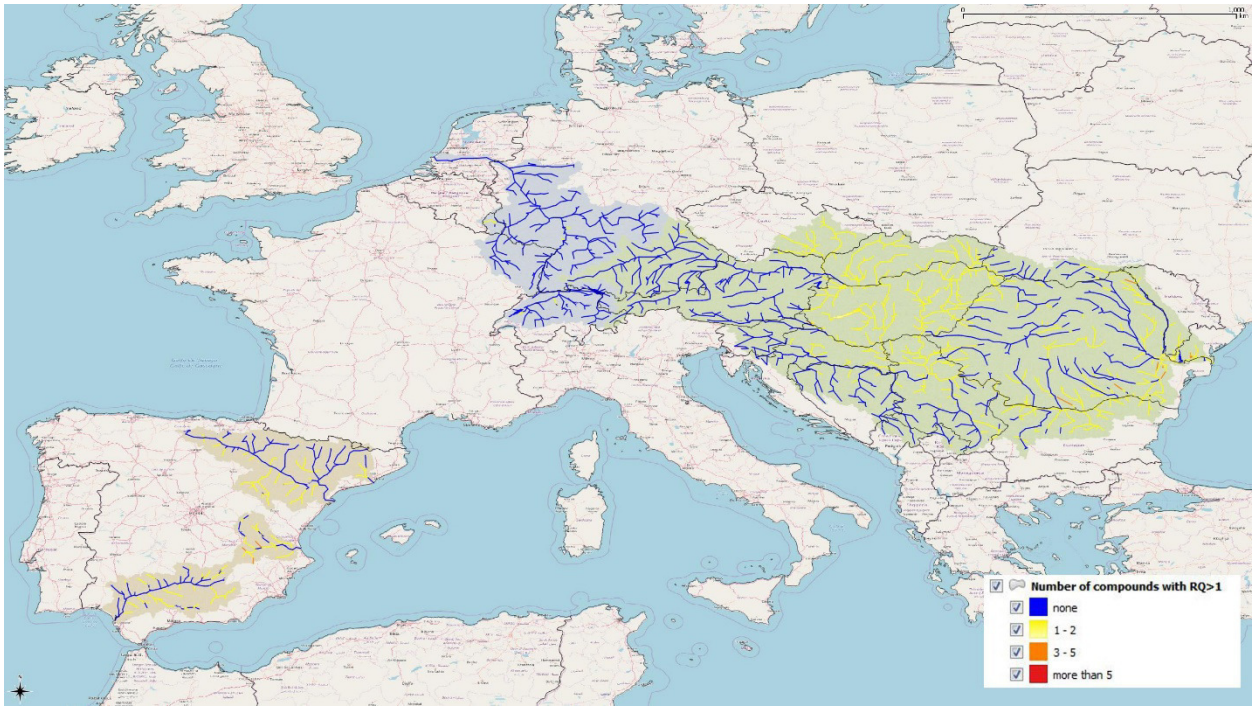

Figure 5.9: Number of chemicals predicted to exceed RQs of 1 for chronic fish reproductive toxicity. Segments coloured yellow, orange and red signify locations signaling the lower boundary of mixture risks of concern in IA-based MRAs in Tier 3A.

As for algae and daphnids, we identified a number of chemicals that contributed substantially to modelled mixture risks for fish, consistently across all river basins. These are listed in **Table 5.4.**

Table 5.4: The 7 Chemicals projected to contribute substantially to modelled mixture risks to fish, across all modelled river basins

CAS_NR	Compound
1912249	atrazine
140669	4-(1,1,3,3-tetramethylbutyl)phenol
57636	Etinylestradiol
137268	thiram
86500	Azinphos-methyl
115297	Endosulfan
50282	estradiol

5.3.4 Human MRA for the exposure pathway drinking water

For 633 of the modelled chemicals (632 for the Danube basin) we retrieved toxicological data for chronic health risks to humans that allowed us to conduct a Tier 2A MRA. Unlike the ecotoxicological MRAs, where we used the 95th percentile of modelled annual concentrations, the analysis was carried out on the basis of median annual concentrations. We assessed whether surface water taken from the river basins in question would be fit for drinking water production without purification. **Figure 5.10** shows the outcome of the analysis by depicting PODIs for the Danube, Rhine and SCARCE basins. The PODI remained < 1 in the majority of river segments of the Spanish basins, upland areas of the Rhine catchment and stretches in Austria, Croatia, Southern Ukraine as well as segments in Northern Romania. In almost all other areas, there are some indications for concern of the water quality when used directly as a resource for drinking water.

Figure 5.10: Predicted chronic combined toxicity to humans for drinking water consumption in the Danube, Rhine and SCARCE river basins, expressed as PODI. Shown is the outcome of a Tier 2A analysis based on median annual modelled water concentrations. For interpretation of colour codes see Material and Methods.

In river segments that signaled little in the way of concern for water quality as a drinking water resource (for the studied set of chemicals and their mixtures), fewer than 10 chemicals contributed significantly to the PODI (**Figure 5.11**). However, in all other areas there were at least 20, and often up to 50 chemicals predicted to make substantial contributions to the PODI.

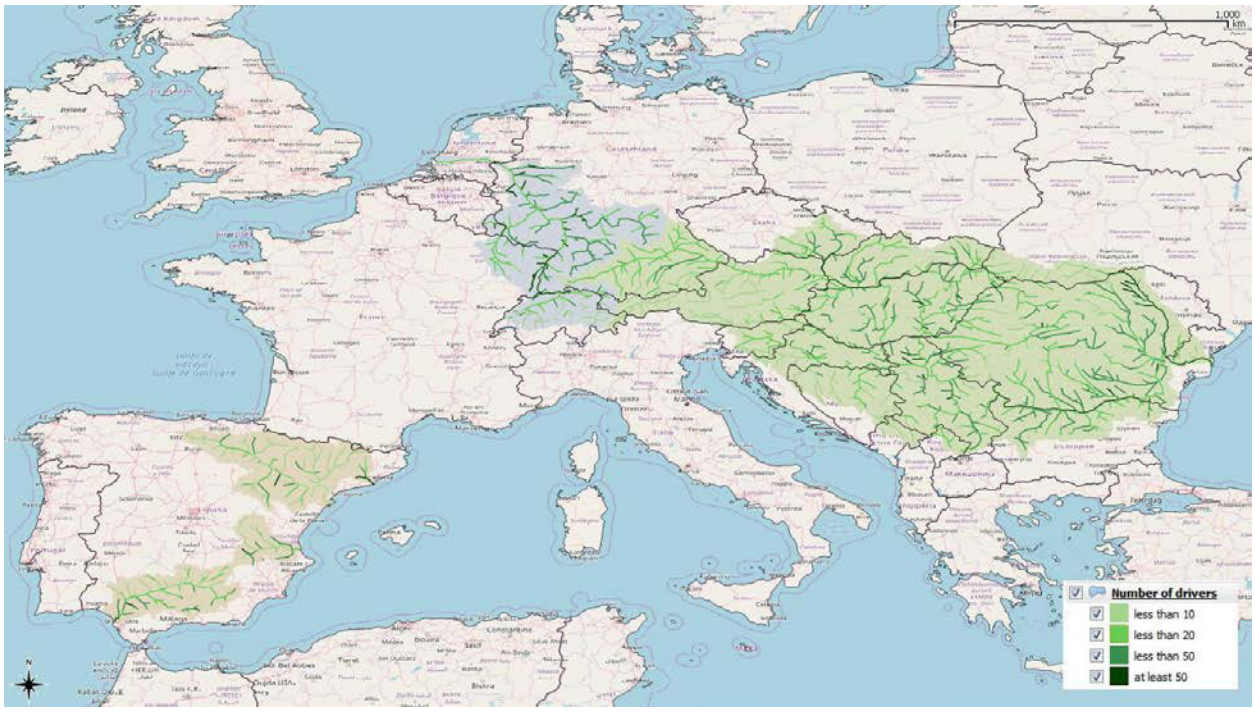

Figure 11: Number of chemicals ("drivers") modelled to contribute significantly to the PODI for human drinking water consumption

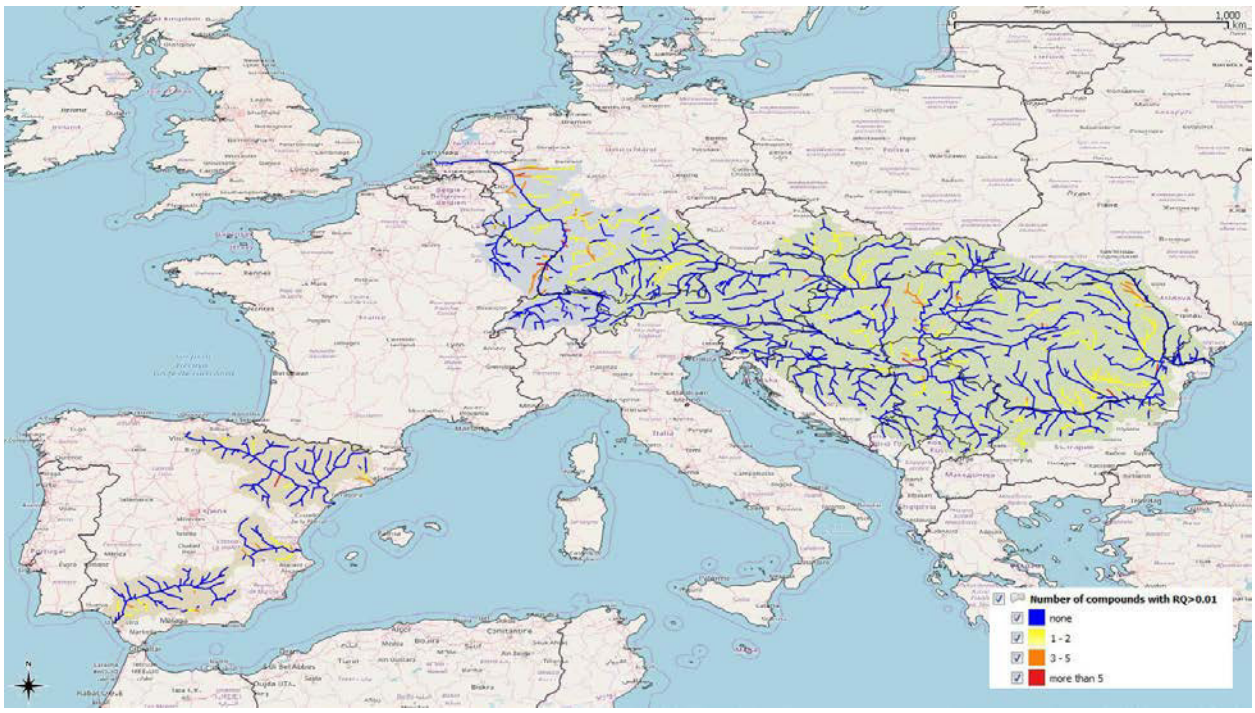

Figure 12: Number of chemicals predicted to exceed RQs of 0.01 for exposures via drinking water. Segments coloured yellow, orange and red signify locations signaling the lower boundary of mixture risks of concern in IA-based MRAs in Tier 3A.

In the majority of river segments, there were no predicted exceedances of the critical RQ of 0.01 (thus maintaining the default margin of exposure of 100 in human risk assessment) for any of the modelled single chemicals. Where there were exceedances, this concerned 1 – 2 chemicals. Only in a few segments were there more than 2 substances with modelled RQs > 0.01 (**Figure 12**).

We identified 7 chemicals that we predicted to make substantial contributions to the modelled combined human health risks, consistently across all river basins (**Table 5.5**).

Table 5.5: The 7 Chemicals projected to contribute substantially to modelled mixture risks to humans for the exposure route drinking water

CAS_NR	Compound
79061	acrylamide
110656	but-2-yne-1,4-diol
80057	4,4'-isopropylidenediphenol
80159	Cumene hydroperoxide
108952	phenol
62533	aniline
96242	3-chloropropane-1,2-diol

5.3.5 Human MRA for consumption of fish caught in the Danube, Rhine and SCARCE river basins

As for the drinking water MRA, we retrieved toxicological data relevant for the assessment of chronic health risks to humans for 633 of the modelled chemicals (632 for the Danube basin). This allowed us to conduct a Tier 2A MRA. The analysis was carried out on the basis of median annual modelled concentrations. We assessed whether fish taken from the river basins in question would be fit for human consumption. As described in Section 3, the analysis was based on 3 prototypical fish with features that mark the lower and upper boundaries of contaminant accumulation via direct uptake from the water column. The MRA conducted for a prototype with features of phytovorous fish revealed a smaller degree of concern. There were only small differences between the predicted combined exposures modelled for consumption of planctivorous and piscivorous fish. In the sections below we only present the results of the analysis for piscivorous fish.

Figure 5.13 shows the outcome of the MRA by depicting the resulting PODIs for the Danube, Rhine and SCARCE basins. The analysis revealed no concerns for fish caught in river stretches of Alpine regions in Switzerland and Austria, in South-West Ukraine, Croatia and streams in the Pyrenees. For all other river segments, the modelled combined exposures that result from consuming fish caught in these waters cannot comply with the margin of exposure normally required in human risk assessment. In some areas, the necessary margin of exposure is predicted to be exhausted almost entirely.

In many river segments between 10 and 20 chemicals contributed significantly to the PODI (**Figure 5.14**).

In those river segments, where there were no concerns regarding consumption of fish there were also no predicted exceedances of the critical RQ of 0.01 for any of the modelled single chemicals (**Figure 5.15**).

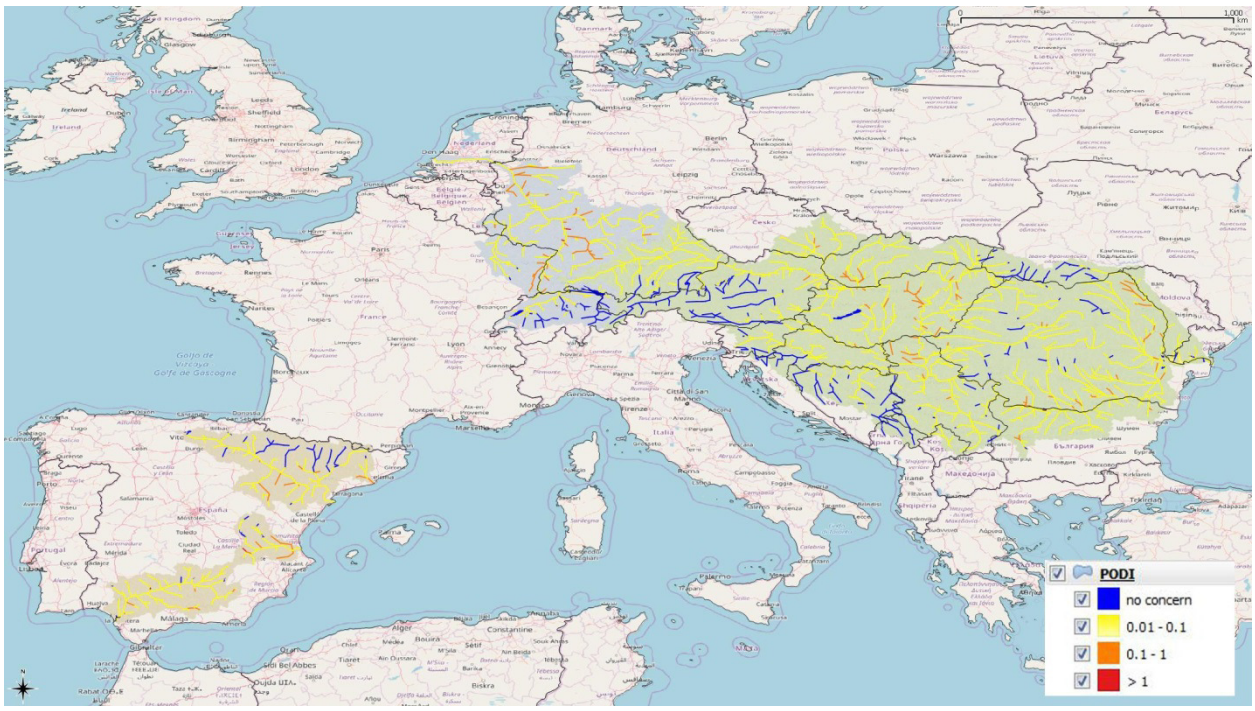

Figure 5.13: Predicted chronic combined toxicity to humans for fish consumption in the Danube, Rhine and SCARCE river basins (piscivorous fish), expressed as PODI Shown is the outcome of a Tier 2A analysis based on median annual modelled water concentrations. For interpretation of colour codes see Material and Methods.

Figure 5.14: Number of chemicals ("drivers") contributing significantly to the PODI for human consumption of piscivorous fish

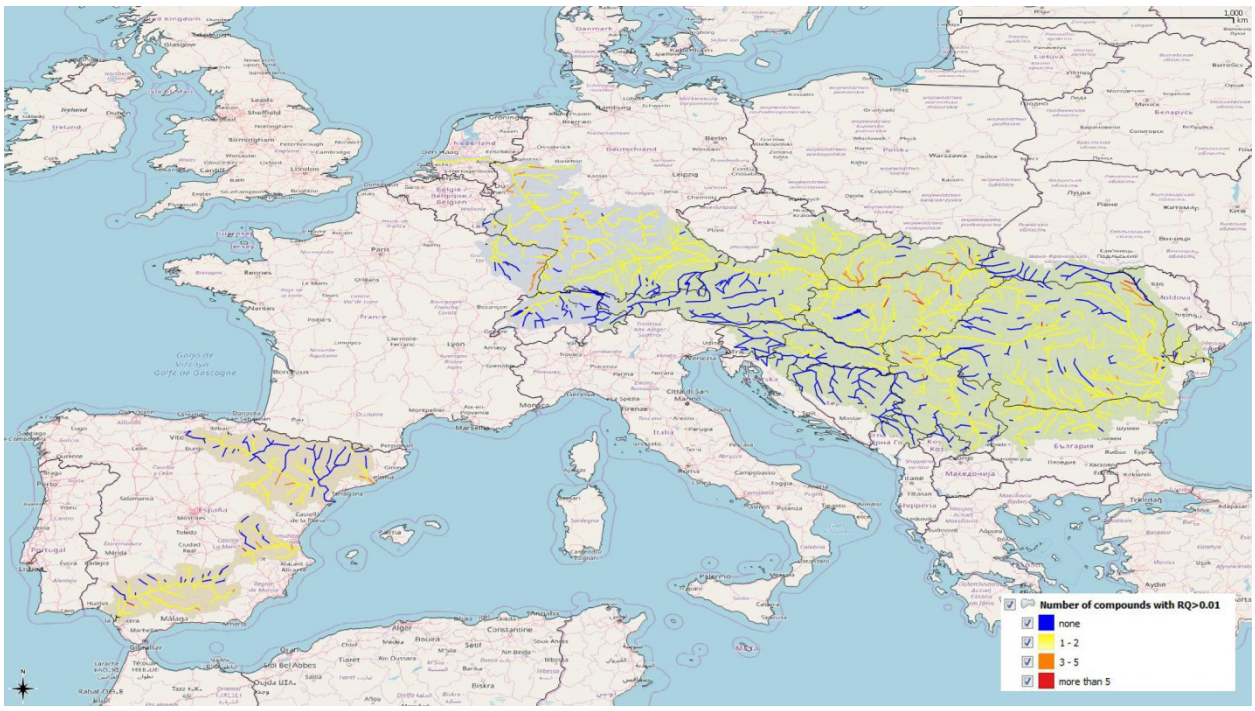

Figure 5.15: Number of chemicals predicted to exceed RQs of 0.01 for exposures via consumption of piscivorous fish. Segments coloured yellow, orange and red signify locations signaling the lower boundary of mixture risks of concern in IA-based MRAs in Tier 3A.

Where there were exceedances of RQs, this concerned 1 – 2 chemicals in the majority of river stretches, with relatively few localized instances where 3 – 5 substances had modelled RQs > 0.01 (**Figure 5.15**).

We identified 7 chemicals that we predicted to make substantial contributions to the modelled combined human health risks via fish consumption, consistently across all river basins (**Table 5.6**). None of these chemicals are among WFD priority substances.

Table 5.6: The 7 Chemicals projected to contribute substantially to modelled mixture risks to humans from fish consumption

CAS_NR	Compound
80057	4,4'-isopropylidenediphenol
80159	Cumene hydroperoxide
34256821	Acetochlor
2921882	Chlorpyrifos
80079	bis(4-chlorophenyl) sulphone
2312358	propargite
793248	N-1,3-dimethylbutyl-N'-phenyl-p-pher

5.4 Discussion

The ecotoxicological MRAs for algae and daphnids revealed a high spatial frequency of insufficiently protective exposures from combined exposures to water-borne pollutants, across all investigated river basins. This was less evident for the MRA for chronic reproductive toxicity in fish, be it that here the estimated values were lower caused by a (far) lower number of compounds being involved in the assessment. To a considerable degree, the outcome of the analyses was determined by the availability of toxicity data for the taxa in question, largest for algae and smallest for fish (**Table 5.1**). It is noteworthy that despite the constraints set by the limited accessibility to relevant toxicity data, exceedances of combined acceptable exposures could also be predicted for daphnids and fish.

Our assumptions and the resulting estimates require confirmation, but the outcome of our analysis supports the conclusion that the potential consequences of co-exposures to multiple water-borne pollutants for aquatic communities and human health are a limiting factor for reaching the goals of the WFD in terms of good water quality (chemical and ecological)status.

Our PODI estimates were influenced by our assumptions regarding the expected contaminant concentrations in surface waters. The uncertainties associated with these estimates were discussed extensively in Deliverables 14.1 and 14.2. Especially for chemicals highlighted as having a strong impact on our PODI estimates (**Tables 5.2 – 5.6**), it will be necessary to conduct targeted confirmatory monitoring exercises. Numerical outcomes of the models are of a screening kind, and outcome data should always be screened before they are interpreted as information for management. We clearly illustrate this along the progressive tiers, which imply an interpretation change from a numerical value below which sites of little concern can be removed from further analyses, to the higher tiers where the numerical outcomes have a clear (or improved) (eco)toxicological meaning.

It is not straightforward to determine how well our estimates approximate the true extent of combined risks to aquatic organisms, considering multiple sources of uncertainty along all steps of the SOLUTIONS model train. However, our least conservative Tier 2C assessments are likely to have underestimated risks because we made the tacit assumption that only the substances for which relevant toxicity data were available contributed to risk, while the remainder of the chemicals predicted to be present in the water column could not be handled other than assuming that they are toxicologically inert. Nevertheless, the Tier 2C PODIs (Tier 2B for fish) are useful as lower-bound estimates of the true risks of combined exposures, which (if all other assumptions about exposures, concentration-additivity, and the

relevance of data from tests with laboratory species are valid) signal non-compliance with WFD protection goals.

Similar considerations apply to the outcome of the human MRAs for drinking water and fish consumption. To substantiate the results of the analysis for fish consumption it would be helpful to carry out confirmatory analytical determinations of the levels in fish of those pollutants that we predicted to make the greatest contribution to the PODIs.

For quantitative interpretations of the PODI values for ecotoxicological MRAs, it is helpful to consider that values greater than 1 suggest that, *ceteris paribus*, the species employed for regulatory testing would experience reproductive toxicity at the borderline of being detectable as statistically significant, if exposed to waters containing the chemicals at their predicted levels. To glean the likely effects of PODIs in excess of 1, it would be necessary to have information about the gradient of the underlying concentration-response relationship of the mixture. Such data are not currently accessible, but can only be obtained through targeted laboratory experiments. Nevertheless, on the basis of available data on the gradient of numerous concentration-response relationships in ecotoxicological studies (analysed by Faust and Scholze in Kortenkamp et al. 2012) it can be anticipated that PODIs approaching 10 – 50 will be associated with significant effects. Further corroboration of this can be found in the context of mixture toxic pressures (Sections 6 and 7), to which these outcomes are quantitatively related. For mixture toxic pressures, it has been shown that increasing values indeed relate to ecological impacts .

Be that as it may, PODIs in excess of 1 can be read as first signals for potential effects, but the associated impacts on aquatic species, evaluated in terms of effect magnitudes, are not accessible through these analyses. To specify ecological consequences, individual-based modelling (IBM) needs to be conducted, analysing the combined impact of chemicals on life history parameters such as viability metrics, to predict the population development of selected sentinel species, or with models assessing effects on species assemblages. These issues will be the topic of Section 6 and 7.

5.5 References

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6 Quantifying expected impacts on assemblages of aquatic species, chemical footprinting and individual-based modelling

6.1 Background

While the previous Sections of this Deliverable deal with a set of tiered assessment approaches that are founded in risk quotients – defined as the ratio between (predicted) exposure concentrations and effect concentrations (so-called risk quotients, RQ) in various formats and abbreviations, see Section 2 – the current chapter considers a method for the prediction of the magnitude of impacts on species assemblages from pollutants in the water column. This is a valuable asset, as this method bridges the gap between MRA methods that build on chemical safety assessment approaches by summing up RQ (see Section 2) and the impact-related approaches to characterize impacts on the ecological status as applied in the Water Framework Directive (which are quantitative impact metrics, expressing damage to Biological Quality Elements). As detailed in Section 2, compliance with combined acceptable levels of chemical pollution of surface water bodies is assessed by summing up RQs of all chemicals present. If the resulting value is smaller than a critical one (often <1), the water body is considered to be sufficiently protected against adverse effects of the chemical(s) present in the water body, as values <1 imply that the exposure level does not exceed the threshold for impacts. If thresholds are defined by the respective Environmental Quality Standards of the chemicals (Tier 1 of the Common Framework), the value implies sufficient protection against adverse effects caused by direct exposure, by secondary poisoning, by specific effects such as endocrine disruption, and by impacts on human health, as those form the background of the threshold value that is used: the EQS for a chemical is aimed to guarantee protection against all these impact types, substantiated by the lowest threshold concentration to define the EQS. Values higher than one imply the opposite, but – due to the inherent mixing of different receptors and toxicity endpoints inherent in EQS – the exceedance has no specific biological interpretation: it marks “insufficient protection”, but does not specify that (Section 2). In this section, the SOLUTIONS description of work expands with a higher-tier approach, that does quantify expected impact magnitudes in two ways:

- By using statistical patterns in the available ecotoxicity data to assess the likelihood that exposures exceed any toxicity endpoint, which translates into a novel metric, the mixture toxic pressure; this was done based on both assessing the likelihood of insufficient protection as well as the likelihood of species loss (again bridging between the chemical safety- and the ecological impact magnitude approaches of REACH and the WFD, respectively)
- By using traits of species to predict for some sentinel species (characterized by dissimilar sets of traits) whether and to what degree mixture exposures would cause population declines.

The former method has been further worked out in the format of summary-chemical footprints for water bodies, which allows to provide summary insights into a water systems-level overview of expected chemical pollution impacts in Europe’s surface water systems.

6.2 Key opportunities offered by the statistical and trait-based approaches

Since the mid-1990s the statistical approach has been defined as a higher-tier method for ecological impact assessment. A high-impact publication by Solomon, Baker et al. (1996) showed a US-wide quantitative risk assessment of a plant protection product at the landscape scale. The method was

evaluated to have changed the discipline and risk assessment practices for chemicals nearly two decades later (Solomon, Giesy et al. 2013). This approach was further developed in SOLUTIONS, with emphasis on the water-systems approach of the WFD, by (a) making the method suitable for use for a large number of chemicals, and (b) assessing mixtures of compounds. The approaches were designed to assist water quality assessors in their task to assess the likelihood that chemical pollution – which encompasses potentially all chemicals and their mixtures (see WFD, Article 2, definitions) – is a factor potentially limiting reaching good water quality status (see WFD, Annex II).

Solomon's approach is based on an overlay of the distribution of exposure concentrations – which is commonly available via monitoring, or via predictive modelling as done in SOLUTIONS (see Deliverable D14.1 and D14.2) – and species sensitivity information. Species sensitivity information is obtained from ecotoxicity tests, and a set of ecotoxicity data – representing the species sensitivities of a set of tested species – has been observed to take the shape of the common bell-shaped distribution. The overlay of the exposure data with the impact data is considered a metric of ecological risk, looking at the fraction of species potentially affected beyond the selected test endpoint that was used to define species sensitivities. The higher the value, the more exposure concentrations exceed the sensitivity thresholds of tested species. In comparison to component-based MRA approaches derived from CA, the bell-shaped species sensitivity distribution (SSD) approach can provide additional insights, for the various reasons discussed by Solomon and Takacs (2002). That is, the outcomes of the statistics-based assessment enable us to estimate the fraction of species affected, whilst the CA-based MRA methods delineate exceedance of acceptable combined exposures, without enabling us to estimate the extent of effects.

The trait-based approaches are capable of delineating expected impacts on species with different trait combinations concerning their reproduction strategies, similar to the sentinel species used in Section 3 for evaluating body residues of chemicals in a variety of typical fish species. As a result of assessing expected quantitative impact magnitudes of chemical pollution, the methods provide a bridge between the CA-derived, component-based MRA approaches and the quantitative ecological impact approaches of the WFD (ecological status). It is key to note, that the SSD-model itself is used both for deriving EQS's for single chemicals (chemical assessment and management policies) as well as toxic pressures of ambient concentrations (environmental assessment and management policies, such as WFD).

6.3 Outcomes of the statistics-based method method to quantify expected impact magnitudes on species assemblages

The statistics-based method was developed prior to the SOLUTIONS project for single compound, landscape based assessments (Solomon, Baker et al. 1996, Solomon, Giesy et al. 2013). So far, however, the chemical safety assessment methods have yielded EQS's for approx. 300 compounds for evaluating water quality under the WFD (EEA 2018), whereby both the target of the policy (all separate chemicals should have exposure concentrations < the respectively EQSs) and the status classification system score and count the frequency of non-compliance. The indicator system of scoring concentrations *vis a vis* the respective EQS-values is combined with a 'one out – all out' principle, to score whether the final goal of the WFD (good water quality, evaluated by at least good ecological and chemical status) is reached: at that point in time, none of the European water bodies has any indicator left at values lower than 'good'. However, using the same indicator system for obtaining information on expected impacts performs poorly. As an example of the relatively poor information on chemical threats to human health or ecosystems, Sweden's surface water bodies scored 100% non-compliant for chemical status, due to the

fact that mercury concentrations exceed the health safety standards (EEA 2012). For the classification, this is a clear signal of non-compliance to the available EQSs for one or more of the compounds monitored and one or more endpoints. However, the indicator system does not inform well on the type and magnitude of the expected impact, altough we showed in the revious Sections that considerable refinements can be reached by utilizing the novel tiered approach for MRA as compared to current formal approaches to report and analyse water quality status and trends (EEA, 2012, 2018).

SOLUTIONS developed a refined diagnostic assessment, to assist the water quality assessor in assessing the likelihood that chemical pollution can be a cause of less than good ecological status. The method is based on SSD-modelling, which can be applied to predicted or monitored concentrations of chemicals. Subsequently, the following steps were made, as explained in Section 7, based on the manuscript "Posthuma, L., Van Gils, J., Zijp, M.C., Van de Meent, D. and De Zwart, D. (2018, submitted). Species sensitivity distributions for use in environmental protection, assessment and management of aquatic ecosystems for 12,386 chemicals. Environ Toxicol Chem.":

1. Collection of ecotoxicity data from an array of global sources
2. Curation of the data, to remove doubles and irrelevant data
3. Operational split of the data set into "chronic" and "acute" test data, to align with the chemical safety assessment approaches and the ecological status approaches, respectively
4. Derivation of Species Sensitivity Distributions (SSD) for 12,386 compounds, both for the chronic and the acute data where possible
5. Use of the SSDs to quantify the likelihood the chemical pollution can be a factor that limits reaching the good ecological status

SOLUTIONS applied the models to case studies performed for the various SOLUTIONS basins. For example, Munz, Burdon et al. (2017) showed that various micropollutants for the Rhine catchment can be found in the water system, based on emissions from waste water treatment plants and agricultural land use. Analyses of the data showed a covariation of instream toxic pressures with upstream land uses, as expected from review and model studies executed partly in liaison to SOLUTIONS (de Zwart, Adams et al. 2018, Holmes, Brown et al. 2018, Posthuma, Brown et al. 2018, Posthuma, Brown et al. 2018). Despite the observation that household chemicals were characterized by the highest regular loads, also episodic pesticide loads occurred, and – based on toxic pressure analyses – these appeared to represent the highest probability that effects on aquatic life would occur. Moreover, expected impacts were dominated by a relatively low number of chemicals, as also found in US-wide studies on a large number of pesticides (Vallotton and Price 2016).

The broadest use of the SOLUTIONS SSD-database was in the Europe-wide assessment of the potential consequences of exposures to mixtures resulting from the use of all chemicals in Europe. In this case, the concentration data were obtained from modelling, rather than from measurement (as in the Rhine case study). The results are detailed in SOLUTIONS Deliverables D14.1 and D14.2, and in Section 6 of this Deliverable. To highlight the type of progress that can be made, we show some examples from the combined integrated SOLUTIONS-model train (which operates from emissions to mixture toxic pressure) for Europe, and thereafter some specific examples – again – the catchment of the Rhine. Typical results that can be obtained are summarized in separate sections (below).

6.4 Europe-wide assessments of mixture toxic pressure: a typical European water body

Europe-wide emission modelling, combined with the methods applied in chemical safety assessment (cf. REACH) resulted in predicted mixture concentrations in a so-called 'typical European water body at steady state', based on multi-media fate modelling. The mixture toxic pressure example was calculated using SSDs based on acute data, as the outcomes of such assessments (expressed as msPAF-acute EC50) have been found to be empirically related to species loss. The predicted acute mixture toxic pressure was found to be approx. 0.23 (fraction), interpreted as the probability that the mixture exposure would exceed the median EC50 of the tested species, with a likely associated species loss of 23%. The study is reported in "Posthuma, L., De Zwart, D. and Van de Meent, D. (2018, subm.) Screening level estimation of release rates of currently used chemicals to the environment - application to solution-oriented assessment of impacts on aquatic ecosystems Environ. Toxicol. Chem.".

6.5 Europe-wide assessments of mixture toxic pressure: SOLUTIONS integrated modelling

Europe-wide emission modelling, combined with the methods of the integrated SOLUTIONS modelling train resulted in predicted mixture concentrations for >20,000 European water bodies on a daily basis. The mixture toxic pressure example was calculated using SSDs based on both chronic and acute data using data for >1800 compounds (REACH-chemicals, pesticides, pharmaceuticals). The former was worked out to provide a Europe-wide map of chronic mixture toxic pressures, and the latter for acute mixture toxic pressures. As reported in the SOLUTIONS-Deliverables on integrated modelling, the analyses showed that many water bodies in Europe would be insufficiently protected against mixture effects, whereby the protection goal was linked to the current studies via logical inference, and that the probability that mixture exposure exceeds the median 50%-effect level was nearly 17% for the Rhine basin. Again, as in both the studies of Munz et al. (2017) and the SOLUTIONS-emissions study cited in the previous section, the contributions of chemicals to the net mixture impacts are highly skewed, with a relatively low number of chemicals contributing to the net mixture toxic pressure. An example of the Europe-wide map is presented in **Figure 6.1**.

It should be noted that the Europe-wide integrated modelling that can be performed by the SOLUTIONS model train provides screening-level information on the probability of mixtures or chemicals to pose harm. Outputs generated by the model are sensitive to the questions posed, and the information entered into the model. For example, scale matters. A Europe-wide assessment of all chemicals may yield a clearly skewed distribution of the relative importance of the chemicals, this distribution will change with lower scale, e.g. towards specific basins, or even to a local water body. The local water body near a site where one single pesticide would evidently be characterized by that pesticide as the chemical with the highest contribution to harm – however, the water body is also part of the higher-scale ranks, which do not necessarily show this pesticide as dominant. Also, time matters. Given the daily basis of using chemicals (e.g., pesticides) and modelling (the SOLUTIONS model train), it is evident that mixture exposure varies over days and seasons. Finally, site matters. We highlight, that the use of the integrated SOLUTIONS model train *first* shows the sites where mixture tend to pose harm to aquatic life (prioritization to site), where after prioritizations to dominant chemicals can be made. In line with the WFD-systems-based approach, the assessor can make the useful interpretation of considering ecotoxicity at the systems scale (e.g., Europe, see **Figure 6.1)**, then to (relative) hot spots, then to

substances. We note a degree of similarity between mixture toxic pressure analyses and the taxa-specific higher-tier analyses based on the PODI approaches (see Section 5), and indeed, aggregated ratio's and mixture toxic pressure data of the same set of sites covary for a part of the exposure level range (a misfit occurs in the range of high aggregated TU-values, which have no upper bound, whereas msPAF are limited to a maximum of 1). The assessor can thus fulfil the task to assess the Annex-II task of assessing the likelihood that chemical pollution poses a threat to aquatic life, so as to derive adequate measures to address the chemical pollution problem. It is of substantial importance, that the models as developed in SOLUTIONS (for 12,386 compounds) liaise both to the chemical safety assessment (EQS, protection goal, WFD-final goal of good chemical status) as well as to ecological impact magnitudes, for a vastly expanded set of compounds (as yet, approx. 300 compounds can be evaluated).

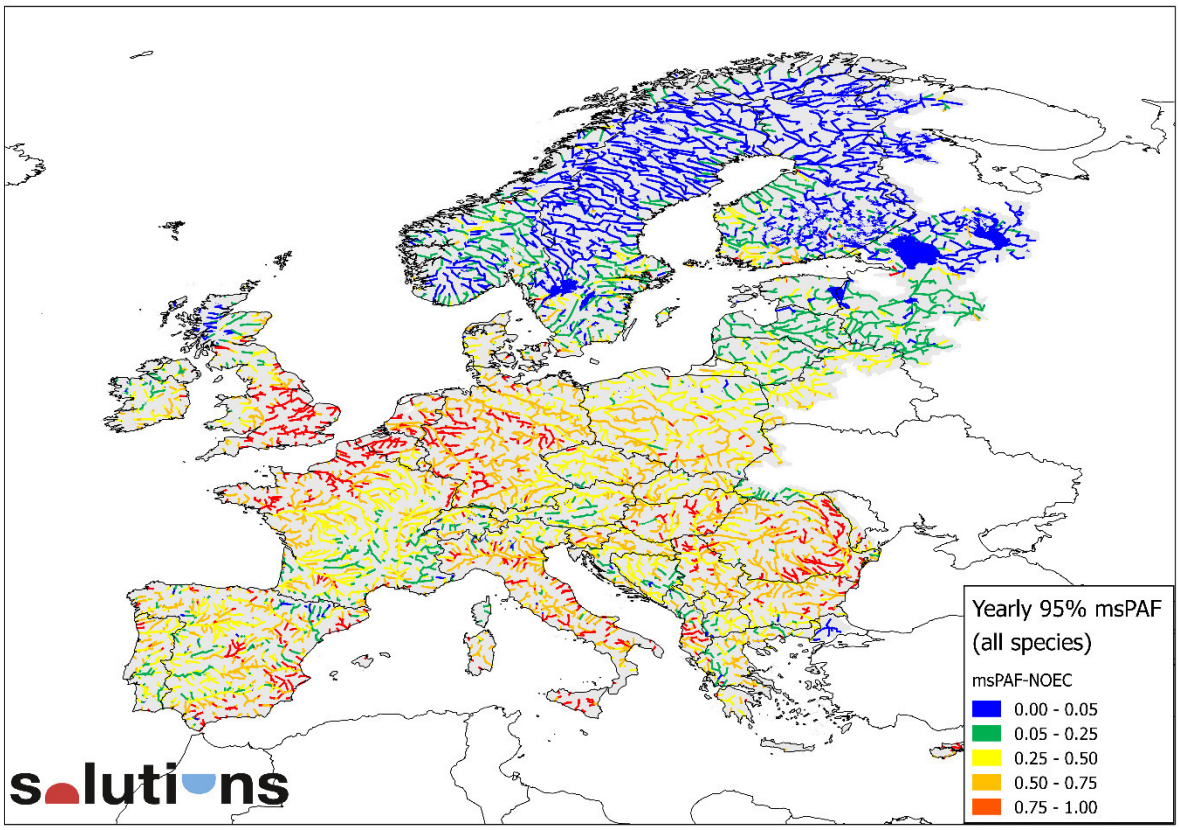

Figure 6.1. **Example of the Europe-wide mapping of mixture toxic pressures, here: the chronic mixture toxic pressure (msPAF-chronic NOEC) for predicted mixture concentrations of >1800 compounds.** Note the relative similarity with earlier maps in Section 5.

6.6 Chemical footprinting: communicating complex information and programs of measures

SOLUTIONS Work Package 18 (risk modelling) also contributed to providing an approach to summarize the mixture toxic pressure data. That was done by deriving chemical footprints. A chemical footprint for a water body summarizes the pollution status in a single number (Posthuma, Bjørn et al. 2014, Zijp, Posthuma et al. 2014), which essentially provides a summary insight into the question whether the amount of water needed to dilute the net chemical emissions to a sufficiently safe level is larger than the amount available (different methods can be used to derive the boundary that discriminates the sufficiently safe level from the insufficiently safe level). In SOLUTIONS, this method was initially defined

in 2014, but it was recently expanded towards a refined assessment for a basin. That is, by considering the separate footprints of the 813 sub-catchments of the Rhine basin, it became possible to summarize the local footprint of each water body, and characterize the relative contributions from upstream sources (prioritization of mixture toxic pressure sources) as well as the ecotoxic outflow to downstream water bodies. Again, this aligns well with the systems-based principles of the WFD, and it helps to assessor to focus on the upstream causes of local impacts, in order to focus effective programs of measures. An example of the footprinting assays is provided in **Figure 6.2**.

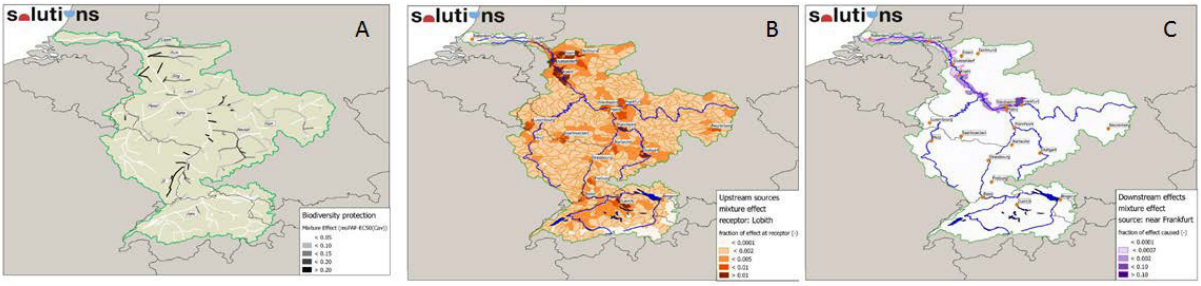

Figure 6.2: **Example of a chemical footprinting analyses, in which the Rhine basin is assessed for local-, upstream sources and downstream affected sub-catchments (details in SOLUTIONS-Deliverables D14.1 and D14.2).** Example results showing the opportunities of using the chemical footprint analyses for water quality assessment and communication and for deriving programs of measures related to mixture risks: (A) Differences of the local mixture toxic pressure across river stretches (local toxic pressure levels), (B) Attribution of the mixture toxic pressure at the German-Dutch border for the Rhine at Lobith to upstream contributions, and (C) downstream effects (relative contribution, -) for a pollution source close to Frankfurt.

6.7 Analysing scenarios of abatement and future emissions

The integrated SOLUTIONS modelling train also allows for evaluating alternative abatement strategies as well as future chemical use scenarios. Those change emissions of multiple chemicals to water systems, and knowing the effects on net mixture toxic pressures can assist in selecting the best abatement strategy, or to anticipate future threats. Details are reported in SOLUTIONS Deliverables D14.1 and D14.2, based on scenarios on abatement and future emissions, defined by the respective SOLUTIONS work packages (Moritz, Bunke et al. 2017, Van Wezel, Ter Laak et al. 2017). Example studies showed that the impact of the various future emission scenarios were largely non-linear, and highly sensitive (effective) for some abatement scenarios as compared to others. This was to be expected from the highly-skewed distributions of the relative contributions of chemicals to mixture problems shown in the various Sections of this report: if those are skewed, abatement strategies focusing on the high-contributing ones will likely yield to largest decrease of harm (chemical footprint). Zijp, Posthuma et al. (2014) already analysed Rhine-basin chemical footprints over time, showing that (a) chemical footprints can show a decreasing tendency over time, which (b) related to associated policy efforts, and (c) measured mixture impacts (using techniques such as Effect-Based Methods applied to time-series water samples).

6.8 Alignment with EQS-protection levels and ecological status

In previous sections, it was argued that the SSD-modelling was designed such that the chronic mixture toxic pressure relates to the chemical safety assessment, and the acute one to species loss. The former has been derived from logical inference. That is, the (historical) operationalisation of the protection goal

("full protection of ecosystem structure and function") has been made via the 95%-protection level per chemical, which is related to 95% of the species being exposed to a single chemical below their chronic no-effect level (this was interpreted as a pragmatic method, to operationalise the protection gaol in terms of critical, protective benchmark concentrations). The same 95%-protection level was used in the SOLUTIONS analyses, for example the one shown in **Figure 6.1.** From these analyses, one can conclude whether the EU-goal of a non-toxic environment (EC 2014) and the WFD-good status has been reached. For the acute mixture toxic pressures, which empirically relate to species loss, the SOLUTIONS project collaborated with the MARS project (www.mars-project.eu). This resulted in an important observation on the relationship between the predicted mixture impacts (msPAF-EC50) for 24 WFD Priority Substances and the Ecological Status classification. It was shown that mixture exposure is a factor that limits reaching or maintaining good or high ecological status, with higher msPAF-EC50 implying higher limitations (**Figure 6.3**). Quantile regression (Cade and Noon 2003) confirmed that this was a statistically highly significant finding. Note that sites that are ecologically in reference conditions (Y-classes 1 and 2) may exhibit relatively high mixture toxic pressures. This likely relates to, first, the modeling of a ' virtual mixture' of all chemicals being present at their 95th percentile expsoure level (which is an over-estimate of values for msPAF of water samples, but which was used as proxy to differentiate inter-site differences in time-variable exposures) and to compensating local factors, such as high food availability (Lassiter and Hallam 1990). Further work is in progress to describe in how far mixture toxic pressure for all studied chemicals (>1800) form a limitation to ecological status. Preliminary analyses suggest that species loss can be attributed – on average – for approx. 20% to chemical pollution (preliminary outputs S. Birk, unpublished). We note that this value has the same order of magnitude as the 23% predicted for the 'typical European water body' (prediction related to the REACH-related modelling approach towards chemical safety assessment) and the approx. 17% species loss reported as average for the Rhine (see above).

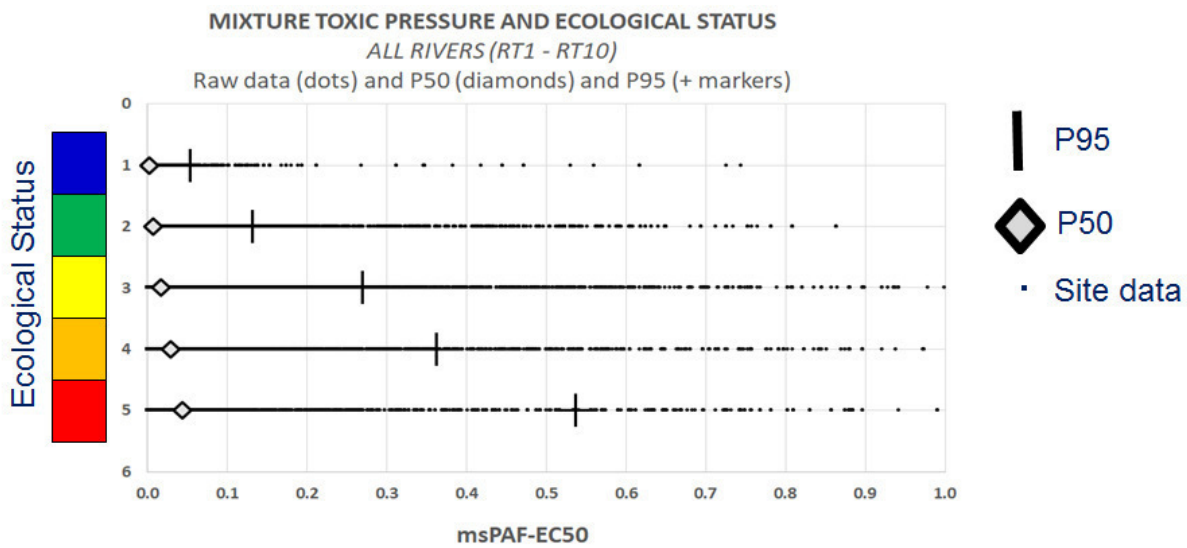

Figure 6.3: The empirical relationship between X=mixture toxic pressure (msPAF-EC50 for 24 priority substances) and Y=Ecological Status class. The study concerned >20,000 European water bodies. The upper right corner contain much fewer data than lower X-values, signalling that the potential stress factor on the X-axis is a limiting factor at higher levels (Cade and Noon 2003), here: chemical pollution. Within each Ecological Status class (Y-axis), the 50th and p5th percentile msPAF-values are marked to highlight the pattern of limitation.

6.9 Refined ecological insights: Individual-Based Models

While SSD-based modelling is a powerful tool to process risk calculations for large numbers of chemicals and their mixtures, this approach considers risks to species assemblages via their sensitivity towards chemicals, negating how impacts proliferate from sensitivity endpoints to population viability of species with different characteristics. Clearly, species with high reproductive output and short generation time will exhibit a different population development, even when their physiological sensitivity for chemical exposure is summarized as the same sensitivity endpoint, such as a similar NOEC or similar EC50. Therefore, an additional tier or ecology- rather than statistics based risk modelling can consider more ecological information, e.g. traits that are related to population dynamics, and can in that way provide the means to consider more than one toxicity endpoint in an integrated way, i.e. assess effects on survival and reproduction in a common frame.

In SOLUTIONS, such an ecological modelling approach was developed and implemented, being more complex than SSD-modelling, but it is still applicable under the SOLUTIONS rationale, i.e. is fit for being applied at the European scale for chemical mixtures. Such modelling approaches can provide the necessary insights in the consequences of statistical exceedance probabilities, in the format of a prognosis of single-chemical and/or mixture effects on single selected sentinel species, in extension of the SSD approach. The sentinel species are selected such that they can be considered a representation of the wide variability of the species occurring in nature.

The development of the corresponding individual-based modeling (IBM) toolbox and the theory behind were described in an internal deliverable (ID M5.3 Progress report on population-level ERA via IBM, Baveco & Focks, 2017). That deliverable describes the method development, a sensitivity analysis and application of IBMs in two example case studies, which were based on preliminary exposure modelling results as produced by the SOLUTIONS model train in early 2017. Individual based models are a form of population modelling, where individuals – and effects of chemicals on individuals – are simulated based on sets of trait-related equations and rules, so as to derive the population level dynamics that emerge from the suite of individual dynamics and chemical impacts. For SOLUTIONS, the considered ecological traits were related to reproduction (age at 1st reproduction, the clutch-size, time between broods, number of broods). Based on the IBM simulations, population growth rates were the main model output. Population-dynamic modelling requires that the population growth rate is – on average – neutral, whilst deviations from that in a systematic downward way can be interpreted as a probability that a species population is eventually likely lost.

After having received updated simulated exposure time series for a list of 1827 chemicals for the SOLUTIONS case study catchments (Danube, Iberian and Rhine) in April 2018, the ecological analyses with the developed IBMs was parameterized for the macroinvertebrate families of *Asellidae, Gammaridae, Chironomidae* and *Baetidae* based on freshwater ecology trait databases. A screening of all available toxicity data for these species resulted, however, in a very reduced share of compounds where toxicity information was available for the selected four macroinvertebrate species, i.e. 17 for *Asellidae,* 26 for *Gammaridae,* 49 for *Chironomidae*, and 25 for *Baetidae* from the set of in total 1827 chemicals. This finding indicates a currently very poor coverage of the 'chemical universe' by the IBM modelling, by the availability of toxicity information for non-standard test species. Despite the idea that an IBM *module* in general enables a refined analysis of and ecological interpretation to lower-tier risk assessments, the current factual application may be limited by data scarcity. Nonetheless, the results as

obtained clearly show that and how IBM outputs enrich the opportunity of assessors to quantify the likelihood of impacts in natural systems, as required under WFD-Annex II (assessment of impacts).

Results of the IBM simulations using the available toxicity and analyses have been presented at conferences, and a corresponding manuscript is in preparation (Baveco et al. in prep.). In that sense, the IBM activities in SOLUTIONS provide a proof of concept showing the potential of the methods, but also that the availability of toxicity information is as yet limiting for non-standard species.

6.10 Modelling field SSDs

SOLUTIONS also investigated whether the basis of SSD assessments of chemical pollution – the observation that species sensitivities form a bell-shaped distribution – can also be found under field conditions. To that end, a data set of measured chemical concentrations, collated from Dutch monitoring data, was analysed. It indeed appeared, that field species exhibit a sensitivity distribution for chemical exposures. A preliminary example of results is shown in **Figure 6.4**. These results imply, that – as expected – sensitive taxon-specific responses may occur before biodiversity is affected. Moreover, the curve clearly shows a field species sensitivity distribution, based on differential effects of chemical pollution on taxon abundances. Further studies of this kind were done by Berger, Haase et al. (2016) (see next section).

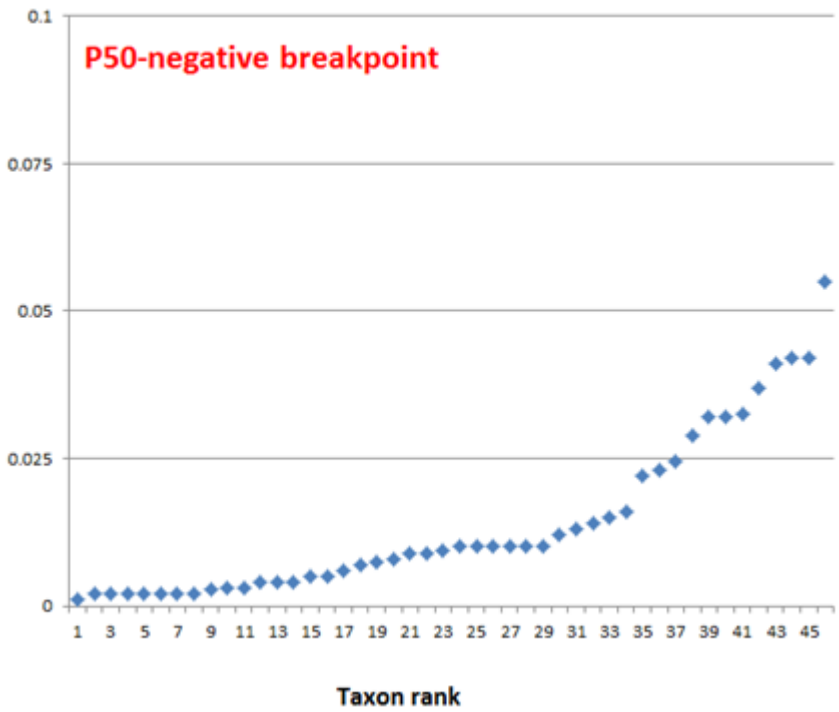

Figure 6.4. Preliminary results of the TITAN analysis of a Dutch monitoring data set, encompassing both chemicals and aquatic invertebrates. The X-axis shows the rank order of taxa regarding the mixture exposure level (Y) at which they exhibit a negative impact of mixture exposure; the breakpoints are expressed on the Y-axis, as derived from laboratory toxicity tests (msPAF-EC50). The field species with the highest sensitivity (lowest X) thus shows a decline of abundance in the field, if approx. 1 in 100 species tested in the laboratory (Y-value) would be affected at the 50%-effect level. The 37th ranked taxon is characterized by an impact of chemical pollution when the 2.5 of 100 species would be affected at the 50%-effect level.

6.11 Modelling Ecosystem Vulnerability Distributions

SOLUTIONS made a final step in the assessment of the likelihood of mixture impacts to aquatic life, considering the fact that different species assemblages exist according to the different definitions of references in the WFD, and that those likely have different vulnerabilities. That is, dependent on the species composition, different (reference) species assemblages will exhibit different stressor responses to the same stressor and stressor level. Evidence for this was published by Mulder, Boit et al. (2012), who constructed food webs from monitoring data (in which all species-to-species and species-to environment relationships were modelled), and who performed artificial (in silico) stressor-impact analyses on those food webs. It appeared that it mattered whether stressors affected the food web randomly (removing species at random, causing indirect effects to other species), or that the stressor influenced the web via bottom-up or top-down impact trajectories (stressing e.g. photosynthesizing species or predators, respectively). Based on that observation, SOLUTIONS developed the Ecosystem Vulnerability Distribution approach, as the ecosystem-level equivalent of the SSD-model, acknowledging that ecosystems from different (reference) sites will exhibit different vulnerabilities to stress. This resulted in a preliminary analyses for a region outside Europe, for which sufficient data were available during the SOLUTIONS project. It appeared that indeed different species assemblages have different vulnerabilities to mixture exposures, and that chemical pollution could be ranked relative to other stressors in their relative role in causing ecological impacts (Zijp, Huijbregts et al. 2017). This finding

implies that the same level of exposure to a chemical or a mixture will imply different magnitudes of impacts in different water bodies. If an EQS is exceeded, this thus implies different levels of responses to that under field conditions. Whilst the EQS is utilized as a key benchmark concentration to classify (chemical) water quality status in the WFD, there are two observations requiring further investigations and improvements. First, Arle, Mohaupt et al. (2016) showed that the EQS itself may be highly uncertain, as the EQS-values for a single chemical in various countries can vary be one or many orders of magnitude (despite standardized EQS-derivation guidance). Moreover, an EQS is also considered as insufficiently protective, given analyses on thresholds of impacts per species (Berger, Haase et al. 2016).

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7 Species-sensitivity distributions for use in environmental protection, assessment and management of aquatic ecosystems for 12,386 chemicals

7.1 Introduction

This Section describes details of SOLUTIONS-progress into SSD-based evaluation of MRA, worked out in a scientific manuscript. The work was prepared to help solving one of the problems of the current WFD implementation, that is: lack of ecotoxicity data for a multitude of compounds. With approx.. 146,000 chemicals in commercial use (ECHA website, visited October 2018), the focus on the 1st tranche of chemicals (45 Priority Substances of Europe-wide concern for water quality status) and the 2nd tranche of compounds (approx. a total of 300 compounds, EEA, 2018), and the chemical pollution definition of the WFD (encompassing any chemical or mixture that may cause harm), we focused on deriving ecotoxicity information for as much chemicals as possible. Apart from adding chemicals we also developed further methods for mixture risk assessment, liaising to both the chemical safety assessment-related concept of 'sufficient protection' as well as the ecological impact assessment of the WFD (ecological status). The manuscript text below shows the details of the method derivation, and an example case study. Human activities cause the emissions of more than 100,000 chemical substances, with expected increases in compound diversity and emitted masses (Bernhardt and others 2017; ECHA 2016; UNEP 2013). This results in diverse ambient concentrations (e.g., EMPODAT, http://www.normandata.eu/empodat/), body residues (USEPA 2009), ecological risks (Malaj and others 2014) and eventual ecological and human health impacts (e.g., (Hoekstra and Wiedmann 2014; Schäfer and others 2016; Vörösmarty and others 2010). Chemicals pollution is considered as one of the main drivers of deterioration of freshwater biodiversity (Vörösmarty and others 2010). Complementary policy approaches are used to prevent and limit impacts of such pollution: chemical safety control, environmental quality assessment and management, and sustainable production and consumption approaches. These require ecotoxicity data and a method to convert these data into estimates of probability of (no-) impact. Species Sensitivity Distributions (SSD) makes such conversions, including such conversion for mixtures (De Zwart and Posthuma 2005a) as required to prevent and limit potential impacts of the 'universe of chemicals' (Bopp and others 2018; Kortenkamp and Faust 2018). Lack of ecotoxicity data is often mentioned as reason for addressing only a small part of the 'universe of chemicals'.

An SSD reflects the observation that inter-species differences in sensitivity to a chemical resemble a bell-shaped distribution (on a log-scale). An SSD is derived by fitting a selected statistical model (e.g., log-normal) to compound ecotoxicity data. Currently, data selection criteria vary amongst policy fields and jurisdictions. Though this complicates practices, SSDs are widely used for decision support purposes (SI-Table 1). This likely relates to ease of use and to an observation association between SSD-predicted and observed biodiversity impacts Posthuma and De Zwart (2012).

The global data set of ecotoxicity tests contains several hundreds of thousands of data (919,123 per 29 sept. 2018, https://cfpub.epa.gov/ecotox/index.cfm), few of which are commonly used to derive SSDs. This results in two trade-offs. Applying strict data selection criteria (e.g., chronic NOECs of particular quality following e.g. Klimisch and others (1997)) results in a low number of compounds with data

numbers are deemed sufficient. Second, when SSDs are thereupon based on fewer data points than available, they become increasingly 'unstable' for simple statistical reasons. In order to enable application of SSDs for as many compounds as possible, we compiled the world's data on species sensitivities. We created a base set of ecotoxicity data on test situations and sensitivities that might occur in nature. These were used to derive of a large set of SSDs, with various qualities. We added a four-digit quality score to each SSD. The score serves the design and/or interpretation of assessments.

The aims of this section (submitted as a manuscript to Environmental Toxicology and Chemistry) are to:

1) build a database with the best available ecotoxicity data for as many chemicals that can be accounted for,
2) derive chemical-specific SSDs, each with a quality score,
3) apply and evaluate various methods to bridge data gaps,
4) illustrate the utility and limitations of using SSDs in practical assessments, and provide the set of SSDs for further use (SI-Table 2).

7.2 Materials and methods

7.2.1 Scope

The study was executed as part of the EU-SOLUTIONS project (www.solutions-project.eu, (Brack and others 2015)). Under the EU-Water Framework Directive (WFD), water pollution is considered to exist when *any chemical or mixture* is or can be harmful to human health or the quality of an aquatic ecosystem. Water quality assessors are suggested to use model results as line of evidence to assess the likelihood that pollution may pose or has caused harm. SSDs particularly fit to this diagnostic task, especially when combined with the step to assess mixtures as that exactly results in those likelihoods! There is also a close association to chemical safety assessment. Protective benchmark concentrations are derived in the context of both REACH and the WFD (named PNEC and EQS, respectively), and represent a chemical exposure level below which adverse ecological impacts of a compound are absent or negligible (EC 2003; 2011). We operationally defined two SSD-models to characterize whether or not water systems are sufficiently protected, and – if not – what level of species loss would likely occur. The latter relates to the WFD 'ecological status' classification, which is based on species loss. Thus, using the two SSDs provides a basis to liaise chemical safety- and water quality assessment practices.

7.2.2 Ecotoxicity database

Ecotoxicity data were collated from many sources and characterized and curated to prepare for the derivation of SSDs:

1. The main body of the existing and well referenced aquatic ecotoxicity database is described in De Zwart (2002). All available toxicity data were designated to represent chronic or acute toxicity criteria (Table 7.1):
    a) records with the endpoints NOEC, LOEC, MATC, EC0, EC5, EC10 and EC20 are marked as "chronic NOEC" (chronic No Observed Effect Concentration) when they have an appropriate taxon-dependent test duration (see Table 7.1) and population relevant effect criterion (e.g., reproduction, growth, population growth, et cetera, next to mortality and immobility).

b) records with a sublethal (EC) or lethal (LC) endpoint ranging for 30% to 70% are marked as "acute EC50" (acute median Effective Concentration) when they have an appropriate taxon-dependent test duration and effect criterion (e.g., mortality and immobility).

This dataset comprised of 30,806 records and contains 2,513 chronic NOEC values and 28,293 acute EC50 values while covering a total of 3,445 substances and 1,556 different taxa. As described by De Zwart (2002), this dataset was comparatively checked for plausible toxicity estimates. At the least suspicion of implausible test results, the original reference was checked for data misinterpretations. Rather often, implausible results were attributable to errors in unit transformations, typing errors and/or tests conducted under less optimal conditions. Obviously erroneous entries were corrected when possible. Data were removed when original sources could not be checked.

Table 7.1. Criteria for operationally characterizing ecotoxicity data as 'chronic' or 'acute' (ECETOC 1993).

Species group	Acute test duration	(sub)chronic test duration
Algae	12 h	> acute
Bacteria	12 h	> acute
Unicellular animals	12-24 h	> acute
Crustaceans	24-48 h	> acute
Fish	4-7 d	> acute
Molluscs, worms, etc.	2-7 d	> acute

2. Further referenced data were added from an analysis and categorization of listed compounds of established and emerging concern under various national and international legislations (see https://www.stowa.nl/publicaties/ecologische-sleutelfactor-toxiciteit-hoofdrapport-deelrapporten-en-rekentools), were checked for plausibility and harmonized in endpoint and data coding whilst removing doubles (see 1). Additionally, also acute NOEC values and chronic EC50 values were identified using the test duration criteria.
   Data were obtained from a variety of sources:

   2.1. The USEPA ECOTOX database (https://cfpub.epa.gov/ecotox/data_download.cfm) as downloaded on October 21st 2014, this addition comprised 58,714 records concerning 1,853 substances, 942 taxa, 15,019 acute EC50 values, 19,875 acute NOEC values, 21,676 chronic NOEC values and 2,144 chronic EC50 values.
   2.2. A total of 952 test results from fish embryo toxicity tests (FET) on 214 substances with 4 different fish species were adopted from the Procter & Gamble Company (Oris and others 2012).
   2.3. Das et al. (2013) and Sandersen et al.(2009) provided 334 records of measured acute EC50 toxicity concerning algae, daphnids and fish for 162 different pharmaceutical active ingredients.
   2.4. A series of reports generated to define preliminary environmental quality criteria for compounds suspected to cause impact provided additional information mainly on pesticides and pharmaceuticals (Harezlak and Keijzers 2011; Osté and others 2010; Smit and Keijzers

2015). This data addition consisted of 1,059 records on acute and chronic ecotoxicity for 37 substances involving 215 different taxa.

2.5. A series of Draft Assessment Reports (DAR) from EFSA (http://dar.efsa.europa.eu/dar-web/provision), and the Pesticide Properties Database (PPDB) (http://sitem.herts.ac.uk/aeru/ppdb/en/search.htm).

2.6. The Swiss Centre for Applied Ecotoxicology at EAWAG provided a large number of dossiers on the ecotoxicity of pharmaceuticals and pesticides (http://www.ecotoxcentre.ch/expert-service/quality-standards/proposals-for-acute-and-chronic-quality-standards/).

2.7. The WikiPharma database (http://www.wikipharma.org/welcome.asp) was downloaded on November 18th 2016 and was used to complement ecotoxicity data for listed pharmaceuticals.

3. Data in the REACH registry (April 24th 2015) after code harmonization added 207,943 records on acute and chronic toxicity on 8,787 different substances, mainly for algae, daphnids and fish. The source data are often unclearly documented regarding test conditions, test duration and exposed taxa, and were not properly referenced to the scientific literature and thus not transparently traceable to (peer reviewed) origin, and is not necessarily comprehensive, complete, accurate or up-to-date (https://echa.europa.eu/legal-notice). This subset of data was therefore analyzed both separately as well as after collation with the other data.

4. Read-across acute ecotoxicity data (baseline, acute LC50) for algae, daphnids and fish were elaborated for 5,201 substances selected for various reasons in the SOLUTIONS project. Toxicity estimates were evaluated as the lowest value derived by two different estimation methods: a) by ECOSAR prediction (Mayo-Bean and others 2017), and b) methods utilized by UFZ, Leipzig, Germany. The UFZ method for acute fish toxicity consists of an automated read-across approach (Schüürmann and others 2011). This model estimates baseline toxicity from log Kow and corrects it by a toxicity enhancement derived from experimental data for similar compounds. Compound similarity is deducted by comparison of atom-centered fragments (Kühne and others 2009). For daphnids, a refined version of this approach has been applied (Kühne and others 2013). For algae, a simple model similar to that for fish was used, but here the acute toxicity was directly derived from experimental data of similar chemicals taken from an internal data set. Again, these data were analyzed both separately as well as after collation with the other data.

7.2.3 SSD derivation

A variety of SSDs was derived to enable quantifying the probability that exposure exceeds a chronic no-effect level (related to regulatory protection targets) or an acute 50%-effect level (related to species loss) for whole species assemblages (all data in a single SSD), and optionally (not analyzed in the case study) for specific taxonomic groups, to assess the likelihood of impacts on specific WFD-'biological quality elements'.

The location and scale parameters of SSDs (mu and sigma) were first derived with optimum data, and resulting SSDs were assigned a high quality score ('1111'). As decreasing test data numbers trades off into limited numbers of compounds and potentially lower SSD-'stability', additional SSDs were derived with various (inter-SSD) extrapolations to bridge data gaps, followed by an evaluation of similarity to the high quality ones (comparing extrapolated and read-across with high quality SSDs).

In line with origin and the use contexts (both chemical safety and environmental quality), data were subdivided according to source quality (literature referenced versus non-referenced, and measured

versus read-across) and to effect endpoints (chronic and acute) with characterization of data that can be used strictly as reported, measured ecotoxicity endpoints.

With the selection of strictly measured data, if more than two different taxa are tested for acute EC50 and chronic NOEC, the summarization process consisted of estimating the two moments of a log-normal SSD (Posthuma and others 2002):

1) mu – the population median of ^{10}log transformed toxicity values with equal weight per taxon, by first calculating the average within taxa and second averaging the averages per taxon over taxa, and
2) sigma – the population standard deviation of ^{10}log transformed toxicity data, without considering taxon weight.

If ecotoxicity data were available for less than 3 taxa, the process was restricted to mu - the average of the population of ^{10}log transformed toxicity values with equal weight per taxon. For the substances with too little data an intermediate median SSD slope (sigma) was adopted with a value of 0.7 (the average slope over all data is 0.71).

The above 'strictly measured' data selection leaves many of the collated data unused. In order to expand the number of compounds with an SSD model, additionally, and similar to the strictly as reported procedure, further test endpoints on acute EC50 and chronic NOEC were obtained after extrapolation from the most prominently available single other test endpoints in the collated data set. Extrapolation factors are summarized in Table 7.2. If more than 4 substances shared the same primary Mode of Action (MoA) in this extrapolation procedure, the SSD slope (sigma) was averaged over all substances with a similar primary MoA. If more than 5 different taxa are tested for either acute EC50 or chronic NOEC, the input data were not further extrapolated. If test data are available in this extrapolation process for less than 3 taxa, the test endpoints (acute EC50 and chronic NOEC) were summarized by extrapolation from all available data, irrespective of the reported test endpoint. This was done according to the scheme and the order presented in Table 7.2, as derived from De Zwart (2002), and approximately reconfirmed by Figure 7.3in the present paper. If in the extrapolation process the maximum coverage of ecotoxicity data is available for less than 3 taxa, the summarization process is based on strictly measured data and restricted to mu - the average of the population of ^{10}log transformed toxicity values with equal weight per taxon.

Table 7.2. SSD-extrapolation scheme by factor From/To.

To / From	Order of extrapolation attempts to acute EC50[1]	Acute EC50 extrapolation factor[2]	Order of extrapolation attempts to chronic NOEC[1]	Chronic NOEC extrapolation factor[2]
Acute EC50	0	Multiply by 1	3	Multiply by 1/10
Acute NOEC	1	Multiply by 3	2	Multiply by 1/3
Chronic EC50	2	Multiply by 3	1	Multiply by 1/3
Chronic NOEC	3	Multiply by 10	0	Multiply by 1

[1] Numbers relate to quality scores in Table 7.3 [2] Numbers express inter-SSD extrapolations (parallel shift).

7.2.4 SSD types and quality criteria

The database contains far more acute EC50- than chronic NOEC data, making the former more robust for the majority of compounds. Also, there are other reasons why some SSDs are likely better estimates of true but unknown sensitivity differences than others. Therefore, we added four-digit quality scores as shown in Table 7.3 with the modality '1111' representing the highest-quality. Derivation of the slope may or not be possible (digit 1). Representation of different taxonomic group was ranked (digit 2). Data origin was classified (digit 3). When SSDs were derived via data-bridging techniques, the method was scored (digit 4). In the latter case, when sufficient acute EC50 or chronic NOEC values are not available but other toxicity endpoints are, those are extrapolated to acute EC50 and chronic NOEC values using empirical derived extrapolation values (Brock and others 2008; De Zwart 2002; Duboudin and others 2004). Mind that this way of bridging data gaps should not be considered as the application of an acute/chronic ratio (ACR) on a per-species basis. The correct interpretation of this extrapolation is a parallel shift in an SSD, which is far more robust than per-species ACR extrapolations.

Table 7.3. Four-digit quality scoring of SSDs, based on underlying data types, quality and numbers.

Digit	Quality aspect	Modality	Meaning
1	SSD fullness	1	Data on full SSD available (Mu and Sigma)
1		2	Not sufficient data to calculate SSD slope
2	Biodiversity coverage	1	Number of taxa evaluated >10
2		2	Number of taxa evaluated >5
2		3	Number of taxa evaluated >2
2		4	Number of taxa evaluated <3
3	Data origin quality	1	Strictly measured
3		2	Extrapolated
3		3	Read-across
4	Extrapolation quality	1	Not extrapolated
4		2	Single-step extrapolation (Table 2)
4		3	Double-step extrapolation (Table 2)
4		4	Triple-step extrapolation (Table 2)
4		5	All available toxicity data extrapolation (Table 2)
4		6	Read-across

7.2.5 Evaluations of SSDs

Various regression of 'other' SSDs on high-quality ones were performed to evaluate quality of the 'other' SSDs (for mu, the SSD midpoint). The regressions involved (A) REACH data, (B) read-across data, and (C) extrapolated acute EC50 or chronic NOEC data (cf. Table 7.2). These were regressed against the geometrical average of high-quality SSDs, defined as strictly measured acute EC50 or chronic NOEC toxicity data over tested taxa derived with the curated and validated data for the substances. Also, the geometrical average of strictly measured chronic NOEC toxicity data over tested taxa was regressed against the geometric average of strictly measured acute EC50 toxicity data.

7.2.6 Case study: assessment questions and associate screening-level outcomes

The case study studied exposure to 1,760 compounds and their mixtures. The selected chemicals (REACH-chemicals, pesticides and pharmaceuticals) have been or are produced, used and emitted in Europe (based on available dossier information), and have sufficient data for all analysis steps. The companion paper (Posthuma and others 2018 (companion paper, submitted sept 2018)) provided emission data. The SOLUTIONS integrated modeling framework provided predicted concentration data.

This model is based on the E-HYPE hydrology model (Donnelly and others 2013), on which the emission data were projected. Predicted were freely dissolved concentrations for 22,278 EU sub-catchments (resolution / median size: 214 km^2) for 365 days. Toxic pressures of the individual chemicals were derived from predicted bioavailable concentrations per sub-catchment/day using the SSDs of the present study, followed by quantification of the chronic and acute mixture toxic pressure per sub-catchment/day (De Zwart and Posthuma 2005b). A simplified approach was applied to derive mixture toxic pressures, by operationally assuming that all chemicals act concentration additively, in formula:

$$(\sum_{i=1}^{1760} HU_i, where\ HU_i\ is: \frac{Predicted\ environmental\ concentration_i}{SSD\ midpoint\ mu_i}).$$

with HU=Hazard Unit, in line with the frequent practice of water quality assessment for mixtures by linearly summed Risk Quotients over compounds. The approach was modeled with the MS-Excel function NORMDIST(^{10}log(ΣHU),0,Average SSD slope = 0.7,1). SSD quality scores for the studied chemicals are relatively high (from '1111' to '1324'or '1325' for chronic and acute, respectively). Model results were summarized using various approaches and statistics.

7.3 Results

7.3.1 Ecotoxicity data

When stripped from repetitive data, the set of measured ecotoxicity data consists of 256,409 records on 11,126 different substances, where 123,630 records pertain to acute EC50 test results, 75,131 to acute NOEC values, 8,404 records cover chronic EC50 values and 49,244 records reflect chronic NOEC values. In total, 2,257 different taxa have been subjected to one or more substances. The number of different taxa tested per substance and type of test ranges from 1 to 271. The addition of the read-across data with estimates of acute EC50 values for green algae and/or daphnids and/or fish, adding 15,273 data records, brought the number of different substances with information on ecotoxicity to 12,386 (as some compounds have both a data-driven and a read-across SSD). Of the 271,682 data records 25% are based on validated data from existing ecotoxicity databases ('strictly measured' and referenced) and 69% are based on untraceable and unreferenced REACH data, while 5% are based on read-across data.

The number of chemicals for which one or more SSDs were derived is 12,386. Multiple SSDs can be available for one compound (e.g., both chronic and acute).

7.3.2 SSDs and quality scores

A variety of SSDs was derived (Table 7.4), with detailed (mu, sigma, quality score) information in SI-Table 2. The mu and sigma can be used for any assessment purpose (see SI-1). The quality scores (varying from '1111' to '1325' or '2324' for acute and chronic SSDs, respectively) are relevant for assessment planning and interpretation. High toxic pressures predicted with low quality SSDs suggest further ecotoxicity data collection or a refined assessment step rather than conclusive evidence of high toxic pressure. Low toxic pressures predicted with low quality scores provide however useful management information, as this

allows to use a practical strategy of 'excluding the innocent' (sites or compounds) for further management attention.

Table 7.4. Types and counts of SSDs. "Measured" = ecotoxicity data are from laboratory toxicity testing, "Traceable" = […] from traceable in the scientific literature, "AllData" = […] from combined traceable and untraceable measurements, "ReadAcross" = […] QSAR extrapolation, "FullSSD-True" = SSD model derived from sufficient data to quantify sigma, "FullSSD-False" = SSD model derived from insufficient data to quantify sigma. All SSDs are derived by combining data on any of the aquatic taxa available.

Origin & Quality	DataType	FullSSD	# of SSDs (# compounds)
Measured & Traceable	Acute EC50	TRUE	4,235
Measured & Traceable	Acute EC50	FALSE	3,669
Measured & Traceable	Chronic NOEC	TRUE	2,518
Measured & Traceable	Chronic NOEC	FALSE	838
Measured & NonTraceable	Acute EC50	TRUE	7,929
Measured & NonTraceable	Acute EC50	FALSE	4,093
Measured & NonTraceable	Chronic NOEC	TRUE	5,376
Measured & NonTraceable	Chronic NOEC	FALSE	2,730
Measured & AllData	Acute EC50	TRUE	11,422
Measured & AllData	Acute EC50	FALSE	6,849
Measured & AllData	Chronic NOEC	TRUE	7,760
Measured & AllData	Chronic NOEC	FALSE	3,233
ReadAcross	Acute EC50	TRUE	4,927
ReadAcross	Acute EC50	FALSE	274

7.3.3 Accuracy of "other" SSDs

EC50-level. The regressions of SSDs derived from various methods ('other') on high-quality ones for the SSD-midpoints were all significant (**Figure 7.1**: REACH (A), overlapping number of compounds 927, $y = 0.8173x + 0.7025$, $R^2 = 0.65$, $P<0.001$; read-across (B), overlapping number of compounds 1,116, $y = 0.5914x + 1.2515$, $R^2 = 0.49$, $P<0.001$; extrapolations with Table (C, overlapping number of compounds 3,827, $y = 0.9611x + 0.1362$, $R^2 = 0.95$, $P<0.001$).The read-across SSDs (related to baseline-toxicity) showed more variability, and appeared to underestimate the mu for the most toxic substances up to a factor of 10 as compared to high-quality SSDs. The reliability of acute-EC50 SSDs based on the other data analysis methods decreases in the sequence Extrapolated SSDs ≈ REACH-based SSDs > Read-across SSDs.

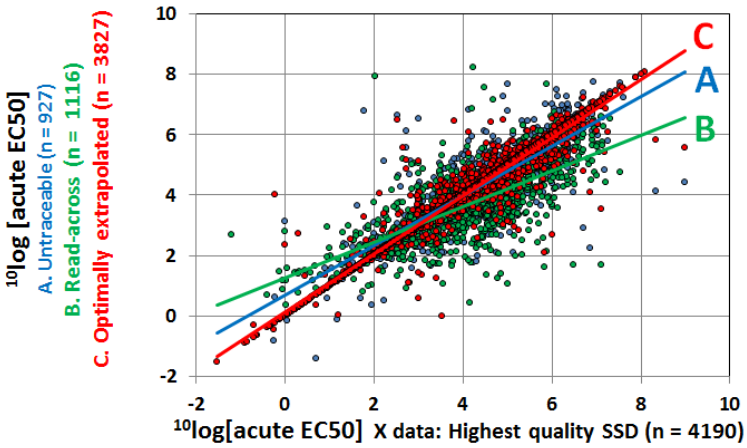

Figure 7.1. Comparison of acute-EC50 SSD midpoint data for three SSD-derivation approaches regressed on highest-quality SSD-midpoint data. X-data: highest-quality SSDs (Traceable data, All taxa, Geometrically averaged, Measured data, Acute EC50). Y-data types: 'other' and 'derived' SSDs (A=Untraceable data [REACH], blue; B=Read-across, green; C=Optimally extrapolated, red).

*NOEC-level.*_Similar analyses for chronic NOEC data are shown in **Figure 7.2.** For REACH-data, the relationship was less strong than for EC50- data, but still highly significant (A, overlapping number of compounds 251, y=0.7448x + 0.8502, R^2=0.60, P<0.001). For the most toxic substances, the REACH data tend to underestimate toxicity as compared to the well-referenced dataset by a factor of up to approximately 30. A highly significant relationship was found between extrapolated chronic data and X-data (B, overlapping number of compounds 1,131, y=0.7941x+0.5902, R^2=0.74, P<0.001). The extrapolated data also tend to underestimate toxicity as compared to the well-referenced dataset by a factor of up to approximately 10. The reliability of chronic-NOEC SSDs based on the other data analysis was relatively similar for both other methods.

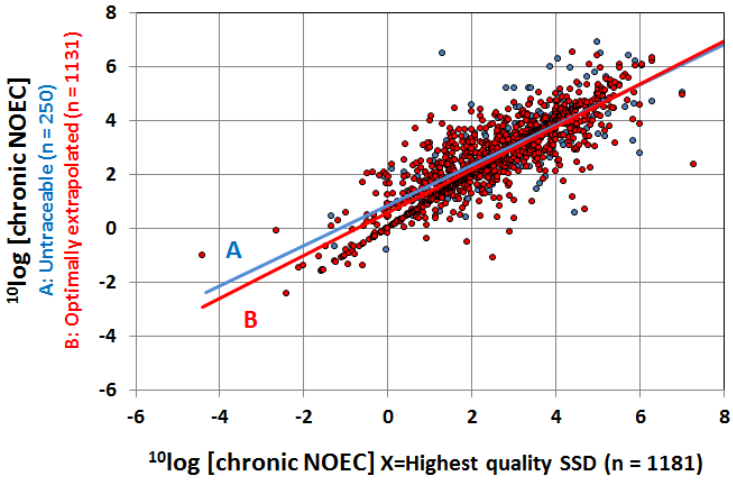

Figure 7.2. Comparison of chronic NOEC SSDs midpoint data for two SSD-derivation approaches regressed on highest-quality midpoint data. X-data: highest-quality SSDs (Traceable data, All taxa, Geometrically averaged, Measured data, Chronic NOEC). Y-data types: other SSDs (A=Untraceable data [REACH], B= Optimally extrapolated, red).

EC50 and NOEC SSDs. The comparison of SSDs based on NOECs versus EC50s showed a significant association between the mu values for the 250 substances for which both aspects are strictly measured and quantified (**Figure 7.3**, n= 250, y=0.7304x - 0.4414, R^2=0.60, P<0.001). On average, the chronic NOEC is less than a factor of 10 lower than the acute EC50, which represents an observed factorial shift of the SSD. A limited number of outliers has a strong influence on this regression. A restriction of the regression to the 5-95 percentile data intervals yielded a factorial difference of about 6.6 and a slope of about 0.85 (n=225, y=0.8509x - 0.8237, R^2 = 0.76, P<0.001). These outcomes suggest that, on average, an SSD-NOEC can be derived from an SSD-EC50 by extrapolation (as shown in **Table 7.4**), but also that the variability around the average should be taken into account when such an extrapolation would be used in practice.

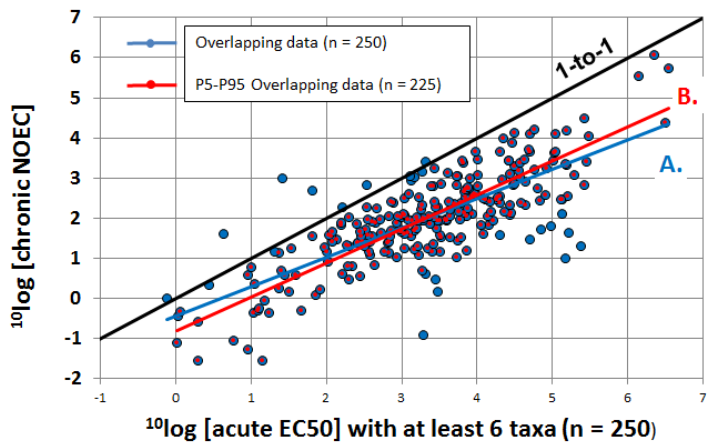

Figure 7.3. Comparison of SSD-midpoints for acute EC50 (X) and chronic NOEC (Y). A: All data points, blue dots and blue line. B: *Ibidem*, restricted to the P5-P95 data ranges, red dots and red line.

Selecting SSDs for an assessment problem. A single compound may be associated to various SSDs, with different scope (e.g., total species assemblages, or algae only), data origins and quality scores. A recommended process would sub-select the SSD for a compound based on the assessment problem

definition (e.g., total assemblage, or algae only) and the quality scores (SI-Table 2), with higher numbers of data and taxa diversity generally representing more reliable SSDs. An average slope with a numeric value of 0.7 is adopted if there are insufficient data to derive the specific slope from the data.

7.3.4 Case study results: illustrating various screening-level outcomes

Note: results and rankings of sites and substances address various practice-oriented questions, but are for illustrative purposes only. They show how the method allows breaking down the effect metrics in contributions per site and substance. Results are *explicitly not intended or to be interpreted* as a list of Europe-wide priority sites or chemicals in a WFD context. That would require methods agreed and approved by all stakeholders, which is clearly beyond the scope of the current paper.

Assessor question 1: how accurate are concentration predictions? The integrated emission + E-Hype modeling yielded 1.5 * 10^{10} predicted concentrations (22,278 sites * 365 days * 1,760 compounds). To evaluate accuracy, predicted concentrations were compared to measured concentrations. Details will be published by J. van Gils (Deltares, Delft, the Netherlands; publication in preparation). Over- and under-prediction of observed concentrations were equally distributed and remained within one order of magnitude for 65% of basin/substance combinations, and within two orders of magnitude for 90% of basin/substance combinations. These results should be interpreted in the context of the wide spatio-temporal variation of measured field concentrations that result from natural processes, human activities (pesticide spraying) and sampling schemes.

Assessor question 2: what is the spatial distribution of the likelihood of mixture impacts? The spatial patterns regarding (in)sufficient protection and ecological impact magnitudes are shown in Figure 7.4 and Figure 7.5, respectively, based on the 95th percentile of predicted toxic pressures over a year (P95-year = 18 days is 5% of a year). The interpretation proceeds as follows:

<u>(1) Statistical</u>. Colours represent the variation of the probability that a randomly selected species from the set of tested species would exposed beyond the selected effect threshold for more than 18 days per year. This probability is the 'Probability of Effects on a Species' (PES) (Suter and others 2002). Higher mixture exposures imply a probability to cause harm to randomly selected test species if reared in the water. Thus, these probabilities are *not* a characteristics of the tested species or of the local species assemblage, but of the polluted water. Colours reflect the relative potential of the pollution of a water body to cause harm to a randomly selected test species.

<u>(2) Biodiversity interpretation</u>. PES-values are logically and quantitatively the same as PAF-values (Potentially Affected Fraction of species). PAF is however the more commonly used metric to characterize pollution, related to the regulatory-defined protection endpoint ('prevent effects on biodiversity'). Colours reflect thus also the relative potential of the pollution of a water body to cause harm to a fraction of species in the assemblage of tested species.

<u>(3) Regulatory interpretation</u>. The WFD-Annex II defines it as an assessors' task "*[to] … carry out an assessment of the likelihood that surface water bodies …. will fail to meet the environmental quality objectives ….*". This likelihood can be established separately, using the two SSDs per compound. This yields two maps, representing the likelihood of insufficient protection and of impacts exceeding the 50%-effect level, respectively.

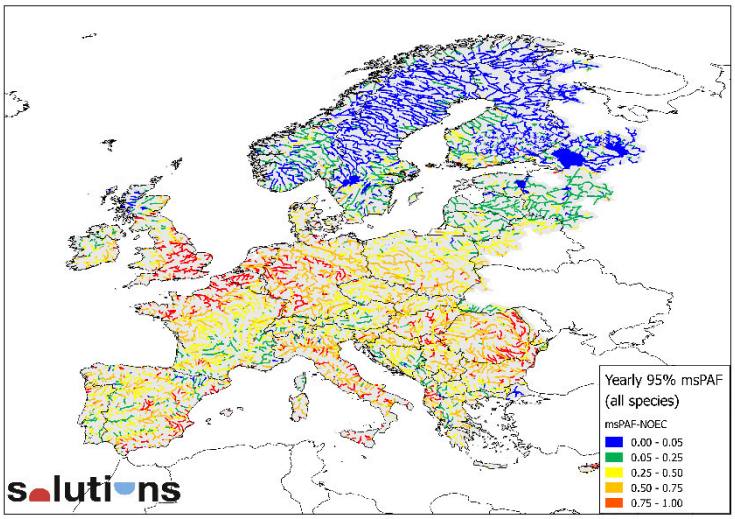

Figure 7.4. Results mapped in relation to the regulatory concept of 'sufficient protection' of aquatic ecosystems, and thus to both REACH and the 'good chemical status' concept of the WFD. The map depicts the relative likelihood that European water bodies are insufficiently protected against exposure to mixtures for 95% of the days (18 days). The blue colour marks sites with sufficient protection against adverse effects of exposure that operate via growth and reproduction, other colours show differences in the likelihood to pose distress to species assemblages (exposure higher than the no-effect level); the chosen colours do not relate to the EU-'ecological status' classification. Technical output specification: numbers are P95-year of msPAF-chronic NOEC per site (n=22,728 water bodies).

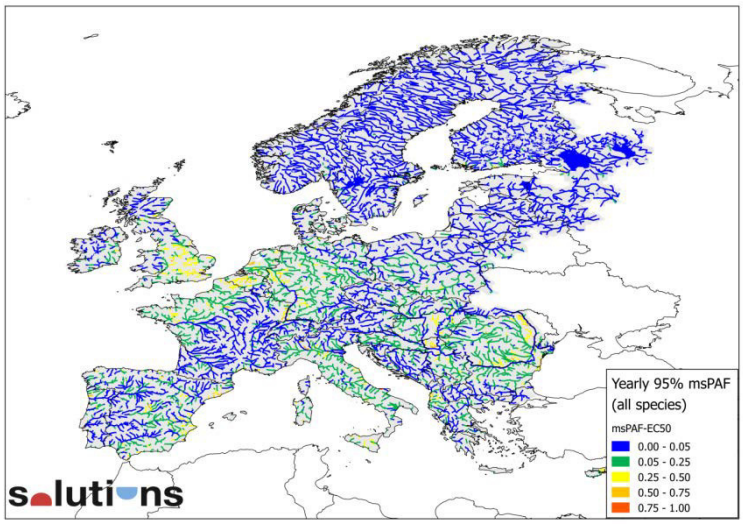

Figure 7.5. Results mapped in relation to the regulatory concept of expected magnitudes of biodiversity impacts, as utilized in the WFD-'ecological status' classes, where impacts on altered aquatic life are characterized as reference (non-altered), moderate, large and severe. The map depicts the relative likelihood that European water pose harm to aquatic ecosystems at the indicated levels for at most 5% of the days (18 days), with numbers relating to expected species loss. Note that this map does not encompass emission peaks. The colour scale boundaries were set at the same numerical values as those of **Figure 23**) and are not related to the EU-'ecological status' classification. Technical output specification: numbers are P95-year msPAF-acute EC50 per site (n=22,728 water bodies).

Assessor question 3: what is the spatial distribution of insufficient protection? The critical value between blue and green Figure 7.4 is related to the EQS-related protection level. The aim of 'full protection of ecosystem structure and function' against exposure to a single chemical has historically been operationalized via the 5th percentile of an SSD-chronic NOEC (HC5-NOEC). This equals the so-called '95%-protection criterion' (at HC5-NOEC, 95% of the species are protected against exceedance of their no-effect level). An msPAF-NOEC=0.05 also reflects the 95%-protection level, but now for mixtures. Water bodies not mapped as blue can thus be considered to be 'insufficiently protected' according to both the REACH (PNEC) and the WFD (EQS) regulation. The fraction of blue coloured water bodies, with potential 'sufficient protection' against mixture effects during 18 days in a year or less, is small. Blue sites are mainly restricted to low-populated Nordic countries. A majority of water bodies appears insufficiently protected.

Assessor question 4: what is the frequency of insufficient protection amongst basins? Cumulative distributions of the probabilities that mixture exposures exceed the no-effect level are shown in Figure 25. Insufficient protection occurs in approx. 65% of the European water bodies (P95-year data). Specific basins have higher fractions of water bodies with insufficiently protection (≈93%, 88% and 79% for Rhine, Danube and Spanish basins, respectively). There are Pareto-type (skewed) distributions of the across-site likelihood that mixtures pose harm: relatively few sites are characterized by a relatively high chronic toxic pressure. Identifying those can support management decisions to reduce harm.

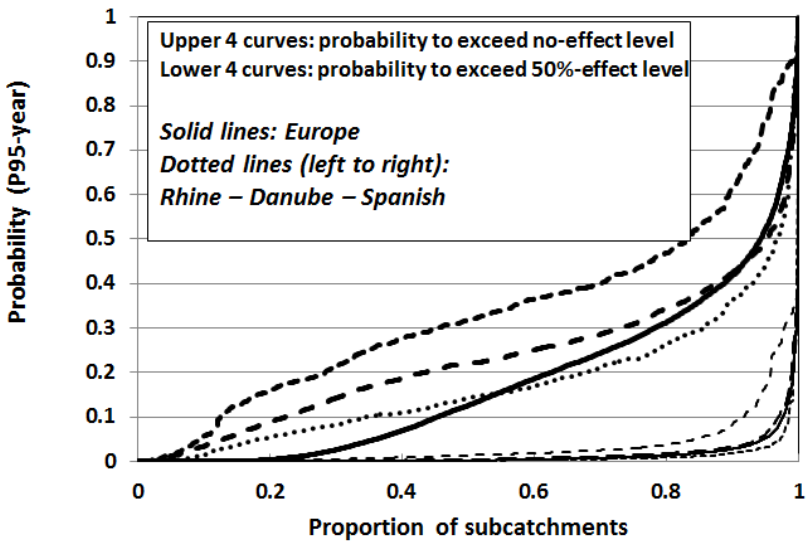

Figure 7.6. Cumulative distributions of mixture toxic pressures of the individual sub-catchments of Europe (n=22,728) and of three specific basins (Rhine: n=813; Danube n=3477; Spanish basins n=696). X-axis=rank-order of the sub-catchments. Y-axis: probability that exposures exceed the no-effect- or 50%-effect level, under the assumption of concentration additivity for all substances in the study.

Assessor question 5: what is the spatial distribution of the likelihood of species loss? Exposures relating to 'insufficient protection' are not predictive of species loss. The relative probability of that is depicted in **Figure 7.5**, again for the P95-year exposures (exposures on 18 days reach the 50%-effect level). A vast fraction of European water bodies is predicted to exhibit chemical pollution-driven species loss. We selected the value of <0.05 to define the blue scale, as a probability at which impacts might not easily be discerned from natural variability (reference variability), although there is wide-spread mixture-related distress (**Figure 7.4**). The non-blue colours in **Figure 7.5** represent increasing species loss predictions. The choice for the P95-year data excludes peak events, such as related to pesticides. Section 3 of the Supporting Information shows the increased probability of impacts when using e.g. the P99-year (4 days peak exposures are covered). The number of sufficiently protected sites is reduced, and the number of sites expected to show species loss increased.

Assessor question 6: can the results help focusing management on sites and compounds? _Yes, but rankings are highly specific to questions asked and situations considered (e.g., the P95 and P99-year example). Rankings of substances and substance groups that pose most harm were derived for the P95-year data, which implies the tendency that pesticides are under-represented in the example ranking. Note that even the chemicals involved in the '1986-red Rhine' incident (massive pesticide emissions from an accident at a chemical factory, Schweizerhalle) would *not* be 'seen' in the P95-based ranking (Giger 2009). Illustrative results for the P95-year data are summarized in **Table 7.5**, related to species loss and relatively short total exposure days (18 days of exceedance of the 50% effect level). Ranks were derived in two steps. In the first step, a relative toxicity score for each compound in a sub-set of samples was determined as the product of the mean compound toxic pressure in the set and the ratio of non-zero values for that compound and the non-zero values for the mixtures (representing magnitude and relative contribution and frequency of increased compound pressures to total mixture pressures). Thereupon, all scores were ranked relatively, with Phorate as base (defined as '1'). The result metric relates to the probability of impacts to species assemblages aggregated over an area and over time. This ranking showed that >99% of the thus-derived relative impact was attributable to approx. 15

compounds. In the example, Bisphenol-A consistently ranks highest. This compound is imported + produced in the largest mass class of the top-15 chemicals and is ubiquitously used by consumers, professional users and manufacturers. The top-15 explains nearly all exceedances of effect levels related to direct effects of exposure. The remaining 1,745 chemicals cause additional relative impacts of <0.5% to this direct species loss. A Pareto-type classification (often referred to as the 80-20 rule) of 1,745 versus 15 chemicals implies that approx. 1% of the compounds causes 99% of the exposure impacts, leading to a Pareto-type '99-1' rule for species loss for the P95-year assessment.

Table 7.5. Example of chemical ranking. The illustration is on the top-15 ranked toxicants, their SSD-quality scores and their relative impact potential to species loss, based on exposures lasting max. 18 days beyond the 50%-effect level, for Europe and the three major case study river basins (relative ranks in columns 6 – 11 defined by anchoring the relative impact of other compounds in river system to Phorate/Europe=1, based on msPAF-EC50). Count: number of counts of a compound in the top-15 in all of Europe and the 3 case study basins, rank=net rank order based on the findings, expressing frequency and level of exposure contributing to likelihood of effects. WFD- and NORMAN priority: see text. Note that the choice for P95 excludes peak exposures of e.g. pesticides.

Substance	CAS	Qual Score (SSD-acute EC50)	WFD priority	Norman priority	All 22 EU Basins	Danube basin	Rhine basin	Spanish basins	Count	Rank
Bisphenol-A	80-05-7	1111	√	√	90316	85935	277239	110079	4	1
N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	793-24-8	1311			2573	2451	20344	3528	4	2
Chlorpyrifos	2921-88-2	1111	√		1629	2755		78285	3	3
Anthracene	120-12-7	1111	√		1502	6675	3528	247	4	4
Octamethylcyclotetrasiloxane	556-67-2	1224		√	1483	6325	1320	92	4	5
N-(4-aminophenyl)aniline	101-54-2	1311			1381	268	15144	393	4	6
Cumene hydroperoxide	80-15-9	1311			1123	4332	2242	634	4	7
Difenylamine	122-39-4	1111		√	589	308	8667	1028	4	8
1-Dodecanol	112-53-8	1211			48	558			2	9
Pyraclostrobin	175013-18-0	1211			41	151	114		3	10
Cyhexatin	13121-70-5	1111			25	8		2821	3	11
p-Phenylenediamine	106-50-3	1311			19	17	97		3	12
Dimoxystrobin	149961-52-4	1311			11	46	37		3	13
Terbufos (not approved for use)	13071-79-9	1111			6	75		96	3	14
Phorate (not approved for use)	298-02-2	1111			1			110	2	15
Count			3	3	15	14	10	11		
Sum relative score op 15 substances					100748	109904	328733	197314		
Sum relative score remaining 1760 substances					208	571	0	0		
Percent of sum relative score in top 15 substances					99.8%	99.5%	100.0%	100.0%		

Given the sensitivity of rankings for choices that can or need be made, we recommend that chemical rankings should be made preferably *within* groups of chemicals. That would better represent true patterns (e.g., not missing pesticides), but it would also fit better to packages of management perspectives, which of course vary vastly between e.g. pharmaceuticals and pesticides. Pharmaceuticals were not found as chemicals for which exposures exceeds the EC50-level via direct effects on growth and reproduction. However, this does not mean they are without harm. The vast number of sites with apparent 'insufficiently protection' in **Figure 7.4** suggests otherwise, even if we consider that even that figure lacks information on specific toxicity and secondary poisoning. Note also, that the EU-wide model operates on a scale of >200 km^2, so that probabilities of impacts at point sources (e.g., downstream waste water treatment plants) are not shown in detail. At such point sources, impacts are (much) higher than shown for whole water bodies (this study).

Assessor question 7: do we miss chemicals in monitoring for the WFD? Yes. Some of the chemicals shown in Table 7.5 are *not* covered by current regulatory prioritization approaches. (Priority Substances and

NORMAN Working Group Prioritisation, https://www.norman-network.com/sites/default/files/files/suspectListExchange/NORMAN_PriorityList_2016.csv, as provided by Valerio Dulio. Further attention in monitoring would be asked for ten additional compounds (in the present illustration).

Assessor question 8: what needs be done before drawing final conclusions for management? Model outputs may be biased when specific compound characteristics and use information is neglected in modeling and interpretation. Critical interpretation is important. For example, screening of the apparent drivers of mixture toxicity in Table 7.5 reveals that two top-15 compounds, Terbufos and Phorate, are not approved in the EU. The model was run on the basis of dossier data, but apparently, the non-approval decision is supported by the current analyses. The other compounds are widely used in agriculture (the pesticides: Chlorpyrifos, Cyhexatin, Pyraclostrobin and Dimoxystrobin) or by consumers and professionals as well as in various industrial processes (remaining compounds). They are classified as "toxic to aquatic life with long lasting effects", as "very toxic to aquatic life / very toxic to aquatic life with long lasting effects", and/or as Substances of Very High Concern. Import+production masses span ranges of large masses (10^6 to10^7 tons per year for Bisphenol-A) to lower masses (10 to 100 tons per year, for Difenylamine). Apparently, chemical safety assessment procedures apparently identify drivers of mixture impacts in the field, and prioritization of that via mass classes and intrinsic hazard characteristics of chemicals (highest numbers have had first priority for regulatory safety assessments) seem to make sense. Further scrutiny should not only consider the chemicals, but also exposure- (not done for the case study) and effect data (inspection of SSD-quality did not reveal poor-quality SSDs).

7.4 Discussion

7.4.1 SSD data, derivation, availability and utility

The collation, curation and classification of ecotoxicity data resulted in a vast expansion of the number of SSDs. The total set of SSDs represents compound-specific SSDs that can be used to assess the probability that ambient exposures exceed a critical effect level for whole species assemblages or – if needed – for specific taxonomic groups. The latter relates to practical questions for the WFD, where pollution may impact specific taxonomic groups (so-called 'biological quality elements'). A case study illustrated the utility for water quality assessment, addressing specific practical questions. Although no case studies are shown for other SSD uses, such as derivation of protective benchmark concentrations or for use in life cycle assessments, the SSDs can also be used for those purposes. Regarding derivation of protective benchmarks, the results of **Figure 7.3** suggest that such benchmarks can be derived from acute test data, due to confirmed across-SSD patterns, potentially expanding the number of EQSs. The use of SSDs to support sustainable production and consumption policies is currently considered to support the design of safer production chains and support buying benign products (Saouter and others 2017).

7.4.2 The case study

The case study outcomes suggested that (1) water quality is insufficiently protected against the direct effects of chemical pollution on species assemblages, with (2) an associated predicted degree of likely species loss, caused by (3) relatively few compounds at the European scale, which are (4) logical outcomes in comparison to compound-specific characteristics (mass used in Europe, ubiquitous use,

hazard characteristics). Clearly, the 'non-toxic environment' has not been reached yet (Figure 7.4), and integrative environmental modeling can support selecting 'best management' to reduce pollution threats.

7.4.3 SSDs and WFD utility

So far, chemical pollution under the WFD is addressed for approx. 200 to 300 individual compounds at maximum (EEA 2018). This is done via evaluating concentration to protective benchmark concentration (EQS) ratios followed by applying a 'one out, all out' approach to water quality classification. Such exceedances are used to trigger management attention (when exposure exceeds the EQS for at least one compound), but in its current form it is incomplete: it neglects 99.7% of the compounds in commerce as well as mixture effects. Moreover, the classification may suffer from undesired across-countries EQS variability, which exceeds one order of magnitude for many compounds (Arle and others 2016). Finally, it reacts sensitively to each added chemical that is monitored, as that increases the probability of non-compliance. As a result, regulatory water quality status evaluations showed substantial and sometimes increasing numbers of water bodies with exceedances of at least one EQS (EEA 2012; 2018). Whilst this approach informs us that the probability of *any* harm from *any* chemical at the time of sampling may not be negligible (as EQSs relate to 'sufficient protection'), it does *not* provide insights in the likelihood of harm – it only discriminates a negligible from a non-negligible likelihood. This is insufficient for evaluating impact magnitudes, and thus insufficient to rank sites and compounds. The use of SSDs, applied to non-compliant sites, provides the necessary, refined diagnostic information. It shows mixture non-compliance (Figure 23) and impact hot spots and ranking (Figure 24). This solves important and complex conundrums of current practice (next section).

SSD results are not stand-alone data for practitioners. An assessment of the likelihood of impacts under the WFD consists of various lines of evidence. Model results are combined with information from an 'assessment of pressures' (human activities causing chemical emissions) and available monitoring data, and/or other information, to come to conclusions. Information may consider sources as diverse as non-target screening of the presence of chemicals (Hollender and Schymanski 2017) to effect-based methods that assess impacts of complex mixtures in water samples (Altenburger and others 2015). River basin management planning is based on all the information. The use of SSDs in this process allows the assessor to obtain highly specific information on the likelihood that chemical pollution causes harm, in line with the holistic principles of the WFD (Voulvoulis and others 2017). That is, the use of the SSD models allows for making an impact-related interpretation sequence that moves from the water system to the best solution, in the sequence "(water) System to Site to Substance to (eventually: management) Solution". This complements the current reductionist EQS-based "Substance-Solution" approach, which operates for approx. 200 compounds.

7.4.4 Improving on pollution classification and communication

There are practical conundrums associated with the present classification system. First, when a site is mapped as non-compliant due to exceedance of an EQS ('red'), it is unclear whether human health or environment would be affected, by which compound(s) or mixtures, and to which extent. Thus, management cannot be focused on priority sites, chemicals or protected endpoints. Second, interpretation and communication on the 'red' classification of chemical pollution is complicated, for scholars, responsible authorities and the general public alike, and it has unforeseen consequences. One

such reaction is to try limiting addition of suspect chemicals to the monitoring effort, as this increases the probability of water systems turning 'red'. Here, more effort results in worse scores. Another is to cease investing in management tracks that appear not helpful ('red' remains 'red'). Here, past effort results in no apparent improvement.

Problems with the current classification relate to interpretation and communication. That is, the current indicators are – in themselves – fine, as they reflect the same level of protection in both REACH and WFD. Moreover, the indicator *system* is designed such that it triggers management attention until the WFD has reached its goal (no single 'flag' is left upon a long-term classification-diagnosis-management cycle), and the 'one out all out' principle of classification serves this long-term strategic goal. For communication and interpretation, however, the current 'flags' should *not* be interpreted and communicated as evidence for 'impact'. A 'flag' only means 'pay attention and diagnose a potential role in impacts'. It is at this point that SSDs provide refined diagnostic information (see case study results as example). The use of modeling, amongst which with SSDs, is thus key to understand the 'red' and refine its meaning, and is explicitly suggested for diagnosis in the WFD (Annex II).

7.4.5 Limitations of SSDs for decision support

The use of SSDs has intrinsic restrictions. They don't help to establish the likelihood of impacts via indirect effects (when e.g. loss of a prey affects the predator) or via specific exposure-effect pathways (such as secondary poisoning or endocrine disruption). If an analysis of pressures suggests that such chemicals are emitted, then the assessor should apply pertinent approaches to assess those (not SSDs).

Further, the prediction of the probability that exposure exceeds a critical threshold has a clear interpretation (see case study results), but at the same time it remains imprecise regarding the 'appearance' of that harm. The *simple* expression of an increased 'probability of exceedance of a critical effect level' has the *complex* interpretation that the species that are exposed may show widely different responses. This has indeed been observed by Berger and others (2016). The probability metrics thus appear to be useful (case study results) and meaningful for designing or updating management plans (relationships to both protection goals and impact classes).

7.4.6 Specific utility of SSDs for ranking

The use of SSDs in landscape-level assessment of risks of a compound was developed some decades ago (Solomon and others 1996), and this has substantially changed and improved assessment practices (Solomon and others 2013). The present study expands on that, by adding many chemicals and their mixtures, and adding ranking of sites and substances within mixtures. Regarding ranking practices, we recommend using a few classes for rankings, because numerical details hide relevant information, whilst in fact being an over-interpretation of data. That is, we propose three classes, viz. (a) a high-ranking class of sites or compounds (where the probability is always high, from various viewpoints) such as "pollution hot spots", (b) an always low-ranking class (where the low probability allows to 'exclude the innocent') and (c) an intermediate class (where the probability depends on the situation). The three management attention classes discriminate three management perspectives (attention, no attention, and possible further lines of evidence needed, respectively).

These classes are populated with highly skewed Pareto-type distributions of probabilities of impacts, both across sites (Figure 7.6) and for compounds within sites (Table 7.5). Skewed distributions should be

expected (Muller 2016; West 2017), and were also found in large-scale monitoring data sets (Vallotton and Price 2016). It is however wrong to consider the contents of e.g. Table 7.5 as a given ranking for Europe. Exposures may vary per region, land use and day, such that downstream of agricultural land use pesticides dominate toxicity during some days in the growing season. Pareto patterns are a key phenomenon in chemical pollution assessments, but most affected sites and most contributing compounds at those sites vary.

7.4.7 Alignment of policy regimes

The use of SSDs can be supportive in complementary policy regimes on chemicals (see Introduction and SI-Table 1). This liaise approaches as diverse as REACH (chemical safety), the WFD (environmental quality) and Sustainable Production and Consumption (product policies). A surprising similarity of results was found in the present study and the companion paper, liaising outputs generated in the phase of chemical safety assessment (e.g., REACH) and environmental assessments (e.g., the WFD). That is, the results of the present study can be summarized as a likelihood of exceeding the 50%-effect level of (on average) 5.3%, 6.1%, 16.7% and 3.2% for the European-, Danube, Rhine and Spanish basins, respectively. In the companion paper, the same metric was estimated as 21% for steady state conditions and a (virtual) 'typical European water body' (Posthuma and others 2018 (companion paper, submitted sept 2018)). The basin-specific outcomes are (slightly) lower than the value for the 'virtual' water body. The latter estimate represents the 100th percentile estimate (P100) for a mixture of 4757 compounds. Despite the much higher number of compounds, we note that the Pareto-distribution of the relative contributions of chemicals means that increases in toxic pressure may be (very) small for chemicals added in an assessment.

Each of regulatory uses of SSDs currently applies specific, historically defined requirements on using data and SSDs. A perceived lack of ecotoxicity data appears closely related to the strictness of data selection criteria (e.g., NOECs are preferred, and there are much fewer NOECs than EC50s). It is the selection criteria that matter most. Those seriously trade off into a disability to consider most compounds in many contemporary assessments and into using 'unstable' SSDs for other compounds. At present, the largest set of data and SSDs is used in LCA. The use of SSDs can be expanded, and SSD quality scores can support to reach a good interpretation of outcomes.

7.4.8 Summarising complex results and trends

One of the conundrums of current chemical pollution problems is: results communication, an example of which was given for the 'red' classification of water quality. Various authors already propose SSD-based chemical footprints for regions to summarize and communicate complex results (Bjørn and others 2014; Zijp and others 2014). The best management scenario can then be evaluated and communicated via selecting the scenario resulting in the smallest footprint. Prospective footprinting may further help exploring consequences of changes in society, such as the implementation of a circular economy or of a sustainable chemistry approach (Blum and others 2017).

SSDs can be used as an effective, though lower-tier approach to water quality protection, assessment and management and a wide diversity of policy fields, with opportunities to explore 'big patterns' (footprints) as well as 'details' (specific chemicals and sites). The use of SSDs provides information

intermediate between generic assessments of chemical safety and more specific impacts assessments based on more complex (ecological) modelling.

7.5 Conclusions

1. Species Sensitivity Distribution (SSD) play a role in current environmental protection, assessment and management practices, currently for a few to a few thousand compounds only
2. SSDs are provided for 12,386 substances, with a quality score to assist in planning and interpretation of assessments
3. The utility of SSDs was illustrated for water quality assessment at the European scale considering 1,760 compounds and their mixtures
4. The role of chemical pollution on aquatic ecosystems could be specified, regarding both the regulatory concept of sufficient protection (REACH and WFD) as well as species loss (WFD, ecological status' classification)
5. The use of models is suggested in the European WFD, and SSDs fit that use as they express the likelihood that pollution causes harm
6. The use of SSDs for water quality assessment follows the holistic principles of the WFD, and supports a "System-Site-Substance-Solution" sequence in the assessment of impacts

The use of SSDs complements the current "Substance-Solution" approach, which substantially refines the diagnosis of and communication on chemical pollution in surface waters.

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Annex 1: Bioconcentration and Bioaccumulation of chemicals in aquatic food-webs

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Introduction

To obtain concentrations of chemicals in fish used for human consumption, bioconcentration modelling is required. We followed the approach of Arnot and Gobas (2004) and Armitage et al. (2013) and extended and adapted it in several ways. Firstly, we enabled the use of concentration time-series as input, calculating fluctuating body concentrations instead of equilibrium concentrations. Secondly, we added a food web perspective, where fish may have different positions in the food web and consume different food items. Internal concentrations are thus calculated for all components in the food web, including plant material-eating (*phytovorous*), zooplankton-eating (*planktivorous*) and predatory (*piscivorous*) fish.

Bioaccumulation model

<u>Modelling uptake and elimination of chemicals in fish</u>

The bioconcentration model described by Armitage et al. (2013) is an extension of the bioaccumulation model for organic compounds described by Arnot and Gobas (2004), extending the applicability of the latter to ionisable organic compounds. Although the Armitage et al. (2013) model enables the calculation of rate constants for uptake from water and total elimination through gill ventilation, faecal egestion, metabolism and growth dilution, it does not include the mathematical description of uptake of organic compounds through consumption of food items. However, the uptake from food as described by Arnot and Gobas (2004) can be easily added to the model given by Armitage et al. (2013).

The bioconcentration model of Armitage et al. (2013) is a one-compartment model described by a first-order differential equation of the concentration of an organic compound in biota:

$$\frac{dC_b}{dt} = k_w C_w + k_d C_d - k_e C_b$$

where C_b is the concentration in biota (mg kg^{-1}), t denotes time (days), k_w is the uptake rate constant for uptake from water (L kg^{-1} day^{-1}), C_w is the concentration (freely dissolved and available for uptake) in water (mg L^{-1}), k_d is the uptake rate constant for uptake from food (diet, kg kg^{-1} day^{-1}), C_d denotes the concentration of the compound in the diet (mg kg^{-1}), and k_e denotes the overall elimination rate constant (day^{-1}).

Uptake through gill ventilation and consumption of food

The uptake rate constant k_w comprises only uptake at the respiratory surface resulting from ventilation of water through the gills:

$$k_w = E_w \frac{G_V}{W_b}$$

Similarly, the uptake rate constant k_d only describes uptake from diet:

$$k_d = E_d \frac{G_d}{W_b}$$

The uptake rate k_w (L kg^{-1} day^{-1}) is a function of the chemical absorption efficiency across the gill E_w (-), the gill ventilation rate G_v (L day^{-1}) and the weight of the organism W_b (kg). Similarly, the uptake rate k_d (kg kg^{-1} day^{-1}) is a function of the absorption efficiency across the gastro-intestinal tract E_d (-), the feeding rate G_d (kg day^{-1}) and the organisms weight W_b (kg)

Absorption efficiencies are estimated for the gill and the gastro-intestinal tract separately:

$$E_w = (R_W + \left(\frac{\mu * R_L}{K_{ow}}\right))^{-1} + \varepsilon$$

$$E_d = (3 * 10^{-7} * K_{ow} + 2)^{-1}$$

where K_{ow} (-) is the octanol-water partition coefficient of the chemical and ε (-) is a constant in the range of 0.005 – 0.005 (the value 0.0005 is used in the present calculations). R_w (-, default value 1.85) and R_L (-, default value 155) characterise the relative resistances of chemical transport through multiple aqueous (water) and organic diffusion layers at and in the gill, resp. (Armitage et al., 2013). The factor μ (-) accounts for ionisation of the compound, and is the ratio of the total concentration (neutral + ionised) to the concentration of the neutral species:

$$\mu = 1 + 10^{(pH - pKa)}$$

The pH of the bulk water phase may be adjusted by the user, the pH at the gill of the fish is assumed to be (equation given by Armitage et al. (2013) in the spreadsheet implementing their model):

$$pH_{Gill} = 0.7141 * pH_{Bulk} + 1.4672$$

Note that the absorption efficiency for the gastro-intestinal tract is assumed not to be influenced by the degree of ionisation.

The estimation of the gill ventilation rate G_v (L day^{-1}) according to Armitage et al. (2013) is based on body weight, temperature and oxygen concentration in the water:

$$G_V = \frac{10^{(2.8 + 0.786\, Log\, W_b + 0.017 * T)}}{0.65 C_{ox}} / W_b$$

where T is the temperature of the water (°C) and C_{ox} is the concentration (mg L^{-1}) of oxygen in the water. The oxygen concentration in water (assuming 90% saturation) is estimated from the equation given by Armitage et al. (2013) in the tools section of the spreadsheet implementing their model:

$$C_{ox} = 0.9 * (14.45 - 0.413 * T + 0.0055 * T^2)$$

The feeding rate G_d (kg day^{-1}) is estimated as a function of weight of the organism (W_b) and temperature T (°C):

$$G_d = 0.022\, W_b^{0.85} e^{0.06 * T}$$

Elimination through gill ventilation, faecal egestion, growth and metabolism

The overall elimination rate constant is the sum of rate constants for depuration through gill ventilation (k_2), faecal egestion (k_e), metabolism (k_b) and growth dilution (k_g), each of which are described in more detail by Armitage et al. (2013) and by Arnot and Gobas (2004).

<u>Gill ventilation</u>

Depuration through gill ventilation k_2 (day^{-1}) is governed by the same processes as uptake from water through the gill, i.e. water ventilation and membrane permeation. For that reason it is estimated from the ratio of the organism-water partition coefficient K_{BW} and the uptake rate constant k_w:

$$k_2 = k_w / K_{BW}$$

The partition coefficient K_{BW} is estimated assuming that lipids, non-lipid organic matter and water within the organism all contribute to the partitioning of the compound from water to the organism, albeit to a different extent.

$$K_{BW} = f_{lipid} K_{ow} + f_{nlom} * \beta * K_{ow} + f_{water}$$

Where f_{lipid}, f_{nlom} and f_{water}, the sum of which equals 1, denote the weight fractions (wet weight) of the lipid, non-lipid organic matter and water fractions within the organism, resp. The factor β expresses the ratio of the sorption capacity of non-lipid organic matter to that of octanol, for which Arnot and Gobas (2004) suggest a value of 0.035 as a first estimate, but Armitage et al. (2013) prefer the value of 0.05 which is also used in the current calculations.

Armitage et al. (2013) have changed this equation slightly, to explicitly account for differences between neutral (storage) lipids and structural (polar) phospholipids, and for differences between the neutral and charged form of ionisable compounds. Instead of K_{BW} they define a distribution ratio D_{BW} which is not governed by the octanol-water partition coefficient, but by an octanol-water distribution rate (D_{OW}, applicable to distribution over neutral storage lipids and non-lipid organic matter) and a membrane-water distribution ratio (D_{MW}, applicable to distribution over polar phospholipds):

$$D_{BW} = f_{SL} D_{OW} + f_{PL} D_{MW} + f_{nlom} * \beta * D_{OW} + f_{water}$$

where f_{SL}, f_{PL}, f_{nlom} and f_{water}, the sum of which equals 1, denote the weight fractions (wet weight) of storage lipids, polar (phospho) lipids, non-lipid organic matter and water within the organism, resp. D_{ow} and D_{MW} represent a weighted average of the octanol-water and membrane-water partition coefficients of neutral and ionised forms of the chemical.

$$D_{OW} = X_N K_{OW,N} + X_I K_{OW,I}$$

$$D_{MW} = X_N K_{MW,N} + X_I K_{MW,I}$$

Where X_N and X_I represent the fraction of neutral and ionised forms of the chemical, $K_{OW,N}$ and $K_{MW,N}$ represent the octanol-water and membrane-water partition coefficients of the neutral form of the chemical, and $K_{OW,I}$ and $K_{MW,I}$ represent the octanol-water and membrane-water partition coefficients of the ionised form of the chemical.

The octanol-water and membrane-water partition coefficients of the ionised form are calculated assuming that it partitions into octanol and membranes less easily than the neutral form:

$$\log K_{OW,I} = log K_{OW,N} - \Delta_{OW}$$

$$\log K_{MW,N} = 1.01 * log K_{OW,N} + 0.12$$

$$\log K_{MW,I} = log K_{MW,N} - \Delta_{MW}$$

With Δ_{OW} and Δ_{MW} assumed to be in the range of 2 – 4 and 0.3 – 2 resp. (values of 3.1 and 2 were used in the calculations).

For a fish of 5% (wet weight) lipid content, the distribution of lipids between storage lipids and polar phospholipids is assumed to be 4 : 1; any increase in fat content is assumed to be attributable to storage lipids only, i.e. every fish is presumed to contain 1% w/w phospholipids with additional lipid content attributed exclusively to storage lipids. Non-lipid organic matter is assumed to account for 15% of the fish wet weight, whereas the remaining fraction is assumed to consist of water.

<u>Faecal egestion</u>

In the original model described by Arnot and Gobas (2004) the faecal egestion rate (k_e, day^{-1}) is estimated from the equation

$$k_e = G_F E_d K_{gb} / W_b$$

Where G_F is the egestion rate (kg faeces/kg organism per day), E_d (-) is the dietary absorption efficiency across the intestinal tract, and K_{gb} (-) is the partition coefficient of the chemical between the gastro-intestinal tract and the organism. Similar to the procedure used in the description of elimination through the gill, the possible presence of the charged form of a compounds is accounted for by replacing K_{gb} by D_{gb}, the apparent distribution coefficient of a compound which weights the partition coefficients of the neutral and charged forms of the compound.

$$k_e = G_F E_d D_{gb} / W_b$$

The faecal egestion rate G_F is a function of the digestibility of the diet, which depends on its composition, making a distinction between a polar (phospholipid) and non-polar (storage) lipid fraction, and non-lipid organic matter:

$$G_F = \{(1 - A_{PL}) f_{PL} + (1 - A_{SL}) f_{SL} + (1 - A_{nlom}) f_{nlom}\} G_D$$

Where f_{PL}, f_{SL} and f_{nlom} denote the fractions phospholipids, storage lipids and non-lipid organic matter in the food resp., and A_{PL}, A_{SL} and A_{NLOM} denote the dietary assimilation efficiencies of phospholipids, storage lipids and non-lipid organic matter (Arnot and Gobas suggest values of 0.92, 0.92 and 0.60, resp. in fish, and a value of 0.75 for all three phases in aquatic non-invertebrates; the assimilation efficiency of water is set at 0.70). G_d is equal to the already previously defined feeding rate:

$$G_d = 0.022\, {W_b}^{0.85} e^{0.06 * T}$$

The absorption efficiency is given by:

$$E_d = (3 * 10^{-7} * K_{ow} + 2)^{-1}$$

The apparent distribution coefficient is given by:

$$D_{GB} = \{\nu_{SL} D_{OW} + \nu_{PL} D_{MW} + \nu_{nlom} * \beta * D_{OW} + \nu_{water}\} / D_{BW}$$

Where D_{BW} represents the previously defined biota-water partition coefficient, and v_{sl}, v_{pl}, v_{nlom} and v_{water} represent the fractions storage lipid, polar lipid, non-lipid organic matter and water in the egested material, resp. These fractions may differ from the respective fractions in the diet itself because of differences in assimilation efficiencies between the various fractions.

$$\nu_{SL} = (1 - A_{SL}\} f_{SL} / \{(1 - A_{SL}) f_{SL} + (1 - A_{PL}) f_{PL} + (1 - A_{nlom}) f_{nlom} + (1 - A_{water}) f_{water}\}$$

$$\nu_{PL} = (1 - A_{PL}\} f_{PL} / \{(1 - A_{SL}) f_{SL} + (1 - A_{PL}) f_{PL} + (1 - A_{nlom}) f_{nlom} + (1 - A_{water}) f_{water}\}$$

$$\nu_{nlom} = (1 - A_{nlom}\} f_{nlom} / \{(1 - A_{SL}) f_{SL} + (1 - A_{PL}) f_{PL} + (1 - A_{nlom}) f_{nlom} + (1 - A_{water}) f_{water}\}$$

$$\nu_{water} = (1 - A_{water}\} f_{water} / \{(1 - A_{SL}) f_{SL} + (1 - A_{PL}) f_{PL} + (1 - A_{nlom}) f_{nlom} + (1 - A_{water}) f_{water}\}$$

<u>Growth</u>

The rate constant for dilution through growth (k_g, day^{-1}) is estimated on the basis of water temperature (T, °C) and organism weight (W_b, kg):

$$k_g = 0.00586 * \{1.113^{(T-20)} * (1000 * W_b)^{-0.2}\}$$

Metabolism

The rate constant for elimination through metabolism (k_b, day^{-1}) depends on the chemical and on the species of fish, and is typically estimated through QSAR-techniques. The rates used in the present investigation were provided by Ralph Kühne and estimated using a method published by Arnot et al. (2008a). Arnot et al. (2008b) investigated the results of this method for the estimation of transformation rates in fish and concluded that correlations between predicted and experimental transformation rates for fish were modest. Estimated transformation rates at 'standard conditions' (assuming a fish of 0.01 kg weight and environmental temperature of 15°C, $k_{b,w=0.01}$) can be transformed to other fish weights W (kg) and temperatures (T, °C) using the equation (Nichols et al., 2007):

$$k_{b,w} = k_{b,w=0.01} * \left(\frac{W}{0.01}\right)^{-0.25} * \exp\{0.01 * (T - 15)\}$$

If no data on metabolism are available, k_b can be assumed zero, i.e. it is assumed that elimination through metabolism is negligible. Similarly, if no information on temperature is available a temperature of 15°C is assumed.

Estimation of concentration in fish food

The concentration in consumed biota, C_d can be estimated in several ways. The first, model-based way to estimate concentrations in various consumed biota is to use the bioconcentration model as given by Arnot and Gobas (2004), starting at the lowest trophic level that is to be incorporated and working towards higher trophic levels. For each level the uptake through food is calculated using concentrations for lower trophic levels (food) already calculated. This ultimately results in the uptake through food in the highest trophic level (in our case a fish) to be calculated on the basis of estimated concentrations in lower trophic levels that are used as food. If food is composed of more than a single lower trophic level prey, a weighted concentration in biota can be used that accounts for diet composition by weighting the concentrations in the various food constituents according to their fraction in the diet.

An alternative approach is based on the concept of the Trophic Magnification Factor (*TMF*) (Fisk et al., 1998; Mackintosh et al., 2004; Kelly et al., 2007; Gobas et al., 2009; Walters et al., 2011; Conder et al., 2012). The *TMF* was developed for screening whether a compound shows biomagnification potential over a range of trophic levels. *TMF* can be understood as an average biomagnification factor over different trophic levels (Jonker, 2012). The *TMF* simply describes by which factor the (lipid normalised) concentration in biota increases when going up in the food web by one trophic level.

The method assumes that phytoplankton is in equilibrium with the surrounding water. The ratio between concentrations of a substance in phytoplankton and water is given by the bioconcentration factor of the compound in phytoplankton BCF_{phyto}. From the concentration in phytoplankton, the concentrations in higher trophic levels can be estimated using the Trophic Magnification Factor (*TMF*). If e.g. a species is ΔTL trophic levels up from phytoplankton, the lipid content (fraction) in the species is $F_{lipid,species}$ and the lipid content (fraction) in the phytoplankton is given by $F_{lipid,phyto}$, the predicted concentration of the substance in that species is:

$$C_{species} = \frac{F_{lipid,species}}{F_{lipid,phyto}} * 10^{\log(TMF)*\Delta\mathrm{TL}} BCF_{phyto} C_w$$

which is equivalent to:

$$C_{species} = \frac{F_{lipid,species}}{F_{lipid,phyto}} TMF^{\Delta\mathrm{TL}} BCF_{phyto} C_w$$

This equation enables a prediction of concentrations of the substance in any species at any trophic level. We use it to predict concentrations in the food items of our fish food-web components. For the fish themselves we use the Armitage et al. (2013) bioconcentration modelling approach. The concentrations in the food of the 'Armitage fish' are calculated from weighted average concentrations in the various food items. Initially, we assume that fish diets consist of a single food item.

Experimental data being scarce, the method can apply estimation methods for the bioconcentration factor of organic chemicals in phytoplankton (*BCFphyto*) and for the TMF of organic chemicals in a more or less 'standard' food web system. For both quantities estimation methods use readily available physico-chemical properties of a compound, in particular the logarithm of its octanol-water partition coefficient, log K_{ow}. In the following section we discuss how bioconcentration in phytoplankton and *TMF* values for whole food-webs can be predicted from substance and species properties.

Estimation of bioconcentration in phytoplankton

Geyer et al. (1984, 1991) have described a relationship between the bioaccumulation in *Chlorella fusca* and the octanol-water partition coefficient of 41 organic chemicals, ranging in Log *Kow* from approx. 0.55 (hydroquinone) to 6.28 (p,p'-DDT). The bioconcentration factor on the basis of wet weight was used to establish the following relationship (N=41, r=0.902):

$$\log BCF_{Chlorella,wet} = 0.681 \log K_{ow} + 0.164$$

Ellgehausen et al. (1980) using *Scenedesmus acutus* and 8 pesticides found a similar relationship between sorption potential and Log *Kow*, the latter ranging from 1.8 – 6.2 (N=8, r^2=0.93):

$$\log K_{Algae} = 0.70 \ \log K_{ow} - 0.26$$

The difference between this equation and the equation given by Geyer et al. (1984) for wet weight is relatively small, and may be caused by differences in surface area and lipid content between species. It is proposed to use the equation given by Geyer et al. (1984) for the estimation of the bioconcentration factor of a compound in phytoplankton, i.e.

$$\log BCF_{Phyto} = 0.681 \log K_{ow} + 0.164$$

Estimation of TMF on the basis of substance properties

Walters et al. (2011) calculated *TMF's* for a large number of polychlorinated biphenyls (PCBs) from linear regression of (logarithm of) lipid normalised concentrations in organisms against trophic position in a food web (Lake Hartwell, invertebrates and fish only). Regression was found to be most reliable (r^2 > 0.5) for compounds with Log K_{ow} ranging from approx. 6.0 to 7.27.

Subsequently they established a relationship between *TMF* and Log K_{ow}:

$$TMF = (1.88 \pm 0.12) * (LogKow - 5.06) + (1.37 \pm 0.17)$$

The equation was established for PCBs with Log K_{ow} ranging from 5.06 to 7.27. Despite the lower reliability of *TMF* established for compounds with Log *Kow* < 6, the *TMF* of these compounds was described by the *TMF*-Log K_{ow} relationship quite well. The r^2 for the *TMF*-Log K_{ow} relationship, including all compounds, was 0.80.

Mackay et al. (2016) compared simulated results of three different theoretical food web models (pelagic, demersal and combined pelagic – demersal) containing up to 7 species. They give an overview of trophic magnification factors for a series of compounds of varying hydrophobicity, where *TMF* increases in a more or less linear fashion with Log K_{ow} for compounds with Log K_{ow} > 4 (see Figure TMFKow1). The values of TMF as simulated by Mackay et al. (2016) are given by the equation:

$$TMF = (1.09 \pm 0.13)LogKow - (3.9 \pm 0.8)$$

The domain of applicability of the equation is 4 < Log K_{ow} < 8, and it seems reasonable to use limiting values for *TMF* of 1.03 ≤ *TMF* ≤ 4.93 (which are the values of *TMF* calculated by Mackay et al. (2016) for compounds with Log K_{ow} equal to 4 and 8 resp.).

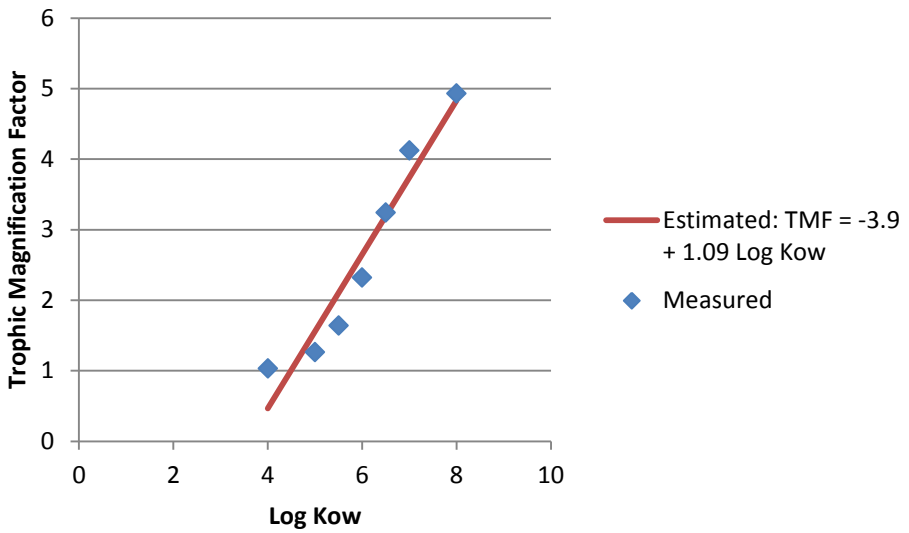

Figure TMFKow1: *TMF* as simulated by Mackay et al. (2016) as a function of hydrophobicity.

Figure TMFKow2 compares the *TMF*-Log K_{ow} relationships given by Walters et al. (2012) and Mackay et al. (2016). For compounds with a Log K_{ow} up to approx. 6, the values for *TMF* calculated by both regression models are quite similar. For compounds with higher Log K_{ow} the model given by Walters et al. (2012) results in somewhat higher estimates of *TMF*, but differences remain relatively small. For a compound with Log K_{ow} = 8, the model gives estimates of *TMF* of 6.9 and 4.8 resp., i.e. less than a factor 1.5 difference.

Given its larger domain of applicability by being based on a wider range of Log *Kow* values, the relationship given by Mackay et al. (2016) is preferred. This equation does not account for possible differences in the extent of metabolism between lower and higher trophic levels, but can be considered to reflect a worst-case scenario.

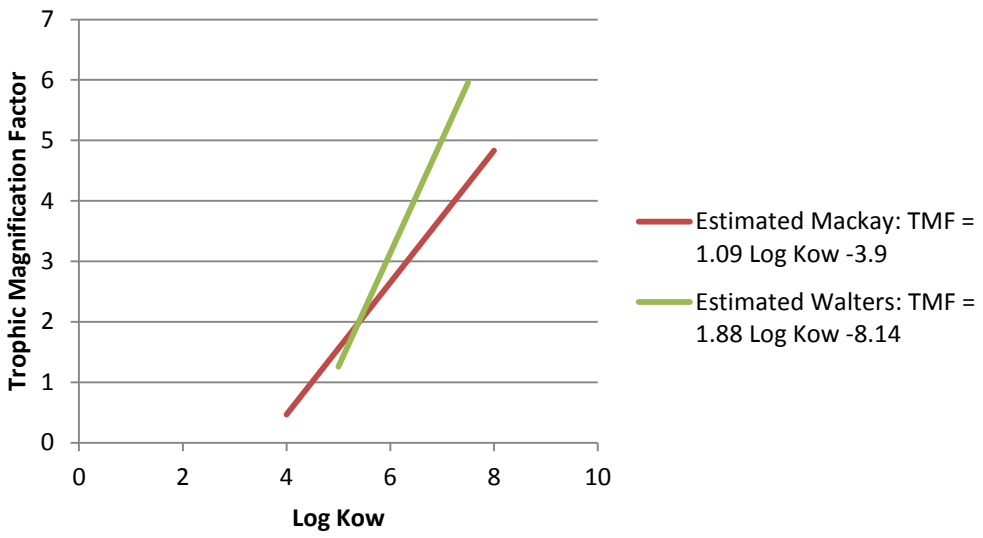

Figure TMFKow2: Comparison between *TMF* estimates derived using the equations given by Mackay et al. (2016) and Walters et al. (2011).

Lipid content in phytoplankton and zooplankton

To extrapolate from phytoplankton to species higher in the food-chain, e.g. zooplankton, applying the trophic magnification concept, differences in lipid content between phytoplankton and zooplankton have to be taken into consideration. Species-specific data are rare; we therefore use average lipid content for phytoplankton and zooplankton estimated from literature data.

Phytoplankton
Ricketts (1966) gives lipid contents of several species of unicellular algae. For the green alga *Pedinomonas minor* a lipid content of 21.1% (dry weight) was established after 20 days of cultivation. Mata et al. (2010) have reported lipid contents for a large number of microalgae considered useful for biodiesel production. For most species the data is given in terms of a range of observed lipid levels. Using only data for freshwater species for which a single lipid content is given, a geometric mean lipid content of 21.5% (dry weight) can be calculated for 4 species (the very low lipid content given for *C. pyrenoidosa* was obtained at a very high areal productivity, and is therefore not used). Feng et al. (2011) report lipid contents of approx. 30% (dry weight) for *Chlorella pyrenoidosa* in batch cultures after at least 10 days of cultivation, whereas Hongyang et al. (2011) report an average lipid content of 37 ± 9% (dry weight) in batch cultures of this same species. Finkel et al. (2016) report a median lipid content of 17.3% (95% interval: 16.2 – 18.2%) on dry weight basis for data on 117 species of microalgae with 591 observations in the stationary phase of growth, taken from AlgaeBase, an online database of terrestrial, marine and freshwater algae (http://www.algaebase.org/). Cañavate et al. (2016) report experimental values for lipid content of microalgae, giving separate values during exponential, late exponential and stationary growth phases for 15 species, i.e. a total of 45 values for 15 different species. On average, the lipid content was 25.0 ± 7.2% of dry weight.

The geometric mean lipid content of phytoplankton from these 6 studies was 24.5% on dry weight basis. Only Ricketts (1966) reported the ratio between dry and wet weight, where dry weight was 14% of wet weight. Unfortunately, the other cited authors did not provide this information. Assuming that the ratio of 0.14 between wet and dry weight applies to the data of the other authors as well, the geometric mean lipid content of fresh water algae from the 6 studies is 3.43% on wet weight basis.

Zooplankton
Bodar et al. (1988) report an average lipid content in *Daphnia magna* of 15.5% (dry weight) for 2 groups of control daphnids at the termination of an experiment investigating the effect of cadmium on several

biochemical parameters. Liu et al. (1996) report an average lipid content for control daphnids of 5.0 ± 0.6% (wet weight). Villarroel et al. (2009) report an average lipid content of 20.3% (dry weight) in adult *D. magna*, whereas Sancho et al. (2009) report an average lipid content of 20.7% (dry weight) for the same strain of daphnids reared in the same laboratory (but used during a different experiment). Kretschmann et al. (2011) report an average lipid content of 1.7 ± 0.1% (wet weight) for *D. magna* cultured with a constant food supply. Looser et al. (1998) report an average lipid content of 0.3% wet weight in control daphnids at the end of a bioconcentration experiment. This lipid content is not used, since these daphnids were not fed during the 3-day exposure period and the lipid content of these daphnids therefore is expected to be lower than for daphnids which had food at their disposal.

Looser et al. (1998) report a ratio between wet and dry weight of *Daphnia magna* of 14 : 1, which was determined for adult daphnids at the end of a bioconcentration experiment. Preuss et al. (2008) report a similar ratio of 15.3 : 1 for adult *D. magna*, whereas Manar et al. (2009) report an average ratio between wet and dry weight of 23 : 1, and Tervonen et al. (2010) established a ratio of 12.5 : 1 in adult *D. magna*. The geometric mean of these values results in an average ratio wet weight : dry weight of 15.8 : 1 for adult *D. magna*. Using this average ratio, the geometric mean of lipid contents in *Daphnia magna* given above 10.74% on dry weight basis, which corresponds to lipid content of 1.70% on the basis of wet weight.

Modelling uptake through ingestion of contaminated sediment

Very little information was found on the amount of sediment ingested by fish, and on the assimilation efficiencies of contaminants from food. In view of the large incertainties uptake of contaminants through ingestion of sediment is not included in the calculations. However, the scarce information that was retrieved is summarised for future reference nonetheless.

Wilson et al. (2003) report data on *Ctenochaetus striatus* originally generated by Polunin et al. (1995). The ingestion rate (food plus inorganic sediment material) of *C. striatus* is given as 223 mg (dw) per gram (ww) of fish per day, noting that this species has a high percentage of inorganic sediment in their diet. Since this value includes food uptake, it is clearly an overestimation of the sediment ingestion rate. This value (22%) might, however, serve as an upper limit of ingestion rate for this species, but might be particular to fish species living and feeding on coral reefs. Similarly, Goatley and Bellwood (2010) describe measurements of sediment ingestion by the surgeonfish *Ctenochaetus striatus* in the Great Barrier Reef (Australia). Sediment feeding rates were estimated either from a combination of bite rates and bite volumes (8.8 ± 2.4 and 11.8 ± 3.3 g sediment per fish per day at 2 different sites) or from defecation rates (66.1 ±14.4 and 24.7 ± 7.1 g sediment per fish per day at the same 2 sites) were observed. Using a third method, based on gut contents and throughput rates, a sediment removal rate of 22.8 ± 3.1 g per fish per day was estimated. However, since the weight of fish is not given, it is difficult to estimate the ingestion rate per gram of fish per day.

Doyle et al. (2011) describe a method to estimate sediment ingestion by fish. However, their study focusses on the question which fraction of the content of the gastro-intestinal (GI) tract consists of sediment, as opposed to other material, concluding that in Shorthead Redhorse Suckers up to 46% of the total mass of GI content may consist of ingested sediments. Unfortunately, no attempt is made to convert these numbers into an ingestion rate in terms of amount of sediment ingested per gram of fish per day.

McCarthy et al. (2003) found that the sediment ingestion rate of Fathead Minnows depended on the organic carbon content, and thus the nutritional value, of the sediment under consideration, a phenomenon that has also been observed for aquatic deposit feeders and detritivores (Cammen, 1979). Sediment ingestion rates for minnows were 1.3% and 0.6% of body weight per day for sediments with low and high organic carbon content resp. Fathead Minnows are known to perturb sediment during feeding, but there are fish species, like bream and mullet, which probably perturb sediment to a larger extent. The ingestion rate found for Fathead Minnow may thus be considered a low estimate.

Moermond et al. (2004), studying the uptake of PCB by benthivorous carp, conclude from their data that benthivorous fish appear to ingest as much sediment as invertebrate food. They therefore propose to use a sediment ingestion rate equal to the food ingestion rate, but corrected for the dry to wet weight ratio

DW of the sediment (a value of 0.34 is suggested for DW). The uptake rate from sediment then corresponds to the uptake rate as defined for uptake from food, k_d: $k_{sed} = k_d$ * DW, where k_d is the uptake rate from food as previously defined (see section on uptake from food). The uptake rate has to be multiplied by the concentration of the contaminant in the sediment (experimental values, or alternatively estimates can be used which depend on water concentration, organic carbon content of the sediment and hydrophobicity of the compound). These model assumptions were also used by van Beusekom et al. (2006) in the modelling of food-chain accumulation of brominated flame retardants in fish.

Ruus et al. (2012) found that polychlorinated biphenyls accumulated in Atlantic Cod after ingestion of contaminated sediment with an assimilation efficiency of 30 – 50%, the higher efficiencies associated with the lower chlorinated congeners. Use of the equations given by Moermond et al. (2004) assumes that assimilation efficiency from sediment is equal to the assimilation efficiency from food, but k_{sed} can be easily corrected if there is reason to assume otherwise.

The food-web context

Fish used for human consumption may belong to different species and age/size-classes, with different positions in the aquatic food-web. Trophic level index (*TL*) defines the position, at least its 'vertical' dimension: primary producers are the first level, primary consumers the second, etc. Trophic level may be derived from the 15N/14N nitrogen isotope ratio in a species, and an increase in this isotope rate of 0.34 – 0.38% corresponds to a 1-unit increase in trophic position (Gobas et al., 2009). Although trophic levels for the species considered in this report are not known, the assumption is made that TL increases one unit when going from phytoplankton to zooplankton. Assumptions about Trophic Levels are only used in the calculations for the transfer of contaminant from phytoplankton to zooplankton. The transfer of contaminant to phytovorous fish feeding on living or dead plant material, planktivorous fish feeding on zooplankton and piscivorous fish being predators feeding on other fish is modelled using the kinetic equations describing uptake from food as given by Arnot et al. (2004).

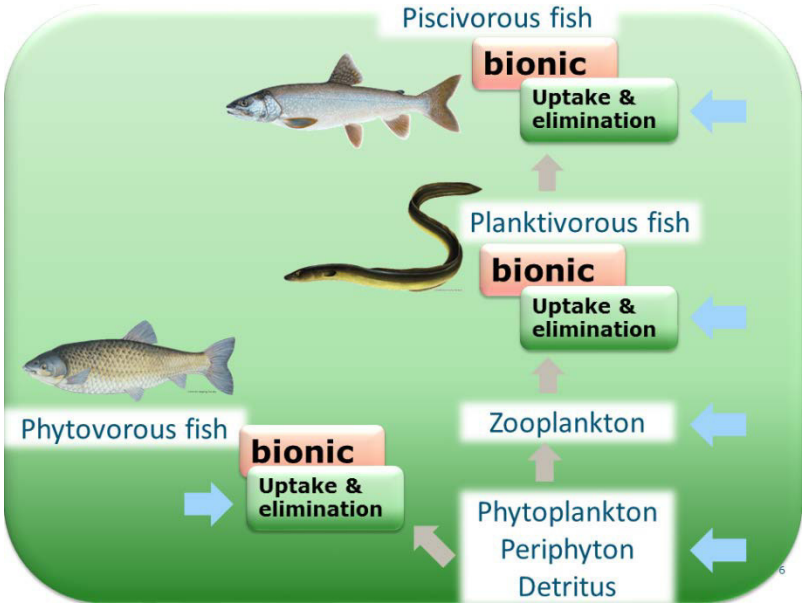

Figure FoodWeb: The food-web with 3 fish components: phytovorous fish feeding on living or dead plant material, planktivorous fish feeding on zooplankton and piscivorous fish being predators feeding on other fish.

For calculation of the uptake of chemicals via food (k_D), it is important to realise that fish species differ in their lipid content, affecting the other uptake and elimination constants. In principle in the model the food-web can be assembled freely, with the restriction that each species' food intake comes from a single food-web component. From the species used for human consumption, data were collected on their trophic level and their lipid content (M. Faust), and a selection was proposed representing two likely worst cases and one best case (Table Cases). For the whole food-web the composition in terms of lipids is summarized in Table Lipid. It should be noted that whether these cases really do represent best and worst cases depends on the characteristics of the chemical.

Table Cases. Selection of fish species, with their trophic level (*TL*) and lipid content (*LC*), and their representation in the model (with integer *TL*).

	Weight [g]	Trophic Level (*TL*)	Lipid Content (*LC*) [% wet weight]			Representative Species (for *TL* and *LC*)	Food-web Component
			Polar	Neutral	Total		
Worst Case I: max TL	20	4.5	0.8	14.2	15.0	Lake trout, River lamprey, Sea lamprey	Piscivorous fish (*TL* 4)
Worst Case II: max LC	20	3.5	0.8	24.2	25.0	Eel	Planktivorous fish (*TL* 3)
Best Case	2,000	2.0	0.8	0.2	1.0	Grass carp, Common nase	Phytovorous fish (*TL* 2)

Table Lipid. The distribution of lipids over polar phospholipids and neutral storage lipids for phytoplankton, zooplankton, and fish of low, intermediate and high fat content.

Component	Total lipid content (% wet weight)	Phospholipids (% wet weight)	Storage lipids (% wet weight)	Non-lipid organic matter (% wet weight)
Phytoplankton	3.43			
Zooplankton	1.70	0.34	1.36	15
Fish, lean	1.00	0.8	0.2	15
Fish, intermediate	15.0	0.8	14.2	15
Fish, fatty	25.0	0.8	24.2	15

Model output

The model can be used with time-series of concentrations, e.g. with daily values for one year as generated by the fate models in the SOLUTIONS modelling train, or be based on an observed/measured concentration. In the first case time-series of daily body concentrations constitute the output. These time-series are summarized in monthly and annual maximum and mean (geometric and arithmetic) values, for use in the human health risk assessment. In the second case, the model is run for one year for a constant water concentration and the 'equilibrium' concentrations reached at the end of the simulation are reported, for each food-web component.

In both cases, the basic time step of the modelling is 1 hour, to account for the combination of large uptake and/or elimination constants and high fluctuations in (daily) concentrations. When available, it is possible to use daily values for temperature and/or pH. However, this requires that the calculation of uptake and elimination constants is done not only once at the start of the simulation, but is repeated at the start of each day (when environmental conditions have changed).

Applications

Scenario I WFD priority substances

Description

26 WFD priority substances (Table Substances); main river catchments in Europe with a total of 24567 sub-catchments; simulated concentration time-series (daily values for 1 year) from the STREAM-EU model (ref).

Results

For each substance and each food-web component, monthly or annual values can be displayed in maps (data in ESRI shape file format), as in Figure Map_1.

Statistics including the 50 and 95-percentile concentration values can be extracted from the distribution of values over all (24567) sub-catchments, as in Figure Dist. These statistics and distributions can be generated also a catchment base, to be able to compare the situation in different catchments.

The 50- and 90-percentiles can be compared for the three fish components. For an overview, results for all substances can be collected in a single graph (Figure Bars); comparison is however meaningless, as long as concentrations are not related to critical levels, e.g., as part of the human health risk assessment.

Table Substances. The 26 WFD priority substances for which simulation data are available for the main European catchments.

CAS	Name
91-20-3	Naphthalene
1582-09-8	2,6-Dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine
62-73-7	Phosphoric acid 2,2-dichloroethenyl dimethyl ester
71-43-2	Benzene
886-50-0	Terbutryne
470-90-6	Phosphoric acid, 2-Chloro-1-(2,4-dichlorophenyl)ethenyl diethyl ester
1912-24-9	Atrazine
67-66-3	Trichloromethane
117-81-7	1,2-Benzenedicarboxylic acid, bis(2-Ethylhexyl)ester
76-44-8	1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H-indene
2921-88-2	Chlorpyrifos
330-54-1	N'-(3,4-Dichlorophenyl)-N,N-dimethylurea
50-28-2	(17beta)Estra-1,3,5(10)triene-3,17-diol
107-06-2	1,2-Dichloroethane
122-34-9	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine
115-32-2	4-Chloro-alpha-(4-chlorophenyl)-alpha-(trichloromethyl)benzenemethanol
25637-99-4	Hexabromocyclododecane
115-29-7	Endosulfan
34123-59-6	N,N-Dimethyl-N'-[4-(1-methylethyl)phenyl]urea
42576-02-3	Bifenox
74070-46-5	Aclonifen
1461-22-9	Tributylchlorostannane
52315-07-8	3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid cyano(3-phenoxyphenyl)methyl ester
75-09-2	Dichloromethane
608-93-5	1,2,3,4,5-Pentachlorobenzene
87-86-5	2,3,4,5,6-Pentachlorophenol

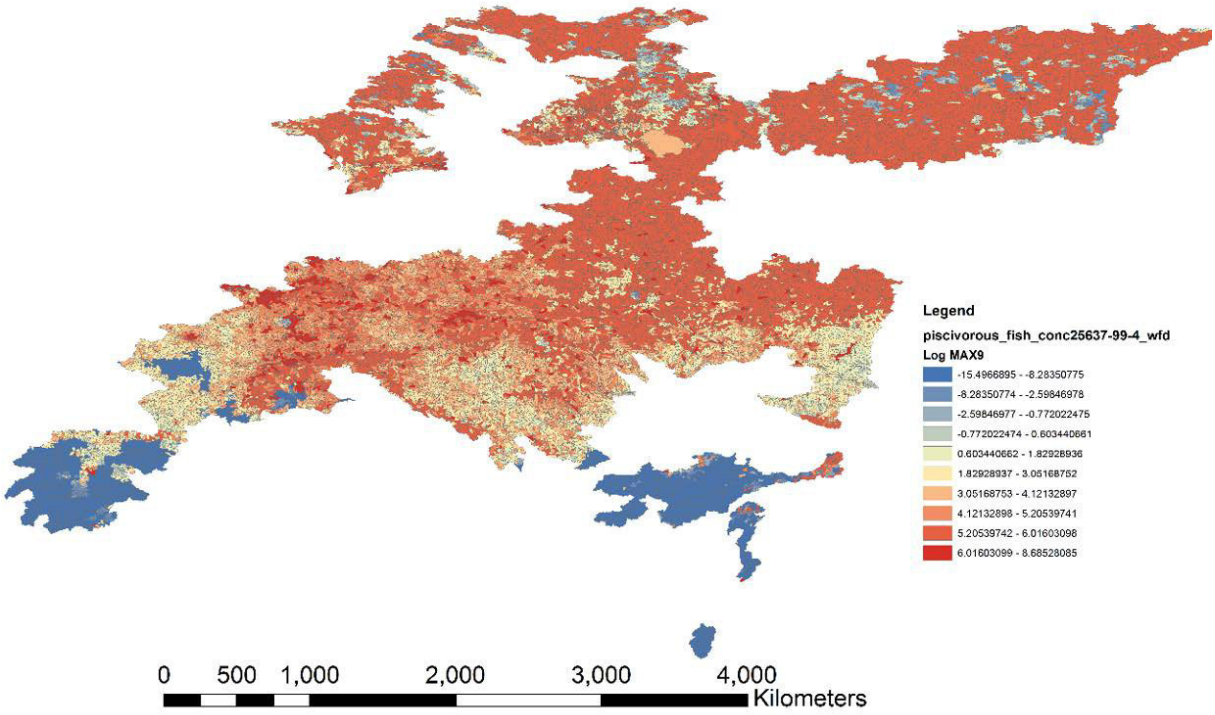

Figure Map_1: Example map of monthly max piscivorous fish concentrations for September, chemical 25637-99-4 (Hexabromocyclododecane).

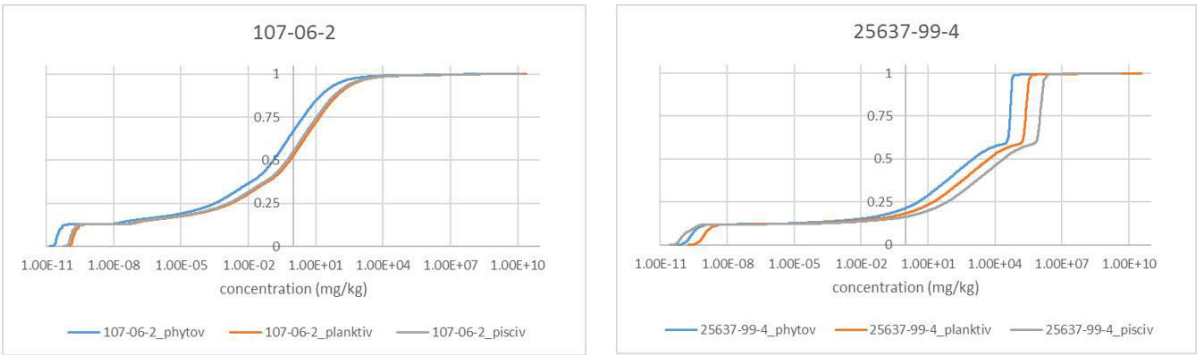

Figure Dist: Example of the distribution of annual maximum values of body concentrations over all sub-catchments, for substances 107-06-2 (1,2-Dichloroethane) and 25637-99-4 (Hexabromocyclododecane), in piscivorous, planktivorous and phytovorous fish.

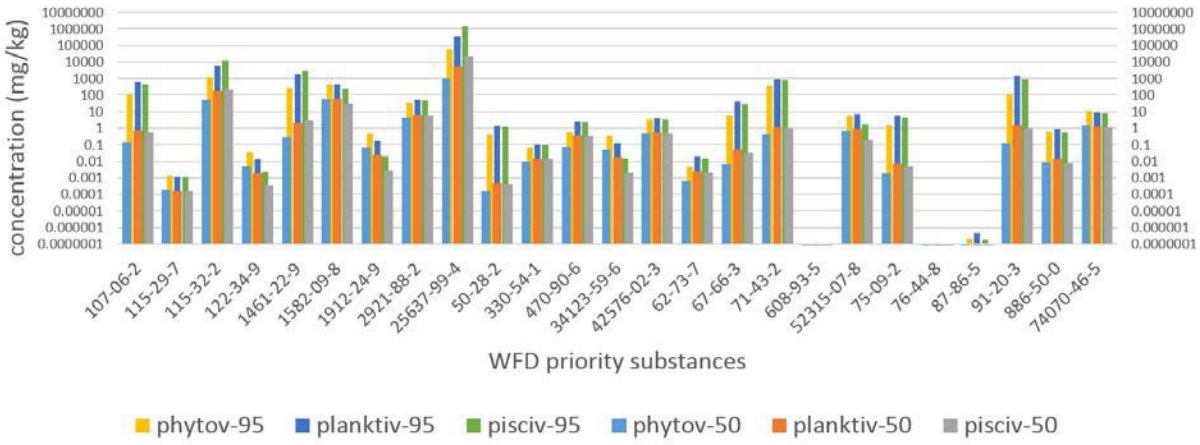

Figure Bars. 50- and 95-percentiles of annual maximum concentration distributions over 24567 WFD sub-catchments, for phytovorous, planktivorous and piscivorous fish.

Scenario II Observations in JDS3

196 chemicals for which observations are available for JDS data set. Single or multiple concentration values? Single -> assume constant concentrations and focus on equilibrium values.

Scenario III Modelling train results for >1800 substances for 3 large catchments in Europe

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ANNEX 2

Sheets

Chemicals:	
Group:	Substance group
Substance:	Substance name
CAS#:	CAS#
Unit:	Unit (µg/l)
zero or no values:	Meaning of 'zero' or 'no values' in JDS3 database (see below for colour code)
LoQ:	Limit of quantification (nv: no value provided)
LoD:	Limit of detection (nv: no value provided)
Organisation:	Institute that performed the measurements
Remarks:	Remarks on method or missing data (overall 4 measurements were missing, they were replace with zero)
Conc with zeros:	Concentrations for all chemicals and all JDS3 sites. Blanks ('no vaules') were replcaced by "0" to facilitate further calculations. Zeros mean either non-detects (<LoD or <LoQ)
Conc with half LoD:	Concentrations for all chemicals and all JDS3 sites. Zeros were replaced with LoD/2 where available. Else LoQ/2 or half the lowest measured value* were used. *the impact of this approach will be closely watched in the risk assessment
Conc with LoD:	Concentrations for all chemicals and all JDS3 sites. Zeros were replaced with LoD where available. Else LoQ or the lowest measured value* were used. *the impact of this approach will be closely watched in the risk assessment

Colour code

Meaning of 'zero' or 'no values'	*In the different scenarios blanks or zeros are replaced with:*
< LoQ or LoD	LoD/2 or LoD
<LoQ	LoQ/2 or LoQ
non detects	Lowest measured value'/2 or 'lowest measured value'*

*(Practical approach which may not provide good approximations, especially when substance was not detected at many sites. The impact of this approach will be watched in the risk assessment)

Chemicals

Group	Substance	CAS#	Unit	zero or no values	LoQ	LoD	Organisation	Remarks
Metals	Arsenic (As) - dissolved	7440-38-2	µg/l	<LoQ	0.03	0.009	CW - Croatian Waters	
Metals	Cadmium (Cd) - dissolved	7440-43-9	µg/l	<LoQ	0.01	0.003	CW - Croatian Waters	
Metals	Chromium (Cr) - dissolved	7440-47-3	µg/l	<LoQ	0.1	0.017	CW - Croatian Waters	
Metals	Copper (Cu) - dissolved	7440-50-8	µg/l	<LoQ	0.027	0.008	CW - Croatian Waters	
Metals	Lead (Pb) - dissolved	7439-92-1	µg/l	<LoQ	0.009	0.002	CW - Croatian Waters	
Metals	Mercury (Hg) - dissolved	7439-97-6	µg/l	<LoQ	0.002	0.0006	CW - Croatian Waters	site 18 is missing!
Metals	Nickel (Ni) - dissolved	7440-02-0	µg/l	<LoQ	0.04	0.012	CW - Croatian Waters	
Metals	Zinc (Zn) - dissolved	7440-66-6	µg/l	<LoQ	0.04	0.012	CW - Croatian Waters	
PAHs	Anthracene	120-12-7	µg/l	<LoQ	0.002	nv	PM - Povodi Moravy, s.p.	
PAHs	Benzo(a)pyrene	50-32-8	µg/l	<LoQ	0.002	nv	PM - Povodi Moravy, s.p.	
PAHs	Benzo(b)fluoranthene	205-99-2	µg/l	<LoQ	0.002	nv	PM - Povodi Moravy, s.p.	
PAHs	Benzo(g,h,i)perylene	191-24-2	µg/l	<LoD	0.0005	nv	PM - Povodi Moravy, s.p.	
PAHs	Benzo(k)fluoranthene	207-08-9	µg/l	<LoQ	0.002	nv	PM - Povodi Moravy, s.p.	
PAHs	Fluoranthene	206-44-0	µg/l	<LoQ	0.002	nv	PM - Povodi Moravy, s.p.	
PAHs	Indeno(1,2,3-c,d)pyrene	193-39-5	µg/l	<LoD	0.0005	nv	PM - Povodi Moravy, s.p.	
PAHs	Naphthalene	91-20-3	µg/l	<LoD	0.002	nv	PM - Povodi Moravy, s.p.	
Herbicides	2,4-D	94-75-7	µg/l	<LoQ	0.00022	0.00009	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Herbicides	2-Methyl-4-chlorphenoxy acetic acid (MCPA)	94-74-6	µg/l	<LoQ	0.00015	0.00006	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Herbicides	Ametryn	834-12-8	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Aminomethylphosphonic acid (AMPA)	1066-51-9	µg/l	<LoD	0.06	0.03	UBAAT - Umweltbundesamt GmbH	
Herbicides	Atrazine	1912-24-9	µg/l	<LoQ	0.005	nv	UFZ - Helmholtz Centre for Environmental Research	
Herbicides	Atrazine-2-hydroxy	2163-68-0	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Atrazine-desethyl	6190-65-4	µg/l	<LoQ	0.00117	0.0005	CW - Croatian Waters	
Herbicides	Atrazine-desisopropyl	1007-28-9	µg/l	<LoQ	0.00108	0.00032	CW - Croatian Waters	
Herbicides	Bentazone	25057-89-0	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Bromacil	314-40-9	µg/l	<LoQ	0.00152	0.00053	CW - Croatian Waters	
Herbicides	Carbetamide	16118-49-3	µg/l	<LoQ	0.00086	0.00025	CW - Croatian Waters	
Herbicides	Chloridazon	1698-60-8	µg/l	<LoQ	0.00036	0.0001	CW - Croatian Waters	
Herbicides	Chloridazon-desphenyl	6339-19-1	µg/l	<LoQ/LoD	0.05	0.025	UBAAT - Umweltbundesamt GmbH	
Herbicides	Chloridazon-methyl-desphenyl	17254-80-7	µg/l	<LoQ/LoD	0.05	0.025	UBAAT - Umweltbundesamt GmbH	
Herbicides	Chloroxuron	1982-47-4	µg/l	<LoQ	0.00165	0.0005	CW - Croatian Waters	
Herbicides	Chlortoluron	15545-48-9	µg/l	<LoQ	0.00052	0.00015	CW - Croatian Waters	
Herbicides	Cyanazine (Fortrol)	21725-46-2	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Herbicides	Cybutryne (Irgarol)	28159-98-0	µg/l	<LoQ	0.00018	0.00007	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Herbicides	Dimefuron	34205-21-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Herbicides	Dimethachlor CGA 369873	1418095-08-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Dimethachlor sulfonic acid CGA 354742	N/A	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Dimethenamid	87674-68-8	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Dinoseb	88-85-7	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Dinoterb	1420-07-1	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Diuron	330-54-1	µg/l	<LoQ	0.00165	0.0005	CW - Croatian Waters	
Herbicides	Ethidimuron (Sulfadiazole)	30043-49-3	µg/l	<LoQ	0.00072	0.00021	CW - Croatian Waters	
Herbicides	Ethofumesate	26225-79-6	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Herbicides	Glyphosate	1071-83-6	µg/l	<LoQ/LoD	0.06	0.03	UBAAT - Umweltbundesamt GmbH	
Herbicides	Hexazinon	51235-04-2	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Isoproturon	34123-59-6	µg/l	<LoQ	0.0003	0.0001	CW - Croatian Waters	
Herbicides	Linuron	330-55-2	µg/l	<LoQ	0.0016	0.0005	CW - Croatian Waters	
Herbicides	Metamitron	41394-05-2	µg/l	<LoQ	0.0028	0.0008	CW - Croatian Waters	
Herbicides	Metazachlor	67129-08-2	µg/l	<LoQ	0.00385	0.0011	CW - Croatian Waters	
Herbicides	Metazachlor ESA	172960-62-2	µg/l	<LoQ/LoD	0.05	0.025	UBAAT - Umweltbundesamt GmbH	
Herbicides	Metazachlor OA	1231244-60-2	µg/l	<LoD	0.05	0.025	UBAAT - Umweltbundesamt GmbH	
Herbicides	Methabenzthiazuron	18691-97-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Herbicides	Metobromuron	3060-89-7	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Herbicides	Metolachlor	51218-45-2	µg/l	<LoQ	0.00173	0.00066	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Herbicides	Metolachlor ESA	171118-09-5	µg/l	<LoQ/LoD	0.05	0.025	UBAAT - Umweltbundesamt GmbH	
Herbicides	Metoxuron	19937-59-8	µg/l	<LoQ	0.0006	0.00018	CW - Croatian Waters	
Herbicides	Monolinuron	1746-81-2	µg/l	<LoQ	0.0012	0.00036	CW - Croatian Waters	
Herbicides	Prometryn	7287-19-6	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Herbicides	Propazine	139-40-2	µg/l	<LoQ	0.00093	0.00028	CW - Croatian Waters	
Herbicides	Propazine-2-hydroxy	7374-53-0	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Simazine	122-34-9	µg/l	<LoQ	0.00087	0.00026	CW - Croatian Waters	
Herbicides	S-Metolachlor CGA 368208	1173021-76-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	S-Metolachlor NOA 413173	1418095-19-8	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Terbutryn	886-50-0	µg/l	<LoQ	0.00064	0.00033	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Herbicides	Terbutylazine	5915-41-3	µg/l	<LoQ	0.00097	0.00029	CW - Croatian Waters	
Herbicides	Terbutylazine CGA 324007	309923-18-0	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Terbutylazine SYN 545666	N/A	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Terbutylazine-2-hydroxy	66753-07-9	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Herbicides	Terbutylazine-desethyl	30125-63-4	µg/l	<LoQ	0.00179	0.00054	CW - Croatian Waters	
Herbicides	Terbutylazine-desethyl-2-hydroxy	66753-06-8	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Insecticides	Diazinone	333-41-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Insecticides	Fipronil	120068-37-3	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	4-Chlorophenol	106-48-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Fungicides	Azoxystrobin	131860-33-8	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Carbendazim	10605-21-7	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Cyproconazol	94361-06-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Flusilazole	85509-19-9	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Metalaxyl NOA 409045	75596-99-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Picoxystrobin	117428-22-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Propiconazole	60207-90-1	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Quinoxyfen	124495-18-7	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Tebuconazol	107534-96-3	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Fungicides	Trifloxystrobin CGA 321113	252913-85-2	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	10,11-Dihydro-10,11-dihydroxycarbamazepine	58955-93-4	µg/l	<LoQ	0.0003	0.00013	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Pharmaceuticals	10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	17-beta Estradiol	50-28-2	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	1-Adamantylamin	768-94-5	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	2-Hydroxycarbamazepine	68011-66-5	µg/l	<LoQ	0.01	nv	UFZ - Helmholtz Centre for Environmental Research	
Pharmaceuticals	3,4-Methylendioxyamphetamine (MDA)	4764-17-4	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	3,4-Methylenedioxyethamphetamine (MDEA)	14089-52-2	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	6-Acetylmorphine	2784-73-8	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	7-Aminoclonazepam	4959-17-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	7-Aminoflunitrazepam	34084-50-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Acetylcodeine	6703-27-1	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Acetyl-sulfamethoxazole	21312-10-7	µg/l	<LoQ	0.02	nv	UFZ - Helmholtz Centre for Environmental Research	
Pharmaceuticals	Alfentanil	71195-58-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	alpha-Hydroxyalprazolam	37115-43-8	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	alpha-Hydroxymidazolam	59468-90-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	alpha-Hydroxytriazolam	37115-45-0	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Alprazolam	28981-97-7	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Amidotrizoic acid	117-96-4	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Amisulpride	71675-85-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Amitriptyline	50-48-6	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Amoxapine	14028-44-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Amoxicillin	26787-78-0	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Amphetamine	300-62-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Atenolol	29122-68-7	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Atropine	51-55-8	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Benzoylecgonine	519-09-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Betaxolol	63659-18-7	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Bezafibrate	41859-67-0	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Bisoprolol	66722-44-9	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Bromazepam	1812-30-2	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Buprenorphine	52485-79-7	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Buprenorphine glucuronide	101224-22-0	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Candesartan	139481-59-7	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Carbamazepine	298-46-4	µg/l	<LoQ	0.00015	0.00022	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Pharmaceuticals	Carbamazepine-10,11-epoxide	36507-30-9	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Carisoprodol	78-44-4	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Cetirizine	83881-51-0	µg/l	<LoQ	0.01	nv	UFZ - Helmholtz Centre for Environmental Research	
Pharmaceuticals	Chlorprothixene	113-59-7	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Citalopram	59729-33-8	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Clobazam (Urbadan)	22316-47-8	µg/l	<LoQ	0.001	nv	UNI Umea - Umeå University	
Pharmaceuticals	Clonazepam	1622-61-3	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Clonidine	4205-90-7	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Clozapine	5786-21-0	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Cocaethylene	529-38-4	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Cocaine	50-36-2	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Codeine	76-57-3	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	CP 47,497	70434-82-1	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	CP 47,497-C8 homologue	70434-92-3	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Crotamiton	483-63-6	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Desalkylflurazepam	2886-65-9	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Desipramine	50-47-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Dextromethorphan (Methorphan)	125-71-3	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Diazepam	439-14-5	µg/l	<LoQ	0.00165	0.0005	CW - Croatian Waters	
Pharmaceuticals	Diclofenac	15307-79-6	µg/l	<LoQ	0.00086	0.00034	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Pharmaceuticals	Digitoxin	71-63-6	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Digoxin	20830-75-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Dihydrocodeine	125-28-0	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Diphenhydramine	58-73-1	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Dothiepin	113-53-1	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Doxepin	1668-19-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	EDDP (metabolite of Methadone)	30223-73-5	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	
Pharmaceuticals	Felbamate	25451-15-4	µg/l	<LoQ	0.003	0.001	CW - Croatian Waters	

Pharmaceuticals	Fenazepam	51753-57-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Fenofibrate	49562-28-9	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Fentanyl	437-38-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Flumazenil	78755-81-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Flunitrazepam	1622-62-4	µg/l	<LoQ	0.001	nv		UNI Umea - Umeå University	
Pharmaceuticals	Flupentixol	2709-56-0	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Flurazepam	17617-23-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Gabapentin	60142-96-3	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Gabapentin-lactam	64744-50-9	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Haloperidol	52-86-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Hydrochlorothiazide	58-93-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Hydrocodone	125-29-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Hydromorphone	466-99-9	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Imipramine	50-49-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Indometacin	53-86-1	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Iohexol	66108-95-0	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Iomeprol	78649-41-9	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Iopamidol	62883-00-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Iopromid	73334-07-3	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Irbesartan	138402-11-6	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	JWH-018 (N-(n-pentanoic acid)	209414-07-3	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	JWH-073 (2-methylnaphthyl analog)	1427325-61-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Ketamine	6740-88-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Ketoprofen	22071-15-4	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Lamotrigine	84057-84-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Librium (Chlordiazepoxide)	58-25-3	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Lidocaine	137-58-6	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Lorazepam	846-49-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Losartan	114798-26-4	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Maprotiline	10262-69-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Medazepam	364-85-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Meperidine (Pethidine)	57-42-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Methamphetamine	537-46-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Methylendioxymethamphetamine (MDMA)	69610-10-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Methylphenidate	113-45-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Metoprolol	37350-58-6	µg/l	<LoQ	0.02	nv		UFZ - Helmholtz Centre for Environmental Research	
Pharmaceuticals	Metroprolol acid	56392-14-4	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Midazolam	59467-70-8	µg/l	<LoQ	0.0005	nv		UNI Umea - Umeå University	
Pharmaceuticals	Mirtazapine	61337-67-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Morphine	57-27-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Morphine glucuronide	20290-10-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	n-Acetyl-4-aminoantipyrine	83-15-8	µg/l	<LoQ	0.01	nv		UFZ - Helmholtz Centre for Environmental Research	
Pharmaceuticals	Nadolol	42200-33-9	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Naltrexone	16590-41-3	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Naproxen	22204-53-1	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	N-Desmethylclozapine	6104-71-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	N-Formyl-4-aminoantipyrine	1672-58-8	µg/l	non detect	nv		nv	ZLBF - LW Langenau	
Pharmaceuticals	Nitrazepam	146-22-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Norbuprenorphine	78715-23-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Nordiazepam	1088-11-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Norfentanyl	1609-66-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Normeperidine (Norpethidine)	77-17-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Norpropoxyphene (Desmethyl propoxyphene)	32504-12-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Nortriptyline	72-69-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	O-Desmethyltramadol	73986-53-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	O-Desmethylvenlafaxine (Desvenlafaxine)	93413-62-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Olanzapine	132539-06-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Opipramol	315-72-0	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Oxazepam	604-75-1	µg/l	<LoQ	0.0005	nv		UNI Umea - Umeå University	
Pharmaceuticals	Oxcarbazepine	28721-07-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Oxycodone	76-42-6	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Oxymorphone	76-41-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Paliperidone (9-Hydroxyrisperidone)	144598-75-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Paroxetine	61869-08-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Pentazocine	359-83-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Pentobarbital	76-74-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Pentoxifylline	6493-05-6	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Phenacetin	62-44-2	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Phenazone	60-80-0	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Phencyclidine (PCP)	77-10-1	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Phentermine	122-09-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Phenytoin	125-59-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Pipamperone	1893-33-0	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Prazepam	2955-38-6	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Pregabalin	148553-50-8	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Primidone	125-33-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Promazine	58-40-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Promethazine	60-87-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Propafenone	54063-53-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Propoxyphene (Dextropropoxyphene)	469-62-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Propranolol	525-66-6	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Propyphenazone	479-92-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Protriptyline	438-60-8	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Quetiapine	111974-69-7	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Risperidone	106266-06-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Ritalinic acid	19395-41-6	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Secobarbital	76-73-3	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Sertraline	79617-96-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Sotalol	3930-20-9	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Strophanthidin	66-28-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Sulfadimidin / Sulfamethazin	57-68-1	µg/l	<LoQ	0.05	nv		UFZ - Helmholtz Centre for Environmental Research	
Pharmaceuticals	Sulfamethoxazole	723-46-6	µg/l	<LoQ	0.0001		0.00005	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Pharmaceuticals	Sulpirid	15676-16-1	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Telmisartan	144701-48-4	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Temazepam	846-50-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Topiramate	97240-79-4	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Tramadol	27203-92-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Trazodone	19794-93-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Triazolam	28911-01-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Trimethoprim	738-70-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Trimipramine	739-71-9	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Valsartan	137862-53-4	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Valsartan acid	164265-78-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Pharmaceuticals	Venlafaxine	93413-69-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Verapamil	52-53-9	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Zolpidem	82626-48-0	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Pharmaceuticals	Zopiclone	43200-80-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Polar compounds	1H-Benzotriazole	95-14-7	µg/l	<LoQ	0.00066		0.00031	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	2-(Methylthio)benzothiazole	615-22-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Polar compounds	2-Ethylhexyl diphenyl phosphate (EHDP)	1241-94-7	µg/l	<LoQ	0.00023		0.00012	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	5,6-Dimethylbenzotriazole	4184-79-6	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Polar compounds	5-Methyl-1H-benzotriazole	136-85-6	µg/l	<LoQ	0.00053	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Benzothiazole-6-carboxylic acid	3622-35-3	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Polar compounds	Nonylphenol (4-Nonylphenol)	104-40-5	µg/l	<LoQ	0.01	nv		UFZ - Helmholtz Centre for Environmental Research	
Polar compounds	Tolyltriazol (mix of isomers)	29385-43-1	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Polar compounds	Triisobutyl phosphate (TIBP)	126-71-6	µg/l	<LoQ	0.000014	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Tri-n-butyl phosphate (TnBP)	126-73-8	µg/l	<LoQ	0.0000085		0.0000042	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Tri-n-propyl phosphate (TnPP)	513-08-6	µg/l	<LoQ	0.00014		0.00007	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Triphenyl phosphate (TPT)	115-86-6	µg/l	<LoQ	0.00001		0.00002	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Tris(1-chloro-2-propyl)phosphate (TCPP)	13674-84-5	µg/l	<LoQ	0.0003	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Tris(2-butoxyethyl)phosphate (TBEP)	78-51-3	µg/l	<LoQ	0.00113	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Tris(2-chloroethyl)phosphate (TCEP)	115-96-8	µg/l	<LoQ	0.00018	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Polar compounds	Tris(3,5-dimethylphenyl)phosphate (T35DMPP)	25653-16-1	µg/l	<LoQ	0.00023	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	3 sites missing
Polar compounds	Tris(methylphenyl)phosphate (TMPP)	1330-78-5	µg/l	<LoQ	0.00017		0.000084	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Organotin compounds	Dibutyltin-cation	1002-53-5	µg/l	<LoQ/LoD	0.0002		0.0001	UBAAT - Umweltbundesamt GmbH	
Organotin compounds	Dioctyltin-cation	94410-05-6	µg/l	<LoQ/LoD	0.0002		0.0001	UBAAT - Umweltbundesamt GmbH	
Organotin compounds	Diphenyltin-cation	6381-06-2	µg/l	<LoQ/LoD	0.0002		0.0001	UBAAT - Umweltbundesamt GmbH	
Organotin compounds	Tetrabutyltin	1461-25-2	µg/l	<LoQ/LoD	0.0000002		0.0000001	UBAAT - Umweltbundesamt GmbH	
Organotin compounds	Tributyltin-cation	36643-28-4	µg/l	<LoQ/LoD	0.0000002		0.0000001	UBAAT - Umweltbundesamt GmbH	
Organotin compounds	Triphenyltin-cation	668-34-8	µg/l	<LoD	0.0002		0.0001	UBAAT - Umweltbundesamt GmbH	
Other	2,4-Dinitrophenol (DNP)	51-28-5	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Other	Acesulfame	33665-90-6	µg/l	<LoQ	0.02	nv		UFZ - Helmholtz Centre for Environmental Research	
Other	Bisphenol A	80-05-7	µg/l	<LoQ	nv		nv	CW - Croatian Waters	
Other	Bisphenol S	80-09-1	µg/l	<LoQ	0.1	nv		UFZ - Helmholtz Centre for Environmental Research	
Other	Caffeine	58-08-2	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Other	Cotinine	486-56-6	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Other	Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	µg/l	<LoQ	0.2	nv		WRISK - Water Research Institute	
Other	N,N-Diethyl-m-toluamid (DEET)	134-62-3	µg/l	<LoQ	0.00193	nv		JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Other	Nicotine	54-11-5	µg/l	<LoQ	0.003		0.001	CW - Croatian Waters	
Other	Perfluorobutanesulfonate (PFBS)	375-73-5	µg/l	<LoQ	0.00055		0.00019	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Other	Perfluoroheptanoic acid (PFHpA)	375-85-9	µg/l	<LoQ	0.0032		0.0015	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Other	Perfluorohexane sulfonate (PFHxS) (anion)	108427-53-8	µg/l	non detect	nv		nv	ZLBF - LW Langenau	Semi-quantitative
Other	Perfluorohexanoic acid (PFHxA)	307-24-4	µg/l	<LoQ	0.0005		0.0011	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	

Other	Perfluorononanoate (PFNA)	375-95-1	µg/l	<LoQ	0.00066	0.00029	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Other	Perfluorooctanesulfonic acid (PFOS)	1763-23-1	µg/l	<LoQ	0.00109	0.00053	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Other	Perfluorooctanoic acid (PFOA)	335-67-1	µg/l	<LoQ	0.00107	0.00046	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability	
Other	Saccharin	81-07-2	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative
Other	Sucralose	56038-13-2	µg/l	non detect	nv	nv	ZLBF - LW Langenau	Semi-quantitative

Concentration with zeros

JDS3 site	Arsenic (As) - dissolved	Cadmium (Cd) - dissolved	Chromium (Cr) - dissolved	Copper (Cu) - dissolved	Lead (Pb) - dissolved	Mercury (Hg) - dissolved	Nickel (Ni) - dissolved	Zinc (Zn) - dissolved	Anthracene	Benzo(a)pyrene	Benzo(b)fluoranthene	Benzo(g,h,i)perylene	Benzo(k)fluoranthene
JDS01	1.1	0	0.48	1.2	0.4	0	0.93	6	0.0027	0	0	0.0015	0
JDS02	1.4	0	0.68	1.1	0.5	0	0.78	4.2	0	0	0	0.001	0
JDS03	1.3	0.024	1.2	2	0.63	0.0027	1.8	13	0.0025	0	0	0.0021	0
JDS04	1.4	0	0.5	1.6	0.73	0.0039	0.8	6.4	0	0	0	0.0013	0
JDS05	1.4	0.014	0.31	1.5	0.7	0.0028	0.81	10	0	0	0	0.0014	0
JDS06	1.5	0.013	0.7	1.6	0.56	0	1.1	8.6	0	0	0	0.001	0
JDS07	1.6	0.038	0.5	1.7	1.4	0	1.1	11	0.0024	0.0024	0	0.0026	0.0022
JDS08	1.4	0	0.97	2.1	0.7	0	1	5.5	0	0	0	0.0016	0
JDS09	1.5	0.066	5.3	1.2	1.6	0	19	6.6	0	0	0	0	0
JDS10	1.5	0.081	0.84	1.2	1.4	0	1.7	5.7	0.0021	0	0	0.0022	0
JDS11	1.5	0.057	6.7	1.3	0.86	0	25	7	0	0	0	0.0015	0
JDS12	3.3	0.073	0.36	1.5	1.2	0	2.8	9.9	0	0	0	0.0014	0
JDS13	1.6	0.048	0.91	1.3	1.3	0	0.95	5.4	0	0	0	0.0011	0
JDS14	1.6	0.015	0.29	1.4	0.26	0	1	8	0	0	0	0.0014	0
JDS15	1.6	0.02	0.5	1.2	0.2	0	1	6.3	0	0	0	0.0019	0
JDS16	2.4	0.096	0.58	1.1	1.8	0	1.2	7.3	0	0	0	0.0023	0
JDS17	1.7	0.034	0.54	1.3	0.38	0.0046	1	5.5	0	0	0	0.0013	0
JDS18	3.6	0.057	0.45	1.4	1	0.0044	1.2	5.7	0	0	0	0.0014	0
JDS19	1.7	0.15	0.62	1.5	8.1	0	1.4	6.6	0	0	0	0.0015	0
JDS20	1.9	0.07	0.42	1.6	4.2	0.0037	1.2	8.6	0	0	0	1.30E-06	0
JDS21	2.3	0.029	2.1	1.3	0.63	0.0056	7.3	6	0	0	0	0	0
JDS22	2	0.024	0.63	1.4	0.66	0.0034	1.9	7	2.50E-06	0	2.10E-06	2.40E-06	0
JDS23	3.5	0.011	0.29	1	0.49	0.0023	1.3	12	2.20E-06	0	0	2.10E-06	0
JDS24	2	0.022	0.34	1.3	0.4	0.0037	1.6	8.5	9.80E-06	2.40E-06	2.70E-06	2.60E-06	0
JDS25	2	0.028	0.47	1.4	0.45	0.0046	1.1	7.7	2.40E-06	0	0	2.10E-06	0
JDS26	2.1	0.033	0.56	1.5	0.97	0.005	1.3	7.7	2.10E-06	0	0	2.40E-06	0
JDS27	2.2	0.025	0.67	1.4	0.72	0.0043	1.2	6.8	2.50E-06	0	0	2.00E-06	0
JDS28	2.2	0.022	0.33	1.3	0.23	0	1.1	5.7	2.50E-06	0	2.30E-06	2.20E-06	0
JDS29	2.4	0.027	0.59	0.74	0.51	0.0045	0.76	5.1	2.10E-06	0	0	1.80E-06	0
JDS30	2.2	0.026	0.52	1.1	0.24	0.0046	0.93	5.7	2.30E-06	0	0	2.20E-06	0
JDS31	2.3	0.028	2.6	1.1	0.49	0.0028	9	6.3	0.002	0	0	0.002	0
JDS32	2.3	0.028	0.67	1.2	0.35	0.0057	1.3	7.1	0.003	0.0023	0.0024	0.029	0
JDS33	2.3	0.03	0.68	1.2	0.52	0.0025	1.4	7.4	0.0029	0	0.0024	0.0031	0
JDS34	2.3	0.029	1.1	1.1	0.27	0.0057	2.2	7.1	0	0	0	0.0015	0
JDS35	4.3	0.033	0.56	1.8	0.4	0.0039	1.3	13	0	0	0	0.0012	0
JDS36	2.4	0.033	0.86	1.3	0.87	0	2.3	8.7	0	0	0	0.0018	0
JDS37	2.5	0.03	1	1.4	0.67	0.0021	1.5	7.1	0	0	0	0.0013	0
JDS38	2.2	0.075	0.88	2	1.6	0.0042	1.2	2.3	0	0	0	0.0014	0
JDS39	2.2	0.048	0.82	2.1	0.59	0.0051	1.1	2.1	0	0	0	0.0013	0
JDS40	2.2	0.044	0.76	1.9	0.29	0.0051	1	1.6	0	0	0	0.0016	0
JDS41	5	0.3	67	2.3	2.6	0	230	3.4	0	0	0	0.0017	0
JDS42	2.2	0.051	0.84	2	0.8	0.0028	1.4	2.2	0	0	0	0.0013	0
JDS43	2.5	0.084	1.6	2	0.38	0.0041	4.7	3.9	0	0	0	0.0014	0
JDS44	2.3	0.04	0.76	2.1	0.47	0	1.3	2.1	0	0	0	0.0017	0
JDS45	2.5	0.043	0.71	2	0.26	0.0056	1.2	1.5	0	0	0	0.0007	0
JDS46	2.4	0.037	0.59	2.1	0.3	0.0047	1.3	1.8	0	0	0	0.0011	0
JDS47	2.4	0.045	0.72	2.2	0.36	0.007	1.3	2.1	0	0	0	0.0013	0
JDS48	1.5	1.1	0.63	283	0.45	0.0023	36	61	0	0	0	0.0012	0
JDS49	2.3	0.04	0.81	9.9	0.29	0.0056	1.2	1.9	0	0	0	0.0013	0
JDS50	2.3	0.041	2.2	5.2	0.25	0.0038	8.7	8.3	0	0	0	0.0013	0
JDS51	5.3	0.11	1.9	13	1	0.0047	6.4	1.8	0	0	0	0.0017	0
JDS52	2.2	0.046	0.71	3.7	0.27	0.0048	1.3	1.7	0	0	0	0.001	0
JDS53	2.4	0.043	0.72	3.5	0.32	0.0054	2.2	4.9	0	0	0	0.0012	0
JDS54	2	0.041	0.61	2.9	0.23	0.0051	1.5	1	0	0	0	0.0015	0
JDS55	2.4	0.039	0.47	3.2	0.35	0.0056	1.2	2.5	0	0	0	0.0012	0
JDS56	3.2	0.025	1.5	4.1	0.41	0.0063	1.6	2.9	0	0	0	0.0012	0
JDS57	2.4	0.037	0.37	3.1	0.41	0.0032	1.4	5.6	0	0	0	0.0012	0
JDS58	2.5	0.024	0.44	5.8	0.43	0.0061	3.3	3.9	0	0	0	0.002	0
JDS59	2.4	0.04	0.5	2.6	0.39	0.0027	1.8	1.3	0	0	0	0.0011	0
JDS60	2.4	0.038	2.2	2.5	0.32	0.0052	8	2.4	0	0	0	0.0011	0
JDS61	2.4	0.046	0.58	2.8	0.33	0.0032	2.8	2.5	0	0	0	0.001	0
JDS62	2.3	0.04	0.67	2.7	0.33	0.0026	1.4	1.5	0	0	0	0.0012	0
JDS63	1.7	0.03	0.23	2.6	0.36	0.0022	1.6	2.7	0	0	0	0.0027	0
JDS64	1.7	0.023	0.71	2.8	0.27	0.0058	2.3	1.4	0	0	0	0.0037	0
JDS65	2.4	0.042	0.33	2.8	0.71	0.0041	1.7	2.9	0	0	0	0.0018	0
JDS66	2.3	0.038	0.39	3.1	0.41	0.0064	1.4	3.6	0	0	0	0.0029	0
JDS67	2.4	0.039	0.7	2.6	0.38	0.0046	1.3	2.5	0	0	0	0.0025	0
JDS68	2.4	0.043	0.73	2.7	0.22	0.0032	1.3	1.1	0	0	0	0.0037	0

Fluoranthene	Indeno(1,2,3-c,d)pyrene	Naphthalene	2,4-D	2-Methyl-4-chlorphenoxy acetic acid (MCPA)	Ametryn	Aminomethylphosphonic acid (AMPA)	Atrazine	Atrazine-2-hydroxy	Atrazine-desethyl	Atrazine-desisopropyl	Bentazone	Bromacil	Carbetamide
0.004	0	0.022	0.00021	0.0057	0	0	0.006	0	0.0098	0	0.004	0.18	0.031
0.0021	0.0024	0	0.0038	0.0056	0	0.26	0.00866667	0	0.01	0	0.004	0.048	0.0078
0.0047	0	0.035	0.0034	0.0061	0	0.27	0.01266667	0	0.014	0	0.003	0.084	0.0017
0.0024	0	0.024	0.0021	0.0063	0	0.3	0.01133333	0	0.016	0.0008	0.005	0.05	0.0015
0.0029	0	0.021	0.0018	0.004	0	0.24	0.01266667	0.002	0.012	0	0.003	0.03	0.0022
0.0027	0	0.014	0.00051	0.0024	0	0.16	0.006	0	0.01	0	0	0.083	0
0.005	0	0.018	0.001	0.0028	0	0.16	0.005	0	0.0077	0.0001	0	0.084	0
0.0028	0	0.0087	0.00087	0.0027	0	0.17	0.005	0	0.0082	0	0	0.057	0.0032
0.0025	0	0.0094	0.001	0.0021	0	0.18	0.005	0	0.007	0	0	0.065	0.0028
0.0043	0.0037	0.03	0.00083	0.0026	0	0.19	0.005	0	0.0072	0.0004	0	0	0
0.0028	0	0.01	0.0016	0.0025	0	0.17	0.005	0.003	0.013	0	0.003	0	0.0017
0.0041	0	0.017	0.0072	0.012	0	0.63	0.014	0.02	0.0079	0	0.01	0	0.011
0.0022	0	0.0072	0.0013	0.0016	0	0.2	0	0	0.0073	0.0003	0	0	0.0016
0.0028	0	0.013	0.002	0.0037	0	0.21	0.006	0.007	0.0092	0.0006	0.004	0.044	0
0.0032	0	0.013	0.0014	0.0028	0	0.21	0.00633333	0.005	0.0099	0.0004	0.005	0	0.0096
0.0035	0	0.015	0.0048	0.0064	0	0.33	0.007	0.01	0.011	0	0.008	0.088	0
0.0024	0	0.0057	0.0014	0.0029	0	0.21	0.00666667	0	0.0088	0.0004	0.004	0.03	0
0.0025	0	0.015	0.0025	0.0036	0	0.4	0.006	0.02	0.008	0	0.009	0.035	0
0.0026	0	0.008	0.0019	0.0038	0	0.21	0.00566667	0.007	0.0095	0	0.005	0.19	0
0.003	0	0.016	0.0047	0.0051	0	0.14	0.00666667	0.01	0.0072	0	0.005	0.077	0.0018
0	0	7.20E-06	0.0017	0.003	0	0.19	0.00566667	0.006	0.007	0	0.004	0.029	0.0012
4.60E-06	0	1.50E-05	0.0015	0.0029	0	0.15	0.00633333	0.005	0.0092	0	0.004	0.068	0.025
4.30E-06	0	1.60E-05	0.0012	0.002	0	0.25	0.006	0.01	0.0048	0	0.004	0.056	0.011
2.00E-05	0	4.00E-05	0.0016	0.0028	0	0.21	0.00733333	0.006	0.0073	0.0006	0.005	0.044	0.0045
5.50E-06	0	1.90E-05	0.001	0.0029	0	0.23	0.00733333	0.007	0.0077	0	0.004	0.048	0.0025
6.10E-06	3.40E-06	1.50E-05	0.0012	0.0029	0	0.26	0.00666667	0.01	0.0064	0	0.005	0	0.0023
5.50E-06	0	1.90E-05	0.0017	0.0025	0	0.25	0.006	0.008	0.0053	0	0.005	0	0.0038
6.20E-06	4.90E-06	1.60E-05	0.0015	0.0031	0	0.27	0.007	0.01	0.0058	0	0.005	0	0.0011
3.10E-06	0	1.50E-05	0.00068	0.00098	0	0.16	0	0.004	0.0034	0	0.003	0	0.0019
4.10E-06	0	1.50E-05	0.001	0.0022	0	0.23	0.005	0.008	0.005	0	0.005	0.067	0.0026
0.0039	0.0031	1.10E-05	0.0013	0.002	0	0.24	0.00533333	0.008	0.0038	0	0.005	0	0.0027
0.0055	0	0.019	0.0016	0.002	0	0.27	0.00666667	0.009	0.0044	0	0.005	0.039	0.003
0.0057	0	0.02	0.0011	0.0013	0	0.27	0.006	0.007	0.0037	0	0.005	0	0
0.0028	0	0.0098	0.00094	0.0017	0	0.26	0.00633333	0.009	0.0033	0	0.004	0	0.0021
0.0022	0	0.006	0.0032	0.00066	0	0.22	0.00633333	0	0.0031	0	0.01	0.051	0.0016
0.003	0	0.0071	0.0013	0.002	0	0.25	0.00633333	0.007	0.0034	0	0.004	0.077	0.0057
0.0025	0.0036	0.0058	0.0016	0	0	0.21	0	0.01	0	0	0	0	0
0.0026	0	0.0055	0.0015	0.0017	0	0.16	0.005	0.007	0	0	0.004	0.11	0.0016
0.0021	0	0.005	0.0019	0.0014	0	0.28	0.006	0.008	0.0035	0	0.005	0	0.0013
0.0024	0	0.0075	0.0013	0.0016	0	0.26	0.00533333	0.01	0.0032	0	0.005	0	0.0028
0.0024	0	0.0095	0.0057	0	0	0.37	0	0	0.0033	0	0.008	0	0.0036
0.0029	0	0.0069	0.0014	0.0015	0	0.25	0.005	0.01	0	0	0.005	0	0.0011
0.0025	0.0026	0.0065	0.0017	0.0014	0	0.24	0.00533333	0.009	0.004	0.0003	0.006	0	0.0014
0.003	0	0.0067	0.0018	0.0015	0	0.27	0.00566667	0.008	0.0048	0.0003	0.006	0	0.0016
0.0031	0.0011	0.0034	0.002	0.0016	0	0.25	0.005	0.01	0.0034	0	0.005	0.024	0.0019
0.0024	0	0.0067	0.0022	0.0016	0	0.29	0.00533333	0.01	0.004	0	0.006	0	0.0019
0.0025	0.0024	0.0064	0.0019	0.0015	0	0.28	0.00566667	0.01	0	0.0011	0.005	0	0
0.0023	0	0.0059	0.016	0	0	0	0.007	0	0	0	0.02	0.066	0
0.0023	0	0.0068	0.0018	0.0013	0	0.24	0.00533333	0.01	0	0	0.006	0.034	0
0.003	0	0.0057	0.0017	0.0012	0	0.25	0.005	0.01	0	0.0015	0.005	0	0.0016
0.003	0	0.0075	0.0017	0.00055	0	0.34	0	0	0.0081	0.0023	0.009	0	0
0	0.0025	0.008	0.0014	0.0014	0	0.25	0.005	0.009	0.0034	0.0004	0.003	0.023	0.0012
0.0022	0	0.011	0.002	0.0015	0	0.25	0.00533333	0.008	0.004	0.0018	0.004	0	0
0.0022	0.0027	0.011	0.004	0.00019	0	0.24	0	0.01	0	0	0.02	0	0.0014
0	0	0.012	0.0031	0.0013	0	0.22	0.005	0.01	0	0	0.006	0	0.001
0.0023	0	0.002	0.021	0.00032	0	0.96	0.005	0.02	0	0	0.02	0	0.0011
0	0	0.011	0.0019	0.0011	0	0.25	0.006	0.009	0.0031	0	0.004	0	0.0012
0.0043	0	0.033	0.0084	0	0.004	0.62	0.07	0.045	0.0035	0	0.1	0	0
0	0	0.0091	0	0.0026	0	0.26	0.006	0.008	0	0	0.005	0	0
0	0.002	0.016	0.0027	0.0015	0	0.25	0.007	0.01	0	0	0.007	0	0.0087
0	0.0021	0.014	0.0018	0.0011	0	0.23	0.007	0.01	0.0032	0	0.006	0	0
0.0021	0	0.015	0	0.0013	0	0.23	0.007	0.01	0.0014	0	0.007	0	0
0.0027	0	0.016	0.0089	0.00039	0	0.13	0	0.02	0	0	0.02	0	0.0014
0	0	0.0094	0.0044	0.0004	0	0.12	0.011	0.03	0	0	0.03	0	0.0011
0	0	0.014	0.0023	0.0015	0	0.24	0.00533333	0.01	0	0	0.007	0	0.0018
0.0025	0.0025	0.012	0.004	0.0022	0	0.24	0.005	0.01	0	0	0.007	0.03	0.0018
0.002	0.0024	0.0097	0	0.0021	0	0.26	0.006	0.01	0	0	0.007	0	0.0019
0.0025	0	0.012	0.0013	0.00059	0	0.23	0.006	0.01	0	0	0.008	0.032	0.0015

Chloridazon	Chloridazon-desphenyl	Chloridazon-methyl-desphenyl	Chloroxuron	Chlortoluron	Cyanazine (Fortrol)	Cybutryne (Irgarol)	Dimefuron	Dimethachlor CGA 369873	Dimethachlor sulfonic acid CGA 354742	Dimethenamid	Dinoseb	Dinoterb	Diuron
0.027	0.14	0	0.012	0	0	0	0.014	0.04	0	0	0	0	0.02
0.0061	0.18	0	0.025	0	0	0.00037	0.015	0.02	0	0	0	0	0.029
0.0064	0.16	0	0.011	0.0015	0	0	0.0096	0.02	0	0	0	0	0.028
0	0.24	0	0.0096	0.0018	0	0	0	0.02	0	0	0	0	0.029
0	0.24	0	0.012	0	0	0.00022	0.0055	0.02	0	0	0	0.07	0.026
0	0.095	0	0.015	0.01	0	0.00043	0	0.01	0	0	0	0.03	0.017
0	0.08	0	0.014	0	0	0	0.0038	0.01	0	0	0	0.08	0.016
0	0.1	0	0.013	0.023	0	0	0	0.01	0	0	0	0.02	0.013
0	0.13	0	0.04	0.01	0.076	0.00034	0.0066	0.01	0	0	0	0.03	0
0	0.095	0	0.023	0.021	0	0	0.026	0.01	0	0	0	0.02	0
0	0.1	0	0.026	0.028	0	0.00032	0.014	0	0	0	0	0.02	0.012
0.0042	0.25	0.055	0.016	0	0	0.00036	0.0086	0.05	0.02	0.004	0	0.05	0
0	0.082	0	0.019	0.033	0	0	0.014	0.01	0	0	0	0.03	0
0.003	0.098	0	0.016	0.019	0	0.00032	0.0075	0	0	0	0	0.04	0
0	0.094	0	0.017	0.014	0	0.0002	0.013	0.02	0	0	0	0.003	0
0	0.074	0	0.0094	0.0014	0	0	0.011	0.02	0	0	0	0.003	0.012
0	0.088	0	0.012	0.013	0	0.0005	0	0.03	0	0	0	0.004	0.016
0.004	0.15	0	0.017	0	0	0.00066	0.038	0.02	0	0	0	0.004	0.012
0	0.12	0	0.011	0.0018	0	0.00047	0.032	0.02	0	0	0	0.003	0
0	0.086	0	0.015	0.0059	0	0.00061	0.041	0.02	0	0	0	0.003	0.012
0	0.089	0	0.0099	0.0067	0	0.00061	0.011	0.02	0	0	0	0.01	0
0.02	0.1	0	0.014	0.008	0	0.00049	0.0097	0.02	0	0	0	0.004	0
0.012	0	0	0.0096	0.0044	0	0.00083	0.041	0.01	0	0	0	0.004	0
0.0032	0.094	0	0.0054	0.0063	0	0.00031	0.017	0.02	0	0	0	0.004	0.011
0.0026	0.085	0	0.0069	0.01	0	0	0.0081	0.02	0	0	0	0.003	0.013
0.0026	0.094	0	0.0077	0.0048	0	0	0.0033	0.02	0	0	0	0.003	0
0.0033	0.081	0	0.0065	0.0052	0	0.00054	0.028	0.02	0	0	0	0.004	0.012
0.0027	0.082	0	0.009	0.004	0	0	0.028	0.02	0	0	0	0.004	0
0.0026	0	0	0.0076	0.0009	0	0	0	0	0	0	0	0.003	0.012
0.0026	0.08	0	0.0062	0.0032	0	0	0.025	0.01	0	0	0	0.004	0
0.0024	0.069	0	0.0071	0.0045	0	0	0.021	0.01	0	0	0	0.004	0
0.0026	0.079	0	0.0086	0.004	0	0	0.009	0.02	0	0	0	0.004	0
0.0026	0.078	0	0.0076	0.0021	0	0	0.018	0.02	0	0	0	0.003	0
0.0027	0.089	0	0.009	0.0039	0	0	0.013	0.02	0	0	0	0.003	0
0.0029	0	0	0.0073	0.0009	0	0	0.038	0	0	0	0	0.01	0.012
0.0031	0.074	0	0.0094	0.0048	0	0	0.022	0.01	0	0	0	0.02	0
0.0028	0	0	0.0065	0.0018	0	0	0.0043	0	0	0	0	0.01	0
0	0.059	0	0.0088	0.0008	0	0	0.0066	0.01	0	0	0	0.03	0
0.0023	0.056	0	0.007	0	0	0	0.00052	0.01	0	0	0	0.01	0
0	0.05	0	0	0	0	0	0.0088	0.01	0	0	0	0.01	0
0.0024	0	0	0.0049	0	0	0	0	0	0	0	0	0.01	0
0	0.056	0	0.0029	0	0	0	0.005	0.01	0	0	0	0.02	0
0	0.06	0	0.0036	0.0049	0	0	0	0.01	0	0	0	0.01	0.012
0.0024	0	0	0.0037	0	0	0	0.0065	0.01	0	0	0	0.01	0
0	0.051	0	0.0043	0.0039	0	0	0.00072	0	0	0	0	0.01	0
0.0025	0	0	0.0031	0.0094	0	0	0	0.01	0	0	0	0.02	0
0	0.059	0	0.0052	0.002	0	0	0.012	0.01	0	0	0	0.02	0
0	0	0	0.004	0.0015	0	0	0.011	0	0	0	0	0.01	0
0	0	0	0.002	0.0006	0	0	0.0064	0.01	0	0	0	0.02	0
0	0.05	0	0	0.0012	0	0	0.011	0	0	0	0	0.01	0
0	0	0	0	0.0021	0	0	0.0054	0	0	0	0	0.01	0
0	0.052	0	0.0052	0.0018	0	0	0.0077	0	0	0	0	0.003	0
0	0	0	0.0031	0.0007	0	0	0	0	0	0	0	0.008	0
0	0	0	0.0099	0.0047	0	0	0.012	0	0	0	0	0.005	0
0	0	0	0.0068	0.0037	0	0	0.0099	0.01	0	0	0	0.004	0
0	0	0	0.0094	0	0	0	0.011	0	0	0	0	0.006	0.056
0	0	0	0.0014	0	0	0	0.006	0	0	0	0	0.004	0
0	0	0	0.0061	0.006	0	0	0	0	0.3	0	0	0.01	0
0	0	0	0.0076	0	0	0	0.0066	0	0	0	0	0.007	0
0	0	0	0.0069	0.0014	0	0	0.0055	0	0	0	0	0.004	0
0	0	0	0.0064	0.0023	0	0	0.0091	0	0	0	0	0.003	0
0	0.05	0	0.0069	0	0	0	0.0038	0	0	0	0	0.003	0
0	0	0	0.0055	0	0	0	0.0083	0	0	0	0.004	0.006	0
0	0	0	0.0071	0	0	0	0.0099	0	0	0	0	0.01	0
0	0	0	0.0066	0	0	0	0.0078	0	0	0	0	0.004	0
0	0	0	0.0057	0.0042	0	0	0.0076	0	0	0	0	0.006	0
0	0.053	0	0.0062	0.019	0	0	0.01	0	0	0	0	0.003	0
0	0	0	0.006	0	0	0	0.0081	0	0	0	0	0.006	0

Ethidimuron (Sulfadiazole)	Ethofumesate	Glyphosate	Hexazinon	Isoproturon	Linuron	Metamitron	Metazachlor	Metazachlor ESA	Metazachlor OA	Methabenzthiazuron	Metobromuron	Metolachlor	Metolachlor ESA
0.0017	0.029	0	0	0.0052	0	0	0.0009	0	0	0.0017	0.068	0	0
0.0026	0.013	0	0	0.01	0	0	0.0008	0	0	0.0023	0	0.005	0.054
0	0.08	0.07	0	0.0094	1.4	0.0021	0.0005	0.052	0	0.0017	0	0.0084	0
0.0016	0.05	0	0	0.0073	1.2	0	0.0019	0.063	0	0.0018	0	0.011	0.057
0.0019	0	0	0	0.0094	0.69	0	0	0	0	0	0	0.0062	0.064
0	0.036	0	0	0.0045	1	0	0	0	0	0.0016	0	0.005	0
0.00042	0.031	0	0	0.0036	0.013	0	0.0006	0	0	0.0017	0	0.007	0.05
0.0022	0.047	0.073	0	0.0021	0.93	0	0.0006	0	0	0	0	0.0058	0.052
0	0.028	0.065	0	0.016	0.083	0.004	0.0026	0	0	0.0016	0	0.0039	0.055
0.00066	0.052	0	0	0	0	0.025	0.0038	0	0	0.0017	0	0.006	0.06
0.00095	0.027	0	0	0.0007	0	0.014	0.0006	0	0	0	0.0082	0.0041	0.052
0	0.036	0	0.007	0.0052	0.021	0.029	0.0028	0.33	0.17	0	0	0.01	0.087
0.00078	0.025	0	0	0	0.0087	0.019	0.0036	0	0	0.0016	0	0.0025	0.054
0.0004	0.015	0	0	0.0034	0.023	0.025	0.0022	0	0	0.0017	0	0.0063	0.051
0.00025	0.017	0	0	0	0.038	0.021	0.0013	0	0	0	0.043	0.0035	0
0.0035	0.042	0	0	0	0	0.0021	0.0014	0	0	0	0	0.0072	0.072
0.00027	0.043	0	0	0	0.015	0	0.0005	0	0	0	0	0.0039	0.051
0.00025	0.044	0	0	0.005	0.03	0.0017	0.023	0	0	0	0	0.0038	0
0	0.041	0	0	0	0.021	0	0.0013	0	0	0	0.016	0.0044	0
6.80E-05	0.028	0	0	0	0.031	0	0.0009	0	0	0	0	0.0038	0
0	0.031	0	0	0.003	0.033	0	0.0005	0	0	0	0.0074	0.0042	0
0.00022	0.029	0	0	0.0051	0.0029	0	0.0006	0	0	0	0	0.0031	0
0.00019	0.042	0	0	0.002	0.02	0	0	0	0	0	0	0.0024	0
0	0.024	0	0	0.0024	0.018	0	0.0005	0	0	0	0.0087	0.0036	0
0	0.036	0	0	0	0.0093	0	0.0006	0	0	0	0.0066	0.0066	0
0.00026	0.022	0	0	0.0041	0.0081	0	0.0008	0	0	0	0.0086	0.008	0
0.00019	0.03	0	0	0	0	0	0.0006	0	0	0	0.0063	0.0043	0
0.00023	0.031	0	0	0.0076	0.0057	0	0	0	0	0	0.0053	0.0091	0
0.00021	0.01	0	0	0.0019	0	0	0	0	0	0	0.0061	0.0046	0
0	0.021	0	0	0	0.0088	0.0019	0	0	0	0	0.0071	0.0078	0
0	0	0	0	0	0	0	0	0	0	0	0.01	0.0058	0
0	0.02	0	0	0.027	0	0	0	0	0	0	0.0055	0.0087	0
0	0.011	0	0	0.0011	0	0	0	0	0	0	0.006	0.011	0
0	0.024	0	0	0.0015	0	0	0	0	0	0	0.0051	0.011	0
0	0.029	0	0	0.0049	0	0	0.0005	0	0	0	0.0047	0.009	0
0.00032	0.0098	0	0	0.0065	0	0	0	0	0	0	0.0077	0.0065	0
0	0.02	0	0	0	0.0064	0	0.0005	0	0	0	0	0.0026	0
0	0.011	0	0	0	0	0	0	0	0	0	0.0089	0.0054	0
0	0.015	0	0	0	0	0.0019	0	0	0	0	0.0047	0.0049	0
0.00022	0	0	0	0.0024	0.011	0	0	0	0	0	0.0057	0.0063	0
0	0.011	0	0	0	0	0.0016	0	0	0	0	0.0049	0.0041	0
0.00025	0.0059	0	0	0	0.012	0.0022	0	0	0	0	0.0051	0.0055	0
0	0.009	0	0	0	0	0	0	0	0	0	0.0048	0.0057	0
0	0.0093	0	0	0.0042	0	0.0017	0	0	0	0	0.0047	0.0058	0
0	0	0	0	0	0	0.0016	0	0	0	0	0.0043	0.0045	0
0	0.021	0	0	0.0011	0	0.0017	0	0	0	0	0	0.0049	0
0.0014	0	0	0	0.0008	0	0	0	0	0	0	0.0051	0.0054	0
0	0	0	0	0.0009	0	0	0	0	0	0	0.0049	0.004	0
0.0015	0	0	0	0.0007	0	0	0	0	0	0	0	0.0054	0
0.0029	0	0	0	0.0038	0	0	0	0	0	0	0	0.0053	0
0.00038	0.029	0	0	0.0016	0	0	0	0	0	0	0	0.0046	0
0.00037	0.1	0	0	0.0005	0	0	0.016	0	0	0	0	0.0053	0
7.50E-05	0.097	0	0	0	0	0	0.013	0	0	0	0	0.0062	0
0.0013	0.026	0.062	0	0.001	0	0	0	0	0	0	0.0058	0.025	0
0.0019	0.013	0	0	0.0007	0.0001	0.0017	0	0	0	0	0.0053	0.0059	0
0	0.01	0.069	0	0.17	0	0.0025	0	0	0	0	0	0.039	0
0	0	0	0	0.0005	0	0	0	0	0	0	0.0051	0.0047	0
0.00056	0	0	0	0.0018	0.0057	0.0035	0	0	0	0	0.0055	0.0031	0
0	0.0094	0	0	0.0011	0	0.0017	0	0	0	0	0.0023	0.0061	0
0	0	0	0	0.0007	0	0.0017	0	0	0	0	0.0052	0.0049	0
0	0.015	0	0	0.0017	0.0086	0.0018	0	0	0	0	0	0.004	0
0.00092	0	0	0	0.0023	0	0.0017	0	0	0	0	0	0.0048	0
0	0.0094	0	0	0.0039	0	0.002	0.0006	0	0	0	0.0052	0.0071	0
0.002	0.011	0	0	0.0037	0	0.0018	0.0097	0	0	0	0.0046	0.0076	0
0.00031	0	0	0	0.0013	0	0.0018	0	0	0	0	0.0029	0.0068	0
0	0	0	0	0.0017	0.022	0.0017	0	0	0	0	0.0046	0.0056	0
0	0.0091	0	0	0.0017	0	0.0019	0	0	0	0	0.0069	0.0063	0
0.00035	0	0	0	0.001	0.0076	0.0019	0	0	0	0	0.0076	0.0043	0

Metoxuron	Monolinuron	Prometryn	Propazine	Propazine-2-hydroxy	Simazine	S-Metolachlor CGA 368208	S-Metolachlor NOA 413173	Terbutryn	Terbutylazine	Terbutylazine CGA 324007	Terbutylazine SYN 545666	Terbutylazine-2-hydroxy	Terbutylazine-desethyl
0.0049	0	0.006	0.01	0	0	0	0	0.0047	0.011	0	0	0	0
0.0056	0	0.0071	0.028	0	0	0	0	0.0044	0.028	0	0.0075	0	0
0.0013	0.0065	0.0098	0.025	0	0	0	0	0.011	0.025	0	0.003	0	0
0.005	0.0025	0.0065	0.021	0	0	0	0	0.0092	0.021	0	0.004	0	0
0.0068	0	0.0081	0.025	0	0.004	0	0	0.0094	0.025	0	0.008	0	0.0062
0.0049	0	0.0039	0.021	0	0.0016	0	0	0.005	0.021	0	0.0035	0	0.0038
0.0056	0.0068	0	0.0039	0	0	0	0	0.004	0.0046	0	0.008	0	0
0.0026	0.038	0.0018	0.0038	0	0	0	0	0.0033	0.0045	0	0.008	0	0
0.0095	0.089	0.0024	0.053	0	0.0033	0	0	0.0039	0.052	0	0.0085	0	0.0056
0.0098	0	0.0018	0.0059	0	0.0073	0	0	0.0031	0.0066	0	0.0065	0	0.0098
0.0096	0	0	0.012	0	0.0063	0	0	0.0033	0.012	0	0.008	0	0.0086
0.01	0	0	0.044	0	0.005	0.03	0.03	0.0075	0.043	0.01	0.01	0.02	0.0073
0.0096	0	0	0.0082	0	0.0011	0	0	0.0029	0.0087	0	0.0095	0	0.0033
0.017	0.0027	0	0.019	0	0	0	0	0.0029	0.019	0	0.0095	0	0
0.011	0.0063	0.0026	0.01	0	0	0	0.03	0.0042	0.011	0	0.0045	0	0
0.0026	0.0084	0.002	0.0008	0	0.0022	0	0.04	0.0034	0.0016	0	0.0045	0	0.0044
0.0014	0.027	0.0021	0.013	0	0	0	0.02	0.005	0.014	0	0.005	0	0
0	0	0.0019	0.0074	0	0.0044	0	0	0.0044	0.0079	0	0.0145	0	0.0067
0.0031	0.028	0	0.008	0	0.0055	0	0.03	0.0029	0.0086	0	0.015	0	0.0078
0.00035	0.0039	0.0017	0.0011	0	0.0052	0	0	0.0035	0.0019	0	0.014	0.006	0.0075
0.0019	0.012	0	0.0075	0	0	0	0.02	0.0035	0.0081	0	0.015	0	0
0.0017	0.014	0	0.0089	0	0	0	0	0.0034	0.0094	0	0.0145	0	0
0.0013	0	0	0.0048	0	0.0014	0	0.02	0.0044	0.0055	0	0.003	0	0.0035
0.00044	0	0	0.0058	0	0	0	0	0.0032	0.0065	0	0.0095	0.004	0
0	0	0.0014	0.0014	0	0	0	0	0.0035	0.0022	0	0.009	0	0
0.001	0	0	0.004	0	0	0	0.03	0.0032	0.0047	0	0.015	0	0
0.001	0	0.0022	0.0025	0	0.011	0	0.03	0.0041	0.0033	0	0.0145	0.005	0.014
0.0023	0.012	0	0.005	0	0	0	0.03	0.0023	0.0057	0	0.015	0	0
0.00019	0	0	0.0017	0	0	0	0	0.002	0.0025	0	0	0	0
0.00093	0	0	0.0024	0	0	0	0.03	0.0035	0.0031	0	0.0135	0	0
0	0	0	0.0015	0	0	0	0	0.0028	0.0023	0	0.0145	0	0
0.019	0	0.0017	0	0	0	0	0	0.0026	0	0	0.01	0	0
0.0032	0	0	0.0017	0	0	0	0.02	0.0041	0.0024	0	0.0095	0	0
0.0053	0	0	0.0008	0	0	0	0	0.0028	0.0016	0	0.0145	0	0
0.0023	0	0	0.0008	0	0	0.01	0	0.0037	0.0017	0	0	0	0
0.0048	0	0	0	0	0	0	0	0.0032	0	0	0.0085	0	0
0.0046	0	0	0.0017	0	0	0	0	0.0016	0.0024	0	0	0	0
0	0	0	0.0024	0	0	0	0	0.003	0.0031	0	0.0075	0	0
0	0	0	0.0004	0	0	0	0.02	0.002	0.0013	0	0.0085	0	0
0	0	0	0.0021	0	0	0	0.03	0.0025	0.0029	0	0.003	0.004	0
0	0	0	0.0003	0	0	0	0.04	0.0018	0.0012	0	0	0	0
0	0	0	0.0019	0	0	0	0.02	0.0026	0.0027	0	0.005	0	0
0	0.007	0.0015	0.0019	0	0	0	0.02	0.0021	0.0027	0	0.008	0	0
0.0025	0.0028	0	0	0	0.0022	0	0.02	0.0021	0	0	0.003	0	0.0044
0	0.003	0	0	0	0	0	0	0.0027	0	0	0.008	0	0
0.0027	0.0026	0.0017	0	0	0	0	0.03	0.0025	0	0	0.009	0	0
0.00031	0	0	0.0057	0	0.0012	0	0.02	0.0028	0.0063	0	0.0095	0.007	0.0034
0.0018	0	0.0051	0.0018	0	0	0	0	0	0.0026	0	0	0.004	0
0	0	0	0.0025	0	0.001	0	0	0.0027	0.0033	0	0.0135	0.008	0.0031
0.00039	0	0.0017	0.0041	0	0	0	0	0.0017	0.0048	0	0.0085	0	0
0.0038	0	0	0	0	0	0	0	0.0039	0	0	0	0	0
0	0	0.0021	0.0083	0	0	0	0	0.0027	0.0086	0	0.007	0.005	0
0.00096	0.012	0.0019	0.0042	0	0.0013	0	0	0.0028	0.0082	0	0.005	0.005	0.0034
0.0017	0.0028	0	0.0014	0	0	0	0	0	0.0022	0	0	0.005	0
0.0064	0.0057	0	0.0019	0	0	0	0	0.002	0.0027	0	0.0045	0.006	0
0.0031	0.0034	0.0029	0.0066	0.01	0	0.01	0	0.0018	0.0072	0	0	0	0
0	0.0005	0	0.0011	0	0	0	0	0.0025	0.0019	0	0.0065	0	0
0	0.0024	0.0038	0.0011	0	0.0013	0	0	0.0029	0.0019	0	0	0.01	0.0034
0	0	0	0.0011	0	0	0	0	0.002	0.0019	0	0.0025	0.006	0
0.00045	0	0	0	0	0	0	0.02	0.0025	0	0	0.0025	0.006	0
0.0018	0.0027	0	0	0	0	0	0	0.0014	0	0	0	0.006	0
0	0	0	0	0	0	0	0	0	0	0	0.003	0.007	0
0	0.0034	0.0026	0.0068	0	0	0	0	0.00088	0.0074	0	0	0.009	0
0	0.0032	0.0092	0.0087	0	0	0.01	0	0.00077	0.0092	0	0	0.01	0
0.0019	0.0027	0	0.0022	0	0	0	0	0.0025	0.003	0	0.005	0	0
0	0.0026	0	0	0	0	0	0	0.0016	0	0	0.0025	0.005	0
0.0044	0.0027	0.0015	0	0	0.0015	0	0	0.0017	0	0	0	0.007	0.0036
0	0	0	0	0	0.0023	0	0	0.0014	0	0	0	0	0.0045

Terbutylazine-desethyl-2-hydroxy	Diazinone	Fipronil	4-Chlorophenol	Azoxystrobin	Carbendazim	Cyproconazol	Flusilazole	Metalaxyl NOA 409045	Picoxystrobin	Propiconazole	Quinoxyfen	Tebuconazol	Trifloxystrobin CGA 321113
0	0.004	0	0	0	0.004	0	0	0	0.04	0	0.01	0	0
0	0.003	0	0	0	0	0	0	0	0.01	0.004	0.008	0	0
0	0.001	0	0.0015	0	0.005	0	0	0	0	0.006	0.005	0	0
0	0	0	0	0.002	0.007	0	0	0	0	0.004	0.004	0	0
0	0	0	0.0005	0	0.004	0	0	0	0	0.004	0	0	0
0	0	0	0.0006	0	0	0	0	0	0	0.003	0	0	0
0	0	0	0.0005	0	0	0	0	0	0	0	0	0	0
0	0	0	0.0005	0	0	0	0	0	0	0	0	0	0
0	0	0	0.0005	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.005	0	0	0	0	0	0	0	0
0	0	0	0	0	0.004	0	0	0	0	0	0	0	0
0	0	0	0	0.004	0	0.005	0	0	0	0	0	0.006	0
0.1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.008	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0.003	0
0	0	0	0	0	0	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0.005	0	0	0
0	0	0	0	0	0	0	0	0	0	0.003	0	0	0
0	0	0	0	0.002	0	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.009	0	0	0	0	0	0	0	0
0	0	0	0	0	0.008	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0.008	0	0	0.006	0	0.003	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0.003	0
0	0	0	0	0	0	0	0	0	0	0.003	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.01	0	0	0	0	0.003	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0.01	0	0	0	0	0.003	0	0.002	0
0	0	0	0	0	0.01	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0.01	0	0	0	0	0	0	0.002	0
0	0.002	0	0	0	0.007	0.005	0	0	0	0	0	0.004	0.005
0	0	0	0	0	0.01	0	0	0	0	0	0	0.002	0
0	0.001	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0.003	0	0.003	0
0	0	0	0	0	0.009	0	0	0	0	0	0	0.003	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0.004	0	0	0.002	0	0	0	0	0	0	0	0	0
0	0.001	0	0	0	0.008	0	0	0	0	0	0	0.003	0
0	0.001	0	0	0	0.01	0	0	0	0	0	0	0.003	0
0	0.001	0	0	0	0.01	0	0	0	0	0	0	0.003	0
0	0	0	0	0.007	0.009	0	0	0	0	0.003	0	0.002	0
0	0.001	0	0	0	0	0	0	0	0	0	0	0.002	0
0	0.001	0	0	0	0	0	0	0	0	0	0	0.003	0
0	0.005	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0.002	0	0	0	0	0	0	0	0.003	0
0	0.001	0	0	0	0.007	0	0	0	0	0	0	0.002	0
0	0.001	0	0	0	0.02	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.007	0	0	0	0	0	0	0	0
0	0	0	0	0	0.02	0	0	0	0	0	0	0	0
0	0	0	0	0	0.008	0	0	0	0	0	0	0	0
0.03	0	0	0	0	0.02	0	0.003	0	0	0	0	0.005	0
0	0	0	0	0	0.006	0	0	0	0	0	0	0	0
0	0.007	0.02	0	0.004	0.04	0	0	0	0	0	0	0.003	0
0	0	0	0	0	0	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0	0	0.002	0
0	0	0	0	0	0	0	0	0	0	0.003	0	0	0
0	0.001	0	0	0	0.007	0	0	0	0	0	0	0	0
0	0.003	0	0	0	0.009	0	0	0	0	0	0	0	0
0	0.002	0	0	0	0	0	0	0	0	0	0	0.005	0
0	0.001	0	0	0	0	0	0	0	0	0	0	0	0
0	0.001	0	0	0	0.007	0	0	0	0	0	0	0	0
0	0.001	0	0	0	0.01	0	0	0	0	0	0	0.003	0
0	0	0	0	0	0.009	0	0	0	0	0	0	0.002	0

10,11-Dihydro-10,11-dihydroxycarbamazepine	10,11-Dihydro-10-hydroxycarbamazepine	17-beta Estradiol	1-Adamantylamin	2-Hydroxycarbamazepine	3,4-Methylendioxyamphetamine (MDA)	3,4-Methylenedioxyethamphetamine (MDEA)	6-Acetylmorphine	7-Aminoclonazepam	7-Aminoflunitrazepam	Acetylcodeine	Acetyl-sulfamethoxazole	Alfentanil	alpha-Hydroxyalprazolam
0.029	0.0054	0.0015	0	0	0.0043	0.0048	0.00095	0.0024	0.00086	0.0035	0	0.001	0.055
0.068	0.0045	0	0	0	0.0018	0.0048	0.0041	0.0021	0.001	0	0	0.00037	0.049
0.045	0.005	0.0052	0.008	0	0.0029	0.015	0.0041	0	0.0013	0.0037	0	0.001	0.08
0.044	0.0024	0.029	0	0	0.0015	0.0042	0.0043	0.0021	0.00074	0	0	0.00065	0.065
0.073	0.0044	0.023	0	0	0	0.0074	0.0027	0.0024	0.00087	0	0	0.00057	0.06
0.05	0.0017	0.0019	0	0	0.0023	0.005	0.0011	0.0034	0.0016	0.0055	0	0.00094	0.099
0.029	0.0012	0.0048	0	0	0	0.005	0.0011	0.0025	0.0015	0.0041	0	0.00024	0.089
0.026	0.0017	0.0078	0	0	0.0079	0.0052	0.00095	0.0038	0.00082	0.003	0	0.00028	0.075
0.055	0.0054	0.0032	0	0	0.0095	0.001	0.0043	0.0032	0.00061	0	0	0.003	0.021
0.03	0	0	0	0	0.011	0.0021	0.00091	0	0.0013	0.0033	0	0.0003	0.15
0.054	0.0027	0	0	0.014	0.0023	0.0028	0	0	0.0015	0	0	0.00016	0.1
0.11	0.0022	0	0	0.011	0.024	0	0.0015	0	0.0012	0	0	0.0075	0.12
0.035	0.0017	0	0	0	0.016	0.002	0.00091	0.0022	0.0013	0	0	0.0076	0.11
0.031	0.0015	0	0	0	0.019	0.0017	0.0011	0.002	0.0014	0	0	0	0.11
0.062	0.0031	0	0	0	0.092	0.0022	0.00087	0.0021	0.00094	0.0038	0	0.0063	0.1
0.15	0.0024	0	0.01	0	0.0035	0	0	0.0029	0	0.0045	0	0.0011	0.15
0.058	0	0	0	0	0	0.0028	0.00073	0.002	0.00084	0	0	0.0019	0.073
0.093	0.0018	0	0.03	0	0.027	0.0024	0	0.0021	0.001	0	0	0.0019	0.046
0.049	0.0015	0	0	0	0	0.00084	0.0011	0.002	0.00097	0.0037	0	0	0.05
0.021	0.0024	0	0	0	0.0019	0.0054	0.00087	0.0019	0.00096	0.0034	0	0.00066	0.069
0.065	0.001	0	0	0	0.054	0.0047	0.00097	0.0034	0.00062	0.0031	0	0	0.063
0.08	0.0027	0	0	0	0	0.0038	0.00097	0	0	0.0031	0	0	0.058
0.14	0.0014	0	0.009	0	0.0058	0.0016	0	0.0019	0.00067	0	0	0	0.099
0.08	0.0023	0	0.006	0	0	0	0.00095	0.0019	0.00065	0.0035	0	0.002	0.053
0.043	0	0	0	0	0.00045	0	0.00095	0	0.00067	0.0033	0	0.00012	0.069
0.042	0.0012	0	0	0	0.0033	0.0017	0.00092	0.002	0.00063	0.0029	0	0	0.098
0.057	0	0	0	0	0.003	0.0076	0.00082	0	0.00062	0.0031	0	0	0.066
0.06	0	0	0.009	0	0.011	0.0034	0.00081	0.0021	0.00063	0.0029	0	0.0036	0.089
0.037	0.0018	0	0	0	0.091	0.0027	0.0008	0.0024	0.00062	0.003	0	0	0.058
0.052	0.0029	0	0	0	0	0.0031	0	0.002	0.0006	0.0029	0	0.00045	0.06
0.036	0	0	0	0	0.0051	0.0038	0	0.0032	0.00066	0	0	0.001	0.052
0.05	0	0	0.01	0	0.013	0.0022	0	0	0.0006	0.003	0	0.0018	0.047
0.051	0	0	0	0	0.072	0.0027	0	0.0028	0.00062	0.003	0	0	0.075
0.045	0.0011	0	0	0	0	0.003	0.00083	0.0025	0.00059	0.003	0	0.00016	0.076
0.084	0	0	0.01	0	0.19	0	0.0009	0.0066	0.0006	0.003	0	0	0.067
0.039	0	0	0.008	0	0.066	0.0031	0	0.0033	0	0	0	0	0.052
0.024	0.001	0	0	0	0.01	0.0063	0	0.0021	0.00059	0	0	0	0.052
0.034	0.0011	0	0.01	0	0	0.00058	0	0	0.00059	0	0	0.00098	0.051
0.039	0.004	0	0.01	0	0.011	0.0024	0	0.002	0.00062	0	0	0	0.057
0.043	0.0009	0	0	0	0.62	0.0045	0	0.014	0.00094	0	0	8.90E-05	0.052
0.11	0.0011	0	0.01	0.011	0.05	0.0015	0.00079	0.0025	0.0006	0.0032	0.063	0.0019	0.052
0.04	0	0	0.009	0	0.44	0.0028	0.00096	0.013	0.00062	0.0031	0.02	0.00042	0.052
0.042	0	0	0.01	0	0.11	0.0016	0	0.0047	0	0	0	0	0.049
0.043	0	0	0.01	0	0.32	0.0046	0	0.0081	0.00061	0	0	0	0.048
0.044	0	0	0	0	0.58	0.0018	0	0.012	0.00071	0	0	0.00091	0.048
0.045	0	0	0	0	0.049	0.0013	0	0.0037	0	0	0	0	0.051
0.041	0.0035	0	0.007	0	0	0.002	0.23	0	0	0.0078	0	0.00022	0.062
0.075	0.0056	0	0.09	0.014	0.00013	0.002	0.22	0	0	0.0075	0.042	0	0.07
0.043	0.0024	0	0	0	7.30E-05	0.002	0.22	0	0	0.0076	0	0.00015	0.056
0.041	0.0054	0	0.008	0	0	0.0016	0.24	0.002	0	0.0064	0	0.00085	0.045
0.13	0.0025	0	0	0.012	5.50E-05	0.002	0.0048	0.0055	0.00078	0.0072	0	0	0.0035
0.04	0	0	0	0	0	0	0.0029	0.0019	0	0.018	0	0	0.005
0.034	0.0009	0	0	0	0.00039	0	0.0028	0.0021	0.00072	0.019	0	8.60E-05	0.0053
0.032	0.001	0	0.01	0	0.013	0.0011	0	0.002	0	0	0	0	0.00024
0.036	0	0	0.005	0	2.90E-06	0	0	0	0	0	0	0	0.00042
0.086	0.004	0	0.01	0.011	0.0068	0.0014	0	0.0019	0	0.003	0.045	0	0.0018
0.035	0	0	0	0	0	0.00099	0	0	0	0	0	0	0.00024
0.16	0.0088	0	0.04	0.045	0.0036	0.0044	0	0	0.00069	0.0053	0.023	0	0.00086
0.038	0	0	0	0	0.024	0.00035	0	0	0	0	0	0	0.12
0.041	0	0	0	0	0	0.00019	0	0	0	0	0	0	0.00022
0.05	0	0	0	0	0	0.00036	0	0	0	0	0	0	0.11
0.043	0	0	0	0	0	0.00069	0	0	0	0	0	0.00029	0.1
0.013	0	0	0	0	0.023	0.00079	0	0	0	0	0	0.00077	0.15
0.016	0.0024	0	0	0	0.0034	0.0016	0	0	0	0	0	0	0.16
0.037	0	0	0	0	0	0.001	0	0	0	0	0	0	0.14
0.036	0	0	0	0	0	0.00032	0	0	0	0	0	0	0.13
0.046	0.0018	0	0	0	0	0.00062	0	0	0	0	0	0	0.14
0.034	0	0	0.007	0	0	0.0011	0	0	0	0	0	0	0.12

alpha-Hydroxymidazolam	alpha-Hydroxytriazolam	Alprazolam	Amidotrizoic acid	Amisulpride	Amitriptyline	Amoxapine	Amoxicillin	Amphetamine	Atenolol	Atropine	Benzoylecgonine	Betaxolol	Bezafibrate
0.00094	0.0056	0.0045	0	0.0093	0.0078	0.00045	0.012	0	0.03	0.016	0.0042	0	0
0.00099	0.0082	0.0067	0	0.0098	0.0092	0.00045	0.017	0	0	0.028	0.005	0	0
0.002	0.0071	0.012	0	0.014	0.012	0.00074	0.035	0	0	0.033	0.00023	0	0
0.00077	0.0055	0.01	0	0.011	0.012	0.00049	0.048	0	0	0.037	0.007	0	0
0.00059	0.0026	0.0066	0	0.014	0.011	0	0.011	0	0	0.031	0.00084	0	0
0.00075	0.0051	0.01	0	0.0092	0.0025	0.00084	0.026	0	0	0.02	0.0051	0	0
0.0019	0.0054	0.0077	0	0.003	0.0047	0.0005	0.0091	0	0	0.016	0.0062	0	0
0.00066	0.0061	0.011	0	0.00054	0.0073	0.00062	0.0096	0	0	0.015	0.0089	0	0
0.0079	0	0.0096	0	0.0044	0.0023	0.0038	0.13	0.004	0	0.16	6.60E-05	0	0
0.0012	0.0076	0.0023	0	0.0034	0	0	0.0092	0	0	0.013	0	0	0
0.0023	0.0061	0.002	0	0.0071	0.0018	0	0.011	0	0	0.004	0.00022	0	0
0.00081	0.006	0.0031	0	0.002	0	0.00047	0.28	0	0	0.021	0	0	0
0.00044	0.01	0.0027	0	0.0048	0	0	0.0088	0	0	0.012	0	0	0
0	0.013	0.002	0	0.0046	0	0.00047	0.017	0	0	0.016	0	0	0
0	0.0066	0.0043	0	0.002	0.0018	0	0.009	0	0	0.013	0	0	0
0	0.0066	0	0.5	0.008	0.0048	0.0022	0.034	0	0.01	0.038	0.0089	0	0
0	0.0059	0	0	0.0029	0.0041	0.00064	0.0096	0	0	0.019	0.0085	0	0.005
0	0.0075	0	0	0.0018	0.0041	0.00028	0.011	0	0.02	0.0038	0.0003	0	0
0.00058	0.0029	0.0063	0	0.0017	0.004	0.00068	0.0098	0.0018	0	0.017	0.00063	0	0
0	0.0065	0.0052	0	0.0015	0.0047	0	0.0089	0	0	0.021	0.0066	0	0
0	0.0056	0	0	0.0024	0.0029	0.0012	0.01	0.0024	0	0.0025	0.0089	0	0
0	0	0.0048	0	0.0035	0.003	0.0009	0.0091	0.0019	0	0.021	0.0056	0	0
0	0	0.0073	0	0	0.0025	0.00061	0.01	0.001	0	0.011	0.0025	0	0
0	0	0.0019	0	0.0008	0.0051	0.00075	0.0095	0.0019	0	0.018	0.007	0	0
0	0.0057	0.0068	0	0.0033	0.0021	0.00036	0.0099	0.00071	0	0.0072	0.0033	0	0
0	0.0067	0.0061	0	0.0026	0.005	0.00064	0.0094	0.001	0	0.02	0.0022	0	0
0	0.0055	0	0	0.0019	0.0048	0.00057	0	0.0027	0	0.02	0.0055	0	0
0	0	0	0	0.0022	0.0019	0.0011	0.018	0.00092	0	0.0097	0.005	0	0
0	0	0.0034	0	0.00059	0.0025	0.0005	0	0.0012	0	0.0081	0.0025	0	0
0	0	0.0012	0	0.0006	0.0038	0.00054	0.009	0	0	0.013	0.0051	0	0
0	0	0.0022	0	0.00064	0.0029	0.00025	0	0.0005	0	0.015	0.0051	0	0
0	0	0.0031	0	0.00032	0.0033	0.00053	0.0015	0.00096	0	0.028	0.0079	0	0
0	0	0.0021	0	0	0.002	0.00054	0	0.0018	0	0.012	0.0024	0	0
0	0	0.0023	0	0.00035	0.0034	0.00084	0	0.00077	0	0.018	0.0051	0	0
0	0	0.0022	0	0.0005	0	0.0014	0.009	0	0.01	0.019	0.0044	0	0
0	0	0.0042	0	0.0011	0.0036	0.00074	0	0.00057	0	0.0096	0.0042	0	0
0	0	0.0043	0	0.00094	0.0034	0	0	0	0	0.02	0.0077	0	0
0	0.0099	0.0035	0	0.0021	0.0042	0	0	0.0017	0	0.0094	5.20E-05	0	0
0	0.0057	0.0034	0	0.00043	0.0035	0.00055	0	0.00084	0.01	0.012	0.0007	0	0
0	0.0095	0	0	0.0021	0.0027	0.001	0	0	0	0.02	0.0014	0	0
0	0.0056	0.0024	0	0.0016	0.0019	0.0015	0	0.00055	0.02	0.011	0.0004	0	0
0	0	0.0016	0	0.00047	0.0029	0.00073	0.009	0.00068	0	0.021	0.0026	0	0
0	0.0063	0.0016	0	0.00091	0.0024	0.00067	0.0091	0.00081	0.01	0.018	0.0043	0	0
0	0	0	0	0.00041	0.0023	0.0005	0.0087	0.00059	0	0.019	0.0065	0	0
0	0	0.0017	0	0.00045	0.0024	0.00052	0	0	0	0.019	0.0036	0	0
0	0	0.0016	0	0.00028	0.0026	0	0	0	0	0.0092	0.00095	0	0
0	0.0071	0.009	0	0.0042	0.0059	0.00039	0	0	0	0.0015	0.0041	0	0
0	0	0.0068	0	0.0042	0.0069	0.00047	0	0	0.02	0.002	0.0048	0	0
0	0	0.0057	0	0.0037	0.0098	0.00044	0	0	0	0.0017	0.0059	0	0
0	0	0.004	0	0.0047	0.0099	0.00046	0	0	0	0.0024	0.0059	0	0
0	0	0.004	0	0.003	0.013	0.00049	0	0	0.01	0.0023	0.0025	0	0
0.00061	0.0075	0	0	0.004	0.013	0.00084	0	0	0	0.0015	0.0081	0	0
0	0.016	0	0	0.0038	0.011	0	0	0	0	0.0017	0.0046	0	0
0	0.01	0.0053	0	0.0011	0	0.0011	0	0	0	0.013	0.0036	0	0
0	0	0.0037	0	0.0005	0.0023	0	0	0	0	0.011	0.0043	0	0
0	0	0.0017	0	0.0083	0.0026	0.00045	0	0	0.03	0.075	0.0031	0	0
0	0	0.0008	0	0	0.0017	0.00054	0	0	0	0.0015	0.0026	0	0
0	0	0.0015	0	0.031	0.006	0	0	0	0.2	0.14	0.0012	0.01	0
0	0.0085	0.0041	0	0.00051	0.0022	0.00046	0	0	0.02	0.0096	0.0032	0	0
0	0	0.0021	0	0.0003	0.0022	0	0	0.011	0.02	0.0093	0.0017	0	0
0	0	0.0015	0	0	0	0	0	0	0.01	0.01	0.0031	0	0
0	0	0.0033	0	0.00064	0	0.0021	0	0.00045	0	0.011	0.0036	0	0
0	0	0.003	0	0.00063	0.002	0.00055	0	0	0	0.0095	0.0033	0	0
0	0	0.0035	0	0.00033	0	0.00046	0	0	0	0.011	0.0039	0	0
0	0	0.0025	0	0.00033	0	0.00075	0	0	0	0.0084	0.0026	0	0
0	0	0.002	0	0	0.0023	0.00049	0	0	0	0.0079	0.0025	0	0
0	0	0.0031	0	0	0	0.00052	0	0	0	0.0083	0.0025	0	0
0	0.012	0.0027	0	0	0	0.00067	0	0	0.01	0.0092	0.0025	0	0

Bisoprolol	Bromazepam	Buprenorphine	Buprenorphine glucuronide	Candesartan	Carbamazepine	Carbamazepine-10,11-epoxide	Carisoprodol	Cetirizine	Chlorprothixene	Citalopram	Clobazam (Urbadan)	Clonazepam	Clonidine
0.009	0	0.025	0	0	0.02	0	0.0025	0	0.0012	0.0018	0	0.04	0.0013
0.005	0.011	0.034	0.2	0.02	0.032	0	0.46	0	0.0013	0.0015	0.011	0.034	0
0.007	0	0.038	0	0	0.03	0	0.02	0	0.0039	0	0	0	0.0013
0.008	0	0.025	0	0.02	0.034	0	0.013	0	0.0013	0	0	0	0
0.006	0	0.0062	0.044	0.01	0.033	0	0.03	0	0.0019	0	0.005	0.0038	0.0013
0.007	0.012	0.011	0	0	0.028	0	0.021	0	0.0015	0.0011	0	0.041	0.0013
0	0	0.0092	0	0.01	0.024	0	0.0019	0	0.00083	0	0	0.042	0.0013
0	0	0.014	0	0.009	0.017	0	0.012	0	0	0	0	0.034	0
0	0.015	0.062	0.039	0.01	0.023	0	0.029	0	0.014	0	0	0.029	0.0013
0	0	0.025	0	0.01	0.019	0	0.003	0	0.00078	0	0	0.28	0
0	0	0.018	0	0.01	0.023	0	0.0026	0	0.0014	0.0014	0	0.26	0.0014
0	0	0.02	0	0.01	0.047	0	0.013	0.018	0.0012	0.0011	0	0.25	0
0	0	0.021	0	0.01	0.016	0	0.0037	0	0	0	0	0.24	0
0	0	0.02	0	0.01	0.022	0	0.0051	0	0.0012	0	0	0.22	0
0	0	0.021	0	0.02	0.025	0	0.015	0	0	0	0	0.21	0
0.008	0.012	0.022	0	0.025	0.059	0.01	0.019	0	0.0015	0	0	0.05	0
0	0	0.017	0	0.02	0.027	0	0.0086	0	0.0018	0	0	0.05	0
0	0.015	0.019	0	0.01	0.031	0	0.025	0.014	0	0	0	0.0029	0.0013
0	0	0.022	0	0.02	0.032	0	0	0.011	0.0013	0	0.0039	0.042	0.0013
0	0	0.018	0	0.02	0.035	0	0.009	0	0	0	0	0.021	0
0	0.018	0.015	0	0.02	0.027	0	0.017	0	0.0012	0	0	0.0079	0
0	0	0.019	0	0.01	0.035	0	0.0073	0	0	0	0	0.022	0
0	0	0.017	0	0	0.043	0	0	0	0	0	0	0.0022	0
0	0	0.0055	0	0.01	0.035	0	0.0063	0	0	0	0.0032	0.018	0
0	0	0.014	0	0.02	0.032	0	0.08	0	0	0	0	0.0055	0
0	0.014	0.016	0	0.02	0.025	0	0.0096	0	0.0013	0	0	0.011	0
0.005	0	0.013	0	0.02	0.032	0	0.015	0	0.0012	0	0	0.0098	0
0.003	0	0.014	0	0.02	0.047	0	0	0	0	0	0	0.009	0
0	0	0.012	0	0.01	0.027	0	0.0022	0	0	0.0017	0.0032	0	0
0	0	0.013	0	0.01	0.029	0	0.034	0	0	0	0	0.0068	0
0	0	0.011	0	0.02	0.021	0	0.0023	0	0	0	0	0	0
0	0	0.012	0	0.02	0.033	0.009	0.22	0	0.0012	0.0057	0.0056	0	0
0	0	0.015	0	0.02	0.036	0	0.0036	0	0	0	0	0	0
0	0.022	0.012	0	0.02	0.031	0	0.018	0	0	0	0	0.0036	0
0	0.012	0.011	0	0	0.034	0.009	0.0075	0	0	0	0	0	0
0	0.01	0.011	0	0.01	0.022	0	0.0032	0	0	0	0	0.0032	0
0	0.017	0.0075	0	0.01	0.0089	0	0	0	0	0	0.0036	0	0
0.004	0.014	0.012	0	0.01	0.022	0.007	0	0	0	0	0	0.0037	0
0	0.012	0.0094	0	0.01	0.02	0	0.0069	0	0	0.0092	0	0	0
0	0.011	0.011	0	0.01	0.023	0	0.0064	0	0	0	0.0026	0	0
0.009	0.012	0.01	0	0	0.027	0.01	0	0	0	0	0.0051	0	0
0	0.012	0.011	0	0.01	0.024	0	0.0087	0	0	0	0.0043	0	0
0	0.013	0.0081	0	0.01	0.025	0	0.0042	0	0	0	0.0041	0.0043	0
0	0.014	0.0099	0	0.01	0.025	0	0.015	0	0	0.0016	0	0	0
0	0.012	0.0091	0	0.02	0.025	0	0.0064	0	0	0	0.01	0	0
0	0.012	0.0078	0	0.02	0.024	0	0.0038	0	0	0	0	0	0
0	0	0.009	0	0.02	0.019	0	0.25	0	0	0	0.0084	0	0
0	0	0.0094	0	0	0.039	0	0.076	0	0	0	0.0096	0	0
0	0	0.0092	0	0.02	0.023	0	0.0032	0	0	0	0.0061	0	0
0	0.011	0.02	0.081	0.01	0.023	0	0.0034	0	0	0	0	0	0
0	0	0.007	0	0	0.034	0.01	0.0056	0.053	0	0	0	0	0
0	0	0.066	0.29	0.01	0.02	0	0.0066	0	0.0035	0.0047	0.0046	0	0
0	0	0.07	0.18	0.01	0.018	0	0.0039	0	0.0085	0.0036	0.0083	0	0
0.007	0.011	0.005	0	0	0.0062	0	0.012	0	0	0.0063	0	0	0
0	0	0.0043	0	0	0.019	0	0	0	0	0	0.01	0	0
0.01	0.011	0.0029	0	0	0.038	0	0	0	0	0.0014	0	0	0
0	0.012	0.001	0	0.01	0.018	0	0.0033	0	0	0	0.0037	0	0
0.03	0.011	0.0032	0	0.065	0.068	0.04	0.042	0	0	0	0.008	0	0
0	0.012	0.0047	0	0.01	0.024	0	0	0	0	0	0	0	0
0	0	0.0045	0	0.02	0.023	0	0	0	0	0	0	0	0
0	0.011	0.0048	0	0.01	0.024	0	0	0	0	0.0056	0	0	0
0	0	0.0043	0.33	0.01	0.02	0	0	0	0	0	0	0	0
0	0	0	0	0.008	0.0036	0	0	0	0	0	0	0	0
0	0	0.0028	0	0	0.005	0	0.011	0	0	0.002	0	0	0
0	0	0.006	0	0.01	0.023	0	0	0	0	0	0.002	0	0
0	0.012	0.0032	0	0.009	0.023	0	0	0	0	0	0	0	0
0	0	0.0037	0	0.01	0.028	0	0.0068	0	0	0	0	0	0
0	0.012	0	0	0	0.017	0	0.014	0	0	0	0	0	0

Clozapine	Cocaethylene	Cocaine	Codeine	CP 47,497	CP 47,497-C8 homologue	Crotamiton	Desalkylflurazepam	Desipramine	Dextromethorphan (Methorphan)	Diazepam	Diclofenac	Digitoxin	Digoxin
0	0.0032	0.019	0.044	0.0091	0.0025	0	0.0052	0.12	0.0029	0.012	0.011	0.042	0.01
0	0.0024	0.029	0.042	0.0023	0.018	0	0.0053	0.048	0.0039	0.018	0.018	0.03	0.024
0.012	0.002	0.024	0.11	0.0015	0.0077	0	0.0087	0.03	0.004	0.016	0.01	0.037	0
0.014	0.00054	0.035	0.041	0.0096	0.026	0	0	0.04	0.0028	0.015	0.0093	0	0
0	0.0012	0.015	0.04	0.011	0.011	0	0.0052	0.064	0.003	0.015	0.016	0.035	0
0.0055	0.0045	0.0071	0.044	0.0073	0.12	0	0.0087	0.058	0.0035	0.022	0.01	0.044	0.01
0	0.00037	0.01	0.044	0.015	0.014	0	0.0091	0.014	0.0034	0.019	0.0051	0.038	0
0	0	0.024	0.06	0.0092	0.028	0	0.0063	0.011	0.0041	0.021	0.0032	0.072	0.013
0.33	0.0016	0.064	0.0016	0.026	0.014	0	0.051	0.0086	0.016	0.021	0	0.05	0.0097
0.0033	0	0	0.0017	0.51	0	0	0.029	0.0097	0.0033	0.012	0.012	0	0
0.0042	0	0	0	0.46	0	0	0	0.019	0.0035	0.011	0.011	0	0
0.0065	0	0	0	0.45	0	0	0	0.026	0.0038	0.0047	0.021	0	0
0.014	0.00072	0	0	0.47	0	0	0	0.023	0.0032	0.009	0.0037	0	0
0.0094	0	0	0	0.46	0	0	0	0.011	0.0033	0.0075	0.0067	0	0
0	0.00071	0	0	0.46	0.0024	0	0.0086	0.015	0.0036	0.0044	0.01	0.094	0
0.092	0.0011	0.0065	0.034	0.07	0.0033	0	0.0094	0.0077	0.0033	0.026	0.016	0	0.014
0.069	0	0.002	0.026	0	0.014	0	0	0.011	0	0.006	0.01	0.074	0
0.005	0	0.02	0.039	0	0.0006	0	0	0.015	0.0029	0	0.0097	0.11	0
0.011	0	0.0061	0.032	0	0.0078	0	0	0.0065	0.003	0	0.0036	0	0
0.022	0	0.005	0.031	0	0.0054	0	0	0.017	0.0029	0	0.051	0.042	0.012
0.019	0	0.004	0.02	0.0024	0.0043	0	0	0.0071	0.0041	0	0.004	0.046	0.011
0.0072	0.00058	0.012	0.021	0	0.0039	0	0	0.0084	0.0029	0	0.015	0	0
0.01	0.00056	0.0034	0.023	0	0.0047	0	0	0.0066	0.0042	0	0	0	0.012
0.013	0.00046	0.0071	0.021	0	0.0027	0	0	0.015	0	0.007	0.0071	0	0
0.054	0	0.0066	0.019	0	0.0023	0	0	0.0085	0.0029	0	0.0076	0	0
0.073	0	0.0052	0.017	0	0	0	0	0.0085	0	0.0058	0.0066	0	0
0.03	0.00066	0.009	0.019	0	0.0003	0	0	0	0	0	0.0045	0	0
0.011	0	0.0047	0.016	0	0	0	0	0.0082	0.0028	0.0053	0.0039	0	0
0.019	0	0.0093	0.017	0	0	0	0.0046	0.017	0.0029	0	0.0039	0	0
0.028	0	0.0063	0.02	0	0	0	0	0.013	0	0	0.0033	0	0
0.06	0	0.0074	0.019	0.0099	0	0	0	0.096	0.0029	0	0.001	0	0
0.0095	0	0.0046	0.022	0	0	0	0	0.012	0.0031	0.0081	0.0036	0	0
0.013	0.00065	0.0082	0.017	0	0	0	0	0.0055	0	0.0049	0.0041	0	0
0.042	0	0.0074	0.016	0	0.0045	0	0	0.0055	0.003	0	0.0037	0	0
0.0056	0	0.0094	0.016	0	0	0	0	0	0	0	0.0021	0	0
0.052	0	0	0.015	0	0.0014	0	0	0.0047	0.003	0	0.0038	0	0
0.021	0	0.014	0.02	0	0	0	0	0.0051	0.0028	0.0048	0	0	0
0.0044	0.0015	0.0094	0.014	0	0.0025	0.003	0	0.016	0	0.0041	0.0037	0	0
0	0	0.0064	0.012	0	0.00079	0	0	0.014	0	0.0042	0	0	0
0	0	0.0061	0.0095	0	0	0	0	0.011	0.0064	0	0.0027	0	0
0	0	0.014	0.011	0.0039	0.0013	0	0	0.014	0	0.0047	0.0057	0	0
0	0	0.011	0.011	0	0.0019	0	0	0.011	0.0082	0	0.0017	0	0
0	0.0019	0.015	0.015	0	0	0	0	0.0099	0.0038	0	0.0017	0	0
0	0.00043	0.011	0.012	0	0.0042	0	0	0.0081	0.003	0	0.0037	0	0
0	0.00063	0.016	0.0096	0	0.0025	0	0.0052	0.01	0.0084	0	0	0	0
0	0.00052	0.007	0.0087	0	0	0	0	0.0092	0.0038	0	0	0	0
0	0.00093	0.038	0.096	0	0.00048	0	0	0.03	0.0055	0	0	0	0
0.0054	0.0025	0.025	0.1	0	0.00011	0	0	0.004	0.0061	0.0043	0.0021	0	0
0	0	0.037	0.098	0	0.0013	0	0	0.006	0.0051	0	0.0014	0	0
0	0.00095	0.0076	0.11	0.00089	0.0017	0	0	0.0037	0.0047	0.0041	0	0	0
0.012	0.00098	0	0.1	0.025	0.0057	0	0	0	0.0039	0	0.00097	0	0.0088
0.0024	0	0.011	0.11	0.027	0.0022	0	0	0.0011	0.0029	0.0047	0	0.037	0
0	0	0.0039	0.11	0.013	0.0026	0	0	0	0.0033	0.0043	0	0.047	0
0	0.00071	0.0082	0.074	0.0076	0.0064	0	0.0053	0.07	0.0031	0	0.0017	0	0
0.0061	0.00085	0.0066	0.062	0.0014	0.0033	0	0	0.07	0.0039	0	0	0	0
0.0042	0.0012	0.0076	0.065	0.013	0.001	0	0.0047	0.054	0.0036	0	0.069	0	0
0.0052	0.0004	0.0014	0.044	0.00092	0	0	0	0	0	0	0	0	0
0.0023	0.00078	0.023	0.058	0.0029	0.00026	0.01	0	0.036	0	0.0041	0.25	0	0
0	0.0006	0.0043	0.058	0.0084	0.00064	0	0.0072	0.02	0	0	0	0	0
0	0.00068	0.0059	0.057	0.0015	0.00022	0	0	0.011	0	0	0.0049	0	0
0	0.00094	0.0059	0.063	0.017	0.00052	0	0	0.0053	0	0	0	0	0
0	0.0011	0.0033	0.068	0.029	0.00088	0	0	0.016	0	0	0.00089	0	0
0.023	0.00073	0.002	0.066	0.0068	0	0	0.0078	0.039	0	0	0.0016	0	0
0.0081	0	0.0017	0.061	0.013	0.00072	0	0	0.031	0	0	0.0017	0	0
0	0.00064	0.0058	0.057	0.0033	0	0	0	0.04	0	0	0	0	0
0.0034	0.00068	0.0066	0.057	0.0077	0	0	0	0.0095	0	0	0	0	0
0.0069	0.00069	0.0058	0.056	0.0065	0	0	0	0.0044	0.0028	0	0.003	0	0
0	0.00075	0.0081	0.061	0.0046	0	0	0.0047	0.0074	0	0	0.0015	0	0

Dihydrocodeine	Diphenhydramine	Dothiepin	Doxepin	EDDP (metabolite of Methadone)	Felbamate	Fenazepam	Fenofibrate	Fentanyl	Flumazenil	Flunitrazepam	Flupentixol	Flurazepam	Gabapentin
0.83	0.0031	0.0059	0	0.0087	0	0	0.02	0	0.0015	0	0.53	0	0.1
0.76	0.0035	0.0071	0.0012	0.01	0	0.11	0.01	0	0	0	0.41	0	0.1
0.63	0.0056	0.011	0.0015	0.013	0	0	0	0	0.0014	0	0.63	0	0.08
0.59	0.0023	0.0017	0	0.013	0.0003	0	0.006	0	0	0	0.43	0	0.09
0.78	0.0026	0.0083	0	0.012	0	0.018	0	0	0	0	0.32	0	0.07
0.95	0.0052	0.00058	0	0.0033	0.0042	0.016	0	0	0	0	0.53	0	0.06
0.39	0.0034	0.0034	0	0.0055	0	0.031	0	0.00027	0	0	0.37	0	0.05
0.51	0.0034	0.00062	0	0.0081	0	0	0	0.00044	0	0	0.29	0	0.06
0.031	0	0.029	0.033	0.003	0	0.0099	0	0	0	0	0.052	0	0.06
0	0	0.0021	0.0018	0	0.00027	0.01	0	0.00057	0	0	0.36	0	0.1
0	0	0.0034	0.0013	0.0024	0.00029	0	0	0.0023	0	0	0.25	0	0.08
0.0017	0	0.0031	0.0012	0	0	0	0	0.001	0	0	0.23	0	0.2
0.0025	0.00034	0.0045	0	0	4.70E-06	0	0	0.0075	0	0	0.2	0	0.07
0.001	0	0.0035	0.0012	0	0	0.01	0	0	0	0	0.2	0	0.1
0	0	0.0035	0.0013	0.0024	0.00031	0	0	0	0	0	0.17	0	0.1
0.52	0.0092	0.00074	0	0.0056	0	0.021	0	0	0	0	0.53	0	0.2
0.34	0.0043	0.0032	0	0.0049	0	0.015	0	0.00052	0	0	0.32	0	0.2
0.56	0	0.0055	0	0.0048	0.0014	0	0	0	0	0	0.22	0	0.2
0.49	0.0049	0.00045	0	0.0048	0.0011	0.011	0	0	0	0	0.2	0	0.2
0.84	0.0042	0.0026	0	0.0054	0	0.014	0	0.00097	0	0	0.17	0	0.2
0.63	0.0042	0.0003	0	0.0036	0.0016	0	0	0	0	0	0.19	0	0.1
0.3	0.0037	0.0041	0	0.0038	0	0	0	0	0	0	0.18	0	0.1
0.8	0.0039	0.001	0.0012	0.0032	0.0035	0	0	0	0	0	0.17	0	0.1
0.67	0.00078	0.0033	0	0.0059	0.0077	0	0	0	0	0	0.17	0	0.1
0.41	0.0066	0.0033	0.00098	0.0028	0	0	0	0	0	0	0.22	0	0.1
0.46	0.0037	0.0035	0	0.0058	0	0.011	0	0	0	0	0.19	0	0.2
0.14	0.0043	0.0035	0	0.0055	0.0009	0	0	0.00052	0	0	0.19	0	0.2
0.62	0.003	0.0032	0	0.0026	0	0	0	0	0	0	0.18	0	0.1
0.23	0.0041	0.00039	0.0013	0.0032	0.00029	0	0	0	0	0	0.18	0	0.1
0.21	0.0029	0.002	0	0.0045	0	0.011	0	0.0051	0	0	0.17	0	0.1
0.2	0.004	0.0021	0	0.0036	0.0068	0.0099	0	0	0	0	0.16	0	0.2
0.19	0.0024	0.0023	0	0.004	0.0058	0	0	0.0021	0	0	0.16	0	0.1
0.47	0.0043	0.0023	0	0.0027	0	0.011	0	0	0	0	0.14	0	0.1
0.083	0.0039	0.0026	0	0.0041	0	0.012	0	0.041	0	0	0.14	0	0.1
0.36	0.0031	0.0039	0	0	0	0.01	0	0	0	0	0.16	0	0.1
0.35	0.00074	0.0007	0	0.0043	0	0.012	0	0	0	0	0.15	0	0.1
0.33	0.00078	0.00064	0	0.0041	0	0	0	0	0	0	0.1	0	0
0.19	0.0033	0.0037	0	0.005	0.0087	0	0	0.002	0	0.002	0.3	0	0.1
0.31	0.0035	0.003	0.001	0.0042	0.0039	0	0	0	0	0.0013	0.26	0	0.1
0.89	0.0017	0.0032	0.0013	0.0034	0.0062	0	0	0	0	0.0012	0.23	0	0.1
0.86	0.004	0.004	0	0.0026	0.0026	0	0	0	0	0	0.19	0	0
0.17	0.00044	0.0031	0	0.0037	0	0	0	0	0	0	0.12	0	0.1
0.36	0.0039	0.0046	0.00094	0.0031	0	0	0	0	0	0	0.1	0	0.1
0.43	0.0032	0.0034	0.0031	0.003	0	0	0	0	0	0	0.098	0	0.1
0.25	0.0034	0.0028	0.00091	0.0031	0	0	0	0	0	0	0.091	0	0.1
0.079	0.00046	0.003	0	0.0033	0.003	0.011	0	0	0	0	0.081	0	0.1
0.58	0.003	0.0036	0	0.0067	0.0043	0.047	0	0.00046	0	0	0.2	0	0.1
0.6	0.002	0.01	0	0.0077	0.12	0	0	0	0	0	0.15	0	0
0.87	0.0006	0.0035	0	0.011	0.0013	0.014	0	0	0	0	0.093	0	0.1
0.67	0.0018	0	0	0.011	0	0.0098	0	0	0	0	0.065	0	0.08
0.5	0	0.0092	0	0.013	0.01	0	0	0.0005	0	0	0.043	0	0.1
0.34	0.00061	0.00029	0	0.014	0	0.0097	0	0	0.0014	0	0.039	0	0.06
0.077	0	0.0007	0.0011	0.012	0	0.0098	0	0	0.0014	0	0.044	0.00091	0.08
0.66	0.0017	0.0014	0.0011	0	0.0006	0.012	0	0.00057	0	0	0.12	0	0.07
0.55	0	0.0021	0.0011	0.003	0.0013	0	0	0	0	0	0.093	0	0.1
0.39	0	0.0055	0	0.003	0.00076	0	0	0	0	0	0.082	0	0.06
0.26	0.0012	0.0022	0.001	0.0025	0	0	0	0	0	0	0.068	0	0.07
0.29	0	0.0093	0	0.0067	0	0	0	0	0	0	0.06	0	0.4
0.34	0	0.0017	0.00097	0.0029	0	0.011	0	0	0	0	0.056	0	0.06
0.25	0.00046	0.0022	0.00095	0.0029	0.00078	0	0	0	0	0	0.053	0	0.09
0.21	0.00093	0.0026	0.0018	0	0	0	0	0	0	0	0.051	0	0.06
0.49	0	0.0022	0	0.0028	0	0	0	0	0	0	0.051	0	0.09
0.21	0.0025	0.0014	0.0011	0.0027	0.0045	0	0	0.0019	0	0	0.077	0	0.05
0.39	0.001	0.0014	0.00098	0	0	0	0	0	0	0	0.062	0	0.06
0.47	0.00085	0.002	0.0012	0	0.00052	0	0	0.00035	0	0	0.053	0	0.06
0.33	0.0011	0.0016	0	0.003	0	0	0	0	0	0	0.048	0	0.07
0.26	0.00092	0.0021	0	0	0	0	0	0	0	0	0.047	0	0.08
0.18	0	0.002	0.0015	0	0.0074	0	0	0	0	0	0.044	0	0.1

Gabapentin-lactam	Haloperidol	Hydrochlorothiazide	Hydrocodone	Hydromorphone	Imipramine	Indometacin	Iohexol	Iomeprol	Iopamidol	Iopromid	Irbesartan	JWH-018 (N-(n-pentanoic acid)	JWH-073 (2-methylnaphthyl analog)
0.03	0.0019	0.05	0.033	0.00092	0	0	0	0.3	0	0	0.0065	0	0.22
0.02	0.002	0.04	0.031	0.0015	0	0	0.1	0.3	0	0.07	0.0065	0	0.14
0.02	0	0	0.081	0	0.0038	0	0	0.1	0	0.1	0.0025	0	0.48
0.02	0.0021	0	0.03	0.00094	0	0	0	0.3	0	0.2	0.0025	0	0.26
0.02	0.0021	0	0.029	0.0015	0	0	0	0	0	0	0.0025	0	0.74
0.01	0.0023	0	0.032	0.00087	0	0	0	0	0	0	0.00375	6.30E-05	0.018
0.02	0.002	0	0.032	0	0.014	0	0	0.1	0	0	0.00175	0	0.027
0.01	0	0	0.044	0.00087	0	0	0	0	0	0	0	0	0.12
0.02	0.0032	0	0.0021	0.01	0.0073	0	0	0	0	0	0.0015	0.0024	0.093
0.02	0.002	0	0.0022	0.00094	0.0086	0	0	0	0	0	0.00175	0	0.0035
0.02	0.0021	0	0	0.0014	0.003	0	0	0	0	0	0	0	0.033
0.1	0	0	0	0.002	0.018	0	0	0	0	0	0.00475	0	0.3
0.02	0	0	0	0.00096	0.014	0	0	0	0	0.09	0	4.70E-05	0.026
0.02	0	0	0	0.00093	0	0	0	0	0	0.1	0	0	0.06
0.04	0	0	0	0.0029	0	0	0	0	0	0	0.0025	0	0.21
0.08	0.002	0.04	0.025	0.0078	0.042	0	0	0	5	0	0.0075	0	0.15
0.04	0.002	0	0.019	0.0026	0.0022	0	0	0	0	0	0.0025	0	0.078
0.08	0.002	0	0.029	0.0019	0.0028	0	0	0	3	0.1	0.0225	0	0.0088
0.04	0	0	0.024	0.0021	0.0018	0	0	0	0	0	0.00425	1.70E-05	0.0043
0.04	0	0	0.023	0.0019	0.0021	0	0	0.1	0	0.1	0.005	0	0.0023
0.04	0	0	0.016	0.0009	0.0032	0	0	0.2	2.2	0.09	0.00725	6.00E-05	0.074
0.04	0.002	0	0.016	0.001	0.053	0	0	0	0	0	0.007	0	0.15
0.03	0.002	0	0.018	0.0069	0	0	0	0	0	0	0.03	0	0.085
0.03	0.002	0	0.016	0.0008	0.1	0	0	0	0	0.09	0.005	8.00E-06	0.079
0.04	0	0	0.014	0.0032	0.0068	0	0	0.1	2.2	0	0.005	0	0.02
0.04	0	0	0.013	0.0014	0.0028	0	0	0.2	2.1	0.08	0.005	0	0.09
0.04	0.002	0	0.015	0.0033	0.003	0	0	0	2.1	0.07	0.00725	3.60E-05	0.3
0.05	0	0	0.013	0	0	0	0	0	0	0.1	0.0075	0	0.0038
0	0	0	0.013	0.0014	0.0097	0	0	0	0	0	0	0	0
0.04	0	0	0.015	0.00089	0.0069	0	0	0.2	0	0	0.007	0	0.033
0.04	0	0	0.015	0.0009	0.003	0	0	0	2.3	0	0.00675	0	0
0.04	0	0	0.017	0	0.019	0	0	0.2	2	0	0.01	3.70E-05	0.0059
0.04	0	0	0.013	0.00095	0.0014	0	0	0.1	2.2	0	0.00675	0	0.048
0.04	0	0	0.013	0.0017	0.0014	0	0	0	2.2	0.1	0.007	0	0
0.04	0	0	0.012	0.0023	0	0	0	0	0	0	0.01	0	0
0.03	0	0	0.011	0	0	0	0	0	0	0	0.00425	0	0.0042
0	0	0	0.015	0	0.0051	0	0	0	0	0	0	0	0.012
0.02	0.002	0	0.011	0.0017	0.023	0	0	0	0	0.07	0.00425	0	0.083
0	0	0	0.0093	0.0009	0.0049	0	0	0	0	0	0.005	0	0
0.03	0	0	0.0078	0	0.0018	0	0	0	0	0	0.00475	0	0.0055
0.007	0	0	0.0089	0.00086	0.005	0	0.4	0	0	0.7	0	0	0.037
0.03	0	0	0.009	0	0	0	0	0	0	0.1	0.0025	0	0.19
0.04	0	0	0.011	0.0039	0.0035	0	0.1	0	0	0.09	0.00475	0	0.088
0.04	0	0	0.0097	0	0	0	0	0	0	0.1	0.009	0	0.11
0.03	0	0	0.0079	0.0014	0.0051	0	0	0	0	0	0.007	0	0.056
0.03	0	0	0.0072	0.00098	0.0076	0	0	0	0	0.08	0.0045	0	0.0036
0.03	0	0	0.063	0	0	0	0.2	0	0	0	0.00725	0	0.15
0	0	0	0.065	0	0	0	0.2	0	0	0	0	0	0.62
0.03	0	0	0.065	0	0.031	0	0	0	0	0.08	0.0075	0	0.23
0.02	0	0	0.08	0	0.032	0	0	0	0	0	0.0025	0	0.09
0.03	0.0019	0	0.077	0.00091	0.0028	0	0.3	1.3	2.5	0	0.0095	0	0
0.02	0.0047	0	0.075	0	0.0017	0	0	0	0	0	0.00225	1.60E-05	0
0.01	0.0054	0	0.064	0	0	0	0	0	0	0	0.00225	0	0
0	0	0	0.054	0	0.0014	0	0	0	2	0	0	0	2.1
0.02	0	0	0.045	0	0.0019	0	0	0	0	0	0	0	0.13
0.02	0	0.08	0.047	0	0.0026	0	0	0	0	0	0	0.00063	0.0048
0.01	0	0	0.046	0	0.0015	0	0	0	0	0	0.00175	0	0.33
0.03	0	0.03	0.042	0.0015	0.0015	0.01	1.1	1.4	11	0.3	0.0575	0	1.2
0.02	0	0	0.042	0.00085	0	0	0	0	0	0	0.0015	0	0.05
0.02	0	0	0.042	0.001	0.0014	0	0	0	0	0	0.00225	0	0.11
0.01	0	0	0.046	0	0.019	0	0	0	0	0	0.0015	0	0.083
0.02	0	0	0.049	0.0008	0.0063	0	0	0	0	0	0.00175	0	0.14
0.008	0	0	0.048	0.001	0.0014	0	0	0	0	0	0	0	0.0061
0.01	0	0	0.045	0.0023	0	0	0	0	0	0	0	0.00085	0.18
0.01	0	0	0.042	0.00093	0.0019	0	0	0	0	0	0	0	0.14
0.01	0	0	0.041	0	0.0013	0	0	0	0	0	0.00225	0	0.1
0.01	0	0	0.041	0.00069	0.0016	0	0	0	0	0	0.002	0	0.14
0.02	0	0	0.045	0.001	0.0014	0	0	0	0	0	0	0	0.35

Ketamine	Ketoprofen	Lamotrigine	Librium (Chlordiazepoxide)	Lidocaine	Lorazepam	Losartan	Maprotiline	Medazepam	Meperidine (Pethidine)	Methamphetamine	Methylendioxymethamphetamine (MDMA)	Methylphenidate	Metoprolol
0.0021	0	0.021	0	0.005	0.035	0	0.0058	0.00064	0.0018	0.0029	0.0069	0.0024	0
0	0	0.027	0	0.0049	0.049	0	0.0071	0.00029	0.00091	0.0027	0.0087	0.013	0.028
0.0026	0	0.03	0.0028	0.0057	0.045	0	0.01	0.0028	0.0058	0.0026	0.0098	0.022	0.041
0.0013	0	0.03	0	0.006	0.051	0	0.0095	0.0012	0.0016	0	0.0082	0.012	0.06233333
0	0	0.034	0	0.0069	0.039	0	0.0092	0.0012	0	0	0.0065	0.01	0.04166667
0	0	0.021	0	0.0052	0.07	0	0.00054	0.00023	0.00065	0	0.0039	0.014	0.04033333
0	0	0.02	0.0026	0.0037	0.081	0	0.0027	0.00096	0	0	0.0062	0.012	0.01333333
0	0	0.019	0	0.0037	0.056	0	0.0052	0.00073	0	0	0.0053	0.012	0
0.0029	0	0.013	0.031	0.042	0	0	0.00026	0.0095	0.022	0	0.2	0.034	0
0.0015	0	0.018	0.023	0.004	0.0023	0	0	0.0016	0.0018	0	0.0039	0	0.00666667
0	0	0.028	0.041	0.0051	0.0006	0	0	0.0014	0.0014	0	0.0049	0.017	0.01533333
0	0	0.046	0.0065	0.0034	0	0	0	0.0012	0.0014	0.014	0.014	0.02	0
0.0014	0	0.019	0.034	0.0056	0.0043	0	0	0.0012	0.001	0	0.0064	0	0
0	0	0.026	0.046	0.005	0.004	0	0	0.0012	0.0015	0.0036	0.0053	0.014	0
0.0011	0	0.026	0.048	0.0049	0	0	0	0.0011	0.0011	0	0.0062	0.015	0
0	0	0.046	0.0029	0.007	0.039	0.01	0.0028	0.002	0.002	0.0045	0.03	0.012	0
0.0014	0	0.024	0	0.0048	0.019	0	0.0021	0.0003	0.0018	0	0.0087	0.0034	0
0.0013	0	0.029	0.0085	0.0037	0.013	0	0.0021	0.00074	0.0017	0	0.027	0	0
0	0	0.023	0	0.0042	0.03	0	0.002	0.00052	0.0017	0	0.0059	0	0
0	0	0.022	0	0.0032	0.014	0	0.0026	0.00016	0	0.0032	0.0095	0.0015	0
0	0	0.021	0.0027	0.0041	0.0029	0	0.0009	0.00023	0.0016	0	0.01	0.0018	0
0.0013	0	0.026	0	0.0055	0.018	0.007	0.001	0	0.0018	0	0.0085	0.011	0
0.0013	0	0.028	0	0.0054	0.018	0.01	0.00046	0.00031	0.0018	0.0026	0.28	0.0016	0
0	0	0.022	0	0.005	0.011	0.007	0.0031	0.00081	0.0022	0.0028	0.0077	0.0079	0.02466667
0.0014	0	0.021	0	0.0045	0.0059	0	0.00014	0.00041	0.0011	0	0.0074	0	0.022
0.0012	0	0.021	0	0.0043	0.0064	0.008	0.003	0.00069	0.0018	0.0027	0.0065	0.0095	0.025
0.0011	0	0.021	0.0026	0.0048	0.0064	0.008	0.0027	0.00017	0.0018	0	0.0072	0.0053	0.024
0.0011	0	0.019	0	0.0047	0.013	0	0	0	0.0014	0.0031	0.0077	0	0.0105
0.0023	0	0.0074	0	0.0035	0.0038	0	0.00051	0	0.0012	0.0031	0.00035	0.0013	0
0	0	0.018	0	0.0038	0.0044	0.008	0.0018	0	0	0	0.006	0.0015	0
0	0	0.016	0	0.0038	0.0068	0.008	0.00086	0	0.0015	0.0049	0.0063	0.001	0
0	0	0.015	0	0.0041	0.0033	0.007	0.0012	0	0.0017	0	0.0068	0.0015	0
0	0	0.016	0	0.0039	0.0048	0.007	0	0.00021	0.0012	0	0.0072	0.0012	0
0	0	0.015	0	0.004	0.0023	0.009	0.0013	0	0.0012	0	0.0064	0.0046	0
0	0	0.009	0	0.0043	0.0007	0	0	0.00069	0.0016	0.0024	0.064	0	0
0.0012	0	0.015	0	0.0043	0.0054	0.007	0.0016	0	0	0	0.01	0.0019	0
0	0	0.0054	0	0.0039	0.0052	0	0.0014	0.00016	0.001	0.0026	0.0056	0	0
0	0	0.013	0	0.0043	0.016	0.007	0.0022	0.00065	0.0015	0.004	0.013	0	0
0	0	0.013	0	0.0037	0.0033	0.007	0.0014	0	0.0015	0.0029	0.0095	0	0.00666667
0	0	0.012	0	0.0043	0.0009	0.008	0.00073	0.0048	0.00038	0.004	0.011	0	0
0.0014	0	0.019	0	0.0037	0.0055	0.03	0	0	0.0031	0.0046	0.049	0	0
0	0	0.014	0	0.0037	0	0	0.00094	0.00028	0.0017	0.0027	0.0098	0	0
0	0	0.013	0	0.0038	0.0006	0.008	0.00041	0.0003	0.00075	0	0.01	0.0011	0
0.0014	0	0.013	0	0.0042	0.0021	0.008	0.00034	0.0002	0.00043	0.0028	0.009	0	0
0	0	0.013	0	0.0037	0.002	0.008	0.00039	0.00038	0.00019	0.0022	0.011	0	0
0	0	0.012	0	0.0034	0	0	0.00056	0.00029	0.00031	0.0023	0.01	0	0
0	0	0.013	0	0.004	0	0	0.0039	0.00033	0.0014	0	0.00054	0.0013	0
0.0014	0	0.012	0	0.0039	0.0021	0	0.0048	0.0014	0.001	0	0.00011	0.0015	0
0.0016	0	0.013	0	0.0038	0.0009	0.006	0.0077	0.00025	0.00085	0	0	0	0
0	0	0	0.0084	0.0036	0	0	0.0078	0.00077	0.00089	0	0.00021	0.0013	0
0	0	0.017	0	0.0067	0	0.03	0.01	0.00062	1.20E-05	0	0.00073	0.0016	0
0	0	0	0.003	0	0	0	0.011	0.005	0	0	0.00014	0.0011	0
0	0	0	0.002	0	0	0	0.0091	0.0021	0	0	8.60E-05	0.0011	0
0	0	0.003	0	0.0035	0	0.02	0	0	0	0	0.011	0.0011	0
0	0	0.008	0	0.0035	0	0	0.00027	0	0.001	0.003	0.0059	0.0011	0
0	0.02	0.0024	0	0.0036	0	0.02	0.00056	0.00046	0.00096	0	0.0042	0.001	0.02
0.00099	0	0.0081	0	0.0029	0	0	0.0003	0	0.00087	0	0.0021	0.0012	0
0	0	0.017	0	0.025	0	0.02	0.0039	0.00014	0.0022	0	0.016	0.0022	0.82
0.0012	0	0.0084	0	0.0033	0	0	0.00022	0	0.0033	0	0.0069	0.0013	0.008
0.0012	0	0.0078	0	0.0034	0	0	0.00016	0	0.00091	0	0.0037	0.0021	0.01466667
0.0012	0	0.0073	0	0.0033	0	0	0	0.00022	0.00073	0	0.0037	0.0011	0
0.0014	0	0.0081	0	0.0034	0	0	5.90E-05	0	0.00087	0.0029	0.0069	0.0013	0
0	0	0.0021	0	0.0035	0	0	2.30E-05	0.0003	0.0011	0	0.0016	0.0019	0
0	0	0.0027	0.0025	0.0041	0	0	0	0.0005	0.00079	0	0.011	0	0
0.0012	0	0.0077	0	0.0036	0	0	0	0	0.00081	0	0.0041	0	0
0	0	0.0072	0	0.0034	0	0	0.00027	0.00039	0.00078	0	0.0045	0.0013	0.021
0.0013	0	0.0077	0.0027	0.0034	0	0	0	0	0.00078	0	0.0038	0	0
0.0013	0	0.0071	0	0.0033	0	0	0	0.0002	0.00036	0	0.0034	0.0011	0

Metroprolol acid	Midazolam	Mirtazapine	Morphine	Morphine glucuronide	n-Acetyl-4-aminoantipyrine	Nadolol	Naltrexone	Naproxen	N-Desmethylclozapine	N-Formyl-4-aminoantipyrine	Nitrazepam	Norbuprenorphine	Nordiazepam
0.03	0	0	0.0021	0	0.091	0	0.00098	0	0	0.1	0	0.023	0.02
0.04	0	0	0.0026	0	0.14333333	0	0	0	0	0.1	0.015	0.022	0.0051
0.03	0	0.0074	0	0	0.18	0	0.0012	0	0	0.1	0.099	0.055	0.0069
0.03	0	0	0.0021	0	0.19	0	0	0	0	0.1	0.022	0.033	0.0034
0.02	0	0.0051	0.0026	0	0.19666667	0	0	0	0	0.09	0.035	0.0048	0.0043
0.02	0.0014	0.0058	0.002	0	0.08033333	0	0.0027	0	0.0044	0.07	0.06	0.01	0.034
0.01	0.0023	0.0029	0	0	0.06933333	0	0.0015	0	0.0025	0.07	0.03	0.0097	0.0086
0.01	0	0.0023	0.002	0	0.06233333	0	0.00059	0	0.0039	0.05	0.034	0.0061	0.021
0.01	0	0.025	0.0099	0	0.06933333	0	0	0	0.014	0.07	0.92	0.14	0.0029
0.01	0	0.0028	0.0021	0	0.07	0	0.00083	0	0.017	0.06	0.041	0.01	0.0049
0.02	0	0.0041	0.0025	0	0.1	0	0	0	0	0.07	0.029	0.012	0.0029
0.04	0	0	0.003	0.06	0.18	0	0	0	0	0.1	0.041	0.0026	0.0048
0.01	0	0.003	0.0021	0	0.058	0	0	0	0	0.07	0.036	0.022	0.0028
0.02	0	0.0054	0.0021	0	0.05333333	0	0	0	0	0.07	0.0089	0.013	0.0046
0.03	0	0.0043	0.0038	0	0.07733333	0	0.0012	0	0.029	0.1	0.016	0.012	0.0031
0.04	0	0.0039	0.008	0	0.12	0	0.0018	0	0.052	0.3	0.031	0	0.0043
0.03	0	0	0.0035	0	0.086	0	0	0	0	0.1	0.018	0	0.0099
0.04	0	0	0.0029	0	0.12	0	0	0	0.015	0.3	0.012	0.0084	0.0095
0.03	0	0.0022	0.0031	0	0.077	0	0.0012	0	0	0.1	0.012	0	0.014
0.03	0	0	0.0029	0	0.08233333	0	0.00094	0	0.035	0.2	0.0093	0	0.017
0.03	0	0	0.002	0	0.077	0	0.00068	0	0.0062	0.1	0.011	0	0.026
0	0	0.0024	0.0021	0	0.08466667	0	0.00071	0	0.022	0.2	0.019	0	0.018
0.04	0	0.0027	0.0073	0	0.075	0	0	0	0.015	0.3	0.016	0.0065	0.022
0.03	0.0018	0	0.002	0	0.08566667	0	0.001	0	0	0.1	0.01	0.01	0.022
0.03	0	0	0.0041	0	0.06766667	0	0.00083	0	0.024	0.1	0.017	0.0037	0.025
0.04	0	0	0.0025	0	0.081	0	0.00052	0	0.034	0.2	0.011	0.0025	0.021
0.03	0	0	0.0041	0	0.06866667	0	0.00066	0	0	0.2	0.014	0.0051	0.026
0.03	0	0.0048	0	0	0.08166667	0	0.00053	0	0	0.2	0.015	0.0024	0.021
0.01	0	0.0022	0.0025	0	0.039	0	0.00063	0	0.18	0.07	0.003	0.002	0.026
0.03	0.0018	0	0.002	0	0.06266667	0	0.00053	0	0.011	0.1	0.014	0.0059	0.025
0.03	0	0.0062	0.0021	0	0.062	0	0	0	0	0.2	0	0.0025	0.022
0.03	0	0.0027	0	0	0.08766667	0	0.00062	0	0	0.2	0	0.0022	0.018
0.03	0	0	0.0021	0	0.062	0	0.00058	0	0.058	0.2	0.01	0.0025	0.0085
0.03	0	0	0.0027	0	0.07966667	0	0.00061	0	0.025	0.2	0.0042	0.0021	0.013
0.03	0	0.0045	0.0033	0	0.19	0.003	0.00059	0	0.056	0.4	0.0043	0.0027	0.016
0.02	0	0.0027	0	0	0.086	0	0	0	0.0054	0.1	0.012	0.0023	0.018
0.02	0	0	0	0	0.041	0	0	0	0.029	0.04	0.0047	0.0021	0.015
0.02	0	0.0022	0.0027	0	0.077	0	0	0	0	0.1	0.044	0.0066	0.024
0.04	0	0.0023	0.002	0	0.07866667	0	0	0	0	0.1	0	0.003	0.013
0.03	0	0	0	0	0.09133333	0	0	0	0	0.2	0	0	0.015
0.3	0	0.0034	0.002	0	0.31	0	0.00072	0	0.0029	0.4	0.0038	0.02	0.019
0.04	0	0	0	0	0.09733333	0	0.00066	0	0	0.2	0	0	0.0096
0.04	0	0.0062	0.0047	0	0.09033333	0	0	0	0.024	0.2	0.004	0.0033	0.0092
0.05	0	0.004	0	0	0.09	0	0	0	0.091	0.2	0.0044	0.0029	0.015
0.04	0	0	0.0024	0	0.07933333	0	0	0	0.01	0.2	0	0.0026	0.016
0.05	0	0	0.0021	0	0.08866667	0	0	0	0.016	0.2	0.039	0	0.012
0.04	0	0.0031	0	0	0.086	0	0.0045	0	0	0.2	0	0.017	0.018
0.4	0	0	0	0	0.73	0	0.0042	0	0.012	0.4	0	0.014	0.025
0.04	0	0	0	0	0.079	0	0.0043	0	0.0024	0.1	0.0044	0.015	0.011
0.03	0	0	0	0	0.08966667	0	0.0034	0	0	0.1	0.0039	0.011	0.012
0.1	0	0	0.0021	0	0.79	0	0.004	0	0.012	1.5	0	0.0028	0.015
0.02	0	0	0	0	0.08733333	0	0.013	0	0	0.09	0.017	0	0.015
0.02	0	0	0	0	0.09633333	0	0.014	0	0	0.1	0.013	0	0.01
0.05	0	0	0	0	0.44	0	0	0	0	0.8	0	0.0048	0.039
0.03	0	0	0	0	0.09333333	0	0	0	0	0.1	0	0.0044	0.038
0.05	0	0	0	0	0.65	0	0.00059	0	0	0.5	0	0	0.04
0.02	0	0	0	0	0.09566667	0	0	0	0	0.1	0	0.0028	0.029
0.7	0	0.0022	0.0025	0	1.5	0	0.0025	0.07	0.0016	1.2	0.0047	0.003	0.031
0.02	0	0	0.002	0	0.08733333	0	0	0	0	0.1	0	0.012	0.034
0.04	0	0.0026	0.0021	0	0.12666667	0	0	0	0	0.2	0	0.0028	0.025
0.03	0	0	0	0	0.08366667	0	0	0	0	0.1	0	0.0093	0.03
0.04	0	0	0.002	0	0.13	0	0	0	0	0.1	0	0.0094	0.03
0.03	0	0	0.0022	0	0.07233333	0	0	0	0	0.1	0	0.011	0.03
0.01	0	0.0033	0.0033	0	0.09	0	0	0	0	0.1	0	0.01	0.037
0.03	0.002	0.003	0.0021	0	0.09133333	0	0	0	0	0.1	0	0.0021	0.024
0.03	0	0.0036	0	0	0.07233333	0	0	0	0.0067	0.1	0	0.0087	0.029
0.03	0	0	0.0019	0	0.091	0	0	0	0	0.1	0	0.0092	0.036
0.03	0.0015	0.029	0.0021	0	0.08566667	0	0	0	0	0.2	0	0.011	0.032

Norfentanyl	Normeperidine (Norpethidine)	Norpropoxyphene (Desmethylpropoxyphene)	Nortriptyline	O-Desmethyltramadol	O-Desmethylvenlafaxine (Desvenlafaxine)	Olanzapine	Opipramol	Oxazepam	Oxcarbazepine	Oxycodone	Oxymorphone	Paliperidone (9-Hydroxyrisperidone)	Paroxetine
0.001	0.0019	0.091	0	0.0074	0.0097	0.011	0.0029	0	0	0.0072	0.0034	0	0.0011
0.0016	0.016	0.094	0	0.0089	0.014	0.0067	0.0054	0.0052	0.0028	0.014	0.0054	0	0.013
0.0012	0.028	0.049	0.004	0.011	0.015	0.0065	0	0	0	0.013	0.0048	0.00087	0.016
0.0011	0.015	0	0.0014	0.011	0.015	0.0081	0	0	0.0024	0.019	0.0056	0.00076	0.017
0	0.012	0.059	0.0019	0.01	0.015	0.0071	0.0061	0.0046	0.0039	0.014	0.0056	0	0.019
0.00082	0.018	0.018	0	0.0075	0.011	0.03	0.0032	0.0032	0.0015	0.012	0.0036	0	0.013
0	0.015	0.16	0.0016	0.0068	0.0083	0.012	0.0044	0.0041	0.0013	0.0077	0.0033	0.00077	0.0082
0.00076	0.015	0.036	0	0.0062	0.0069	0.013	0.0025	0.0062	0.0011	0.015	0.007	0	0.0084
0	0.045	0.75	0	0.014	0.0042	0.19	0	0.0044	0.015	0.0031	0.0058	0.0014	0.0021
0.0012	0	0	0.0027	0.0073	0.0068	0.011	0	0.015	0	0.0029	0.0035	0	0.0053
0.00096	0.022	0.012	0.0032	0.011	0.011	0.02	0	0.012	0	0.0037	0.0074	0	0.0074
0.0017	0.026	0.22	0.013	0.011	0.0051	0.008	0	0.0059	0.002	0	0	0	0.0087
0.001	0	0.49	0	0.0081	0.0072	0.0086	0.0029	0.0059	0.0044	0.0034	0.0056	0	0.0046
0	0.018	0.21	0	0.0089	0.0099	0.013	0	0.011	0.0023	0.0088	0	0	0.0056
0	0.019	0	0.012	0.0074	0.0077	0.0096	0	0.012	0	0.0069	0.0066	0	0.0037
0.0025	0.014	0.21	0	0.012	0.014	0.011	0.023	0.013	0.00078	0.019	0	0.00072	0.0009
0.0017	0.0033	0.28	0.0023	0.0077	0.0079	0.012	0	0.0092	0	0.011	0.0061	0	0.017
0.0088	0	0	0.0029	0.012	0.0081	0	0.0052	0.0042	0.00086	0.021	0	0	0
0.0044	0	0.13	0.0019	0.0071	0.0071	0	0	0.0037	0	0.015	0.0062	0	0
0.0049	0.00075	0.15	0	0.0074	0.0058	0.0049	0	0.0064	0	0.01	0.0041	0	0
0.0026	0.0012	0.093	0.0076	0.0066	0.0054	0.0042	0	0.0063	0.0011	0.012	0.0041	0	0
0.0025	0.013	0.21	0.0071	0.0078	0.0074	0.0078	0	0.0072	0.0013	0.013	0.0037	0	0.0057
0.0026	0.00091	0.068	0	0.004	0.00087	0.0016	0	0	0	0.0036	0.004	0.0016	0
0.0015	0.0095	0.56	0	0.0072	0.0063	0.0069	0	0.0074	0	0.013	0.004	0	0.0035
0	0	0.24	0.0037	0.0072	0.0066	0.0057	0	0.0057	0	0.011	0.0035	0.00085	0
0.0035	0.012	0.15	0.041	0.0066	0.0057	0.0087	0	0.0055	0	0.0078	0.0033	0.00098	0
0.0027	0.0059	0.27	0	0.007	0.0058	0.012	0	0.0078	0	0.0066	0.0034	0.00096	0.0032
0	0	0.66	0.018	0.0068	0.0051	0.0021	0	0.0077	0	0.0083	0.0034	0.00084	0.0053
0	0.00042	0.11	0.015	0.0077	0.0034	0	0	0.012	0	0.011	0	0.0008	0.002
0.0019	0.00074	0.0065	0.0055	0.0071	0.0042	0.0042	0	0.0067	0	0.007	0	0.00078	0.0049
0	7.40E-05	0.041	0.026	0.0061	0.0039	0	0	0.0079	0	0.0057	0	0	0
0.0017	0.00067	0.024	0.0048	0.0063	0.0038	0.0093	0	0.008	0	0.005	0	0.0008	0.0028
0	0.0003	0.36	0.0036	0.006	0.0039	0.0029	0	0.0052	0	0.0029	0.0032	0.0008	0.0028
0.00086	0.0049	0.015	0.0016	0.0064	0.0032	0.0053	0	0.0068	0	0.0045	0	0.00092	0.0047
0.0027	0	0.13	0	0.004	0.006	0	0.043	0	0	0.0063	0.0032	0.00085	0.0018
0	0.0013	0.013	0.02	0.0057	0.0026	0	0.0035	0.0066	0	0.005	0	0.00098	0.0035
0.0012	0	0.42	0.0054	0.0053	0.0035	0	0.0031	0.0052	0	0.0026	0	0	0
0.0012	0	0.31	0.02	0.0055	0.0033	0.0091	0	0.0067	0	0.0048	0	0	0.0016
0.00084	0	0.21	0.0019	0.0052	0.0026	0.0058	0.0064	0.0024	0	0.0043	0	0.00085	0
0.0011	0	0.0092	0.0038	0.0055	0.0027	0	0	0.0056	0	0.0044	0	0.00077	0.005
0	0	0.036	0.0051	0.085	0.0013	0	0.0043	0.0037	0	0.01	0.0034	0.00092	0
0	0	0.4	0	0.0052	0.0022	0.0028	0.0035	0.0035	0	0.0038	0	0.00081	0.0033
0.0011	0.00017	0.52	0.0025	0.0052	0.0023	0.0041	0	0.0062	0	0.0038	0	0.00079	0.0028
0.00077	0	0.027	0.011	0.0049	0.0019	0.0045	0	0.0042	0	0.0042	0	0.00079	0.0046
0	0	0.05	0.0038	0.0041	0.00077	0.0045	0	0.0043	0	0.0029	0	0	0.0037
0.00095	0	0.093	0.0018	0.0085	0.00083	0.0054	0	0.0042	0	0.0048	0.0032	0.0008	0.0036
0.00066	0.00042	0	0	0.0064	0.0061	0.0053	0	0.0063	0.0055	0.0042	0.0032	0	0.011
0	0.00065	0.027	0	0.0053	0.0012	0	0.11	0.0048	0.0059	0.0061	0	0	0.0094
0	0	0.018	0.028	0.0078	0.0055	0.0021	0.0026	0.0041	0.0054	0.0069	0.0032	0	0.014
0	0.00042	0.022	0	0.0034	0	0.0019	0.0032	0	0.014	0.0035	0.0034	0	0
0	0.00087	0	0	0.01	0.00062	0.0048	0	0	0	0.0029	0.0044	0	0.011
0	0.00021	0.015	0	0	0	0.011	0	0.0031	0	0.56	1.4	0	0.013
0	0.00016	0	0	0	0	0.013	0	0.0029	0.0047	0.64	1.2	0.00072	0.0089
0.00082	0.0002	0.0094	0.0014	0.0045	0.00049	0.0076	0	0	0.0016	0.0042	0.0032	0	0.0031
0.00081	0.00013	0.0039	0.0016	0.0046	0.0033	0.003	0.0034	0.0046	0.0017	0.0024	0	0	0.0011
0.0011	4.90E-05	0.0018	0.0015	0.013	0.0014	0.0017	0	0	0.0011	0.028	0	0.00083	0.0031
0.00064	0.00032	0	0.0016	0.0046	0.0031	0.0012	0.0028	0.0065	0.0013	0	0	0	0.0022
0.0011	0.0016	0	0.0017	0.015	0.017	0.02	0.0041	0.011	0.004	0.0024	0	0	0.014
0.00066	0.00045	0	0.02	0.0045	0.0036	0.0019	0	0.0023	0.0011	0.0023	0	0	0.0008
0.00066	0.0016	0	0.0019	0.0042	0.0028	0.0023	0.0029	0.0043	0	0	0	0	0.001
0.00072	0.00012	0	0	0.005	0.0028	0.0032	0.037	0.0019	0	0	0	0	0.0012
0.0007	0.00049	0	0	0.0048	0.0025	0.0015	0.0066	0.0025	0	0	0.0034	0	0.0017
0.00085	0.0012	0	0.0036	0.0038	0.00058	0	0	0.0028	0	0.0081	0	0	0.001
0.00082	0	0	0.013	0.0035	0.0011	0.0019	0	0	0	0.014	0	0	0
0.00077	0	0	0.003	0.0044	0.0025	0.0014	0	0.0041	0	0.0023	0.0031	0	0.0007
0.00069	0.00045	0	0.0016	0.004	0.0024	0.0022	0.059	0.0035	0	0	0.004	0	0.001
0.00068	0	0	0.0017	0.0045	0.0025	0.0026	0.032	0.0028	0	0	0	0	0
0	0.00023	0	0.0015	0.0042	0.0026	0.0021	0.043	0.0045	0	0	0	0	0

Pentazocine	Pentobarbital	Pentoxifylline	Phenacetin	Phenazone	Phencyclidine (PCP)	Phentermine	Phenytoin	Pipamperone	Prazepam	Pregabalin	Primidone	Promazine	Promethazine
0	0	0	0	0.005	0.0059	0.0012	0	0	0.028	0	0.7	0.0018	0.0067
0	0	0	0	0.004	0.0037	0.00097	0.0027	0	0.028	0.008	0.047	0	0
0	0	0	0	0.003	0.0049	0.00096	0	0.01	0.068	0	1.7	0	0
0	0	0	0	0.004	0.0032	0	0.0022	0	0.04	0	1	0.0026	0.0077
0	0	0	0	0.008	0.0042	0	0.0038	0	0.038	0	0.8	0	0
0	0	0	0.01	0.008	0.0082	0	0.0013	0.017	0.047	0	0.62	0	0
0	0	0	0.006	0.01	0.0055	0	0.0012	0.012	0.05	0	0.69	0	0
0	0	0	0	0.01	0.0036	0	0.00094	0.0033	0.05	0	0.61	0.002	0.0069
0.03	0	0	0	0.005	0.11	0	0.015	0.037	0.006	0	1.5	0.094	0.12
0	0	0	0	0.008	0.0038	0	0	0.0037	0.0021	0	0.81	0.0021	0.007
0	0	0	0	0.01	0.0035	0	0	0	0.0022	0	0.78	0.0024	0.0074
0	0	0	0.02	0	0.0047	0.012	0.0018	0.0047	0.0006	0	0.79	0.002	0.007
0	0	0	0	0.01	0.0012	0	0.0043	0	0.0015	0	1.1	0	0
0.00026	0	0	0	0.01	0.0049	0.0019	0.0022	0.0039	0.0021	0	1	0	0
0	0	0	0	0.02	0.0039	0	0	0	0.0009	0	0.83	0.0027	0.0078
0	0	0	0	0.008	0.0095	0.0028	0.00061	0.0028	0.036	0	0.95	0	0
0	0	0	0	0.02	0.0091	0	0	0.0034	0.03	0	0.83	0	0
0	0	0	0	0	0.0016	0	0.00069	0.0037	0.036	0	0.95	0	0
0	0	0	0	0.02	0.0088	0	0	0.0016	0.029	0	0.67	0.0019	0.0068
0.00014	0	0	0	0.02	0.021	0.0015	0	0.0012	0.0039	0.008	0.69	0	0
0	0	0	0	0.01	0.0085	0	0.00092	0.0074	0.035	0	1.1	0	0
0	0.0046	0	0	0.01	0.0093	0	0.0012	0.003	0.007	0	0.76	0.0026	0.0077
0	0	0	0	0.02	0.0034	0.00091	0	0.0034	0.0066	0	0.77	0.0027	0.0078
0	0	0	0	0.01	0	0.0011	0	0.0032	0.008	0	1	0	0
0	0.12	0	0	0.01	0.0058	0	0	0.0015	0.017	0.007	0.8	0	0
0	0	0	0	0.01	0.0049	0.00098	0	0.00075	0.019	0	0.8	0	0
0	0	0	0	0.01	0.0044	0	0	0	0.0051	0	0.27	0.0076	0.014
0	0	0	0	0.01	0.0012	0.0014	0	0	0.0053	0	0.89	0.0028	0.008
0	0	0	0	0	0.0054	0.0014	0	0.00076	0.0071	0	0.72	0.0029	0.008
0	0	0	0	0.01	0.0057	0	0	0.0015	0.013	0.007	0.46	0	0
0	0	0	0	0.01	0.0029	0.0033	0	0.008	0.011	0	0.69	0	0
0	0	0	0	0.01	0	0	0	0.0018	0.018	0	0.62	0	0
0	0	0	0	0.01	0.0022	0	0	0	0.016	0.008	0.61	0.0023	0.0073
0	0	0	0	0.01	0.0033	0	0	0	0.013	0	0.54	0	0
0	0	0	0	0.01	0.0055	0.00072	0	0	0.012	0	0.98	0.0019	0.0068
0	0	0	0	0.007	0.0023	0	0	0.0019	0.011	0.006	0.56	0.0019	0.0068
0	0	0	0	0.002	0.0043	0.00091	0	0	0.0094	0	0.6	0	0
0	0	0	0	0.006	0.002	0.0023	0	0	0.021	0	0.66	0	0
0	0	0	0	0	0.0037	0.0012	0	0	0.0028	0	0.59	0.0025	0.0075
0.0011	0	0	0	0.006	0.0038	0.0023	0	0	0.012	0	0.74	0	0
0	0	0	0	0.02	0.0052	0.0029	0	0.0047	0.014	0	0.6	0.0054	0.011
0.00038	0	0	0	0	0.017	0.0011	0	0	0.011	0	0.59	0	0
0	0	0	0	0.006	0.0031	0	0	0	0.023	0.007	0.48	0	0
0.0003	0	0	0	0.007	0.015	0.0011	0	0	0.022	0	0.61	0.002	0.007
0.0011	0	0	0	0.009	0.02	0.00056	0	0	0.021	0	0.64	0	0
0	0	0	0	0.007	0.0022	0.00064	0	0	0.021	0	0.53	0	0
0	0	0	0	0.006	0.0018	0	0.0055	0	0.033	0	0	0.0024	0.0074
0	0	0	0	0.05	0.0045	0	0.0059	0	0.034	0	0.11	0.0021	0.0071
0	0	0	0	0.008	0.0041	0	0.0053	0	0.036	0	0.018	0.0031	0.0083
0	0	0	0	0.006	0.0054	0	0.014	0.013	0.03	0	0.32	0.002	0.0069
0	0	0	0	0.2	0.0022	0	0	0.0062	0.021	0	0	0	0
0	0	0	0	0.006	0.0027	0	0	0.0068	0.011	0	0.019	0	0
0	0	0	0	0.006	0.0012	0	0.0046	0	0.011	0	0	0	0
0	0	0	0	0.02	0.0017	0	0.0014	0.0096	0.011	0	0.0025	0	0
0	0	0	0	0.006	0.0016	0.0013	0.0016	0.0052	0.0066	0	0.0026	0	0
0	0	0	0	0.02	0.0017	0	0.00099	0.014	0.02	0	0.0028	0.0024	0.0074
0	0	0	0	0.005	0.0017	0	0.0012	0.0061	0.017	0	0.0022	0.0023	0.0074
0	0	0.2	0	0.07	0	0	0.0039	0.0031	0.036	0.02	0.0023	0.0034	0.0086
0	0	0	0	0.006	0	0	0.00091	0.005	0.014	0	0.21	0.0027	0.0078
0	0	0	0	0.009	0.0012	0	0	0.0042	0.014	0	0.0018	0.0043	0.0098
0	0	0	0	0.008	0	0	0	0.0066	0.014	0	0.43	0	0
0	0	0	0	0.009	0	0.0012	0	0.0073	0.012	0	0.28	0	0
0	0	0	0	0.006	0	0	0	0.021	0.01	0	0.36	0	0
0	0	0	0	0	0.0009	0	0	0.0047	0.01	0	0.4	0	0
0	0	0	0	0.008	0	0	0	0.0036	0.006	0	0.25	0	0
0	0	0	0	0.007	0	0	0	0.0089	0.01	0	0.47	0.0022	0.0072
0	0	0	0	0.007	0.0014	0	0	0.0052	0.008	0	0.16	0.0021	0.0071
0	0	0	0	0.008	0	0	0	0.0049	0.01	0	0.029	0.008	0.014

Propafenone	Propoxyphene (Dextropropoxyphene)	Propranolol	Propyphenazone	Protriptyline	Quetiapine	Risperidone	Ritalinic acid	Secobarbital	Sertraline	Sotalol	Strophanthidin	Sulfadimidin / Sulfamethazin	Sulfamethoxazole
0.0037	0	0.01	0	0	0	0	0	0.011	0.0049	0	0	0	0.04
0.0035	0	0	0	0	0.00064	0.015	0.0019	0.0052	0.005	0	0.0035	0	0.036
0.0062	0	0	0	0.0024	0	0.011	0	0	0.0084	0	0	0	0.034
0.0021	0	0	0	0	0	0	0	0.02	0	0	0	0	0.043
0.0023	3.20E-05	0	0	0.00033	0	0.0018	0	0.015	0.0049	0	0	0	0.043
0	0.00083	0	0.003	0	0.00048	0	0.001	0	0.0084	0	0	0	0.021
0.003	0	0	0.003	0	0	0	0	0	0.0088	0	0.0027	0	0.024
0.0041	0	0	0	0	0.00061	0	0	0.0054	0.006	0	0	0	0.018
0.021	0.0091	0	0.001	0.037	0	0	0.00062	0.0052	0.05	0	0	0	0.031
0	0	0	0.001	0.0012	0.001	0	0.0022	0.12	0.029	0	0	0	0.021
0.0036	0	0	0.001	0.0017	0	0	0.0049	0.0071	0	0	0	0	0.025
0	0	0	0	0.011	0.00086	0	0.0096	0.0051	0	0	0.0038	0	0.047
0.003	0	0	0.001	0	0.00046	0.0018	0.00052	0	0	0	0.0029	0	0.015
0	0	0	0.002	0	0.00018	0.007	0.001	0	0	0	0	0	0.02
0.0032	0	0	0.002	0.011	0.00038	0	0.0019	0.015	0.0082	0	0.0037	0	0.025
0	0	0	0	0	0.00033	0	0.0045	0	0.0091	0	0	0	0.032
0	0	0	0.002	0.00072	0.00039	0	0	0.0052	0	0	0	0	0.029
0.0022	0	0	0	0.0014	0	0.0017	0	0	0	0	0	0	0.023
0	0	0	0.003	0.00035	0.0019	0.0028	0	0.018	0	0	0	0	0.024
0.002	0	0	0.003	0	0.00012	0.0038	0	0	0	0	0	0	0.025
0.0019	0	0	0.002	0.0062	0	0	0.0029	0	0	0	0	0	0.026
0	0	0	0.002	0.0057	0.00035	0	0	0.016	0	0	0	0	0.027
0.0023	0	0	0	0	0.0013	0.0044	0	0.007	0	0	0	0	0.011
0.0023	0.00064	0	0.003	0	0.00017	0	0.0047	0	0	0	0	0	0.023
0	0	0	0.003	0.0022	0.00038	0	0.00084	0.0093	0	0	0.003	0	0.019
0	0	0	0.003	0.041	0	0	0	0	0	0	0.0025	0	0.017
0	0.017	0	0.003	0	0	0	0	0	0	0	0.0031	0	0.024
0.002	0	0	0.003	0.016	0	0	0	0	0	0	0	0	0.02
0.0022	0	0	0	0.014	0.00091	0	0.00029	0	0.0043	0	0.003	0	0.0037
0	0	0	0.002	0.0041	0	0.0021	0	0	0	0	0	0	0.016
0.0023	0	0	0.003	0.026	0	0	0.00067	0	0	0	0.0024	0	0.012
0	0	0	0.003	0.0033	0	0	0.0016	0	0	0	0	0	0.016
0.0019	0	0	0.002	0.002	0	0	0.0014	0	0	0	0.0028	0	0.013
0.0017	0	0	0.002	0	0.0002	0.0022	0.0006	0	0	0	0.0028	0	0.015
0.002	0	0	0	0	0	0.0018	0	0	0	0	0.0029	0	0.018
0.0018	5.90E-05	0	0	0.019	0	0	0.002	0	0	0	0.0035	0	0.011
0	4.60E-05	0	0.002	0.0039	0	0	0.00025	0	0	0	0	0	0.016
0	0	0	0.002	0.019	0	0.0032	0.00081	0	0	0	0.0029	0	0.012
0	0	0	0.003	0.00026	0	0.002	0.00013	0	0	0	0.003	0	0.013
0.0019	0.0022	0	0.002	0.0022	0	0	0.0047	0	0	0	0.0028	0	0.013
0	0	0	0.007	0.0036	0	0.014	0	0	0	0	0.0033	0	0.051
0	0.0029	0	0.003	0	0.00024	0.0021	0.0015	0	0	0	0	0	0.012
0	0	0	0.002	0.00093	0	0	0.0021	0	0	0	0.0025	0	0.015
0	0.0027	0	0.003	0.0096	0	0.0015	0.0034	0	0	0	0.0029	0	0.011
0.0018	0.00088	0	0.002	0.0023	0.00018	0	0.001	0	0.0049	0	0	0	0.016
0.0019	0	0	0.002	0.00024	0.00021	0.002	0	0	0	0	0	0	0.017
0	0	0	0.002	0	0	0.0016	0.00029	0	0	0	0	0	0.017
0	0	0.005	0.006	0	0	0.0017	0.00022	0	0	0.04	0	0	0.04
0.002	0	0	0.003	0.027	0	0.0017	0	0	0	0	0	0	0.018
0	0.0096	0	0.002	0	0	0	0.00031	0	0	0	0	0	0.015
0.0021	0	0	0	0	0.00019	0.0081	0.00071	0	0	0	0	0	0.065
0.003	0.00066	0	0.001	0	0.00053	0.0014	0	0	0	0	0	0	0.015
0.002	0	0	0	0	0	0.0025	0.00042	0	0	0	0.0029	0	0.014
0	0	0	0	0	0.0002	0.002	0.00016	0	0.005	0	0.0028	0	0.017
0	0	0	0.002	1.10E-05	0.00024	0	0.0002	0	0	0	0	0	0.013
0	0	0	0	0	0.00016	0	0.00039	0	0.0044	0	0.0029	0	0.047
0	0	0	0.001	0	0.00017	0	9.10E-05	0	0	0	0	0	0.016
0	0	0.06	0	9.20E-05	0.00018	0.025	0.0027	0	0	0.09	0	0.073	0.14
0	0	0	0.002	0.019	0.00018	0	0.00071	0	0.0069	0	0	0	0.018
0	0	0	0.001	0.00028	0.0002	0	0.0038	0	0	0	0	0	0.02
0	0	0	0.001	0	0.00016	0	0.0015	0	0	0	0	0	0.016
0	0	0	0	0	0	0.0016	0	0	0	0	0	0	0.015
0.0021	0	0	0.001	0.0021	0	0.002	0.0019	0	0.0075	0	0	0	0.0088
0	0	0	0	0.012	0.00021	0.0017	0.0027	0	0	0	0	0	0.013
0	0	0	0.001	0.0014	0.00021	0	0.0017	0	0	0	0	0	0.015
0	0	0	0	2.60E-05	0.00016	0	0.0025	0	0	0	0	0	0.016
0.0033	0	0	0.002	0.00015	0.00017	0	0.0022	0	0	0	0	0	0.021
0	0	0	0.002	0	0	0	0.0027	0	0.0044	0	0	0	0.015

Sulpirid	Telmisartan	Temazepam	Topiramate	Tramadol	Trazodone	Triazolam	Trimethoprim	Trimipramine	Valsartan	Valsartan acid	Venlafaxine	Verapamil	Zolpidem
0.02	0.03	0.0034	0.00064	0.0094	0	0.0027	0	0.011	0.02	0.05	0.0047	0	0.0017
0.02	0.03	0.0034	0.00098	0.014	0.0016	0.0038	0	0.17	0.02	0.06	0.0061	0.041	0.0017
0.02	0.03	0	0.0012	0.014	0	0.0035	0	0.015	0.02	0.06	0.007	0	0.0017
0.02	0.03	0.0035	0.00098	0.015	0	0.0034	0	0.15	0.02	0.065	0.0067	0	0.0018
0.02	0.02	0.0029	0	0.015	0	0.0038	0	0.18	0.015	0.055	0.0072	0.0099	0
0.01	0.02	0.0035	0	0.011	0.0018	0.0049	0	0.041	0.005	0.04	0.0044	0.0069	0.0018
0.01	0.02	0.0039	0	0.008	0.0016	0.0055	0	0.16	0.005	0.04	0.0022	0	0.0017
0.009	0.02	0.0037	0	0.0066	0.0016	0.0048	0	0.027	0.005	0.035	0.0019	0	0.0017
0.009	0.02	0.012	0	0.0038	0.0051	0.0077	0	0.69	0.005	0.045	0.078	0.15	0
0.01	0.02	0.0039	0	0.0065	0.0016	0.0033	0	0.13	0.0045	0.04	0.0022	0.0056	0
0.01	0.02	0.0034	0	0.01	0.0016	0.0037	0	0.11	0.01	0.045	0.0033	0.008	0.0017
0.04	0.2	0	0	0.0048	0.0016	0.0019	0	0.16	0.0095	0.1	0.0015	0	0
0.01	0.02	0.0035	0	0.0069	0.0017	0.0028	0	0.063	0.0095	0.04	0.0026	0.0056	0.0019
0.01	0.03	0.0033	0	0.0096	0.0015	0.0011	0	0.1	0.01	0.05	0.0026	0.0054	0
0.02	0.04	0	0	0.0074	0.0016	0.0016	0	0.1	0.015	0.08	0.0024	0	0
0.02	0.05	0.0035	0.00059	0.013	0	0.0032	0	0.36	0.035	0.2	0.0037	0.0074	0
0.02	0.02	0	0	0.0075	0	0.0021	0	0.32	0.015	0.075	0.0026	0.0043	0.0017
0.03	0.1	0.01	0.00067	0.0077	0	0.0024	0	0.27	0.025	0.2	0.0027	0	0.0017
0	0.04	0.0035	0	0.0068	0.0017	0.0026	0	0.22	0.02	0.08	0.0023	0.0054	0.0018
0.02	0.05	0.0034	0	0.0055	0.0016	0.0018	0	0.079	0.015	0.095	0.0021	0	0
0.02	0.03	0.0032	0.00094	0.0051	0.0017	0.0022	0	0.024	0.015	0.08	0.0022	0	0.0018
0.02	0.04	0.0038	0	0.0071	0.0015	0.0017	0	0.028	0.02	0.085	0.003	0	0
0	0.06	0.0032	0.0019	0.0006	0	0.0023	0	0.053	0.025	0.2	0.0004	0.0047	0
0.02	0.05	0.0031	0	0.006	0.0017	0.0017	0	0.06	0.02	0.085	0.0026	0	0
0.01	0.04	0.0033	0	0.0062	0.0016	0.00023	0	0.053	0.02	0.09	0.0026	0	0
0.02	0.05	0.0033	0	0.0054	0.0016	0.0015	0	0.18	0.02	0.1	0.0023	0	0.0017
0.02	0.04	0.0033	0	0.0055	0.0017	0.00076	0	0.079	0.02	0.095	0.0023	0	0
0.01	0.05	0	0.00065	0.0047	0.0016	0.00053	0	0.085	0.02	0.1	0.0022	0	0
0	0.02	0.0031	0	0.0031	0.0016	0.00092	0	0.032	0.0095	0.055	0.0014	0	0
0.01	0.04	0.0034	0	0.0039	0.0016	0.0013	0	0.24	0.015	0.095	0.0017	0	0
0.01	0.04	0	0	0.0035	0.0016	0.0015	0	0.24	0.02	0.095	0.0015	0	0
0.02	0.05	0	0	0.0035	0.0017	0.0016	0	0.022	0.02	0.095	0.0014	0	0.0018
0.02	0.04	0	0	0.0036	0.0016	0.0012	0	0.33	0.02	0.095	0.0016	0	0.0019
0.02	0.04	0	0	0.0029	0.0015	0	0	0.27	0.015	0.095	0.0014	0	0
0	0.04	0.0031	0	0.0056	0.0016	0.0015	0	0.33	0.008	0.095	0.0004	0	0.0018
0.01	0.03	0	0	0.0023	0.0016	0.00094	0	0.033	0.015	0.085	0.0014	0	0
0	0	0.0031	0	0.0032	0.0016	0.00092	0	0.31	0.004	0.01	0.0016	0	0.0017
0.02	0.03	0	0	0.003	0.0017	0.0002	0	0.019	0.01	0.065	0.0029	0	0
0.02	0.04	0	0.00063	0.0023	0.0016	0	0	0	0.015	0.08	0.0014	0.0054	0
0.02	0.03	0	0	0.0024	0.0016	0	0	0.0073	0.015	0.09	0.002	0	0.0017
0.04	0	0	0	0.001	0.0016	0	0	0.091	0.025	0	0.0006	0	0
0.02	0.04	0	0	0.0019	0.0015	0	0	0.13	0.01	0.095	0.0014	0	0.0018
0.02	0.03	0	0	0.002	0	0	0	0.17	0.015	0.085	0.0016	0	0.0019
0.02	0.03	0	0	0.0016	0	0	0	0.14	0.009	0.09	0.0018	0	0
0.02	0.03	0	0	0.0005	0	0	0	0.011	0.004	0.095	0.0009	0	0.0017
0.02	0.03	0	0	0.0005	0	0	0	0.034	0.004	0.095	0.0013	0	0.0017
0.02	0.03	0	0	0.0058	0.0016	0	0	0.019	0.0045	0.09	0.0013	0	0
0.08	0	0	0	0.0009	0.0016	0	0	0.15	0	0	0.0004	0	0.0017
0.02	0.02	0.003	0	0.0052	0.0016	0	0	0	0.0045	0.085	0.0014	0	0
0.01	0.03	0	0	0	0	0	0	0.0094	0.0035	0.07	0.0004	0	0.0017
0	0.3	0	0	0.0003	0.0016	0	0	0	0.1	0.4	0.0005	0	0
0.01	0.02	0.0033	0	0	0.0017	0	0	0	0	0.06	0	0	0
0.01	0.02	0.0032	0	0	0.0016	0	0	0	0.0035	0.075	0	0	0
0	0.05	0	0	0.0002	0.0016	0	0	0.27	0.035	0.2	0	0	0.0017
0.01	0.02	0	0	0.003	0	0	0	0.096	0.005	0.065	0.0008	0	0
0	0.07	0.0032	0	0.0011	0.0026	0	0.009	0.28	0.07	0.15	0.0006	0	0.0017
0.01	0.02	0	0	0.0028	0	0	0	0.24	0	0.06	0.0007	0	0.0017
0.02	0.3	0.0063	0.00088	0.016	0	0	0	0.23	0.1	0.05	0.0028	0.0052	0
0.01	0.02	0	0	0.0033	0	0	0	0.26	0.0035	0.055	0.0007	0	0.0017
0.01	0.03	0	0	0.0025	0	0	0	0.18	0.009	0.065	0.0006	0	0.0017
0.01	0.02	0	0	0.0025	0	0	0	0.2	0.01	0.06	0.0005	0	0.0017
0	0.02	0	0	0.0022	0	0	0	0.27	0.0095	0.07	0.0006	0	0
0	0.02	0	0	0.0003	0.0016	0	0	0.37	0	0	0	0	0.0017
0	0	0	0	0.0008	0.0029	0	0	0.35	0	0	0	0	0
0	0.02	0	0	0.0022	0	0	0	0.38	0	0.055	0.0006	0	0.0017
0.009	0.02	0	0	0.0021	0	0	0	0.3	0	0.055	0.0005	0	0.0017
0	0.02	0	0	0.0022	0	0	0	0.28	0.005	0.065	0.0006	0	0
0.01	0.02	0	0	0.0023	0	0	0	0.29	0.0095	0.07	0	0	0.0017

Zopiclone	1H-Benzotriazole	2-(Methylthio)benzothiazole	2-Ethylhexyl diphenyl phosphate (EHDP)	5,6-Dimethylbenzotriazole	5-Methyl-1H-benzotriazole	Benzothiazole-6-carboxylic acid	Nonylphenol (4-Nonylphenol)	Tolyltriazol (mix of isomers)	Triisobutyl phosphate (TIBP)	Tri-n-butyl phosphate (TnBP)	Tri-n-propyl phosphate (TnPP)	Triphenyl phosphate (TPT)	Tris(1-chloro-2-propyl)phosphate (TCPP)
0.0036	0.23	0	0	0	0.052	0	0	0.2	0.011	0.004	0	0.0014	0.11
0.0033	0.46	0.03	0.0014	0	0.097	0	0	0.25	0.048	0.0038	0.00074	0.0056	0.095
0	0.32	0	0	0	0.07	0	0	0.2	0.023	0.0018	0	0.0042	0.17
0.0063	0.34	0.04	0	0	0.057	0	0	0.2	0.024	0.0038	0	0.0015	0.18
0.0062	0.48	0.03	0.0016	0	0.092	0	0	0.1	0.02	0.0051	0	0.0031	0.12
0.0032	0.28	0.03	0.0059	0	0.049	0	0	0.045	0.017	0.0018	0.00085	0.0034	0.064
0.0022	0.26	0.04	0	0	0.02	0	0	0.045	0.015	0.0033	0	0.001	0.09
0.00074	0.21	0.04	0	0	0.029	0	0	0.05	0.013	0.0028	0	0	0.24
0.019	0.31	0	0	0	0.052	0	0	0.05	0.0085	0.0039	0	0.0012	0.056
0.003	0.29	0.03	0	0	0.055	0	0	0.2	0.022	0.0035	0	0.0012	0.092
0.0054	0.32	0.04	0.00056	0	0.061	0	0	0.15	0.016	0.0041	0	0.001	0.058
0	0.38	0	0.0018	0	0.15	0	0	0.25	0.012	0.0051	0	0.0076	0.13
0.0023	0.21	0.04	0	0	0.038	0	0	0.15	0.014	0.0031	0	0.0017	0.045
0.0024	0.27	0	0	0	0.039	0	0	0.15	0.015	0.0039	0	0.0011	0.11
0.0024	0.35	0.04	0.00052	0	0.074	0	0	0.3	0.015	0.004	0	0.0012	0.059
0.036	0.54	0	0.0015	0.007	0.14	0	0	0.4	0.017	0.0045	0	0.00099	0.095
0	0.36	0.05	0.00054	0	0.097	0	0	0.3	0.017	0.0062	0.00081	0.001	0.058
0.019	1.6	0	0.00093	0	0.1	0	0	0.35	0.049	0.07	0.00089	0.0012	0.086
0	0.36	0	0.00068	0	0.099	0	0	0.25	0.016	0.0039	0	0.0031	0.052
0	0.55	0.04	0	0	0.1	0	0	0.2	0.018	0.0094	0	0.0021	0.099
0	0.45	0	0.00056	0	0.088	0	0	0.25	0.017	0.006	0.00071	0.0013	0.073
0	0.47	0	0.0034	0	0.093	0	0	0.25	0.018	0.0072	0	0.0014	0.077
0	0.4	0	0.004	0.02	0.051	0	0	0.2	0.026	0.0057	0	0.00095	0.15
0	0.47	0	0.0042	0	0.19	0	0.00866667	0.3	0.015	0.005	0	0.002	0.079
0	0.39	0	0	0	0.054	0	0	0.2	0.017	0.0034	0	0.0009	0.11
0	0.38	0.03	0	0	0.06	0	0	0.4	0.018	0.0035	0	0.0013	0.12
0	0.5	0	0.002	0	0.12	0	0	0.3	0.015	0.0058	0	0.0022	0.079
0.0095	0.36	0	0.0003	0	0.1	0	0	0.3	0.016	0.005	0	0.00085	0.092
0	0.13	0	0	0	0.033	0	0	0.05	0.021	0	0	0.001	0.036
0	0.3	0.03	0	0	0.087	0	0	0.25	0.017	0.0031	0	0.00093	0.074
0.0065	0.3	0	0	0	0.036	0	0	0.25	0.019	0.0046	0	0.00074	0.084
0.0072	0.35	0.04	0	0	0.043	0	0	0.25	0.0095	0.0033	0	0	0.58
0.0063	0.3	0.04	0	0	0.071	0	0	0.25	0.03	0.00042	0	0.00074	0.082
0	0.28	0.04	0	0	0.077	0	0	0.2	0.023	0.0035	0	0.0014	0.081
0.0064	0.061	0.05	0.00069	0.02	0.08	0	0	0.3	0.013	0.0028	0	0.0052	0.072
0.0071	0.28	0.04	0	0.007	0.037	0	0	0.3	0.023	0.0024	0	0	0.066
0.0011	0.063	0	0	0	0.018	0	0	0.04	0.0047	0.0045	0	0	0.028
0.0036	0.21	0	0	0	0.027	0	0	0.15	0.016	0.0041	0	0	0.057
0.0022	0.21	0.05	0	0	0.043	0	0	0.25	0.015	0.005	0	0.0009	0.059
0.0027	0.23	0	0	0	0.043	0	0	0.2	0.018	0.0044	0	0	0.065
0.0026	0.14	0.04	0	0	0.065	0	0	0.3	0.024	0.0029	0	0.0012	0.084
0	0.23	0	0	0	0.041	0	0	0.2	0.015	0.0041	0	0.00062	0.061
0	0.25	0.04	0	0	0.05	0	0	0.25	0.015	0.0042	0.0021	0.0018	0.12
0	0.25	0	0	0	0.036	0	0	0.25	0.015	0.002	0	0.00058	0.1
0.00072	0.25	0.03	0	0	0.068	0	0	0.25	0.014	0.0038	0	0.00067	0.11
0.0022	0.25	0.03	0	0.007	0.074	0	0.00466667	0.35	0.015	0.0042	0	0	0.12
0.0022	0.21	0	0	0.005	0.05	0	0	0.3	0.019	0.0037	0	0.00063	0.067
0.0045	0.0015	0.03	0	0	0.0095	0.01	0.02	0	0.0025	0.0029	0	0	0.6
0	0.26	0	0	0	0.093	0	0	0.3	0.019	0.0051	0	0.00064	0.074
0	0.26	0	0	0.005	0.031	0	0	0.2	0.022	0.0037	0	0.0012	0.11
0.0022	0.16	0	0	0	0.11	0	0	0.2	0.037	0.019	0	0	0.28
0.0037	0.27	0.06	0	0	0.12	0	0.00433333	0.05	0.025	0.0042	0	0.00058	0.069
0.0035	0.25	0.03	0	0	0.072	0	0	0.2	0.021	0.0066	0	0.00076	0.11
0	0.024	0.05	0	0	0.021	0	0	0	0.015	0.0024	0	0.0058	0.074
0.0023	0.23	0	0	0	0.073	0	0	0.2	0.021	0.0041	0	0	0.086
0.0018	0.11	0.04	0.00038	0	0.025	0	0.018	0	0.0085	0.0073	0	0.0016	0.11
0	0.24	0.06	0	0	0.12	0.04	0	0.2	0.021	0.0044	0	0.00074	0.085
0	0.26	0.09	0	0.01	0.29	0	0.012	0.25	0.097	0.012	0.001	0.0073	0.3
0.0019	0.28	0	0	0	0.083	0	0	0.2	0.023	0.0046	0.00073	0.00091	0.11
0	0.27	0.04	0.0012	0	0.08	0	0	0.2	0.025	0.0014	0	0.00074	0.1
0.0019	0.22	0	0	0	0.019	0	0	0.15	0.019	0.0052	0	0	0.12
0.0019	0.24	0.04	0	0.005	0.071	0	0	0.15	0.022	0.0042	0	0.00064	0.12
0	0.027	0	0	0	0.046	0	0.009	0.035	0.021	0.0066	0	0	0.096
0.0019	0.0073	0.03	0.00068	0	0.024	0	0	0.005	0.0074	0.011	0	0.00055	0.035
0.002	0.25	0.03	0	0	0.057	0	0	0.05	0.0068	0.0059	0	0	0.29
0	0.24	0.05	0	0	0.052	0	0	0.15	0.027	0.0068	0	0.0038	0.079
0.0024	0.26	0	0	0.005	0.077	0	0	0.2	0.027	0.0082	0	0.0017	0.12
0	0.18	0.05	0	0	0.027	0	0	0.2	0.019	0.0046	0	0	0.054

Tris(2-butoxyethyl) phosphate (TBEP)	Tris(2-chloroethyl) phosphate (TCEP)	Tris(3,5-dimethylphenyl)phosphate (T35DMPP)	Tris(methylphenyl)phosphate (TMPP)	Dibutyltin-cation	Dioctyltin-cation	Diphenyltin-cation	Tetrabutyltin	Tributyltin-cation	Triphenyltin-cation	2,4-Dinitrophenol (DNP)	Acesulfame	Bisphenol A	Bisphenol S
0.025	0.011	0	0	0.0025	0	0	3.00E-07	2.00E-07	0	0.02	0.43	0.05	0
0.049	0.018	0.01	0.0013	0	0	0	0	0	0	0.03	0.51333333	0.013	0
0.034	0.023	0	0	0	0	0	0	0	0	0.02	0.62	0.03	0
0.04	0.023	0	0	0.00053	0	0	0	5.00E-07	0	0.02	0.64666667	0.55	0
0.042	0.017	0.014	0	0.00056	0	0	0	0	0	0.01	0.70666667	0.065	0
0.023	0.0068	0.024	0.0093	0.00077	0	0	0	0	0	0.01	0.47	0.0083	0
0.018	0.011	0	0	0	0	0	2.00E-07	7.00E-07	0	0.02	0.46333333	0.0095	0
0.054	0.028	0	0	0.00059	0	0	0	0	0	0.02	0.43	0.24	0
0.024	0.0096	0	0	0.00046	0	0	0	3.00E-07	0	0.01	0.48666667	0.14	0
0.02	0.012	0	0	0.00036	0	0	0	4.00E-07	0	0.01	0.41	1.3	0
0.022	0.0081	0	0.0032	0	0	0	0	0	0	0.02	0.45666667	0.039	0.21
0.007	0.012	0	0.013	0.00023	0	0.00034	0	7.00E-07	0.00021	0.02	0.69	0.014	0
0.02	0.004	0	0	0.00021	0	0	0	0	0	0.02	0.4	0.039	0
0.018	0.011	0	0	0	0	0	0	0	0	0.02	0.385	0.021	0
0.019	0.0094	0.008	0.00086	0	0	0	0	0	0	0.02	0.49	0.14	0
0.02	0.013	0.054	0.0088	0	0	0	0	0	0	0.02	0.53	0.017	0
0.018	0.0099	0	0	0	0	0	0	0	0	0.02	0.51333333	0.049	0
0.011	0.012	0	0	0.00086	0	0	0	0	0	0.02	0.59	0.032	0
0.016	0.0086	0	0.0022	0	0	0	0	3.00E-07	0	0.02	0.46666667	0.17	0
0.015	0.011	0	0	0.00062	0	0	0	0	0	0.03	0.49	0.08	0
0.019	0.0097	0	0.00082	0.00037	0	0	0	0	0	0.02	0.46	0.024	0
0.018	0.0087	0.011	0.0088	0.00028	0	0	0	0	0	0.02	0.50666667	0.65	0
0.0093	0.0093	0.017	0.0079	0.00025	0	0	0	0	0	0.02	0.58	0.064	0
0.018	0.0092	0.042	0.011	0.00031	0	0	0	0	0	0.02	0.49	0	0
0.0097	0.01	0	0	0.00022	0	0	0	0	0	0.03	0.45	0.055	0
0.0096	0.011	0	0	0.00027	0	0	0	0	0	0.03	0.49666667	0.0056	0
0.017	0.009	0.016	0	0.00028	0	0	0	0	0	0.03	0.45666667	0.0093	0.27
0.015	0.012	0	0	0	0	0	0	0	0	0.03	0.54333333	0	0
0.0095	0.0034	0	0	0	0	0	0	0	0	0.04	0.20666667	0	0
0.0077	0.0077	0	0	0.00038	0	0	0	0	0	0.03	0.4	0	0
0	0.0096	0	0	0	0	0	0	0	0	0.03	0.36666667	0	0
0	0.012	0	0	0.00034	0	0	0	0	0	0.04	0.47333333	0	0
0.0076	0.0081	0	0	0.00044	0	0	0	0	0	0.04	0.41333333	0	0
0.0061	0.0082	0	0	0.00021	0.00027	0	0	0	0	0.04	0.47	0	0
0	0.01	0	0	0.00024	0	0	0	0	0	0.02	0.44	0	0
0	0.0069	0	0	0.00023	0	0	0	0	0	0.03	0.43333333	0	0
0	0.0024	0	0	0	0	0	0	0	0	0.02	0.19666667	0	0
0	0.0059	0	0	0.00027	0	0	0	0	0	0.02	0.41	0	0
0	0.0058	0	0	0.00053	0.00023	0	0	0	0	0.03	0.48666667	0	0
0	0.0059	0	0	0	0	0	0	0	0	0.04	0.43	0	0
0	0.013	0	0	0.00051	0	0	0	0	0	0.02	0.58	0	0
0	0.0063	0	0	0.00035	0	0	0	0	0	0.03	0.40333333	0	0
0.051	0.033	0	0	0.00027	0	0	0	0	0	0.03	0.45666667	0	0
0.011	0.015	0	0	0.00045	0	0	0	0	0	0.03	0.44	0	0
0.011	0.011	0	0	0.00022	0	0	0	0	0	0.03	0.44333333	0	0
0.0086	0.0096	0	0	0.00024	0	0	0	0	0	0.03	0.46	0	0
0	0.0049	0	0	0.00062	0	0	0	0	0	0.03	0.49	0	0
0	0.01	0	0	0	0	0	0	0	0	0.06	0.69	0	0
0	0.0091	0	0.00087	0.00022	0	0	0	0	0	0.03	0.45	0	0
0.0057	0.01	0	0	0	0	0	0	0	0	0.02	0.47333333	0	0
0	0.041	0	0	0	0	0	0	0	0	0.02	1	0	0
0	0.0062	0	0	0	0	0	0	0	0	0.02	0.42666667	0	0
0	0.011	0	0	0	0	0	0	0	0	0.02	0.45666667	0	0
0	0.015	0	0	0	0	0	0	0	0	0.02	0.98	0	0
0	0.0079	0	0	0	0	0	0	0	0	0.02	0.48	0	0
0.012	0.017	0	0	0	0	0	0	0	0	0.01	1.2	0	0
0	0.0098	0	0	0	0	0	0	0	0	0.02	0.42333333	0	0
0.093	0.029	0	0	0	0	0	0	0	0	0.01	1.1	0	0
0	0.007	0	0	0	0	0	0	0	0	0.02	0.46666667	0	0
0.0052	0.0081	0	0	0	0	0	0	0	0	0.02	0.52	0	0
0.0084	0.0087	0	0	0	0	0	0	0	0	0.02	0.4	0	0
0	0.0048	0	0	0	0	0	0	0	0	0.02	0.50333333	0	0
0	0.0083	0	0	0.00027	0	0	0	0	0	0.04	0.25333333	0	0
0.0089	0.01	0	0	0	0	0	0	0	0	0.04	0.23	0	0
0.006	0.0094	0	0	0	0	0	0	0	0	0.02	0.46333333	0	0
0.0053	0.0081	0	0	0	0	0	0	0	0	0.02	0.37666667	0	0.14
0.01	0.021	0	0	0	0	0	0	0	0	0.02	0.43666667	0	0
0	0.0054	0	0	0.00021	0.00028	0	0	0	0	0.02	0.51	0	0

Caffeine	Cotinine	Di(2-ethylhexyl)phthalate (DEHP)	N,N-Diethyl-m-toluamid (DEET)	Nicotine	Perfluorobutanesulfonate (PFBS)	Perfluoroheptanoic acid (PFHpA)	Perfluorohexane sulfonate (PFHxS) (anion)	Perfluorohexanoic acid (PFHxA)	Perfluorononanoate (PFNA)	Perfluorooctanesulfonic acid (PFOS)	Perfluorooctanoic acid (PFOA)	Saccharin	Sucralose
0.1	0.041	0	0.015	0.2	0.0022	0	0.002	0.0021	0.00085	0.0069	0.0019	0.07	0
0.16	0.046	0.21	0.022	0.29	0.0021	0	0.003	0.0042	0.0014	0.023	0.0034	0.07	0
0.2	0.14	0.28	0.018	0.3	0.0022	0	0	0.0031	0.0019	0.011	0.003	0.05	0
0.14	0.036	0.22	0.022	0.26	0.0023	0	0	0.0034	0.0018	0.013	0.0041	0.07	0
0.14	0.034	0	0.023	0.27	0.0018	0	0	0.0049	0.0018	0.015	0.0047	0.04	0
0.1	0.039	0	0.016	0.24	0.0011	0	0	0.006	0.0027	0.016	0.0091	0.1	0
0.12	0.031	0	0.013	0.27	0.0016	0.0035	0	0.0066	0.0013	0.0056	0.007	0.04	0
0.092	0.042	0.22	0.011	0.61	0.0013	0	0	0.0054	0.0015	0.0054	0.0063	0.04	0
0.19	0.036	0	0.016	0	0.0021	0.0066	0	0.0067	0.002	0.01	0.02	0.06	0
0.11	0.079	0	0.012	0.38	0.0013	0	0	0.005	0.0016	0.0058	0.006	0.04	0
0.2	0.052	0.28	0.017	0.33	0.002	0.0062	0	0.0079	0.0025	0.0069	0.018	0.04	0
0.09	0.079	0.24	0.081	0.28	0.0028	0.0042	0	0.0032	0	0.011	0.0047	0.04	0.2
0.12	0.037	0.24	0.012	0.38	0.0016	0.0067	0	0.0047	0.002	0.0089	0.032	0.04	0
0.15	0.053	0.28	0.015	0.29	0.0014	0.0041	0	0.006	0.0013	0.0061	0.0063	0.05	0
0.22	0.12	0.55	0.02	0.36	0	0	0	0.0067	0	0	0.021	0.07	0.1
0.27	0.041	0.41	0.023	0.1	0	0	0	0.0056	0	0.0053	0.017	0.1	0.3
0.073	0.03	0	0.017	0.14	0.0021	0	0	0.0074	0.001	0.0089	0.008	0.06	0.1
0.12	0.041	0.48	0.028	0.091	0.0015	0	0	0.0034	0.00079	0.0095	0.0043	0.1	0.3
0.069	0.021	0.23	0.02	0.21	0.0021	0.0081	0	0.0085	0.0017	0.02	0.025	0.06	0.1
0.098	0.026	0.23	0.023	0.28	0.0021	0	0	0.0078	0	0.026	0.011	0.07	0.1
0.093	0.025	0	0.019	0.056	0.002	0.0074	0	0.0068	0.0014	0.0058	0.026	0.07	0.1
0.095	0.022	0	0.019	0.16	0.0033	0.01	0	0.0077	0	0.0024	0.037	0.06	0
0.067	0.03	0	0.038	0.2	0.0037	0.0057	0	0.0052	0.0007	0.013	0.015	0.04	0.5
0.069	0.023	0.24	0.018	0.25	0.0021	0.0055	0	0.0071	0.00095	0.0082	0.018	0.06	0.2
0.052	0.02	0.39	0.013	0.2	0.0016	0.0052	0	0.0052	0.0014	0.0078	0.0071	0.07	0.1
0.072	0.018	0.26	0.011	0.1	0.0016	0.004	0	0.0055	0.001	0.0071	0.0057	0.1	0.2
0.078	0.015	0	0.018	0.19	0.0022	0.0058	0	0.0065	0.0008	0.0084	0.017	0.08	0.2
0.08	0.016	0.28	0.005	0.074	0.003	0.0065	0	0.0049	0	0.0082	0.018	0.08	0.2
0.085	0.022	0	0.00076	0.011	0.0025	0	0	0.0016	0.00093	0.005	0.012	0.04	0.1
0.09	0.031	0	0.0028	0.14	0.0028	0.0054	0	0.0044	0	0.0075	0.019	0.06	0.2
0.056	0.018	0	0.0095	0.13	0.0016	0.019	0	0.0059	0.0013	0.0063	0.0052	0.08	0.2
0.11	0.025	0.84	0.012	0.15	0.0022	0.0079	0	0.0052	0.0014	0.0076	0.0061	0.09	0.2
0.06	0.023	0	0.002	0.14	0.003	0.0052	0	0.0042	0.00073	0.013	0.012	0.08	0.2
0.11	0.011	0	0.002	0.11	0.0021	0.0059	0	0.0039	0.0011	0.0097	0.014	0.07	0.2
0.075	0.024	0	0.0032	0.091	0.0012	0	0	0.0014	0.001	0	0.0082	0.1	0.2
0.094	0.031	0	0.0088	0.1	0.003	0.0068	0	0.0031	0.00095	0.0052	0.012	0.06	0.2
0.11	0.027	0	0.0039	0.1	0.00074	0.0065	0	0	0	0.0036	0	0.07	0
0.19	0.038	0.26	0.0079	0.19	0.00076	0.0046	0	0.0029	0.0008	0.0037	0.0033	0.06	0.2
0.16	0.036	0.2	0.0089	0.2	0.00087	0.0052	0	0.0031	0.00074	0.0048	0.0043	0.08	0.1
0.16	0.035	0	0.0093	0.14	0.0012	0.0065	0	0.003	0.0027	0.0056	0.0037	0.09	0.2
0.25	0.046	0.26	0.018	0.15	0.00063	0.0046	0	0.0015	0	0.0047	0.0049	0.6	0.3
0.14	0.034	0.35	0.0014	0.19	0.00094	0	0	0.0043	0.00072	0.0049	0.0042	0.1	0.2
0.2	0.037	0.26	0.0098	0.15	0.0014	0	0	0.0031	0.0013	0.006	0.0044	0.1	0.2
0.12	0.039	0	0.0087	0.17	0.0015	0	0	0.0033	0.0015	0.0055	0.0037	0.1	0.2
0.11	0.034	0	0.0099	0.13	0.0014	0	0	0.0038	0.0016	0.0062	0.0043	0.1	0.2
0.12	0.035	0	0.0099	0.16	0.0011	0	0	0.0033	0.0015	0.0061	0.0041	0.08	0.2
0.021	0.0001	0	0.0072	0	0.0012	0	0	0.0035	0	0.0041	0.0039	0.09	0.2
0.066	0.012	0	0.014	0	0	0	0	0	0	0.0037	0.0018	0	0.2
0.027	0.002	0	0.012	0.0016	0.0014	0	0	0.0038	0	0.0055	0.0051	0.08	0.2
0.013	0.013	0	0.02	0	0.0011	0	0	0.0036	0.0017	0.0064	0.0046	0.07	0.1
0.026	0.015	0.2	0.025	0	0.00073	0	0	0	0.00088	0.0024	0.0048	0.2	0.4
0.023	0	0	0.0094	0	0.0014	0	0	0.004	0.00075	0.0054	0.0051	0.05	0.1
0.024	0	0	0.0094	0	0.0013	0	0	0.0038	0.00097	0.0047	0.0044	0.05	0.2
0.036	0.028	0.35	0.0066	0.021	0.0019	0	0	0.0031	0.00093	0.008	0.0029	0.3	0
0.048	0.017	0.21	0.0077	0.091	0.0011	0	0	0.004	0.00081	0.0048	0.0032	0.06	0.2
0.32	0.055	0.46	0.0076	0.051	0	0	0	0	0	0	0.0032	0.6	0
0.059	0.0092	0.37	0.0085	0.089	0.0014	0	0	0.0038	0	0.0047	0.0038	0.05	0.2
1.3	0.34	0.48	0.037	0.075	0.0018	0	0	0.0018	0.0011	0.0059	0.0026	1.7	0.4
0.14	0.019	0	0.0092	0.015	0.0011	0	0	0.005	0.0033	0.0063	0.0057	0.04	0.1
0.049	0.024	0.26	0.0093	0.038	0.0013	0	0	0.0042	0.003	0.0054	0.0044	0.09	0.2
0.042	0.021	0	0.0051	0.082	0.0013	0	0	0.0032	0.0014	0.0057	0.0038	0.07	0.1
0.031	0.023	0	0.0082	0.065	0.00084	0	0	0.0044	0.0029	0.005	0.0051	0.06	0.2
0.027	0.028	0	0.0023	0.077	0	0	0	0	0.0016	0.0043	0.0012	0.05	0
0.029	0.022	0	0.0015	0.089	0	0	0	0	0.0011	0	0.0015	0.04	0
0.039	0.02	0	0.0093	0.063	0.0013	0	0	0.004	0.0031	0.0057	0.005	0.06	0.1
0.03	0.023	0	0.0095	0.11	0.00093	0	0	0.0024	0.003	0.0069	0.0043	0.08	0.1
0.044	0.012	0.23	0.017	0.073	0.0014	0	0	0.004	0.0033	0.0069	0.0064	0.07	0.2
0.04	0.021	0	0.0048	0.11	0.001	0	0	0.0023	0	0.0052	0.0033	0.1	0.1

Concentration with half LoD

JDS3 site	Arsenic (As) - dissolved	Cadmium (Cd) - dissolved	Chromium (Cr) - dissolved	Copper (Cu) - dissolved	Lead (Pb) - dissolved	Mercury (Hg) - dissolved	Nickel (Ni) - dissolved	Zinc (Zn) - dissolved	Anthracene	Benzo(a)pyrene	Benzo(b)fluoranthene	Benzo(g,h,i)perylene	Benzo(k)fluoranthene
JDS01	1.1	0.0015	0.48	1.2	0.4	0.0003	0.93	6	0.0027	0.001	0.001	0.0015	0.001
JDS02	1.4	0.0015	0.68	1.1	0.5	0.0003	0.78	4.2	0.001	0.001	0.001	0.001	0.001
JDS03	1.3	0.024	1.2	2	0.63	0.0027	1.8	13	0.0025	0.001	0.001	0.0021	0.001
JDS04	1.4	0.0015	0.5	1.6	0.73	0.0039	0.8	6.4	0.001	0.001	0.001	0.0013	0.001
JDS05	1.4	0.014	0.31	1.5	0.7	0.0028	0.81	10	0.001	0.001	0.001	0.0014	0.001
JDS06	1.5	0.013	0.7	1.6	0.56	0.0003	1.1	8.6	0.001	0.001	0.001	0.001	0.001
JDS07	1.6	0.038	0.5	1.7	1.4	0.0003	1.1	11	0.0024	0.0024	0.001	0.0026	0.0022
JDS08	1.4	0.0015	0.97	2.1	0.7	0.0003	1	5.5	0.001	0.001	0.001	0.0016	0.001
JDS09	1.5	0.066	5.3	1.2	1.6	0.0003	19	6.6	0.001	0.001	0.001	0.00025	0.001
JDS10	1.5	0.081	0.84	1.2	1.4	0.0003	1.7	5.7	0.0021	0.001	0.001	0.0022	0.001
JDS11	1.5	0.057	6.7	1.3	0.86	0.0003	25	7	0.001	0.001	0.001	0.0015	0.001
JDS12	3.3	0.073	0.36	1.5	1.2	0.0003	2.8	9.9	0.001	0.001	0.001	0.0014	0.001
JDS13	1.6	0.048	0.91	1.3	1.3	0.0003	0.95	5.4	0.001	0.001	0.001	0.0011	0.001
JDS14	1.6	0.015	0.29	1.4	0.26	0.0003	1	8	0.001	0.001	0.001	0.0014	0.001
JDS15	1.6	0.02	0.5	1.2	0.2	0.0003	1	6.3	0.001	0.001	0.001	0.0019	0.001
JDS16	2.4	0.096	0.58	1.1	1.8	0.0003	1.2	7.3	0.001	0.001	0.001	0.0023	0.001
JDS17	1.7	0.034	0.54	1.3	0.38	0.0046	1	5.5	0.001	0.001	0.001	0.0013	0.001
JDS18	3.6	0.057	0.45	1.4	1	0.0044	1.2	5.7	0.001	0.001	0.001	0.0014	0.001
JDS19	1.7	0.15	0.62	1.5	8.1	0.0003	1.4	6.6	0.001	0.001	0.001	0.0015	0.001
JDS20	1.9	0.07	0.42	1.6	4.2	0.0037	1.2	8.6	0.001	0.001	0.001	1.30E-06	0.001
JDS21	2.3	0.029	2.1	1.3	0.63	0.0056	7.3	6	0.001	0.001	0.001	0.00025	0.001
JDS22	2	0.024	0.63	1.4	0.66	0.0034	1.9	7	2.50E-06	0.001	2.10E-06	2.40E-06	0.001
JDS23	3.5	0.011	0.29	1	0.49	0.0023	1.3	12	2.20E-06	0.001	0.001	2.10E-06	0.001
JDS24	2	0.022	0.34	1.3	0.4	0.0037	1.6	8.5	9.80E-06	2.40E-06	2.70E-06	2.60E-06	0.001
JDS25	2	0.028	0.47	1.4	0.45	0.0046	1.1	7.7	2.40E-06	0.001	0.001	2.10E-06	0.001
JDS26	2.1	0.033	0.56	1.5	0.97	0.005	1.3	7.7	2.10E-06	0.001	0.001	2.40E-06	0.001
JDS27	2.2	0.025	0.67	1.4	0.72	0.0043	1.2	6.8	2.50E-06	0.001	0.001	2.00E-06	0.001
JDS28	2.2	0.022	0.33	1.3	0.23	0.0003	1.1	5.7	2.50E-06	0.001	2.30E-06	2.20E-06	0.001
JDS29	2.4	0.027	0.59	0.74	0.51	0.0045	0.76	5.1	2.10E-06	0.001	0.001	1.80E-06	0.001
JDS30	2.2	0.026	0.52	1.1	0.24	0.0046	0.93	5.7	2.30E-06	0.001	0.001	2.20E-06	0.001
JDS31	2.3	0.028	2.6	1.1	0.49	0.0028	9	6.3	0.002	0.001	0.001	0.002	0.001
JDS32	2.3	0.028	0.67	1.2	0.35	0.0057	1.3	7.1	0.003	0.0023	0.0024	0.029	0.001
JDS33	2.3	0.03	0.68	1.2	0.52	0.0025	1.4	7.4	0.0029	0.001	0.0024	0.0031	0.001
JDS34	2.3	0.029	1.1	1.1	0.27	0.0057	2.2	7.1	0.001	0.001	0.001	0.0015	0.001
JDS35	4.3	0.033	0.56	1.8	0.4	0.0039	1.3	13	0.001	0.001	0.001	0.0012	0.001
JDS36	2.4	0.033	0.86	1.3	0.87	0.0003	2.3	8.7	0.001	0.001	0.001	0.0018	0.001
JDS37	2.5	0.03	1	1.4	0.67	0.0021	1.5	7.1	0.001	0.001	0.001	0.0013	0.001
JDS38	2.2	0.075	0.88	2	1.6	0.0042	1.2	2.3	0.001	0.001	0.001	0.0014	0.001
JDS39	2.2	0.048	0.82	2.1	0.59	0.0051	1.1	2.1	0.001	0.001	0.001	0.0013	0.001
JDS40	2.2	0.044	0.76	1.9	0.29	0.0051	1	1.6	0.001	0.001	0.001	0.0016	0.001
JDS41	5	0.3	67	2.3	2.6	0.0003	230	3.4	0.001	0.001	0.001	0.0017	0.001
JDS42	2.2	0.051	0.84	2	0.8	0.0028	1.4	2.2	0.001	0.001	0.001	0.0013	0.001
JDS43	2.5	0.084	1.6	2	0.38	0.0041	4.7	3.9	0.001	0.001	0.001	0.0014	0.001
JDS44	2.3	0.04	0.76	2.1	0.47	0.0003	1.3	2.1	0.001	0.001	0.001	0.0017	0.001
JDS45	2.5	0.043	0.71	2	0.26	0.0056	1.2	1.5	0.001	0.001	0.001	0.0007	0.001
JDS46	2.4	0.037	0.59	2.1	0.3	0.0047	1.3	1.8	0.001	0.001	0.001	0.0011	0.001
JDS47	2.4	0.045	0.72	2.2	0.36	0.007	1.3	2.1	0.001	0.001	0.001	0.0013	0.001
JDS48	1.5	1.1	0.63	283	0.45	0.0023	36	61	0.001	0.001	0.001	0.0012	0.001
JDS49	2.3	0.04	0.81	9.9	0.29	0.0056	1.2	1.9	0.001	0.001	0.001	0.0013	0.001
JDS50	2.3	0.041	2.2	5.2	0.25	0.0038	8.7	8.3	0.001	0.001	0.001	0.0013	0.001
JDS51	5.3	0.11	1.9	13	1	0.0047	6.4	1.8	0.001	0.001	0.001	0.0017	0.001
JDS52	2.2	0.046	0.71	3.7	0.27	0.0048	1.3	1.7	0.001	0.001	0.001	0.001	0.001
JDS53	2.4	0.043	0.72	3.5	0.32	0.0054	2.2	4.9	0.001	0.001	0.001	0.0012	0.001
JDS54	2	0.041	0.61	2.9	0.23	0.0051	1.5	1	0.001	0.001	0.001	0.0015	0.001
JDS55	2.4	0.039	0.47	3.2	0.35	0.0056	1.2	2.5	0.001	0.001	0.001	0.0012	0.001
JDS56	3.2	0.025	1.5	4.1	0.41	0.0063	1.6	2.9	0.001	0.001	0.001	0.0012	0.001
JDS57	2.4	0.037	0.37	3.1	0.41	0.0032	1.4	5.6	0.001	0.001	0.001	0.0012	0.001
JDS58	2.5	0.024	0.44	5.8	0.43	0.0061	3.3	3.9	0.001	0.001	0.001	0.002	0.001
JDS59	2.4	0.04	0.5	2.6	0.39	0.0027	1.8	1.3	0.001	0.001	0.001	0.0011	0.001
JDS60	2.4	0.038	2.2	2.5	0.32	0.0052	8	2.4	0.001	0.001	0.001	0.0011	0.001
JDS61	2.4	0.046	0.58	2.8	0.33	0.0032	2.8	2.5	0.001	0.001	0.001	0.001	0.001
JDS62	2.3	0.04	0.67	2.7	0.33	0.0026	1.4	1.5	0.001	0.001	0.001	0.0012	0.001
JDS63	1.7	0.03	0.23	2.6	0.36	0.0022	1.6	2.7	0.001	0.001	0.001	0.0027	0.001
JDS64	1.7	0.023	0.71	2.8	0.27	0.0058	2.3	1.4	0.001	0.001	0.001	0.0037	0.001
JDS65	2.4	0.042	0.33	2.8	0.71	0.0041	1.7	2.9	0.001	0.001	0.001	0.0018	0.001
JDS66	2.3	0.038	0.39	3.1	0.41	0.0064	1.4	3.6	0.001	0.001	0.001	0.0029	0.001
JDS67	2.4	0.039	0.7	2.6	0.38	0.0046	1.3	2.5	0.001	0.001	0.001	0.0025	0.001
JDS68	2.4	0.043	0.73	2.7	0.22	0.0032	1.3	1.1	0.001	0.001	0.001	0.0037	0.001

Fluoranthene	Indeno(1,2,3-c,d)pyrene	Naphthalene	2,4-D	2-Methyl-4-chlorphenoxy acetic acid (MCPA)	Ametryn	Aminomethylphosphonic acid (AMPA)	Atrazine	Atrazine-2-hydroxy	Atrazine-desethyl	Atrazine-desisopropyl	Bentazone	Bromacil	Carbetamide
0.004	0.00025	0.022	0.00021	0.0057	0.002	0.015	0.006	0.001	0.0098	0.000165	0.004	0.18	0.031
0.0021	0.0024	0.001	0.0038	0.0056	0.002	0.26	0.00866667	0.001	0.01	0.000165	0.004	0.048	0.0078
0.0047	0.00025	0.035	0.0034	0.0061	0.002	0.27	0.01266667	0.001	0.014	0.000165	0.003	0.084	0.0017
0.0024	0.00025	0.024	0.0021	0.0063	0.002	0.3	0.01133333	0.001	0.016	0.0008	0.005	0.05	0.0015
0.0029	0.00025	0.021	0.0018	0.004	0.002	0.24	0.01266667	0.002	0.012	0.000165	0.003	0.03	0.0022
0.0027	0.00025	0.014	0.00051	0.0024	0.002	0.16	0.006	0.001	0.01	0.000165	0.0015	0.083	0.000125
0.005	0.00025	0.018	0.001	0.0028	0.002	0.16	0.005	0.001	0.0077	0.0001	0.0015	0.084	0.000125
0.0028	0.00025	0.0087	0.00087	0.0027	0.002	0.17	0.005	0.001	0.0082	0.000165	0.0015	0.057	0.0032
0.0025	0.00025	0.0094	0.001	0.0021	0.002	0.18	0.005	0.001	0.007	0.000165	0.0015	0.065	0.0028
0.0043	0.0037	0.03	0.00083	0.0026	0.002	0.19	0.005	0.001	0.0072	0.0004	0.0015	0.000265	0.000125
0.0028	0.00025	0.01	0.0016	0.0025	0.002	0.17	0.005	0.003	0.013	0.000165	0.003	0.000265	0.0017
0.0041	0.00025	0.017	0.0072	0.012	0.002	0.63	0.014	0.02	0.0079	0.000165	0.01	0.000265	0.011
0.0022	0.00025	0.0072	0.0013	0.0016	0.002	0.2	0.0025	0.001	0.0073	0.0003	0.0015	0.000265	0.0016
0.0028	0.00025	0.013	0.002	0.0037	0.002	0.21	0.006	0.007	0.0092	0.0006	0.004	0.044	0.000125
0.0032	0.00025	0.013	0.0014	0.0028	0.002	0.21	0.00633333	0.005	0.0099	0.0004	0.005	0.000265	0.0096
0.0035	0.00025	0.015	0.0048	0.0064	0.002	0.33	0.007	0.01	0.011	0.000165	0.008	0.088	0.000125
0.0024	0.00025	0.0057	0.0014	0.0029	0.002	0.21	0.00666667	0.001	0.0088	0.0004	0.004	0.03	0.000125
0.0025	0.00025	0.015	0.0025	0.0036	0.002	0.4	0.006	0.02	0.008	0.000165	0.009	0.035	0.000125
0.0026	0.00025	0.008	0.0019	0.0038	0.002	0.21	0.00566667	0.007	0.0095	0.000165	0.005	0.19	0.000125
0.003	0.00025	0.016	0.0047	0.0051	0.002	0.14	0.00666667	0.01	0.0072	0.000165	0.005	0.077	0.0018
0.001	0.00025	7.20E-06	0.0017	0.003	0.002	0.19	0.00566667	0.006	0.007	0.000165	0.004	0.029	0.0012
4.60E-06	0.00025	1.50E-05	0.0015	0.0029	0.002	0.15	0.00633333	0.005	0.0092	0.000165	0.004	0.068	0.025
4.30E-06	0.00025	1.60E-05	0.0012	0.002	0.002	0.25	0.006	0.01	0.0048	0.000165	0.004	0.056	0.011
2.00E-05	0.00025	4.00E-05	0.0016	0.0028	0.002	0.21	0.00733333	0.006	0.0073	0.0006	0.005	0.044	0.0045
5.50E-06	0.00025	1.90E-05	0.001	0.0029	0.002	0.23	0.00733333	0.007	0.0077	0.000165	0.004	0.048	0.0025
6.10E-06	3.40E-06	1.50E-05	0.0012	0.0029	0.002	0.26	0.00666667	0.01	0.0064	0.000165	0.005	0.000265	0.0023
5.50E-06	0.00025	1.90E-05	0.0017	0.0025	0.002	0.25	0.006	0.008	0.0053	0.000165	0.005	0.000265	0.0038
6.20E-06	4.90E-06	1.60E-05	0.0015	0.0031	0.002	0.27	0.007	0.01	0.0058	0.000165	0.005	0.000265	0.0011
3.10E-06	0.00025	1.50E-05	0.00068	0.00098	0.002	0.16	0.0025	0.004	0.0034	0.000165	0.003	0.000265	0.0019
4.10E-06	0.00025	1.50E-05	0.001	0.0022	0.002	0.23	0.005	0.008	0.005	0.000165	0.005	0.067	0.0026
0.0039	0.0031	1.10E-05	0.0013	0.002	0.002	0.24	0.00533333	0.008	0.0038	0.000165	0.005	0.000265	0.0027
0.0055	0.00025	0.019	0.0016	0.002	0.002	0.27	0.00666667	0.009	0.0044	0.000165	0.005	0.039	0.003
0.0057	0.00025	0.02	0.0011	0.0013	0.002	0.27	0.006	0.007	0.0037	0.000165	0.005	0.000265	0.000125
0.0028	0.00025	0.0098	0.00094	0.0017	0.002	0.26	0.00633333	0.009	0.0033	0.000165	0.004	0.000265	0.0021
0.0022	0.00025	0.006	0.0032	0.00066	0.002	0.22	0.00633333	0.001	0.0031	0.000165	0.01	0.051	0.0016
0.003	0.00025	0.0071	0.0013	0.002	0.002	0.25	0.00633333	0.007	0.0034	0.000165	0.004	0.077	0.0057
0.0025	0.0036	0.0058	0.0016	0.00003	0.002	0.21	0.0025	0.01	0.00025	0.000165	0.0015	0.000265	0.000125
0.0026	0.00025	0.0055	0.0015	0.0017	0.002	0.16	0.005	0.007	0.00025	0.000165	0.004	0.11	0.0016
0.0021	0.00025	0.005	0.0019	0.0014	0.002	0.28	0.006	0.008	0.0035	0.000165	0.005	0.000265	0.0013
0.0024	0.00025	0.0075	0.0013	0.0016	0.002	0.26	0.00533333	0.01	0.0032	0.000165	0.005	0.000265	0.0028
0.0024	0.00025	0.0095	0.0057	0.00003	0.002	0.37	0.0025	0.001	0.0033	0.000165	0.008	0.000265	0.0036
0.0029	0.00025	0.0069	0.0014	0.0015	0.002	0.25	0.005	0.01	0.00025	0.000165	0.005	0.000265	0.0011
0.0025	0.0026	0.0065	0.0017	0.0014	0.002	0.24	0.00533333	0.009	0.004	0.0003	0.006	0.000265	0.0014
0.003	0.00025	0.0067	0.0018	0.0015	0.002	0.27	0.00566667	0.008	0.0048	0.0003	0.006	0.000265	0.0016
0.0031	0.0011	0.0034	0.002	0.0016	0.002	0.25	0.005	0.01	0.0034	0.000165	0.005	0.024	0.0019
0.0024	0.00025	0.0067	0.0022	0.0016	0.002	0.29	0.00533333	0.01	0.004	0.000165	0.006	0.000265	0.0019
0.0025	0.0024	0.0064	0.0019	0.0015	0.002	0.28	0.00566667	0.01	0.00025	0.0011	0.005	0.000265	0.000125
0.0023	0.00025	0.0059	0.016	0.00003	0.002	0.015	0.007	0.001	0.00025	0.000165	0.02	0.066	0.000125
0.0023	0.00025	0.0068	0.0018	0.0013	0.002	0.24	0.00533333	0.01	0.00025	0.000165	0.006	0.034	0.000125
0.003	0.00025	0.0057	0.0017	0.0012	0.002	0.25	0.005	0.01	0.00025	0.0015	0.005	0.000265	0.0016
0.003	0.00025	0.0075	0.0017	0.00055	0.002	0.34	0.0025	0.001	0.0081	0.0023	0.009	0.000265	0.000125
0.001	0.0025	0.008	0.0014	0.0014	0.002	0.25	0.005	0.009	0.0034	0.0004	0.003	0.023	0.0012
0.0022	0.00025	0.011	0.002	0.0015	0.002	0.25	0.00533333	0.008	0.004	0.0018	0.004	0.000265	0.000125
0.0022	0.0027	0.011	0.004	0.00019	0.002	0.24	0.0025	0.01	0.00025	0.000165	0.02	0.000265	0.0014
0.001	0.00025	0.012	0.0031	0.0013	0.002	0.22	0.005	0.01	0.00025	0.000165	0.006	0.000265	0.001
0.0023	0.00025	0.002	0.021	0.00032	0.002	0.96	0.005	0.02	0.00025	0.000165	0.02	0.000265	0.0011
0.001	0.00025	0.011	0.0019	0.0011	0.002	0.25	0.006	0.009	0.0031	0.000165	0.004	0.000265	0.0012
0.0043	0.00025	0.033	0.0084	0.00003	0.004	0.62	0.07	0.045	0.0035	0.000165	0.1	0.000265	0.000125
0.001	0.00025	0.0091	0.000045	0.0026	0.002	0.26	0.006	0.008	0.00025	0.000165	0.005	0.000265	0.000125
0.001	0.002	0.016	0.0027	0.0015	0.002	0.25	0.007	0.01	0.00025	0.000165	0.007	0.000265	0.0087
0.001	0.0021	0.014	0.0018	0.0011	0.002	0.23	0.007	0.01	0.0032	0.000165	0.006	0.000265	0.000125
0.0021	0.00025	0.015	0.000045	0.0013	0.002	0.23	0.007	0.01	0.0014	0.000165	0.007	0.000265	0.000125
0.0027	0.00025	0.016	0.0089	0.00039	0.002	0.13	0.0025	0.02	0.00025	0.000165	0.02	0.000265	0.0014
0.001	0.00025	0.0094	0.0044	0.0004	0.002	0.12	0.011	0.03	0.00025	0.000165	0.03	0.000265	0.0011
0.001	0.00025	0.014	0.0023	0.0015	0.002	0.24	0.00533333	0.01	0.00025	0.000165	0.007	0.000265	0.0018
0.0025	0.0025	0.012	0.004	0.0022	0.002	0.24	0.005	0.01	0.00025	0.000165	0.007	0.03	0.0018
0.002	0.0024	0.0097	0.000045	0.0021	0.002	0.26	0.006	0.01	0.00025	0.000165	0.007	0.000265	0.0019
0.0025	0.00025	0.012	0.0013	0.00059	0.002	0.23	0.006	0.01	0.00025	0.000165	0.008	0.032	0.0015

Chloridazon	Chloridazon-desphenyl	Chloridazon-methyl-desphenyl	Chloroxuron	Chlortoluron	Cyanazine (Fortrol)	Cybutryne (Irgarol)	Dimefuron	Dimethachlor CGA 369873	Dimethachlor sulfonic acid CGA 354742	Dimethenamid	Dinoseb	Dinoterb	Diuron
0.027	0.14	0.0125	0.012	0.000075	0.0005	0.000035	0.014	0.04	0.01	0.002	0.002	0.0015	0.02
0.0061	0.18	0.0125	0.025	0.000075	0.0005	0.00037	0.015	0.02	0.01	0.002	0.002	0.0015	0.029
0.0064	0.16	0.0125	0.011	0.0015	0.0005	0.000035	0.0096	0.02	0.01	0.002	0.002	0.0015	0.028
0.00005	0.24	0.0125	0.0096	0.0018	0.0005	0.000035	0.0005	0.02	0.01	0.002	0.002	0.0015	0.029
0.00005	0.24	0.0125	0.012	0.000075	0.0005	0.00022	0.0055	0.02	0.01	0.002	0.002	0.07	0.026
0.00005	0.095	0.0125	0.015	0.01	0.0005	0.00043	0.0005	0.01	0.01	0.002	0.002	0.03	0.017
0.00005	0.08	0.0125	0.014	0.000075	0.0005	0.000035	0.0038	0.01	0.01	0.002	0.002	0.08	0.016
0.00005	0.1	0.0125	0.013	0.023	0.0005	0.000035	0.0005	0.01	0.01	0.002	0.002	0.02	0.013
0.00005	0.13	0.0125	0.04	0.01	0.076	0.00034	0.0066	0.01	0.01	0.002	0.002	0.03	0.00025
0.00005	0.095	0.0125	0.023	0.021	0.0005	0.000035	0.026	0.01	0.01	0.002	0.002	0.02	0.00025
0.00005	0.1	0.0125	0.026	0.028	0.0005	0.00032	0.014	0.005	0.01	0.002	0.002	0.02	0.012
0.0042	0.25	0.055	0.016	0.000075	0.0005	0.00036	0.0086	0.05	0.02	0.004	0.002	0.05	0.00025
0.00005	0.082	0.0125	0.019	0.033	0.0005	0.000035	0.014	0.01	0.01	0.002	0.002	0.03	0.00025
0.003	0.098	0.0125	0.016	0.019	0.0005	0.00032	0.0075	0.005	0.01	0.002	0.002	0.04	0.00025
0.00005	0.094	0.0125	0.017	0.014	0.0005	0.0002	0.013	0.02	0.01	0.002	0.002	0.003	0.00025
0.00005	0.074	0.0125	0.0094	0.0014	0.0005	0.000035	0.011	0.02	0.01	0.002	0.002	0.003	0.012
0.00005	0.088	0.0125	0.012	0.013	0.0005	0.0005	0.0005	0.03	0.01	0.002	0.002	0.004	0.016
0.004	0.15	0.0125	0.017	0.000075	0.0005	0.00066	0.038	0.02	0.01	0.002	0.002	0.004	0.012
0.00005	0.12	0.0125	0.011	0.0018	0.0005	0.00047	0.032	0.02	0.01	0.002	0.002	0.003	0.00025
0.00005	0.086	0.0125	0.015	0.0059	0.0005	0.00061	0.041	0.02	0.01	0.002	0.002	0.003	0.012
0.00005	0.089	0.0125	0.0099	0.0067	0.0005	0.00061	0.011	0.02	0.01	0.002	0.002	0.01	0.00025
0.02	0.1	0.0125	0.014	0.008	0.0005	0.00049	0.0097	0.02	0.01	0.002	0.002	0.004	0.00025
0.012	0.0125	0.0125	0.0096	0.0044	0.0005	0.00083	0.041	0.01	0.01	0.002	0.002	0.004	0.00025
0.0032	0.094	0.0125	0.0054	0.0063	0.0005	0.00031	0.017	0.02	0.01	0.002	0.002	0.004	0.011
0.0026	0.085	0.0125	0.0069	0.01	0.0005	0.000035	0.0081	0.02	0.01	0.002	0.002	0.003	0.013
0.0026	0.094	0.0125	0.0077	0.0048	0.0005	0.000035	0.0033	0.02	0.01	0.002	0.002	0.003	0.00025
0.0033	0.081	0.0125	0.0065	0.0052	0.0005	0.00054	0.028	0.02	0.01	0.002	0.002	0.004	0.012
0.0027	0.082	0.0125	0.009	0.004	0.0005	0.000035	0.028	0.02	0.01	0.002	0.002	0.004	0.00025
0.0026	0.0125	0.0125	0.0076	0.0009	0.0005	0.000035	0.0005	0.005	0.01	0.002	0.002	0.003	0.012
0.0026	0.08	0.0125	0.0062	0.0032	0.0005	0.000035	0.025	0.01	0.01	0.002	0.002	0.004	0.00025
0.0024	0.069	0.0125	0.0071	0.0045	0.0005	0.000035	0.021	0.01	0.01	0.002	0.002	0.004	0.00025
0.0026	0.079	0.0125	0.0086	0.004	0.0005	0.000035	0.009	0.02	0.01	0.002	0.002	0.004	0.00025
0.0026	0.078	0.0125	0.0076	0.0021	0.0005	0.000035	0.018	0.02	0.01	0.002	0.002	0.003	0.00025
0.0027	0.089	0.0125	0.009	0.0039	0.0005	0.000035	0.013	0.02	0.01	0.002	0.002	0.003	0.00025
0.0029	0.0125	0.0125	0.0073	0.0009	0.0005	0.000035	0.038	0.005	0.01	0.002	0.002	0.01	0.012
0.0031	0.074	0.0125	0.0094	0.0048	0.0005	0.000035	0.022	0.01	0.01	0.002	0.002	0.02	0.00025
0.0028	0.0125	0.0125	0.0065	0.0018	0.0005	0.000035	0.0043	0.005	0.01	0.002	0.002	0.01	0.00025
0.00005	0.059	0.0125	0.0088	0.0008	0.0005	0.000035	0.0066	0.01	0.01	0.002	0.002	0.03	0.00025
0.0023	0.056	0.0125	0.007	0.000075	0.0005	0.000035	0.00052	0.01	0.01	0.002	0.002	0.01	0.00025
0.00005	0.05	0.0125	0.00025	0.000075	0.0005	0.000035	0.0088	0.01	0.01	0.002	0.002	0.01	0.00025
0.0024	0.0125	0.0125	0.0049	0.000075	0.0005	0.000035	0.0005	0.005	0.01	0.002	0.002	0.01	0.00025
0.00005	0.056	0.0125	0.0029	0.000075	0.0005	0.000035	0.005	0.01	0.01	0.002	0.002	0.02	0.00025
0.00005	0.06	0.0125	0.0036	0.0049	0.0005	0.000035	0.0005	0.01	0.01	0.002	0.002	0.01	0.012
0.0024	0.0125	0.0125	0.0037	0.000075	0.0005	0.000035	0.0065	0.01	0.01	0.002	0.002	0.01	0.00025
0.00005	0.051	0.0125	0.0043	0.0039	0.0005	0.000035	0.00072	0.005	0.01	0.002	0.002	0.01	0.00025
0.0025	0.0125	0.0125	0.0031	0.0094	0.0005	0.000035	0.0005	0.01	0.01	0.002	0.002	0.02	0.00025
0.00005	0.059	0.0125	0.0052	0.002	0.0005	0.000035	0.012	0.01	0.01	0.002	0.002	0.02	0.00025
0.00005	0.0125	0.0125	0.004	0.0015	0.0005	0.000035	0.011	0.005	0.01	0.002	0.002	0.01	0.00025
0.00005	0.0125	0.0125	0.002	0.0006	0.0005	0.000035	0.0064	0.01	0.01	0.002	0.002	0.02	0.00025
0.00005	0.05	0.0125	0.00025	0.0012	0.0005	0.000035	0.011	0.005	0.01	0.002	0.002	0.01	0.00025
0.00005	0.0125	0.0125	0.00025	0.0021	0.0005	0.000035	0.0054	0.005	0.01	0.002	0.002	0.01	0.00025
0.00005	0.052	0.0125	0.0052	0.0018	0.0005	0.000035	0.0077	0.005	0.01	0.002	0.002	0.003	0.00025
0.00005	0.0125	0.0125	0.0031	0.0007	0.0005	0.000035	0.0005	0.005	0.01	0.002	0.002	0.008	0.00025
0.00005	0.0125	0.0125	0.0099	0.0047	0.0005	0.000035	0.012	0.005	0.01	0.002	0.002	0.005	0.00025
0.00005	0.0125	0.0125	0.0068	0.0037	0.0005	0.000035	0.0099	0.01	0.01	0.002	0.002	0.004	0.00025
0.00005	0.0125	0.0125	0.0094	0.000075	0.0005	0.000035	0.011	0.005	0.01	0.002	0.002	0.006	0.056
0.00005	0.0125	0.0125	0.0014	0.000075	0.0005	0.000035	0.006	0.005	0.01	0.002	0.002	0.004	0.00025
0.00005	0.0125	0.0125	0.0061	0.006	0.0005	0.000035	0.0005	0.005	0.3	0.002	0.002	0.01	0.00025
0.00005	0.0125	0.0125	0.0076	0.000075	0.0005	0.000035	0.0066	0.005	0.01	0.002	0.002	0.007	0.00025
0.00005	0.0125	0.0125	0.0069	0.0014	0.0005	0.000035	0.0055	0.005	0.01	0.002	0.002	0.004	0.00025
0.00005	0.0125	0.0125	0.0064	0.0023	0.0005	0.000035	0.0091	0.005	0.01	0.002	0.002	0.003	0.00025
0.00005	0.05	0.0125	0.0069	0.000075	0.0005	0.000035	0.0038	0.005	0.01	0.002	0.002	0.003	0.00025
0.00005	0.0125	0.0125	0.0055	0.000075	0.0005	0.000035	0.0083	0.005	0.01	0.002	0.004	0.006	0.00025
0.00005	0.0125	0.0125	0.0071	0.000075	0.0005	0.000035	0.0099	0.005	0.01	0.002	0.002	0.01	0.00025
0.00005	0.0125	0.0125	0.0066	0.000075	0.0005	0.000035	0.0078	0.005	0.01	0.002	0.002	0.004	0.00025
0.00005	0.0125	0.0125	0.0057	0.0042	0.0005	0.000035	0.0076	0.005	0.01	0.002	0.002	0.006	0.00025
0.00005	0.053	0.0125	0.0062	0.019	0.0005	0.000035	0.01	0.005	0.01	0.002	0.002	0.003	0.00025
0.00005	0.0125	0.0125	0.006	0.000075	0.0005	0.000035	0.0081	0.005	0.01	0.002	0.002	0.006	0.00025

Ethidimuron (Sulfadiazole)	Ethofumesate	Glyphosate	Hexazinon	Isoproturon	Linuron	Metamitron	Metazachlor	Metazachlor ESA	Metazachlor OA	Methabenzthiazuron	Metobromuron	Metolachlor	Metolachlor ESA
0.0017	0.029	0.015	0.0035	0.0052	0.00025	0.0004	0.0009	0.0125	0.0125	0.0017	0.068	0.00033	0.0125
0.0026	0.013	0.015	0.0035	0.01	0.00025	0.0004	0.0008	0.0125	0.0125	0.0023	0.0005	0.005	0.054
0.000105	0.08	0.07	0.0035	0.0094	1.4	0.0021	0.0005	0.052	0.0125	0.0017	0.0005	0.0084	0.0125
0.0016	0.05	0.015	0.0035	0.0073	1.2	0.0004	0.0019	0.063	0.0125	0.0018	0.0005	0.011	0.057
0.0019	0.0005	0.015	0.0035	0.0094	0.69	0.0004	0.00055	0.0125	0.0125	0.0005	0.0005	0.0062	0.064
0.000105	0.036	0.015	0.0035	0.0045	1	0.0004	0.00055	0.0125	0.0125	0.0016	0.0005	0.005	0.0125
0.00042	0.031	0.015	0.0035	0.0036	0.013	0.0004	0.0006	0.0125	0.0125	0.0017	0.0005	0.007	0.05
0.0022	0.047	0.073	0.0035	0.0021	0.93	0.0004	0.0006	0.0125	0.0125	0.0005	0.0005	0.0058	0.052
0.000105	0.028	0.065	0.0035	0.016	0.083	0.004	0.0026	0.0125	0.0125	0.0016	0.0005	0.0039	0.055
0.00066	0.052	0.015	0.0035	0.00005	0.00025	0.025	0.0038	0.0125	0.0125	0.0017	0.0005	0.006	0.06
0.00095	0.027	0.015	0.0035	0.0007	0.00025	0.014	0.0006	0.0125	0.0125	0.0005	0.0082	0.0041	0.052
0.000105	0.036	0.015	0.007	0.0052	0.021	0.029	0.0028	0.33	0.17	0.0005	0.0005	0.01	0.087
0.00078	0.025	0.015	0.0035	0.00005	0.0087	0.019	0.0036	0.0125	0.0125	0.0016	0.0005	0.0025	0.054
0.0004	0.015	0.015	0.0035	0.0034	0.023	0.025	0.0022	0.0125	0.0125	0.0017	0.0005	0.0063	0.051
0.00025	0.017	0.015	0.0035	0.00005	0.038	0.021	0.0013	0.0125	0.0125	0.0005	0.043	0.0035	0.0125
0.0035	0.042	0.015	0.0035	0.00005	0.00025	0.0021	0.0014	0.0125	0.0125	0.0005	0.0005	0.0072	0.072
0.00027	0.043	0.015	0.0035	0.00005	0.015	0.0004	0.0005	0.0125	0.0125	0.0005	0.0005	0.0039	0.051
0.00025	0.044	0.015	0.0035	0.005	0.03	0.0017	0.023	0.0125	0.0125	0.0005	0.0005	0.0038	0.0125
0.000105	0.041	0.015	0.0035	0.00005	0.021	0.0004	0.0013	0.0125	0.0125	0.0005	0.016	0.0044	0.0125
6.80E-05	0.028	0.015	0.0035	0.00005	0.031	0.0004	0.0009	0.0125	0.0125	0.0005	0.0005	0.0038	0.0125
0.000105	0.031	0.015	0.0035	0.003	0.033	0.0004	0.0005	0.0125	0.0125	0.0005	0.0074	0.0042	0.0125
0.00022	0.029	0.015	0.0035	0.0051	0.0029	0.0004	0.0006	0.0125	0.0125	0.0005	0.0005	0.0031	0.0125
0.00019	0.042	0.015	0.0035	0.002	0.02	0.0004	0.00055	0.0125	0.0125	0.0005	0.0005	0.0024	0.0125
0.000105	0.024	0.015	0.0035	0.0024	0.018	0.0004	0.0005	0.0125	0.0125	0.0005	0.0087	0.0036	0.0125
0.000105	0.036	0.015	0.0035	0.00005	0.0093	0.0004	0.0006	0.0125	0.0125	0.0005	0.0066	0.0066	0.0125
0.00026	0.022	0.015	0.0035	0.0041	0.0081	0.0004	0.0008	0.0125	0.0125	0.0005	0.0086	0.008	0.0125
0.00019	0.03	0.015	0.0035	0.00005	0.00025	0.0004	0.0006	0.0125	0.0125	0.0005	0.0063	0.0043	0.0125
0.00023	0.031	0.015	0.0035	0.0076	0.0057	0.0004	0.00055	0.0125	0.0125	0.0005	0.0053	0.0091	0.0125
0.00021	0.01	0.015	0.0035	0.0019	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0061	0.0046	0.0125
0.000105	0.021	0.015	0.0035	0.00005	0.0088	0.0019	0.00055	0.0125	0.0125	0.0005	0.0071	0.0078	0.0125
0.000105	0.0005	0.015	0.0035	0.00005	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.01	0.0058	0.0125
0.000105	0.02	0.015	0.0035	0.027	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0055	0.0087	0.0125
0.000105	0.011	0.015	0.0035	0.0011	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.006	0.011	0.0125
0.000105	0.024	0.015	0.0035	0.0015	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0051	0.011	0.0125
0.000105	0.029	0.015	0.0035	0.0049	0.00025	0.0004	0.0005	0.0125	0.0125	0.0005	0.0047	0.009	0.0125
0.00032	0.0098	0.015	0.0035	0.0065	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0077	0.0065	0.0125
0.000105	0.02	0.015	0.0035	0.00005	0.0064	0.0004	0.0005	0.0125	0.0125	0.0005	0.0005	0.0026	0.0125
0.000105	0.011	0.015	0.0035	0.00005	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0089	0.0054	0.0125
0.000105	0.015	0.015	0.0035	0.00005	0.00025	0.0019	0.00055	0.0125	0.0125	0.0005	0.0047	0.0049	0.0125
0.00022	0.0005	0.015	0.0035	0.0024	0.011	0.0004	0.00055	0.0125	0.0125	0.0005	0.0057	0.0063	0.0125
0.000105	0.011	0.015	0.0035	0.00005	0.00025	0.0016	0.00055	0.0125	0.0125	0.0005	0.0049	0.0041	0.0125
0.00025	0.0059	0.015	0.0035	0.00005	0.012	0.0022	0.00055	0.0125	0.0125	0.0005	0.0051	0.0055	0.0125
0.000105	0.009	0.015	0.0035	0.00005	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0048	0.0057	0.0125
0.000105	0.0093	0.015	0.0035	0.0042	0.00025	0.0017	0.00055	0.0125	0.0125	0.0005	0.0047	0.0058	0.0125
0.000105	0.0005	0.015	0.0035	0.00005	0.00025	0.0016	0.00055	0.0125	0.0125	0.0005	0.0043	0.0045	0.0125
0.000105	0.021	0.015	0.0035	0.0011	0.00025	0.0017	0.00055	0.0125	0.0125	0.0005	0.0005	0.0049	0.0125
0.0014	0.0005	0.015	0.0035	0.0008	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0051	0.0054	0.0125
0.000105	0.0005	0.015	0.0035	0.0009	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0049	0.004	0.0125
0.0015	0.0005	0.015	0.0035	0.0007	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0005	0.0054	0.0125
0.0029	0.0005	0.015	0.0035	0.0038	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0005	0.0053	0.0125
0.00038	0.029	0.015	0.0035	0.0016	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0005	0.0046	0.0125
0.00037	0.1	0.015	0.0035	0.0005	0.00025	0.0004	0.016	0.0125	0.0125	0.0005	0.0005	0.0053	0.0125
7.50E-05	0.097	0.015	0.0035	0.00005	0.00025	0.0004	0.013	0.0125	0.0125	0.0005	0.0005	0.0062	0.0125
0.0013	0.026	0.062	0.0035	0.001	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0058	0.025	0.0125
0.0019	0.013	0.015	0.0035	0.0007	0.0001	0.0017	0.00055	0.0125	0.0125	0.0005	0.0053	0.0059	0.0125
0.000105	0.01	0.069	0.0035	0.17	0.00025	0.0025	0.00055	0.0125	0.0125	0.0005	0.0005	0.039	0.0125
0.000105	0.0005	0.015	0.0035	0.0005	0.00025	0.0004	0.00055	0.0125	0.0125	0.0005	0.0051	0.0047	0.0125
0.00056	0.0005	0.015	0.0035	0.0018	0.0057	0.0035	0.00055	0.0125	0.0125	0.0005	0.0055	0.0031	0.0125
0.000105	0.0094	0.015	0.0035	0.0011	0.00025	0.0017	0.00055	0.0125	0.0125	0.0005	0.0023	0.0061	0.0125
0.000105	0.0005	0.015	0.0035	0.0007	0.00025	0.0017	0.00055	0.0125	0.0125	0.0005	0.0052	0.0049	0.0125
0.000105	0.015	0.015	0.0035	0.0017	0.0086	0.0018	0.00055	0.0125	0.0125	0.0005	0.0005	0.004	0.0125
0.00092	0.0005	0.015	0.0035	0.0023	0.00025	0.0017	0.00055	0.0125	0.0125	0.0005	0.0005	0.0048	0.0125
0.000105	0.0094	0.015	0.0035	0.0039	0.00025	0.002	0.0006	0.0125	0.0125	0.0005	0.0052	0.0071	0.0125
0.002	0.011	0.015	0.0035	0.0037	0.00025	0.0018	0.0097	0.0125	0.0125	0.0005	0.0046	0.0076	0.0125
0.00031	0.0005	0.015	0.0035	0.0013	0.00025	0.0018	0.00055	0.0125	0.0125	0.0005	0.0029	0.0068	0.0125
0.000105	0.0005	0.015	0.0035	0.0017	0.022	0.0017	0.00055	0.0125	0.0125	0.0005	0.0046	0.0056	0.0125
0.000105	0.0091	0.015	0.0035	0.0017	0.00025	0.0019	0.00055	0.0125	0.0125	0.0005	0.0069	0.0063	0.0125
0.00035	0.0005	0.015	0.0035	0.001	0.0076	0.0019	0.00055	0.0125	0.0125	0.0005	0.0076	0.0043	0.0125

Metoxuron	Monolinuron	Prometryn	Propazine	Propazine-2-hydroxy	Simazine	S-Metolachlor CGA 368208	S-Metolachlor NOA 413173	Terbutryn	Terbutylazine	Terbutylazine CGA 324007	Terbutylazine SYN 545666	Terbutylazine-2-hydroxy	Terbutylazine-desethyl
0.0049	0.00018	0.006	0.01	0.005	0.00013	0.005	0.01	0.0047	0.011	0.005	0.00125	0.002	0.00027
0.0056	0.00018	0.0071	0.028	0.005	0.00013	0.005	0.01	0.0044	0.028	0.005	0.0075	0.002	0.00027
0.0013	0.0065	0.0098	0.025	0.005	0.00013	0.005	0.01	0.011	0.025	0.005	0.003	0.002	0.00027
0.005	0.0025	0.0065	0.021	0.005	0.00013	0.005	0.01	0.0092	0.021	0.005	0.004	0.002	0.00027
0.0068	0.00018	0.0081	0.025	0.005	0.004	0.005	0.01	0.0094	0.025	0.005	0.008	0.002	0.0062
0.0049	0.00018	0.0039	0.021	0.005	0.0016	0.005	0.01	0.005	0.021	0.005	0.0035	0.002	0.0038
0.0056	0.0068	0.0005	0.0039	0.005	0.00013	0.005	0.01	0.004	0.0046	0.005	0.008	0.002	0.00027
0.0026	0.038	0.0018	0.0038	0.005	0.00013	0.005	0.01	0.0033	0.0045	0.005	0.008	0.002	0.00027
0.0095	0.089	0.0024	0.053	0.005	0.0033	0.005	0.01	0.0039	0.052	0.005	0.0085	0.002	0.0056
0.0098	0.00018	0.0018	0.0059	0.005	0.0073	0.005	0.01	0.0031	0.0066	0.005	0.0065	0.002	0.0098
0.0096	0.00018	0.0005	0.012	0.005	0.0063	0.005	0.01	0.0033	0.012	0.005	0.008	0.002	0.0086
0.01	0.00018	0.0005	0.044	0.005	0.005	0.03	0.03	0.0075	0.043	0.01	0.01	0.02	0.0073
0.0096	0.00018	0.0005	0.0082	0.005	0.0011	0.005	0.01	0.0029	0.0087	0.005	0.0095	0.002	0.0033
0.017	0.0027	0.0005	0.019	0.005	0.00013	0.005	0.01	0.0029	0.019	0.005	0.0095	0.002	0.00027
0.011	0.0063	0.0026	0.01	0.005	0.00013	0.005	0.03	0.0042	0.011	0.005	0.0045	0.002	0.00027
0.0026	0.0084	0.002	0.0008	0.005	0.0022	0.005	0.04	0.0034	0.0016	0.005	0.0045	0.002	0.0044
0.0014	0.027	0.0021	0.013	0.005	0.00013	0.005	0.02	0.005	0.014	0.005	0.005	0.002	0.00027
0.00009	0.00018	0.0019	0.0074	0.005	0.0044	0.005	0.01	0.0044	0.0079	0.005	0.0145	0.002	0.0067
0.0031	0.028	0.0005	0.008	0.005	0.0055	0.005	0.03	0.0029	0.0086	0.005	0.015	0.002	0.0078
0.00035	0.0039	0.0017	0.0011	0.005	0.0052	0.005	0.01	0.0035	0.0019	0.005	0.014	0.006	0.0075
0.0019	0.012	0.0005	0.0075	0.005	0.00013	0.005	0.02	0.0035	0.0081	0.005	0.015	0.002	0.00027
0.0017	0.014	0.0005	0.0089	0.005	0.00013	0.005	0.01	0.0034	0.0094	0.005	0.0145	0.002	0.00027
0.0013	0.00018	0.0005	0.0048	0.005	0.0014	0.005	0.02	0.0044	0.0055	0.005	0.003	0.002	0.0035
0.00044	0.00018	0.0005	0.0058	0.005	0.00013	0.005	0.01	0.0032	0.0065	0.005	0.0095	0.004	0.00027
0.00009	0.00018	0.0014	0.0014	0.005	0.00013	0.005	0.01	0.0035	0.0022	0.005	0.009	0.002	0.00027
0.001	0.00018	0.0005	0.004	0.005	0.00013	0.005	0.03	0.0032	0.0047	0.005	0.015	0.002	0.00027
0.001	0.00018	0.0022	0.0025	0.005	0.011	0.005	0.03	0.0041	0.0033	0.005	0.0145	0.005	0.014
0.0023	0.012	0.0005	0.005	0.005	0.00013	0.005	0.03	0.0023	0.0057	0.005	0.015	0.002	0.00027
0.00019	0.00018	0.0005	0.0017	0.005	0.00013	0.005	0.01	0.002	0.0025	0.005	0.00125	0.002	0.00027
0.00093	0.00018	0.0005	0.0024	0.005	0.00013	0.005	0.03	0.0035	0.0031	0.005	0.0135	0.002	0.00027
0.00009	0.00018	0.0005	0.0015	0.005	0.00013	0.005	0.01	0.0028	0.0023	0.005	0.0145	0.002	0.00027
0.019	0.00018	0.0017	0.00014	0.005	0.00013	0.005	0.01	0.0026	0.000145	0.005	0.01	0.002	0.00027
0.0032	0.00018	0.0005	0.0017	0.005	0.00013	0.005	0.02	0.0041	0.0024	0.005	0.0095	0.002	0.00027
0.0053	0.00018	0.0005	0.0008	0.005	0.00013	0.005	0.01	0.0028	0.0016	0.005	0.0145	0.002	0.00027
0.0023	0.00018	0.0005	0.0008	0.005	0.00013	0.01	0.01	0.0037	0.0017	0.005	0.00125	0.002	0.00027
0.0048	0.00018	0.0005	0.00014	0.005	0.00013	0.005	0.01	0.0032	0.000145	0.005	0.0085	0.002	0.00027
0.0046	0.00018	0.0005	0.0017	0.005	0.00013	0.005	0.01	0.0016	0.0024	0.005	0.00125	0.002	0.00027
0.00009	0.00018	0.0005	0.0024	0.005	0.00013	0.005	0.01	0.003	0.0031	0.005	0.0075	0.002	0.00027
0.00009	0.00018	0.0005	0.0004	0.005	0.00013	0.005	0.02	0.002	0.0013	0.005	0.0085	0.002	0.00027
0.00009	0.00018	0.0005	0.0021	0.005	0.00013	0.005	0.03	0.0025	0.0029	0.005	0.003	0.004	0.00027
0.00009	0.00018	0.0005	0.0003	0.005	0.00013	0.005	0.04	0.0018	0.0012	0.005	0.00125	0.002	0.00027
0.00009	0.00018	0.0005	0.0019	0.005	0.00013	0.005	0.02	0.0026	0.0027	0.005	0.005	0.002	0.00027
0.00009	0.007	0.0015	0.0019	0.005	0.00013	0.005	0.02	0.0021	0.0027	0.005	0.008	0.002	0.00027
0.0025	0.0028	0.0005	0.00014	0.005	0.0022	0.005	0.02	0.0021	0.000145	0.005	0.003	0.002	0.0044
0.00009	0.003	0.0005	0.00014	0.005	0.00013	0.005	0.01	0.0027	0.000145	0.005	0.008	0.002	0.00027
0.0027	0.0026	0.0017	0.00014	0.005	0.00013	0.005	0.03	0.0025	0.000145	0.005	0.009	0.002	0.00027
0.00031	0.00018	0.0005	0.0057	0.005	0.0012	0.005	0.02	0.0028	0.0063	0.005	0.0095	0.007	0.0034
0.0018	0.00018	0.0051	0.0018	0.005	0.00013	0.005	0.01	0.000165	0.0026	0.005	0.00125	0.004	0.00027
0.00009	0.00018	0.0005	0.0025	0.005	0.001	0.005	0.01	0.0027	0.0033	0.005	0.0135	0.008	0.0031
0.00039	0.00018	0.0017	0.0041	0.005	0.00013	0.005	0.01	0.0017	0.0048	0.005	0.0085	0.002	0.00027
0.0038	0.00018	0.0005	0.00014	0.005	0.00013	0.005	0.01	0.0039	0.000145	0.005	0.00125	0.002	0.00027
0.00009	0.00018	0.0021	0.0083	0.005	0.00013	0.005	0.01	0.0027	0.0086	0.005	0.007	0.005	0.00027
0.00096	0.012	0.0019	0.0042	0.005	0.0013	0.005	0.01	0.0028	0.0082	0.005	0.005	0.005	0.0034
0.0017	0.0028	0.0005	0.0014	0.005	0.00013	0.005	0.01	0.000165	0.0022	0.005	0.00125	0.005	0.00027
0.0064	0.0057	0.0005	0.0019	0.005	0.00013	0.005	0.01	0.002	0.0027	0.005	0.0045	0.006	0.00027
0.0031	0.0034	0.0029	0.0066	0.01	0.00013	0.01	0.01	0.0018	0.0072	0.005	0.00125	0.002	0.00027
0.00009	0.0005	0.0005	0.0011	0.005	0.00013	0.005	0.01	0.0025	0.0019	0.005	0.0065	0.002	0.00027
0.00009	0.0024	0.0038	0.0011	0.005	0.0013	0.005	0.01	0.0029	0.0019	0.005	0.00125	0.01	0.0034
0.00009	0.00018	0.0005	0.0011	0.005	0.00013	0.005	0.01	0.002	0.0019	0.005	0.0025	0.006	0.00027
0.00045	0.00018	0.0005	0.00014	0.005	0.00013	0.005	0.02	0.0025	0.000145	0.005	0.0025	0.006	0.00027
0.0018	0.0027	0.0005	0.00014	0.005	0.00013	0.005	0.01	0.0014	0.000145	0.005	0.00125	0.006	0.00027
0.00009	0.00018	0.0005	0.00014	0.005	0.00013	0.005	0.01	0.000165	0.000145	0.005	0.003	0.007	0.00027
0.00009	0.0034	0.0026	0.0068	0.005	0.00013	0.005	0.01	0.00088	0.0074	0.005	0.00125	0.009	0.00027
0.00009	0.0032	0.0092	0.0087	0.005	0.00013	0.01	0.01	0.00077	0.0092	0.005	0.00125	0.01	0.00027
0.0019	0.0027	0.0005	0.0022	0.005	0.00013	0.005	0.01	0.0025	0.003	0.005	0.005	0.002	0.00027
0.00009	0.0026	0.0005	0.00014	0.005	0.00013	0.005	0.01	0.0016	0.000145	0.005	0.0025	0.005	0.00027
0.0044	0.0027	0.0015	0.00014	0.005	0.0015	0.005	0.01	0.0017	0.000145	0.005	0.00125	0.007	0.0036
0.00009	0.00018	0.0005	0.00014	0.005	0.0023	0.005	0.01	0.0014	0.000145	0.005	0.00125	0.002	0.0045

Terbutylazine-desethyl-2-hydroxy	Diazinone	Fipronil	4-Chlorophenol	Azoxystrobin	Carbendazim	Cyproconazol	Flusilazole	Metalaxyl NOA 409045	Picoxystrobin	Propiconazole	Quinoxyfen	Tebuconazol	Trifloxystrobin CGA 321113
0.015	0.004	0.01	0.0005	0.001	0.004	0.0025	0.0015	0.003	0.04	0.0015	0.01	0.001	0.0025
0.015	0.003	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.01	0.004	0.008	0.001	0.0025
0.015	0.001	0.01	0.0015	0.001	0.005	0.0025	0.0015	0.003	0.005	0.006	0.005	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.002	0.007	0.0025	0.0015	0.003	0.005	0.004	0.004	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.004	0.0025	0.0015	0.003	0.005	0.004	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0006	0.001	0.002	0.0025	0.0015	0.003	0.005	0.003	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.005	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.004	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.004	0.002	0.005	0.0015	0.003	0.005	0.0015	0.002	0.006	0.0025
0.1	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.008	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.005	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.003	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.002	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.009	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.008	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.008	0.0025	0.0015	0.006	0.005	0.003	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.003	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.003	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.003	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.002	0.01	0.0005	0.001	0.007	0.005	0.0015	0.003	0.005	0.0015	0.002	0.004	0.005
0.015	0.0005	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.001	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.003	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.009	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.004	0.01	0.0005	0.002	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.001	0.01	0.0005	0.001	0.008	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.001	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.001	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.007	0.009	0.0025	0.0015	0.003	0.005	0.003	0.002	0.002	0.0025
0.015	0.001	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.001	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.002	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.001	0.01	0.0005	0.001	0.007	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.001	0.01	0.0005	0.001	0.02	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.007	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.02	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.008	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.03	0.0005	0.01	0.0005	0.001	0.02	0.0025	0.003	0.003	0.005	0.0015	0.002	0.005	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.006	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.007	0.02	0.0005	0.004	0.04	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.003	0.002	0.001	0.0025
0.015	0.001	0.01	0.0005	0.001	0.007	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.003	0.01	0.0005	0.001	0.009	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.002	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.005	0.0025
0.015	0.001	0.01	0.0005	0.001	0.002	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.001	0.01	0.0005	0.001	0.007	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.001	0.0025
0.015	0.001	0.01	0.0005	0.001	0.01	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.003	0.0025
0.015	0.0005	0.01	0.0005	0.001	0.009	0.0025	0.0015	0.003	0.005	0.0015	0.002	0.002	0.0025

10,11-Dihydro-10,11-dihydroxycarbamazepine	10,11-Dihydro-10-hydroxycarbamazepine	17-beta Estradiol	1-Adamantylamin	2-Hydroxycarbamazepine	3,4-Methylendioxyamphetamine (MDA)	3,4-Methylenedioxyethamphetamine (MDEA)	6-Acetylmorphine	7-Aminoclonazepam	7-Aminoflunitrazepam	Acetylcodeine	Acetyl-sulfamethoxazole	Alfentanil	alpha-Hydroxyalprazolam
0.029	0.0054	0.0015	0.0025	0.005	0.0043	0.0048	0.00095	0.0024	0.00086	0.0035	0.01	0.001	0.055
0.068	0.0045	0.0005	0.0025	0.005	0.0018	0.0048	0.0041	0.0021	0.001	0.0005	0.01	0.00037	0.049
0.045	0.005	0.0052	0.008	0.005	0.0029	0.015	0.0041	0.0005	0.0013	0.0037	0.01	0.001	0.08
0.044	0.0024	0.029	0.0025	0.005	0.0015	0.0042	0.0043	0.0021	0.00074	0.0005	0.01	0.00065	0.065
0.073	0.0044	0.023	0.0025	0.005	0.0005	0.0074	0.0027	0.0024	0.00087	0.0005	0.01	0.00057	0.06
0.05	0.0017	0.0019	0.0025	0.005	0.0023	0.005	0.0011	0.0034	0.0016	0.0055	0.01	0.00094	0.099
0.029	0.0012	0.0048	0.0025	0.005	0.0005	0.005	0.0011	0.0025	0.0015	0.0041	0.01	0.00024	0.089
0.026	0.0017	0.0078	0.0025	0.005	0.0079	0.0052	0.00095	0.0038	0.00082	0.003	0.01	0.00028	0.075
0.055	0.0054	0.0032	0.0025	0.005	0.0095	0.001	0.0043	0.0032	0.00061	0.0005	0.01	0.003	0.021
0.03	0.0005	0.0005	0.0025	0.005	0.011	0.0021	0.00091	0.0005	0.0013	0.0033	0.01	0.0003	0.15
0.054	0.0027	0.0005	0.0025	0.014	0.0023	0.0028	0.0005	0.0005	0.0015	0.0005	0.01	0.00016	0.1
0.11	0.0022	0.0005	0.0025	0.011	0.024	0.0005	0.0015	0.0005	0.0012	0.0005	0.01	0.0075	0.12
0.035	0.0017	0.0005	0.0025	0.005	0.016	0.002	0.00091	0.0022	0.0013	0.0005	0.01	0.0076	0.11
0.031	0.0015	0.0005	0.0025	0.005	0.019	0.0017	0.0011	0.002	0.0014	0.0005	0.01	0.0005	0.11
0.062	0.0031	0.0005	0.0025	0.005	0.092	0.0022	0.00087	0.0021	0.00094	0.0038	0.01	0.0063	0.1
0.15	0.0024	0.0005	0.01	0.005	0.0035	0.0005	0.0005	0.0029	0.0005	0.0045	0.01	0.0011	0.15
0.058	0.0005	0.0005	0.0025	0.005	0.0005	0.0028	0.00073	0.002	0.00084	0.0005	0.01	0.0019	0.073
0.093	0.0018	0.0005	0.03	0.005	0.027	0.0024	0.0005	0.0021	0.001	0.0005	0.01	0.0019	0.046
0.049	0.0015	0.0005	0.0025	0.005	0.0005	0.00084	0.0011	0.002	0.00097	0.0037	0.01	0.0005	0.05
0.021	0.0024	0.0005	0.0025	0.005	0.0019	0.0054	0.00087	0.0019	0.00096	0.0034	0.01	0.00066	0.069
0.065	0.001	0.0005	0.0025	0.005	0.054	0.0047	0.00097	0.0034	0.00062	0.0031	0.01	0.0005	0.063
0.08	0.0027	0.0005	0.0025	0.005	0.0005	0.0038	0.00097	0.0005	0.0005	0.0031	0.01	0.0005	0.058
0.14	0.0014	0.0005	0.009	0.005	0.0058	0.0016	0.0005	0.0019	0.00067	0.0005	0.01	0.0005	0.099
0.08	0.0023	0.0005	0.006	0.005	0.0005	0.0005	0.00095	0.0019	0.00065	0.0035	0.01	0.002	0.053
0.043	0.0005	0.0005	0.0025	0.005	0.00045	0.0005	0.00095	0.0005	0.00067	0.0033	0.01	0.00012	0.069
0.042	0.0012	0.0005	0.0025	0.005	0.0033	0.0017	0.00092	0.002	0.00063	0.0029	0.01	0.0005	0.098
0.057	0.0005	0.0005	0.0025	0.005	0.003	0.0076	0.00082	0.0005	0.00062	0.0031	0.01	0.0005	0.066
0.06	0.0005	0.0005	0.009	0.005	0.011	0.0034	0.00081	0.0021	0.00063	0.0029	0.01	0.0036	0.089
0.037	0.0018	0.0005	0.0025	0.005	0.091	0.0027	0.0008	0.0024	0.00062	0.003	0.01	0.0005	0.058
0.052	0.0029	0.0005	0.0025	0.005	0.0005	0.0031	0.0005	0.002	0.0006	0.0029	0.01	0.00045	0.06
0.036	0.0005	0.0005	0.0025	0.005	0.0051	0.0038	0.0005	0.0032	0.00066	0.0005	0.01	0.001	0.052
0.05	0.0005	0.0005	0.01	0.005	0.013	0.0022	0.0005	0.0005	0.0006	0.003	0.01	0.0018	0.047
0.051	0.0005	0.0005	0.0025	0.005	0.072	0.0027	0.0005	0.0028	0.00062	0.003	0.01	0.0005	0.075
0.045	0.0011	0.0005	0.0025	0.005	0.0005	0.003	0.00083	0.0025	0.00059	0.003	0.01	0.00016	0.076
0.084	0.0005	0.0005	0.01	0.005	0.19	0.0005	0.0009	0.0066	0.0006	0.003	0.01	0.0005	0.067
0.039	0.0005	0.0005	0.008	0.005	0.066	0.0031	0.0005	0.0033	0.0005	0.0005	0.01	0.0005	0.052
0.024	0.001	0.0005	0.0025	0.005	0.01	0.0063	0.0005	0.0021	0.00059	0.0005	0.01	0.0005	0.052
0.034	0.0011	0.0005	0.01	0.005	0.0005	0.00058	0.0005	0.0005	0.00059	0.0005	0.01	0.00098	0.051
0.039	0.004	0.0005	0.01	0.005	0.011	0.0024	0.0005	0.002	0.00062	0.0005	0.01	0.0005	0.057
0.043	0.0009	0.0005	0.0025	0.005	0.62	0.0045	0.0005	0.014	0.00094	0.0005	0.01	8.90E-05	0.052
0.11	0.0011	0.0005	0.01	0.011	0.05	0.0015	0.00079	0.0025	0.0006	0.0032	0.063	0.0019	0.052
0.04	0.0005	0.0005	0.009	0.005	0.44	0.0028	0.00096	0.013	0.00062	0.0031	0.02	0.00042	0.052
0.042	0.0005	0.0005	0.01	0.005	0.11	0.0016	0.0005	0.0047	0.0005	0.0005	0.01	0.0005	0.049
0.043	0.0005	0.0005	0.01	0.005	0.32	0.0046	0.0005	0.0081	0.00061	0.0005	0.01	0.0005	0.048
0.044	0.0005	0.0005	0.0025	0.005	0.58	0.0018	0.0005	0.012	0.00071	0.0005	0.01	0.00091	0.048
0.045	0.0005	0.0005	0.0025	0.005	0.049	0.0013	0.0005	0.0037	0.0005	0.0005	0.01	0.0005	0.051
0.041	0.0035	0.0005	0.007	0.005	0.0005	0.002	0.23	0.0005	0.0005	0.0078	0.01	0.00022	0.062
0.075	0.0056	0.0005	0.09	0.014	0.00013	0.002	0.22	0.0005	0.0005	0.0075	0.042	0.0005	0.07
0.043	0.0024	0.0005	0.0025	0.005	7.30E-05	0.002	0.22	0.0005	0.0005	0.0076	0.01	0.00015	0.056
0.041	0.0054	0.0005	0.008	0.005	0.0005	0.0016	0.24	0.002	0.0005	0.0064	0.01	0.00085	0.045
0.13	0.0025	0.0005	0.0025	0.012	5.50E-05	0.002	0.0048	0.0055	0.00078	0.0072	0.01	0.0005	0.0035
0.04	0.0005	0.0005	0.0025	0.005	0.0005	0.0005	0.0029	0.0019	0.0005	0.018	0.01	0.0005	0.005
0.034	0.0009	0.0005	0.0025	0.005	0.00039	0.0005	0.0028	0.0021	0.00072	0.019	0.01	8.60E-05	0.0053
0.032	0.001	0.0005	0.01	0.005	0.013	0.0011	0.0005	0.002	0.0005	0.0005	0.01	0.0005	0.00024
0.036	0.0005	0.0005	0.005	0.005	2.90E-06	0.0005	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.00042
0.086	0.004	0.0005	0.01	0.011	0.0068	0.0014	0.0005	0.0019	0.0005	0.003	0.045	0.0005	0.0018
0.035	0.0005	0.0005	0.0025	0.005	0.0005	0.00099	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.00024
0.16	0.0088	0.0005	0.04	0.045	0.0036	0.0044	0.0005	0.0005	0.00069	0.0053	0.023	0.0005	0.00086
0.038	0.0005	0.0005	0.0025	0.005	0.024	0.00035	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.12
0.041	0.0005	0.0005	0.0025	0.005	0.0005	0.00019	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.00022
0.05	0.0005	0.0005	0.0025	0.005	0.0005	0.00036	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.11
0.043	0.0005	0.0005	0.0025	0.005	0.0005	0.00069	0.0005	0.0005	0.0005	0.0005	0.01	0.00029	0.1
0.013	0.0005	0.0005	0.0025	0.005	0.023	0.00079	0.0005	0.0005	0.0005	0.0005	0.01	0.00077	0.15
0.016	0.0024	0.0005	0.0025	0.005	0.0034	0.0016	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.16
0.037	0.0005	0.0005	0.0025	0.005	0.0005	0.001	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.14
0.036	0.0005	0.0005	0.0025	0.005	0.0005	0.00032	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.13
0.046	0.0018	0.0005	0.0025	0.005	0.0005	0.00062	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.14
0.034	0.0005	0.0005	0.007	0.005	0.0005	0.0011	0.0005	0.0005	0.0005	0.0005	0.01	0.0005	0.12

alpha-Hydroxymidazolam	alpha-Hydroxytriazolam	Alprazolam	Amidotrizoic acid	Amisulpride	Amitriptyline	Amoxapine	Amoxicillin	Amphetamine	Atenolol	Atropine	Benzoylecgonine	Betaxolol	Bezafibrate
0.00094	0.0056	0.0045	0.25	0.0093	0.0078	0.00045	0.012	0.0005	0.03	0.016	0.0042	0.005	0.0025
0.00099	0.0082	0.0067	0.25	0.0098	0.0092	0.00045	0.017	0.0005	0.005	0.028	0.005	0.005	0.0025
0.002	0.0071	0.012	0.25	0.014	0.012	0.00074	0.035	0.0005	0.005	0.033	0.00023	0.005	0.0025
0.00077	0.0055	0.01	0.25	0.011	0.012	0.00049	0.048	0.0005	0.005	0.037	0.007	0.005	0.0025
0.00059	0.0026	0.0066	0.25	0.014	0.011	0.0005	0.011	0.0005	0.005	0.031	0.00084	0.005	0.0025
0.00075	0.0051	0.01	0.25	0.0092	0.0025	0.00084	0.026	0.0005	0.005	0.02	0.0051	0.005	0.0025
0.0019	0.0054	0.0077	0.25	0.003	0.0047	0.0005	0.0091	0.0005	0.005	0.016	0.0062	0.005	0.0025
0.00066	0.0061	0.011	0.25	0.00054	0.0073	0.00062	0.0096	0.0005	0.005	0.015	0.0089	0.005	0.0025
0.0079	0.0005	0.0096	0.25	0.0044	0.0023	0.0038	0.13	0.004	0.005	0.16	6.60E-05	0.005	0.0025
0.0012	0.0076	0.0023	0.25	0.0034	0.0005	0.0005	0.0092	0.0005	0.005	0.013	0.0005	0.005	0.0025
0.0023	0.0061	0.002	0.25	0.0071	0.0018	0.0005	0.011	0.0005	0.005	0.004	0.00022	0.005	0.0025
0.00081	0.006	0.0031	0.25	0.002	0.0005	0.00047	0.28	0.0005	0.005	0.021	0.0005	0.005	0.0025
0.00044	0.01	0.0027	0.25	0.0048	0.0005	0.0005	0.0088	0.0005	0.005	0.012	0.0005	0.005	0.0025
0.0005	0.013	0.002	0.25	0.0046	0.0005	0.00047	0.017	0.0005	0.005	0.016	0.0005	0.005	0.0025
0.0005	0.0066	0.0043	0.25	0.002	0.0018	0.0005	0.009	0.0005	0.005	0.013	0.0005	0.005	0.0025
0.0005	0.0066	0.0005	0.5	0.008	0.0048	0.0022	0.034	0.0005	0.01	0.038	0.0089	0.005	0.0025
0.0005	0.0059	0.0005	0.25	0.0029	0.0041	0.00064	0.0096	0.0005	0.005	0.019	0.0085	0.005	0.005
0.0005	0.0075	0.0005	0.25	0.0018	0.0041	0.00028	0.011	0.0005	0.02	0.0038	0.0003	0.005	0.0025
0.00058	0.0029	0.0063	0.25	0.0017	0.004	0.00068	0.0098	0.0018	0.005	0.017	0.00063	0.005	0.0025
0.0005	0.0065	0.0052	0.25	0.0015	0.0047	0.0005	0.0089	0.0005	0.005	0.021	0.0066	0.005	0.0025
0.0005	0.0056	0.0005	0.25	0.0024	0.0029	0.0012	0.01	0.0024	0.005	0.0025	0.0089	0.005	0.0025
0.0005	0.0005	0.0048	0.25	0.0035	0.003	0.0009	0.0091	0.0019	0.005	0.021	0.0056	0.005	0.0025
0.0005	0.0005	0.0073	0.25	0.0005	0.0025	0.00061	0.01	0.001	0.005	0.011	0.0025	0.005	0.0025
0.0005	0.0005	0.0019	0.25	0.0008	0.0051	0.00075	0.0095	0.0019	0.005	0.018	0.007	0.005	0.0025
0.0005	0.0057	0.0068	0.25	0.0033	0.0021	0.00036	0.0099	0.00071	0.005	0.0072	0.0033	0.005	0.0025
0.0005	0.0067	0.0061	0.25	0.0026	0.005	0.00064	0.0094	0.001	0.005	0.02	0.0022	0.005	0.0025
0.0005	0.0055	0.0005	0.25	0.0019	0.0048	0.00057	0.0005	0.0027	0.005	0.02	0.0055	0.005	0.0025
0.0005	0.0005	0.0005	0.25	0.0022	0.0019	0.0011	0.018	0.00092	0.005	0.0097	0.005	0.005	0.0025
0.0005	0.0005	0.0034	0.25	0.00059	0.0025	0.0005	0.0005	0.0012	0.005	0.0081	0.0025	0.005	0.0025
0.0005	0.0005	0.0012	0.25	0.0006	0.0038	0.00054	0.009	0.0005	0.005	0.013	0.0051	0.005	0.0025
0.0005	0.0005	0.0022	0.25	0.00064	0.0029	0.00025	0.0005	0.0005	0.005	0.015	0.0051	0.005	0.0025
0.0005	0.0005	0.0031	0.25	0.00032	0.0033	0.00053	0.0015	0.00096	0.005	0.028	0.0079	0.005	0.0025
0.0005	0.0005	0.0021	0.25	0.0005	0.002	0.00054	0.0005	0.0018	0.005	0.012	0.0024	0.005	0.0025
0.0005	0.0005	0.0023	0.25	0.00035	0.0034	0.00084	0.0005	0.00077	0.005	0.018	0.0051	0.005	0.0025
0.0005	0.0005	0.0022	0.25	0.0005	0.0005	0.0014	0.009	0.0005	0.01	0.019	0.0044	0.005	0.0025
0.0005	0.0005	0.0042	0.25	0.0011	0.0036	0.00074	0.0005	0.00057	0.005	0.0096	0.0042	0.005	0.0025
0.0005	0.0005	0.0043	0.25	0.00094	0.0034	0.0005	0.0005	0.0005	0.005	0.02	0.0077	0.005	0.0025
0.0005	0.0099	0.0035	0.25	0.0021	0.0042	0.0005	0.0005	0.0017	0.005	0.0094	5.20E-05	0.005	0.0025
0.0005	0.0057	0.0034	0.25	0.00043	0.0035	0.00055	0.0005	0.00084	0.01	0.012	0.0007	0.005	0.0025
0.0005	0.0095	0.0005	0.25	0.0021	0.0027	0.001	0.0005	0.0005	0.005	0.02	0.0014	0.005	0.0025
0.0005	0.0056	0.0024	0.25	0.0016	0.0019	0.0015	0.0005	0.00055	0.02	0.011	0.0004	0.005	0.0025
0.0005	0.0005	0.0016	0.25	0.00047	0.0029	0.00073	0.009	0.00068	0.005	0.021	0.0026	0.005	0.0025
0.0005	0.0063	0.0016	0.25	0.00091	0.0024	0.00067	0.0091	0.00081	0.01	0.018	0.0043	0.005	0.0025
0.0005	0.0005	0.0005	0.25	0.00041	0.0023	0.0005	0.0087	0.00059	0.005	0.019	0.0065	0.005	0.0025
0.0005	0.0005	0.0017	0.25	0.00045	0.0024	0.00052	0.0005	0.0005	0.005	0.019	0.0036	0.005	0.0025
0.0005	0.0005	0.0016	0.25	0.00028	0.0026	0.0005	0.0005	0.0005	0.005	0.0092	0.00095	0.005	0.0025
0.0005	0.0071	0.009	0.25	0.0042	0.0059	0.00039	0.0005	0.0005	0.005	0.0015	0.0041	0.005	0.0025
0.0005	0.0005	0.0068	0.25	0.0042	0.0069	0.00047	0.0005	0.0005	0.02	0.002	0.0048	0.005	0.0025
0.0005	0.0005	0.0057	0.25	0.0037	0.0098	0.00044	0.0005	0.0005	0.005	0.0017	0.0059	0.005	0.0025
0.0005	0.0005	0.004	0.25	0.0047	0.0099	0.00046	0.0005	0.0005	0.005	0.0024	0.0059	0.005	0.0025
0.0005	0.0005	0.004	0.25	0.003	0.013	0.00049	0.0005	0.0005	0.01	0.0023	0.0025	0.005	0.0025
0.00061	0.0075	0.0005	0.25	0.004	0.013	0.00084	0.0005	0.0005	0.005	0.0015	0.0081	0.005	0.0025
0.0005	0.016	0.0005	0.25	0.0038	0.011	0.0005	0.0005	0.0005	0.005	0.0017	0.0046	0.005	0.0025
0.0005	0.01	0.0053	0.25	0.0011	0.0005	0.0011	0.0005	0.0005	0.005	0.013	0.0036	0.005	0.0025
0.0005	0.0005	0.0037	0.25	0.0005	0.0023	0.0005	0.0005	0.0005	0.005	0.011	0.0043	0.005	0.0025
0.0005	0.0005	0.0017	0.25	0.0083	0.0026	0.00045	0.0005	0.0005	0.03	0.075	0.0031	0.005	0.0025
0.0005	0.0005	0.0008	0.25	0.0005	0.0017	0.00054	0.0005	0.0005	0.005	0.0015	0.0026	0.005	0.0025
0.0005	0.0005	0.0015	0.25	0.031	0.006	0.0005	0.0005	0.0005	0.2	0.14	0.0012	0.01	0.0025
0.0005	0.0085	0.0041	0.25	0.00051	0.0022	0.00046	0.0005	0.0005	0.02	0.0096	0.0032	0.005	0.0025
0.0005	0.0005	0.0021	0.25	0.0003	0.0022	0.0005	0.0005	0.011	0.02	0.0093	0.0017	0.005	0.0025
0.0005	0.0005	0.0015	0.25	0.0005	0.0005	0.0005	0.0005	0.0005	0.01	0.01	0.0031	0.005	0.0025
0.0005	0.0005	0.0033	0.25	0.00064	0.0005	0.0021	0.0005	0.00045	0.005	0.011	0.0036	0.005	0.0025
0.0005	0.0005	0.003	0.25	0.00063	0.002	0.00055	0.0005	0.0005	0.005	0.0095	0.0033	0.005	0.0025
0.0005	0.0005	0.0035	0.25	0.00033	0.0005	0.00046	0.0005	0.0005	0.005	0.011	0.0039	0.005	0.0025
0.0005	0.0005	0.0025	0.25	0.00033	0.0005	0.00075	0.0005	0.0005	0.005	0.0084	0.0026	0.005	0.0025
0.0005	0.0005	0.002	0.25	0.0005	0.0023	0.00049	0.0005	0.0005	0.005	0.0079	0.0025	0.005	0.0025
0.0005	0.0005	0.0031	0.25	0.0005	0.0005	0.00052	0.0005	0.0005	0.005	0.0083	0.0025	0.005	0.0025
0.0005	0.012	0.0027	0.25	0.0005	0.0005	0.00067	0.0005	0.0005	0.01	0.0092	0.0025	0.005	0.0025

Bisoprolol	Bromazepam	Buprenorphine	Buprenorphine glucuronide	Candesartan	Carbamazepine	Carbamazepine-10,11-epoxide	Carisoprodol	Cetirizine	Chlorprothixene	Citalopram	Clobazam (Urbadan)	Clonazepam	Clonidine
0.009	0.0005	0.025	0.0005	0.004	0.02	0.0035	0.0025	0.005	0.0012	0.0018	0.0005	0.04	0.0013
0.005	0.011	0.034	0.2	0.02	0.032	0.0035	0.46	0.005	0.0013	0.0015	0.011	0.034	0.0005
0.007	0.0005	0.038	0.0005	0.004	0.03	0.0035	0.02	0.005	0.0039	0.0005	0.0005	0.0005	0.0013
0.008	0.0005	0.025	0.0005	0.02	0.034	0.0035	0.013	0.005	0.0013	0.0005	0.0005	0.0005	0.0005
0.006	0.0005	0.0062	0.044	0.01	0.033	0.0035	0.03	0.005	0.0019	0.0005	0.005	0.0038	0.0013
0.007	0.012	0.011	0.0005	0.004	0.028	0.0035	0.021	0.005	0.0015	0.0011	0.0005	0.041	0.0013
0.0015	0.0005	0.0092	0.0005	0.01	0.024	0.0035	0.0019	0.005	0.00083	0.0005	0.0005	0.042	0.0013
0.0015	0.0005	0.014	0.0005	0.009	0.017	0.0035	0.012	0.005	0.0005	0.0005	0.0005	0.034	0.0005
0.0015	0.015	0.062	0.039	0.01	0.023	0.0035	0.029	0.005	0.014	0.0005	0.0005	0.029	0.0013
0.0015	0.0005	0.025	0.0005	0.01	0.019	0.0035	0.003	0.005	0.00078	0.0005	0.0005	0.28	0.0005
0.0015	0.0005	0.018	0.0005	0.01	0.023	0.0035	0.0026	0.005	0.0014	0.0014	0.0005	0.26	0.0014
0.0015	0.0005	0.02	0.0005	0.01	0.047	0.0035	0.013	0.018	0.0012	0.0011	0.0005	0.25	0.0005
0.0015	0.0005	0.021	0.0005	0.01	0.016	0.0035	0.0037	0.005	0.0005	0.0005	0.0005	0.24	0.0005
0.0015	0.0005	0.02	0.0005	0.01	0.022	0.0035	0.0051	0.005	0.0012	0.0005	0.0005	0.22	0.0005
0.0015	0.0005	0.021	0.0005	0.02	0.025	0.0035	0.015	0.005	0.0005	0.0005	0.0005	0.21	0.0005
0.008	0.012	0.022	0.0005	0.025	0.059	0.01	0.019	0.005	0.0015	0.0005	0.0005	0.05	0.0005
0.0015	0.0005	0.017	0.0005	0.02	0.027	0.0035	0.0086	0.005	0.0018	0.0005	0.0005	0.05	0.0005
0.0015	0.015	0.019	0.0005	0.01	0.031	0.0035	0.025	0.014	0.0005	0.0005	0.0005	0.0029	0.0013
0.0015	0.0005	0.022	0.0005	0.02	0.032	0.0035	0.0005	0.011	0.0013	0.0005	0.0039	0.042	0.0013
0.0015	0.0005	0.018	0.0005	0.02	0.035	0.0035	0.009	0.005	0.0005	0.0005	0.0005	0.021	0.0005
0.0015	0.018	0.015	0.0005	0.02	0.027	0.0035	0.017	0.005	0.0012	0.0005	0.0005	0.0079	0.0005
0.0015	0.0005	0.019	0.0005	0.01	0.035	0.0035	0.0073	0.005	0.0005	0.0005	0.0005	0.022	0.0005
0.0015	0.0005	0.017	0.0005	0.004	0.043	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.0022	0.0005
0.0015	0.0005	0.0055	0.0005	0.01	0.035	0.0035	0.0063	0.005	0.0005	0.0005	0.0032	0.018	0.0005
0.0015	0.0005	0.014	0.0005	0.02	0.032	0.0035	0.08	0.005	0.0005	0.0005	0.0005	0.0055	0.0005
0.0015	0.014	0.016	0.0005	0.02	0.025	0.0035	0.0096	0.005	0.0013	0.0005	0.0005	0.011	0.0005
0.005	0.0005	0.013	0.0005	0.02	0.032	0.0035	0.015	0.005	0.0012	0.0005	0.0005	0.0098	0.0005
0.003	0.0005	0.014	0.0005	0.02	0.047	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.009	0.0005
0.0015	0.0005	0.012	0.0005	0.01	0.027	0.0035	0.0022	0.005	0.0005	0.0017	0.0032	0.0005	0.0005
0.0015	0.0005	0.013	0.0005	0.01	0.029	0.0035	0.034	0.005	0.0005	0.0005	0.0005	0.0068	0.0005
0.0015	0.0005	0.011	0.0005	0.02	0.021	0.0035	0.0023	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.012	0.0005	0.02	0.033	0.009	0.22	0.005	0.0012	0.0057	0.0056	0.0005	0.0005
0.0015	0.0005	0.015	0.0005	0.02	0.036	0.0035	0.0036	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.022	0.012	0.0005	0.02	0.031	0.0035	0.018	0.005	0.0005	0.0005	0.0005	0.0036	0.0005
0.0015	0.012	0.011	0.0005	0.004	0.034	0.009	0.0075	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.01	0.011	0.0005	0.01	0.022	0.0035	0.0032	0.005	0.0005	0.0005	0.0005	0.0032	0.0005
0.0015	0.017	0.0075	0.0005	0.01	0.0089	0.0035	0.0005	0.005	0.0005	0.0005	0.0036	0.0005	0.0005
0.004	0.014	0.012	0.0005	0.01	0.022	0.007	0.0005	0.005	0.0005	0.0005	0.0005	0.0037	0.0005
0.0015	0.012	0.0094	0.0005	0.01	0.02	0.0035	0.0069	0.005	0.0005	0.0092	0.0005	0.0005	0.0005
0.0015	0.011	0.011	0.0005	0.01	0.023	0.0035	0.0064	0.005	0.0005	0.0005	0.0026	0.0005	0.0005
0.009	0.012	0.01	0.0005	0.004	0.027	0.01	0.0005	0.005	0.0005	0.0005	0.0051	0.0005	0.0005
0.0015	0.012	0.011	0.0005	0.01	0.024	0.0035	0.0087	0.005	0.0005	0.0005	0.0043	0.0005	0.0005
0.0015	0.013	0.0081	0.0005	0.01	0.025	0.0035	0.0042	0.005	0.0005	0.0005	0.0041	0.0043	0.0005
0.0015	0.014	0.0099	0.0005	0.01	0.025	0.0035	0.015	0.005	0.0005	0.0016	0.0005	0.0005	0.0005
0.0015	0.012	0.0091	0.0005	0.02	0.025	0.0035	0.0064	0.005	0.0005	0.0005	0.01	0.0005	0.0005
0.0015	0.012	0.0078	0.0005	0.02	0.024	0.0035	0.0038	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.009	0.0005	0.02	0.019	0.0035	0.25	0.005	0.0005	0.0005	0.0084	0.0005	0.0005
0.0015	0.0005	0.0094	0.0005	0.004	0.039	0.0035	0.076	0.005	0.0005	0.0005	0.0096	0.0005	0.0005
0.0015	0.0005	0.0092	0.0005	0.02	0.023	0.0035	0.0032	0.005	0.0005	0.0005	0.0061	0.0005	0.0005
0.0015	0.011	0.02	0.081	0.01	0.023	0.0035	0.0034	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.007	0.0005	0.004	0.034	0.01	0.0056	0.053	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.066	0.29	0.01	0.02	0.0035	0.0066	0.005	0.0035	0.0047	0.0046	0.0005	0.0005
0.0015	0.0005	0.07	0.18	0.01	0.018	0.0035	0.0039	0.005	0.0085	0.0036	0.0083	0.0005	0.0005
0.007	0.011	0.005	0.0005	0.004	0.0062	0.0035	0.012	0.005	0.0005	0.0063	0.0005	0.0005	0.0005
0.0015	0.0005	0.0043	0.0005	0.004	0.019	0.0035	0.0005	0.005	0.0005	0.0005	0.01	0.0005	0.0005
0.01	0.011	0.0029	0.0005	0.004	0.038	0.0035	0.0005	0.005	0.0005	0.0014	0.0005	0.0005	0.0005
0.0015	0.012	0.001	0.0005	0.01	0.018	0.0035	0.0033	0.005	0.0005	0.0005	0.0037	0.0005	0.0005
0.03	0.011	0.0032	0.0005	0.065	0.068	0.04	0.042	0.005	0.0005	0.0005	0.008	0.0005	0.0005
0.0015	0.012	0.0047	0.0005	0.01	0.024	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.0045	0.0005	0.02	0.023	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.011	0.0048	0.0005	0.01	0.024	0.0035	0.0005	0.005	0.0005	0.0056	0.0005	0.0005	0.0005
0.0015	0.0005	0.0043	0.33	0.01	0.02	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.0005	0.0005	0.008	0.0036	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.0028	0.0005	0.004	0.005	0.0035	0.011	0.005	0.0005	0.002	0.0005	0.0005	0.0005
0.0015	0.0005	0.006	0.0005	0.01	0.023	0.0035	0.0005	0.005	0.0005	0.0005	0.002	0.0005	0.0005
0.0015	0.012	0.0032	0.0005	0.009	0.023	0.0035	0.0005	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.0005	0.0037	0.0005	0.01	0.028	0.0035	0.0068	0.005	0.0005	0.0005	0.0005	0.0005	0.0005
0.0015	0.012	0.0005	0.0005	0.004	0.017	0.0035	0.014	0.005	0.0005	0.0005	0.0005	0.0005	0.0005

Clozapine	Cocaethylene	Cocaine	Codeine	CP 47,497	CP 47,497-C8 homologue	Crotamiton	Desalkylflurazepam	Desipramine	Dextromethorphan (Methorphan)	Diazepam	Diclofenac	Digitoxin	Digoxin
0.0005	0.0032	0.019	0.044	0.0091	0.0025	0.0015	0.0052	0.12	0.0029	0.012	0.011	0.042	0.01
0.0005	0.0024	0.029	0.042	0.0023	0.018	0.0015	0.0053	0.048	0.0039	0.018	0.018	0.03	0.024
0.012	0.002	0.024	0.11	0.0015	0.0077	0.0015	0.0087	0.03	0.004	0.016	0.01	0.037	0.0005
0.014	0.00054	0.035	0.041	0.0096	0.026	0.0015	0.0005	0.04	0.0028	0.015	0.0093	0.0005	0.0005
0.0005	0.0012	0.015	0.04	0.011	0.011	0.0015	0.0052	0.064	0.003	0.015	0.016	0.035	0.0005
0.0055	0.0045	0.0071	0.044	0.0073	0.12	0.0015	0.0087	0.058	0.0035	0.022	0.01	0.044	0.01
0.0005	0.00037	0.01	0.044	0.015	0.014	0.0015	0.0091	0.014	0.0034	0.019	0.0051	0.038	0.0005
0.0005	0.0005	0.024	0.06	0.0092	0.028	0.0015	0.0063	0.011	0.0041	0.021	0.0032	0.072	0.013
0.33	0.0016	0.064	0.0016	0.026	0.014	0.0015	0.051	0.0086	0.016	0.021	0.00017	0.05	0.0097
0.0033	0.0005	0.0005	0.0017	0.51	0.0005	0.0015	0.029	0.0097	0.0033	0.012	0.012	0.0005	0.0005
0.0042	0.0005	0.0005	0.0005	0.46	0.0005	0.0015	0.0005	0.019	0.0035	0.011	0.011	0.0005	0.0005
0.0065	0.0005	0.0005	0.0005	0.45	0.0005	0.0015	0.0005	0.026	0.0038	0.0047	0.021	0.0005	0.0005
0.014	0.00072	0.0005	0.0005	0.47	0.0005	0.0015	0.0005	0.023	0.0032	0.009	0.0037	0.0005	0.0005
0.0094	0.0005	0.0005	0.0005	0.46	0.0005	0.0015	0.0005	0.011	0.0033	0.0075	0.0067	0.0005	0.0005
0.0005	0.00071	0.0005	0.0005	0.46	0.0024	0.0015	0.0086	0.015	0.0036	0.0044	0.01	0.094	0.0005
0.092	0.0011	0.0065	0.034	0.07	0.0033	0.0015	0.0094	0.0077	0.0033	0.026	0.016	0.0005	0.014
0.069	0.0005	0.002	0.026	0.0005	0.014	0.0015	0.0005	0.011	0.0005	0.006	0.01	0.074	0.0005
0.005	0.0005	0.02	0.039	0.0005	0.0006	0.0015	0.0005	0.015	0.0029	0.00025	0.0097	0.11	0.0005
0.011	0.0005	0.0061	0.032	0.0005	0.0078	0.0015	0.0005	0.0065	0.003	0.00025	0.0036	0.0005	0.0005
0.022	0.0005	0.005	0.031	0.0005	0.0054	0.0015	0.0005	0.017	0.0029	0.00025	0.051	0.042	0.012
0.019	0.0005	0.004	0.02	0.0024	0.0043	0.0015	0.0005	0.0071	0.0041	0.00025	0.004	0.046	0.011
0.0072	0.00058	0.012	0.021	0.0005	0.0039	0.0015	0.0005	0.0084	0.0029	0.00025	0.015	0.0005	0.0005
0.01	0.00056	0.0034	0.023	0.0005	0.0047	0.0015	0.0005	0.0066	0.0042	0.00025	0.00017	0.0005	0.012
0.013	0.00046	0.0071	0.021	0.0005	0.0027	0.0015	0.0005	0.015	0.0005	0.007	0.0071	0.0005	0.0005
0.054	0.0005	0.0066	0.019	0.0005	0.0023	0.0015	0.0005	0.0085	0.0029	0.00025	0.0076	0.0005	0.0005
0.073	0.0005	0.0052	0.017		0.0005	0.0015	0.0005	0.0085	0.0005	0.0058	0.0066	0.0005	0.0005
0.03	0.00066	0.009	0.019	0.0005	0.0003	0.0015	0.0005	0.0005	0.0005	0.00025	0.0045	0.0005	0.0005
0.011	0.0005	0.0047	0.016	0.0005	0.0005	0.0015	0.0005	0.0082	0.0028	0.0053	0.0039	0.0005	0.0005
0.019	0.0005	0.0093	0.017	0.0005	0.0005	0.0015	0.0046	0.017	0.0029	0.00025	0.0039	0.0005	0.0005
0.028	0.0005	0.0063	0.02	0.0005	0.0005	0.0015	0.0005	0.013	0.0005	0.00025	0.0033	0.0005	0.0005
0.06	0.0005	0.0074	0.019	0.0099	0.0005	0.0015	0.0005	0.096	0.0029	0.00025	0.001	0.0005	0.0005
0.0095	0.0005	0.0046	0.022	0.0005	0.0005	0.0015	0.0005	0.012	0.0031	0.0081	0.0036	0.0005	0.0005
0.013	0.00065	0.0082	0.017	0.0005	0.0005	0.0015	0.0005	0.0055	0.0005	0.0049	0.0041	0.0005	0.0005
0.042	0.0005	0.0074	0.016	0.0005	0.0045	0.0015	0.0005	0.0055	0.003	0.00025	0.0037	0.0005	0.0005
0.0056	0.0005	0.0094	0.016	0.0005	0.0005	0.0015	0.0005	0.0005	0.0005	0.00025	0.0021	0.0005	0.0005
0.052	0.0005	0.0005	0.015	0.0005	0.0014	0.0015	0.0005	0.0047	0.003	0.00025	0.0038	0.0005	0.0005
0.021	0.0005	0.014	0.02	0.0005	0.0005	0.0015	0.0005	0.0051	0.0028	0.0048	0.00017	0.0005	0.0005
0.0044	0.0015	0.0094	0.014	0.0005	0.0025	0.003	0.0005	0.016	0.0005	0.0041	0.0037	0.0005	0.0005
0.0005	0.0005	0.0064	0.012	0.0005	0.00079	0.0015	0.0005	0.014	0.0005	0.0042	0.00017	0.0005	0.0005
0.0005	0.0005	0.0061	0.0095	0.0005	0.0005	0.0015	0.0005	0.011	0.0064	0.00025	0.0027	0.0005	0.0005
0.0005	0.0005	0.014	0.011	0.0039	0.0013	0.0015	0.0005	0.014	0.0005	0.0047	0.0057	0.0005	0.0005
0.0005	0.0005	0.011	0.011	0.0005	0.0019	0.0015	0.0005	0.011	0.0082	0.00025	0.0017	0.0005	0.0005
0.0005	0.0019	0.015	0.015	0.0005	0.0005	0.0015	0.0005	0.0099	0.0038	0.00025	0.0017	0.0005	0.0005
0.0005	0.00043	0.011	0.012	0.0005	0.0042	0.0015	0.0005	0.0081	0.003	0.00025	0.0037	0.0005	0.0005
0.0005	0.00063	0.016	0.0096	0.0005	0.0025	0.0015	0.0052	0.01	0.0084	0.00025	0.00017	0.0005	0.0005
0.0005	0.00052	0.007	0.0087	0.0005	0.0005	0.0015	0.0005	0.0092	0.0038	0.00025	0.00017	0.0005	0.0005
0.0005	0.00093	0.038	0.096	0.0005	0.00048	0.0015	0.0005	0.03	0.0055	0.00025	0.00017	0.0005	0.0005
0.0054	0.0025	0.025	0.1	0.0005	0.00011	0.0015	0.0005	0.004	0.0061	0.0043	0.0021	0.0005	0.0005
0.0005	0.0005	0.037	0.098	0.0005	0.0013	0.0015	0.0005	0.006	0.0051	0.00025	0.0014	0.0005	0.0005
0.0005	0.00095	0.0076	0.11	0.00089	0.0017	0.0015	0.0005	0.0037	0.0047	0.0041	0.00017	0.0005	0.0005
0.012	0.00098	0.0005	0.1	0.025	0.0057	0.0015	0.0005	0.0005	0.0039	0.00025	0.00097	0.0005	0.0088
0.0024	0.0005	0.011	0.11	0.027	0.0022	0.0015	0.0005	0.0011	0.0029	0.0047	0.00017	0.037	0.0005
0.0005	0.0005	0.0039	0.11	0.013	0.0026	0.0015	0.0005	0.0005	0.0033	0.0043	0.00017	0.047	0.0005
0.0005	0.00071	0.0082	0.074	0.0076	0.0064	0.0015	0.0053	0.07	0.0031	0.00025	0.0017	0.0005	0.0005
0.0061	0.00085	0.0066	0.062	0.0014	0.0033	0.0015	0.0005	0.07	0.0039	0.00025	0.00017	0.0005	0.0005
0.0042	0.0012	0.0076	0.065	0.013	0.001	0.0015	0.0047	0.054	0.0036	0.00025	0.069	0.0005	0.0005
0.0052	0.0004	0.0014	0.044	0.00092	0.0005	0.0015	0.0005	0.0005	0.0005	0.00025	0.00017	0.0005	0.0005
0.0023	0.00078	0.023	0.058	0.0029	0.00026	0.01	0.0005	0.036	0.0005	0.0041	0.25	0.0005	0.0005
0.0005	0.0006	0.0043	0.058	0.0084	0.00064	0.0015	0.0072	0.02	0.0005	0.00025	0.00017	0.0005	0.0005
0.0005	0.00068	0.0059	0.057	0.0015	0.00022	0.0015	0.0005	0.011	0.0005	0.00025	0.0049	0.0005	0.0005
0.0005	0.00094	0.0059	0.063	0.017	0.00052	0.0015	0.0005	0.0053	0.0005	0.00025	0.00017	0.0005	0.0005
0.0005	0.0011	0.0033	0.068	0.029	0.00088	0.0015	0.0005	0.016	0.0005	0.00025	0.00089	0.0005	0.0005
0.023	0.00073	0.002	0.066	0.0068	0.0005	0.0015	0.0078	0.039	0.0005	0.00025	0.0016	0.0005	0.0005
0.0081	0.0005	0.0017	0.061	0.013	0.00072	0.0015	0.0005	0.031	0.0005	0.00025	0.0017	0.0005	0.0005
0.0005	0.00064	0.0058	0.057	0.0033	0.0005	0.0015	0.0005	0.04	0.0005	0.00025	0.00017	0.0005	0.0005
0.0034	0.00068	0.0066	0.057	0.0077	0.0005	0.0015	0.0005	0.0095	0.0005	0.00025	0.00017	0.0005	0.0005
0.0069	0.00069	0.0058	0.056	0.0065	0.0005	0.0015	0.0005	0.0044	0.0028	0.00025	0.003	0.0005	0.0005
0.0005	0.00075	0.0081	0.061	0.0046	0.0005	0.0015	0.0047	0.0074	0.0005	0.00025	0.0015	0.0005	0.0005

Dihydrocodeine	Diphenhydramine	Dothiepin	Doxepin	EDDP (metabolite of Methadone)	Felbamate	Fenazepam	Fenofibrate	Fentanyl	Flumazenil	Flunitrazepam	Flupentixol	Flurazepam	Gabapentin
0.83	0.0031	0.0059	0.0005	0.0087	0.0005	0.0005	0.02	0.0005	0.0015	0.0005	0.53	0.0005	0.1
0.76	0.0035	0.0071	0.0012	0.01	0.0005	0.11	0.01	0.0005	0.0005	0.0005	0.41	0.0005	0.1
0.63	0.0056	0.011	0.0015	0.013	0.0005	0.0005	0.003	0.0005	0.0014	0.0005	0.63	0.0005	0.08
0.59	0.0023	0.0017	0.0005	0.013	0.0003	0.0005	0.006	0.0005	0.0005	0.0005	0.43	0.0005	0.09
0.78	0.0026	0.0083	0.0005	0.012	0.0005	0.018	0.003	0.0005	0.0005	0.0005	0.32	0.0005	0.07
0.95	0.0052	0.00058	0.0005	0.0033	0.0042	0.016	0.003	0.0005	0.0005	0.0005	0.53	0.0005	0.06
0.39	0.0034	0.0034	0.0005	0.0055	0.0005	0.031	0.003	0.00027	0.0005	0.0005	0.37	0.0005	0.05
0.51	0.0034	0.00062	0.0005	0.0081	0.0005	0.0005	0.003	0.00044	0.0005	0.0005	0.29	0.0005	0.06
0.031	0.0005	0.029	0.033	0.003	0.0005	0.0099	0.003	0.0005	0.0005	0.0005	0.052	0.0005	0.06
0.0005	0.0005	0.0021	0.0018	0.0005	0.00027	0.01	0.003	0.00057	0.0005	0.0005	0.36	0.0005	0.1
0.0005	0.0005	0.0034	0.0013	0.0024	0.00029	0.0005	0.003	0.0023	0.0005	0.0005	0.25	0.0005	0.08
0.0017	0.0005	0.0031	0.0012	0.0005	0.0005	0.0005	0.003	0.001	0.0005	0.0005	0.23	0.0005	0.2
0.0025	0.00034	0.0045	0.0005	0.0005	4.70E-06	0.0005	0.003	0.0075	0.0005	0.0005	0.2	0.0005	0.07
0.001	0.0005	0.0035	0.0012	0.0005	0.0005	0.01	0.003	0.0005	0.0005	0.0005	0.2	0.0005	0.1
0.0005	0.0005	0.0035	0.0013	0.0024	0.00031	0.0005	0.003	0.0005	0.0005	0.0005	0.17	0.0005	0.1
0.52	0.0092	0.00074	0.0005	0.0056	0.0005	0.021	0.003	0.0005	0.0005	0.0005	0.53	0.0005	0.2
0.34	0.0043	0.0032	0.0005	0.0049	0.0005	0.015	0.003	0.00052	0.0005	0.0005	0.32	0.0005	0.2
0.56	0.0005	0.0055	0.0005	0.0048	0.0014	0.0005	0.003	0.0005	0.0005	0.0005	0.22	0.0005	0.2
0.49	0.0049	0.00045	0.0005	0.0048	0.0011	0.011	0.003	0.0005	0.0005	0.0005	0.2	0.0005	0.2
0.84	0.0042	0.0026	0.0005	0.0054	0.0005	0.014	0.003	0.00097	0.0005	0.0005	0.17	0.0005	0.2
0.63	0.0042	0.0003	0.0005	0.0036	0.0016	0.0005	0.003	0.0005	0.0005	0.0005	0.19	0.0005	0.1
0.3	0.0037	0.0041	0.0005	0.0038	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.18	0.0005	0.1
0.8	0.0039	0.001	0.0012	0.0032	0.0035	0.0005	0.003	0.0005	0.0005	0.0005	0.17	0.0005	0.1
0.67	0.00078	0.0033	0.0005	0.0059	0.0077	0.0005	0.003	0.0005	0.0005	0.0005	0.17	0.0005	0.1
0.41	0.0066	0.0033	0.00098	0.0028	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.22	0.0005	0.1
0.46	0.0037	0.0035	0.0005	0.0058	0.0005	0.011	0.003	0.0005	0.0005	0.0005	0.19	0.0005	0.2
0.14	0.0043	0.0035	0.0005	0.0055	0.0009	0.0005	0.003	0.00052	0.0005	0.0005	0.19	0.0005	0.2
0.62	0.003	0.0032	0.0005	0.0026	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.18	0.0005	0.1
0.23	0.0041	0.00039	0.0013	0.0032	0.00029	0.0005	0.003	0.0005	0.0005	0.0005	0.18	0.0005	0.1
0.21	0.0029	0.002	0.0005	0.0045	0.0005	0.011	0.003	0.0051	0.0005	0.0005	0.17	0.0005	0.1
0.2	0.004	0.0021	0.0005	0.0036	0.0068	0.0099	0.003	0.0005	0.0005	0.0005	0.16	0.0005	0.2
0.19	0.0024	0.0023	0.0005	0.004	0.0058	0.0005	0.003	0.0021	0.0005	0.0005	0.16	0.0005	0.1
0.47	0.0043	0.0023	0.0005	0.0027	0.0005	0.011	0.003	0.0005	0.0005	0.0005	0.14	0.0005	0.1
0.083	0.0039	0.0026	0.0005	0.0041	0.0005	0.012	0.003	0.041	0.0005	0.0005	0.14	0.0005	0.1
0.36	0.0031	0.0039	0.0005	0.0005	0.0005	0.01	0.003	0.0005	0.0005	0.0005	0.16	0.0005	0.1
0.35	0.00074	0.0007	0.0005	0.0043	0.0005	0.012	0.003	0.0005	0.0005	0.0005	0.15	0.0005	0.1
0.33	0.00078	0.00064	0.0005	0.0041	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.1	0.0005	0.0025
0.19	0.0033	0.0037	0.0005	0.005	0.0087	0.0005	0.003	0.002	0.0005	0.002	0.3	0.0005	0.1
0.31	0.0035	0.003	0.001	0.0042	0.0039	0.0005	0.003	0.0005	0.0005	0.0013	0.26	0.0005	0.1
0.89	0.0017	0.0032	0.0013	0.0034	0.0062	0.0005	0.003	0.0005	0.0005	0.0012	0.23	0.0005	0.1
0.86	0.004	0.004	0.0005	0.0026	0.0026	0.0005	0.003	0.0005	0.0005	0.0005	0.19	0.0005	0.0025
0.17	0.00044	0.0031	0.0005	0.0037	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.12	0.0005	0.1
0.36	0.0039	0.0046	0.00094	0.0031	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.1	0.0005	0.1
0.43	0.0032	0.0034	0.0031	0.003	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.098	0.0005	0.1
0.25	0.0034	0.0028	0.00091	0.0031	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.091	0.0005	0.1
0.079	0.00046	0.003	0.0005	0.0033	0.003	0.011	0.003	0.0005	0.0005	0.0005	0.081	0.0005	0.1
0.58	0.003	0.0036	0.0005	0.0067	0.0043	0.047	0.003	0.00046	0.0005	0.0005	0.2	0.0005	0.1
0.6	0.002	0.01	0.0005	0.0077	0.12	0.0005	0.003	0.0005	0.0005	0.0005	0.15	0.0005	0.0025
0.87	0.0006	0.0035	0.0005	0.011	0.0013	0.014	0.003	0.0005	0.0005	0.0005	0.093	0.0005	0.1
0.67	0.0018	0.0005	0.0005	0.011	0.0005	0.0098	0.003	0.0005	0.0005	0.0005	0.065	0.0005	0.08
0.5	0.0005	0.0092	0.0005	0.013	0.01	0.0005	0.003	0.0005	0.0005	0.0005	0.043	0.0005	0.1
0.34	0.00061	0.00029	0.0005	0.014	0.0005	0.0097	0.003	0.0005	0.0014	0.0005	0.039	0.0005	0.06
0.077	0.0005	0.0007	0.0011	0.012	0.0005	0.0098	0.003	0.0005	0.0014	0.0005	0.044	0.00091	0.08
0.66	0.0017	0.0014	0.0011	0.0005	0.0006	0.012	0.003	0.00057	0.0005	0.0005	0.12	0.0005	0.07
0.55	0.0005	0.0021	0.0011	0.003	0.0013	0.0005	0.003	0.0005	0.0005	0.0005	0.093	0.0005	0.1
0.39	0.0005	0.0055	0.0005	0.003	0.00076	0.0005	0.003	0.0005	0.0005	0.0005	0.082	0.0005	0.06
0.26	0.0012	0.0022	0.001	0.0025	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.068	0.0005	0.07
0.29	0.0005	0.0093	0.0005	0.0067	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.06	0.0005	0.4
0.34	0.0005	0.0017	0.00097	0.0029	0.0005	0.011	0.003	0.0005	0.0005	0.0005	0.056	0.0005	0.06
0.25	0.00046	0.0022	0.00095	0.0029	0.00078	0.0005	0.003	0.0005	0.0005	0.0005	0.053	0.0005	0.09
0.21	0.00093	0.0026	0.0018	0.0005	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.051	0.0005	0.06
0.49	0.0005	0.0022	0.0005	0.0028	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.051	0.0005	0.09
0.21	0.0025	0.0014	0.0011	0.0027	0.0045	0.0005	0.003	0.0019	0.0005	0.0005	0.077	0.0005	0.05
0.39	0.001	0.0014	0.00098	0.0005	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.062	0.0005	0.06
0.47	0.00085	0.002	0.0012	0.0005	0.00052	0.0005	0.003	0.00035	0.0005	0.0005	0.053	0.0005	0.06
0.33	0.0011	0.0016	0.0005	0.003	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.048	0.0005	0.07
0.26	0.00092	0.0021	0.0005	0.0005	0.0005	0.0005	0.003	0.0005	0.0005	0.0005	0.047	0.0005	0.08
0.18	0.0005	0.002	0.0015	0.0005	0.0074	0.0005	0.003	0.0005	0.0005	0.0005	0.044	0.0005	0.1

Gabapentin-lactam	Haloperidol	Hydrochlorothiazide	Hydrocodone	Hydromorphone	Imipramine	Indometacin	Iohexol	Iomeprol	Iopamidol	Iopromid	Irbesartan	JWH-018 (N-(n-pentanoic acid)	JWH-073 (2-methylnaphthyl analog)
0.03	0.0019	0.05	0.033	0.00092	0.0005	0.005	0.05	0.3	1	0.035	0.0065	0.0005	0.22
0.02	0.002	0.04	0.031	0.0015	0.0005	0.005	0.1	0.3	1	0.07	0.0065	0.0005	0.14
0.02	0.0005	0.015	0.081	0.0005	0.0038	0.005	0.05	0.1	1	0.1	0.0025	0.0005	0.48
0.02	0.0021	0.015	0.03	0.00094	0.0005	0.005	0.05	0.3	1	0.2	0.0025	0.0005	0.26
0.02	0.0021	0.015	0.029	0.0015	0.0005	0.005	0.05	0.05	1	0.035	0.0025	0.0005	0.74
0.01	0.0023	0.015	0.032	0.00087	0.0005	0.005	0.05	0.05	1	0.035	0.00375	6.30E-05	0.018
0.02	0.002	0.015	0.032	0.0005	0.014	0.005	0.05	0.1	1	0.035	0.00175	0.0005	0.027
0.01	0.0005	0.015	0.044	0.00087	0.0005	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.12
0.02	0.0032	0.015	0.0021	0.01	0.0073	0.005	0.05	0.05	1	0.035	0.0015	0.0024	0.093
0.02	0.002	0.015	0.0022	0.00094	0.0086	0.005	0.05	0.05	1	0.035	0.00175	0.0005	0.0035
0.02	0.0021	0.015	0.0005	0.0014	0.003	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.033
0.1	0.0005	0.015	0.0005	0.002	0.018	0.005	0.05	0.05	1	0.035	0.00475	0.0005	0.3
0.02	0.0005	0.015	0.0005	0.00096	0.014	0.005	0.05	0.05	1	0.09	0.00075	4.70E-05	0.026
0.02	0.0005	0.015	0.0005	0.00093	0.0005	0.005	0.05	0.05	1	0.1	0.00075	0.0005	0.06
0.04	0.0005	0.015	0.0005	0.0029	0.0005	0.005	0.05	0.05	1	0.035	0.0025	0.0005	0.21
0.08	0.002	0.04	0.025	0.0078	0.042	0.005	0.05	0.05	5	0.035	0.0075	0.0005	0.15
0.04	0.002	0.015	0.019	0.0026	0.0022	0.005	0.05	0.05	1	0.035	0.0025	0.0005	0.078
0.08	0.002	0.015	0.029	0.0019	0.0028	0.005	0.05	0.05	3	0.1	0.0225	0.0005	0.0088
0.04	0.0005	0.015	0.024	0.0021	0.0018	0.005	0.05	0.05	1	0.035	0.00425	1.70E-05	0.0043
0.04	0.0005	0.015	0.023	0.0019	0.0021	0.005	0.05	0.1	1	0.1	0.005	0.0005	0.0023
0.04	0.0005	0.015	0.016	0.0009	0.0032	0.005	0.05	0.2	2.2	0.09	0.00725	6.00E-05	0.074
0.04	0.002	0.015	0.016	0.001	0.053	0.005	0.05	0.05	1	0.035	0.007	0.0005	0.15
0.03	0.002	0.015	0.018	0.0069	0.0005	0.005	0.05	0.05	1	0.035	0.03	0.0005	0.085
0.03	0.002	0.015	0.016	0.0008	0.1	0.005	0.05	0.05	1	0.09	0.005	8.00E-06	0.079
0.04	0.0005	0.015	0.014	0.0032	0.0068	0.005	0.05	0.1	2.2	0.035	0.005	0.0005	0.02
0.04	0.0005	0.015	0.013	0.0014	0.0028	0.005	0.05	0.2	2.1	0.08	0.005	0.0005	0.09
0.04	0.002	0.015	0.015	0.0033	0.003	0.005	0.05	0.05	2.1	0.07	0.00725	3.60E-05	0.3
0.05	0.0005	0.015	0.013	0.0005	0.0005	0.005	0.05	0.05	1	0.1	0.0075	0.0005	0.0038
0.0035	0.0005	0.015	0.013	0.0014	0.0097	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.0005
0.04	0.0005	0.015	0.015	0.00089	0.0069	0.005	0.05	0.2	1	0.035	0.007	0.0005	0.033
0.04	0.0005	0.015	0.015	0.0009	0.003	0.005	0.05	0.05	2.3	0.035	0.00675	0.0005	0.0005
0.04	0.0005	0.015	0.017	0.0005	0.019	0.005	0.05	0.2	2	0.035	0.01	3.70E-05	0.0059
0.04	0.0005	0.015	0.013	0.00095	0.0014	0.005	0.05	0.1	2.2	0.035	0.00675	0.0005	0.048
0.04	0.0005	0.015	0.013	0.0017	0.0014	0.005	0.05	0.05	2.2	0.1	0.007	0.0005	0.0005
0.04	0.0005	0.015	0.012	0.0023	0.0005	0.005	0.05	0.05	1	0.035	0.01	0.0005	0.0005
0.03	0.0005	0.015	0.011	0.0005	0.0005	0.005	0.05	0.05	1	0.035	0.00425	0.0005	0.0042
0.0035	0.0005	0.015	0.015	0.0005	0.0051	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.012
0.02	0.002	0.015	0.011	0.0017	0.023	0.005	0.05	0.05	1	0.07	0.00425	0.0005	0.083
0.0035	0.0005	0.015	0.0093	0.0009	0.0049	0.005	0.05	0.05	1	0.035	0.005	0.0005	0.0005
0.03	0.0005	0.015	0.0078	0.0005	0.0018	0.005	0.05	0.05	1	0.035	0.00475	0.0005	0.0055
0.007	0.0005	0.015	0.0089	0.00086	0.005	0.005	0.4	0.05	1	0.7	0.00075	0.0005	0.037
0.03	0.0005	0.015	0.009	0.0005	0.0005	0.005	0.05	0.05	1	0.1	0.0025	0.0005	0.19
0.04	0.0005	0.015	0.011	0.0039	0.0035	0.005	0.1	0.05	1	0.09	0.00475	0.0005	0.088
0.04	0.0005	0.015	0.0097	0.0005	0.0005	0.005	0.05	0.05	1	0.1	0.009	0.0005	0.11
0.03	0.0005	0.015	0.0079	0.0014	0.0051	0.005	0.05	0.05	1	0.035	0.007	0.0005	0.056
0.03	0.0005	0.015	0.0072	0.00098	0.0076	0.005	0.05	0.05	1	0.08	0.0045	0.0005	0.0036
0.03	0.0005	0.015	0.063	0.0005	0.0005	0.005	0.2	0.05	1	0.035	0.00725	0.0005	0.15
0.0035	0.0005	0.015	0.065	0.0005	0.0005	0.005	0.2	0.05	1	0.035	0.00075	0.0005	0.62
0.03	0.0005	0.015	0.065	0.0005	0.031	0.005	0.05	0.05	1	0.08	0.0075	0.0005	0.23
0.02	0.0005	0.015	0.08	0.0005	0.032	0.005	0.05	0.05	1	0.035	0.0025	0.0005	0.09
0.03	0.0019	0.015	0.077	0.00091	0.0028	0.005	0.3	1.3	2.5	0.035	0.0095	0.0005	0.0005
0.02	0.0047	0.015	0.075	0.0005	0.0017	0.005	0.05	0.05	1	0.035	0.00225	1.60E-05	0.0005
0.01	0.0054	0.015	0.064	0.0005	0.0005	0.005	0.05	0.05	1	0.035	0.00225	0.0005	0.0005
0.0035	0.0005	0.015	0.054	0.0005	0.0014	0.005	0.05	0.05	2	0.035	0.00075	0.0005	2.1
0.02	0.0005	0.015	0.045	0.0005	0.0019	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.13
0.02	0.0005	0.08	0.047	0.0005	0.0026	0.005	0.05	0.05	1	0.035	0.00075	0.00063	0.0048
0.01	0.0005	0.015	0.046	0.0005	0.0015	0.005	0.05	0.05	1	0.035	0.00175	0.0005	0.33
0.03	0.0005	0.03	0.042	0.0015	0.0015	0.01	1.1	1.4	11	0.3	0.0575	0.0005	1.2
0.02	0.0005	0.015	0.042	0.00085	0.0005	0.005	0.05	0.05	1	0.035	0.0015	0.0005	0.05
0.02	0.0005	0.015	0.042	0.001	0.0014	0.005	0.05	0.05	1	0.035	0.00225	0.0005	0.11
0.01	0.0005	0.015	0.046	0.0005	0.019	0.005	0.05	0.05	1	0.035	0.0015	0.0005	0.083
0.02	0.0005	0.015	0.049	0.0008	0.0063	0.005	0.05	0.05	1	0.035	0.00175	0.0005	0.14
0.008	0.0005	0.015	0.048	0.001	0.0014	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.0061
0.01	0.0005	0.015	0.045	0.0023	0.0005	0.005	0.05	0.05	1	0.035	0.00075	0.00085	0.18
0.01	0.0005	0.015	0.042	0.00093	0.0019	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.14
0.01	0.0005	0.015	0.041	0.0005	0.0013	0.005	0.05	0.05	1	0.035	0.00225	0.0005	0.1
0.01	0.0005	0.015	0.041	0.00069	0.0016	0.005	0.05	0.05	1	0.035	0.002	0.0005	0.14
0.02	0.0005	0.015	0.045	0.001	0.0014	0.005	0.05	0.05	1	0.035	0.00075	0.0005	0.35

Ketamine	Ketoprofen	Lamotrigine	Librium (Chlordiazepoxide)	Lidocaine	Lorazepam	Losartan	Maprotiline	Medazepam	Meperidine (Pethidine)	Methamphetamine	Methylendioxymethamphetamine (MDMA)	Methylphenidate	Metoprolol
0.0021	0.01	0.021	0.0005	0.005	0.035	0.003	0.0058	0.00064	0.0018	0.0029	0.0069	0.0024	0.01
0.0005	0.01	0.027	0.0005	0.0049	0.049	0.003	0.0071	0.00029	0.00091	0.0027	0.0087	0.013	0.028
0.0026	0.01	0.03	0.0028	0.0057	0.045	0.003	0.01	0.0028	0.0058	0.0026	0.0098	0.022	0.041
0.0013	0.01	0.03	0.0005	0.006	0.051	0.003	0.0095	0.0012	0.0016	0.0005	0.0082	0.012	0.06233333
0.0005	0.01	0.034	0.0005	0.0069	0.039	0.003	0.0092	0.0012	0.0005	0.0005	0.0065	0.01	0.04166667
0.0005	0.01	0.021	0.0005	0.0052	0.07	0.003	0.00054	0.00023	0.00065	0.0005	0.0039	0.014	0.04033333
0.0005	0.01	0.02	0.0026	0.0037	0.081	0.003	0.0027	0.00096	0.0005	0.0005	0.0062	0.012	0.01333333
0.0005	0.01	0.019	0.0005	0.0037	0.056	0.003	0.0052	0.00073	0.0005	0.0005	0.0053	0.012	0.01
0.0029	0.01	0.013	0.031	0.042	0.0005	0.003	0.00026	0.0095	0.022	0.0005	0.2	0.034	0.01
0.0015	0.01	0.018	0.023	0.004	0.0023	0.003	0.0005	0.0016	0.0018	0.0005	0.0039	0.0005	0.00666667
0.0005	0.01	0.028	0.041	0.0051	0.0006	0.003	0.0005	0.0014	0.0014	0.0005	0.0049	0.017	0.01533333
0.0005	0.01	0.046	0.0065	0.0034	0.0005	0.003	0.0005	0.0012	0.0014	0.014	0.014	0.02	0.01
0.0014	0.01	0.019	0.034	0.0056	0.0043	0.003	0.0005	0.0012	0.001	0.0005	0.0064	0.0005	0.01
0.0005	0.01	0.026	0.046	0.005	0.004	0.003	0.0005	0.0012	0.0015	0.0036	0.0053	0.014	0.01
0.0011	0.01	0.026	0.048	0.0049	0.0005	0.003	0.0005	0.0011	0.0011	0.0005	0.0062	0.015	0.01
0.0005	0.01	0.046	0.0029	0.007	0.039	0.01	0.0028	0.002	0.002	0.0045	0.03	0.012	0.01
0.0014	0.01	0.024	0.0005	0.0048	0.019	0.003	0.0021	0.0003	0.0018	0.0005	0.0087	0.0034	0.01
0.0013	0.01	0.029	0.0085	0.0037	0.013	0.003	0.0021	0.00074	0.0017	0.0005	0.027	0.0005	0.01
0.0005	0.01	0.023	0.0005	0.0042	0.03	0.003	0.002	0.00052	0.0017	0.0005	0.0059	0.0005	0.01
0.0005	0.01	0.022	0.0005	0.0032	0.014	0.003	0.0026	0.00016	0.0005	0.0032	0.0095	0.0015	0.01
0.0005	0.01	0.021	0.0027	0.0041	0.0029	0.003	0.0009	0.00023	0.0016	0.0005	0.01	0.0018	0.01
0.0013	0.01	0.026	0.0005	0.0055	0.018	0.007	0.001	0.0005	0.0018	0.0005	0.0085	0.011	0.01
0.0013	0.01	0.028	0.0005	0.0054	0.018	0.01	0.00046	0.00031	0.0018	0.0026	0.28	0.0016	0.01
0.0005	0.01	0.022	0.0005	0.005	0.011	0.007	0.0031	0.00081	0.0022	0.0028	0.0077	0.0079	0.02466667
0.0014	0.01	0.021	0.0005	0.0045	0.0059	0.003	0.00014	0.00041	0.0011	0.0005	0.0074	0.0005	0.022
0.0012	0.01	0.021	0.0005	0.0043	0.0064	0.008	0.003	0.00069	0.0018	0.0027	0.0065	0.0095	0.025
0.0011	0.01	0.021	0.0026	0.0048	0.0064	0.008	0.0027	0.00017	0.0018	0.0005	0.0072	0.0053	0.024
0.0011	0.01	0.019	0.0005	0.0047	0.013	0.003	0.0005	0.0005	0.0014	0.0031	0.0077	0.0005	0.0105
0.0023	0.01	0.0074	0.0005	0.0035	0.0038	0.003	0.00051	0.0005	0.0012	0.0031	0.00035	0.0013	0.01
0.0005	0.01	0.018	0.0005	0.0038	0.0044	0.008	0.0018	0.0005	0.0005	0.0005	0.006	0.0015	0.01
0.0005	0.01	0.016	0.0005	0.0038	0.0068	0.008	0.00086	0.0005	0.0015	0.0049	0.0063	0.001	0.01
0.0005	0.01	0.015	0.0005	0.0041	0.0033	0.007	0.0012	0.0005	0.0017	0.0005	0.0068	0.0015	0.01
0.0005	0.01	0.016	0.0005	0.0039	0.0048	0.007	0.0005	0.00021	0.0012	0.0005	0.0072	0.0012	0.01
0.0005	0.01	0.015	0.0005	0.004	0.0023	0.009	0.0013	0.0005	0.0012	0.0005	0.0064	0.0046	0.01
0.0005	0.01	0.009	0.0005	0.0043	0.0007	0.003	0.0005	0.00069	0.0016	0.0024	0.064	0.0005	0.01
0.0012	0.01	0.015	0.0005	0.0043	0.0054	0.007	0.0016	0.0005	0.0005	0.0005	0.01	0.0019	0.01
0.0005	0.01	0.0054	0.0005	0.0039	0.0052	0.003	0.0014	0.00016	0.001	0.0026	0.0056	0.0005	0.01
0.0005	0.01	0.013	0.0005	0.0043	0.016	0.007	0.0022	0.00065	0.0015	0.004	0.013	0.0005	0.01
0.0005	0.01	0.013	0.0005	0.0037	0.0033	0.007	0.0014	0.0005	0.0015	0.0029	0.0095	0.0005	0.00666667
0.0005	0.01	0.012	0.0005	0.0043	0.0009	0.008	0.00073	0.0048	0.00038	0.004	0.011	0.0005	0.01
0.0014	0.01	0.019	0.0005	0.0037	0.0055	0.03	0.0005	0.0005	0.0031	0.0046	0.049	0.0005	0.01
0.0005	0.01	0.014	0.0005	0.0037	0.0005	0.003	0.00094	0.00028	0.0017	0.0027	0.0098	0.0005	0.01
0.0005	0.01	0.013	0.0005	0.0038	0.0006	0.008	0.00041	0.0003	0.00075	0.0005	0.01	0.0011	0.01
0.0014	0.01	0.013	0.0005	0.0042	0.0021	0.008	0.00034	0.0002	0.00043	0.0028	0.009	0.0005	0.01
0.0005	0.01	0.013	0.0005	0.0037	0.002	0.008	0.00039	0.00038	0.00019	0.0022	0.011	0.0005	0.01
0.0005	0.01	0.012	0.0005	0.0034	0.0005	0.003	0.00056	0.00029	0.00031	0.0023	0.01	0.0005	0.01
0.0005	0.01	0.013	0.0005	0.004	0.0005	0.003	0.0039	0.00033	0.0014	0.0005	0.00054	0.0013	0.01
0.0014	0.01	0.012	0.0005	0.0039	0.0021	0.003	0.0048	0.0014	0.001	0.0005	0.00011	0.0015	0.01
0.0016	0.01	0.013	0.0005	0.0038	0.0009	0.006	0.0077	0.00025	0.00085	0.0005	0.0005	0.0005	0.01
0.0005	0.01	0.0005	0.0084	0.0036	0.0005	0.003	0.0078	0.00077	0.00089	0.0005	0.00021	0.0013	0.01
0.0005	0.01	0.017	0.0005	0.0067	0.0005	0.03	0.01	0.00062	1.20E-05	0.0005	0.00073	0.0016	0.01
0.0005	0.01	0.0005	0.003	0.0005	0.0005	0.003	0.011	0.005	0.0005	0.0005	0.00014	0.0011	0.01
0.0005	0.01	0.0005	0.002	0.0005	0.0005	0.003	0.0091	0.0021	0.0005	0.0005	8.60E-05	0.0011	0.01
0.0005	0.01	0.003	0.0005	0.0035	0.0005	0.02	0.0005	0.0005	0.0005	0.0005	0.011	0.0011	0.01
0.0005	0.01	0.008	0.0005	0.0035	0.0005	0.003	0.00027	0.0005	0.001	0.003	0.0059	0.0011	0.01
0.0005	0.02	0.0024	0.0005	0.0036	0.0005	0.02	0.00056	0.00046	0.00096	0.0005	0.0042	0.001	0.02
0.00099	0.01	0.0081	0.0005	0.0029	0.0005	0.003	0.0003	0.0005	0.00087	0.0005	0.0021	0.0012	0.01
0.0005	0.01	0.017	0.0005	0.025	0.0005	0.02	0.0039	0.00014	0.0022	0.0005	0.016	0.0022	0.82
0.0012	0.01	0.0084	0.0005	0.0033	0.0005	0.003	0.00022	0.0005	0.0033	0.0005	0.0069	0.0013	0.008
0.0012	0.01	0.0078	0.0005	0.0034	0.0005	0.003	0.00016	0.0005	0.00091	0.0005	0.0037	0.0021	0.01466667
0.0012	0.01	0.0073	0.0005	0.0033	0.0005	0.003	0.0005	0.00022	0.00073	0.0005	0.0037	0.0011	0.01
0.0014	0.01	0.0081	0.0005	0.0034	0.0005	0.003	5.90E-05	0.0005	0.00087	0.0029	0.0069	0.0013	0.01
0.0005	0.01	0.0021	0.0005	0.0035	0.0005	0.003	2.30E-05	0.0003	0.0011	0.0005	0.0016	0.0019	0.01
0.0005	0.01	0.0027	0.0025	0.0041	0.0005	0.003	0.0005	0.0005	0.00079	0.0005	0.011	0.0005	0.01
0.0012	0.01	0.0077	0.0005	0.0036	0.0005	0.003	0.0005	0.0005	0.00081	0.0005	0.0041	0.0005	0.01
0.0005	0.01	0.0072	0.0005	0.0034	0.0005	0.003	0.00027	0.00039	0.00078	0.0005	0.0045	0.0013	0.021
0.0013	0.01	0.0077	0.0027	0.0034	0.0005	0.003	0.0005	0.0005	0.00078	0.0005	0.0038	0.0005	0.01
0.0013	0.01	0.0071	0.0005	0.0033	0.0005	0.003	0.0005	0.0002	0.00036	0.0005	0.0034	0.0011	0.01

Metroprolol acid	Midazolam	Mirtazapine	Morphine	Morphine glucuronide	n-Acetyl-4-aminoantipyrine	Nadolol	Naltrexone	Naproxen	N-Desmethylclozapine	N-Formyl-4-aminoantipyrine	Nitrazepam	Norbuprenorphine	Nordiazepam
0.03	0.00025	0.0005	0.0021	0.0005	0.091	0.0015	0.00098	0.035	0.0005	0.1	0.0005	0.023	0.02
0.04	0.00025	0.0005	0.0026	0.0005	0.14333333	0.0015	0.0005	0.035	0.0005	0.1	0.015	0.022	0.0051
0.03	0.00025	0.0074	0.0005	0.0005	0.18	0.0015	0.0012	0.035	0.0005	0.1	0.099	0.055	0.0069
0.03	0.00025	0.0005	0.0021	0.0005	0.19	0.0015	0.0005	0.035	0.0005	0.1	0.022	0.033	0.0034
0.02	0.00025	0.0051	0.0026	0.0005	0.19666667	0.0015	0.0005	0.035	0.0005	0.09	0.035	0.0048	0.0043
0.02	0.0014	0.0058	0.002	0.0005	0.08033333	0.0015	0.0027	0.035	0.0044	0.07	0.06	0.01	0.034
0.01	0.0023	0.0029	0.0005	0.0005	0.06933333	0.0015	0.0015	0.035	0.0025	0.07	0.03	0.0097	0.0086
0.01	0.00025	0.0023	0.002	0.0005	0.06233333	0.0015	0.00059	0.035	0.0039	0.05	0.034	0.0061	0.021
0.01	0.00025	0.025	0.0099	0.0005	0.06933333	0.0015	0.0005	0.035	0.014	0.07	0.92	0.14	0.0029
0.01	0.00025	0.0028	0.0021	0.0005	0.07	0.0015	0.00083	0.035	0.017	0.06	0.041	0.01	0.0049
0.02	0.00025	0.0041	0.0025	0.0005	0.1	0.0015	0.0005	0.035	0.0005	0.07	0.029	0.012	0.0029
0.04	0.00025	0.0005	0.003	0.06	0.18	0.0015	0.0005	0.035	0.0005	0.1	0.041	0.0026	0.0048
0.01	0.00025	0.003	0.0021	0.0005	0.058	0.0015	0.0005	0.035	0.0005	0.07	0.036	0.022	0.0028
0.02	0.00025	0.0054	0.0021	0.0005	0.05333333	0.0015	0.0005	0.035	0.0005	0.07	0.0089	0.013	0.0046
0.03	0.00025	0.0043	0.0038	0.0005	0.07733333	0.0015	0.0012	0.035	0.029	0.1	0.016	0.012	0.0031
0.04	0.00025	0.0039	0.008	0.0005	0.12	0.0015	0.0018	0.035	0.052	0.3	0.031	0.0005	0.0043
0.03	0.00025	0.0005	0.0035	0.0005	0.086	0.0015	0.0005	0.035	0.0005	0.1	0.018	0.0005	0.0099
0.04	0.00025	0.0005	0.0029	0.0005	0.12	0.0015	0.0005	0.035	0.015	0.3	0.012	0.0084	0.0095
0.03	0.00025	0.0022	0.0031	0.0005	0.077	0.0015	0.0012	0.035	0.0005	0.1	0.012	0.0005	0.014
0.03	0.00025	0.0005	0.0029	0.0005	0.08233333	0.0015	0.00094	0.035	0.035	0.2	0.0093	0.0005	0.017
0.03	0.00025	0.0005	0.002	0.0005	0.077	0.0015	0.00068	0.035	0.0062	0.1	0.011	0.0005	0.026
0.005	0.00025	0.0024	0.0021	0.0005	0.08466667	0.0015	0.00071	0.035	0.022	0.2	0.019	0.0005	0.018
0.04	0.00025	0.0027	0.0073	0.0005	0.075	0.0015	0.0005	0.035	0.015	0.3	0.016	0.0065	0.022
0.03	0.0018	0.0005	0.002	0.0005	0.08566667	0.0015	0.001	0.035	0.0005	0.1	0.01	0.01	0.022
0.03	0.00025	0.0005	0.0041	0.0005	0.06766667	0.0015	0.00083	0.035	0.024	0.1	0.017	0.0037	0.025
0.04	0.00025	0.0005	0.0025	0.0005	0.081	0.0015	0.00052	0.035	0.034	0.2	0.011	0.0025	0.021
0.03	0.00025	0.0005	0.0041	0.0005	0.06866667	0.0015	0.00066	0.035	0.0005	0.2	0.014	0.0051	0.026
0.03	0.00025	0.0048	0.0005	0.0005	0.08166667	0.0015	0.00053	0.035	0.0005	0.2	0.015	0.0024	0.021
0.01	0.00025	0.0022	0.0025	0.0005	0.039	0.0015	0.00063	0.035	0.18	0.07	0.003	0.002	0.026
0.03	0.0018	0.0005	0.002	0.0005	0.06266667	0.0015	0.00053	0.035	0.011	0.1	0.014	0.0059	0.025
0.03	0.00025	0.0062	0.0021	0.0005	0.062	0.0015	0.0005	0.035	0.0005	0.2	0.0005	0.0025	0.022
0.03	0.00025	0.0027	0.0005	0.0005	0.08766667	0.0015	0.00062	0.035	0.0005	0.2	0.0005	0.0022	0.018
0.03	0.00025	0.0005	0.0021	0.0005	0.062	0.0015	0.00058	0.035	0.058	0.2	0.01	0.0025	0.0085
0.03	0.00025	0.0005	0.0027	0.0005	0.07966667	0.0015	0.00061	0.035	0.025	0.2	0.0042	0.0021	0.013
0.03	0.00025	0.0045	0.0033	0.0005	0.19	0.003	0.00059	0.035	0.056	0.4	0.0043	0.0027	0.016
0.02	0.00025	0.0027	0.0005	0.0005	0.086	0.0015	0.0005	0.035	0.0054	0.1	0.012	0.0023	0.018
0.02	0.00025	0.0005	0.0005	0.0005	0.041	0.0015	0.0005	0.035	0.029	0.04	0.0047	0.0021	0.015
0.02	0.00025	0.0022	0.0027	0.0005	0.077	0.0015	0.0005	0.035	0.0005	0.1	0.044	0.0066	0.024
0.04	0.00025	0.0023	0.002	0.0005	0.07866667	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.003	0.013
0.03	0.00025	0.0005	0.0005	0.0005	0.09133333	0.0015	0.0005	0.035	0.0005	0.2	0.0005	0.0005	0.015
0.3	0.00025	0.0034	0.002	0.0005	0.31	0.0015	0.00072	0.035	0.0029	0.4	0.0038	0.02	0.019
0.04	0.00025	0.0005	0.0005	0.0005	0.09733333	0.0015	0.00066	0.035	0.0005	0.2	0.0005	0.0005	0.0096
0.04	0.00025	0.0062	0.0047	0.0005	0.09033333	0.0015	0.0005	0.035	0.024	0.2	0.004	0.0033	0.0092
0.05	0.00025	0.004	0.0005	0.0005	0.09	0.0015	0.0005	0.035	0.091	0.2	0.0044	0.0029	0.015
0.04	0.00025	0.0005	0.0024	0.0005	0.07933333	0.0015	0.0005	0.035	0.01	0.2	0.0005	0.0026	0.016
0.05	0.00025	0.0005	0.0021	0.0005	0.08866667	0.0015	0.0005	0.035	0.016	0.2	0.039	0.0005	0.012
0.04	0.00025	0.0031	0.0005	0.0005	0.086	0.0015	0.0045	0.035	0.0005	0.2	0.0005	0.017	0.018
0.4	0.00025	0.0005	0.0005	0.0005	0.73	0.0015	0.0042	0.035	0.012	0.4	0.0005	0.014	0.025
0.04	0.00025	0.0005	0.0005	0.0005	0.079	0.0015	0.0043	0.035	0.0024	0.1	0.0044	0.015	0.011
0.03	0.00025	0.0005	0.0005	0.0005	0.08966667	0.0015	0.0034	0.035	0.0005	0.1	0.0039	0.011	0.012
0.1	0.00025	0.0005	0.0021	0.0005	0.79	0.0015	0.004	0.035	0.012	1.5	0.0005	0.0028	0.015
0.02	0.00025	0.0005	0.0005	0.0005	0.08733333	0.0015	0.013	0.035	0.0005	0.09	0.017	0.0005	0.015
0.02	0.00025	0.0005	0.0005	0.0005	0.09633333	0.0015	0.014	0.035	0.0005	0.1	0.013	0.0005	0.01
0.05	0.00025	0.0005	0.0005	0.0005	0.44	0.0015	0.0005	0.035	0.0005	0.8	0.0005	0.0048	0.039
0.03	0.00025	0.0005	0.0005	0.0005	0.09333333	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.0044	0.038
0.05	0.00025	0.0005	0.0005	0.0005	0.65	0.0015	0.00059	0.035	0.0005	0.5	0.0005	0.0005	0.04
0.02	0.00025	0.0005	0.0005	0.0005	0.09566667	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.0028	0.029
0.7	0.00025	0.0022	0.0025	0.0005	1.5	0.0015	0.0025	0.07	0.0016	1.2	0.0047	0.003	0.031
0.02	0.00025	0.0005	0.002	0.0005	0.08733333	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.012	0.034
0.04	0.00025	0.0026	0.0021	0.0005	0.12666667	0.0015	0.0005	0.035	0.0005	0.2	0.0005	0.0028	0.025
0.03	0.00025	0.0005	0.0005	0.0005	0.08366667	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.0093	0.03
0.04	0.00025	0.0005	0.002	0.0005	0.13	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.0094	0.03
0.03	0.00025	0.0005	0.0022	0.0005	0.07233333	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.011	0.03
0.01	0.00025	0.0033	0.0033	0.0005	0.09	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.01	0.037
0.03	0.002	0.003	0.0021	0.0005	0.09133333	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.0021	0.024
0.03	0.00025	0.0036	0.0005	0.0005	0.07233333	0.0015	0.0005	0.035	0.0067	0.1	0.0005	0.0087	0.029
0.03	0.00025	0.0005	0.0019	0.0005	0.091	0.0015	0.0005	0.035	0.0005	0.1	0.0005	0.0092	0.036
0.03	0.0015	0.029	0.0021	0.0005	0.08566667	0.0015	0.0005	0.035	0.0005	0.2	0.0005	0.011	0.032

Norfentanyl	Normeperidine (Norpethidine)	Norpropoxyphene (Desmethylpropoxyphene)	Nortriptyline	O-Desmethyltramadol	O-Desmethylvenlafaxine (Desvenlafaxine)	Olanzapine	Opipramol	Oxazepam	Oxcarbazepine	Oxycodone	Oxymorphone	Paliperidone (9-Hydroxyrisperidone)	Paroxetine
0.001	0.0019	0.091	0.0005	0.0074	0.0097	0.011	0.0029	0.00025	0.0005	0.0072	0.0034	0.0005	0.0011
0.0016	0.016	0.094	0.0005	0.0089	0.014	0.0067	0.0054	0.0052	0.0028	0.014	0.0054	0.0005	0.013
0.0012	0.028	0.049	0.004	0.011	0.015	0.0065	0.0005	0.00025	0.0005	0.013	0.0048	0.00087	0.016
0.0011	0.015	0.0005	0.0014	0.011	0.015	0.0081	0.0005	0.00025	0.0024	0.019	0.0056	0.00076	0.017
0.0005	0.012	0.059	0.0019	0.01	0.015	0.0071	0.0061	0.0046	0.0039	0.014	0.0056	0.0005	0.019
0.00082	0.018	0.018	0.0005	0.0075	0.011	0.03	0.0032	0.0032	0.0015	0.012	0.0036	0.0005	0.013
0.0005	0.015	0.16	0.0016	0.0068	0.0083	0.012	0.0044	0.0041	0.0013	0.0077	0.0033	0.00077	0.0082
0.00076	0.015	0.036	0.0005	0.0062	0.0069	0.013	0.0025	0.0062	0.0011	0.015	0.007	0.0005	0.0084
0.0005	0.045	0.75	0.0005	0.014	0.0042	0.19	0.0005	0.0044	0.015	0.0031	0.0058	0.0014	0.0021
0.0012	0.0005	0.0005	0.0027	0.0073	0.0068	0.011	0.0005	0.015	0.0005	0.0029	0.0035	0.0005	0.0053
0.00096	0.022	0.012	0.0032	0.011	0.011	0.02	0.0005	0.012	0.0005	0.0037	0.0074	0.0005	0.0074
0.0017	0.026	0.22	0.013	0.011	0.0051	0.008	0.0005	0.0059	0.002	0.0005	0.0005	0.0005	0.0087
0.001	0.0005	0.49	0.0005	0.0081	0.0072	0.0086	0.0029	0.0059	0.0044	0.0034	0.0056	0.0005	0.0046
0.0005	0.018	0.21	0.0005	0.0089	0.0099	0.013	0.0005	0.011	0.0023	0.0088	0.0005	0.0005	0.0056
0.0005	0.019	0.0005	0.012	0.0074	0.0077	0.0096	0.0005	0.012	0.0005	0.0069	0.0066	0.0005	0.0037
0.0025	0.014	0.21	0.0005	0.012	0.014	0.011	0.023	0.013	0.00078	0.019	0.0005	0.00072	0.0009
0.0017	0.0033	0.28	0.0023	0.0077	0.0079	0.012	0.0005	0.0092	0.0005	0.011	0.0061	0.0005	0.017
0.0088	0.0005	0.0005	0.0029	0.012	0.0081	0.0005	0.0052	0.0042	0.00086	0.021	0.0005	0.0005	0.0005
0.0044	0.0005	0.13	0.0019	0.0071	0.0071	0.0005	0.0005	0.0037	0.0005	0.015	0.0062	0.0005	0.0005
0.0049	0.00075	0.15	0.0005	0.0074	0.0058	0.0049	0.0005	0.0064	0.0005	0.01	0.0041	0.0005	0.0005
0.0026	0.0012	0.093	0.0076	0.0066	0.0054	0.0042	0.0005	0.0063	0.0011	0.012	0.0041	0.0005	0.0005
0.0025	0.013	0.21	0.0071	0.0078	0.0074	0.0078	0.0005	0.0072	0.0013	0.013	0.0037	0.0005	0.0057
0.0026	0.00091	0.068	0.0005	0.004	0.00087	0.0016	0.0005	0.00025	0.0005	0.0036	0.004	0.0016	0.0005
0.0015	0.0095	0.56	0.0005	0.0072	0.0063	0.0069	0.0005	0.0074	0.0005	0.013	0.004	0.0005	0.0035
0.0005	0.0005	0.24	0.0037	0.0072	0.0066	0.0057	0.0005	0.0057	0.0005	0.011	0.0035	0.00085	0.0005
0.0035	0.012	0.15	0.041	0.0066	0.0057	0.0087	0.0005	0.0055	0.0005	0.0078	0.0033	0.00098	0.0005
0.0027	0.0059	0.27	0.0005	0.007	0.0058	0.012	0.0005	0.0078	0.0005	0.0066	0.0034	0.00096	0.0032
0.0005	0.0005	0.66	0.018	0.0068	0.0051	0.0021	0.0005	0.0077	0.0005	0.0083	0.0034	0.00084	0.0053
0.0005	0.00042	0.11	0.015	0.0077	0.0034	0.0005	0.0005	0.012	0.0005	0.011	0.0005	0.0008	0.002
0.0019	0.00074	0.0065	0.0055	0.0071	0.0042	0.0042	0.0005	0.0067	0.0005	0.007	0.0005	0.00078	0.0049
0.0005	7.40E-05	0.041	0.026	0.0061	0.0039	0.0005	0.0005	0.0079	0.0005	0.0057	0.0005	0.0005	0.0005
0.0017	0.00067	0.024	0.0048	0.0063	0.0038	0.0093	0.0005	0.008	0.0005	0.005	0.0005	0.0008	0.0028
0.0005	0.0003	0.36	0.0036	0.006	0.0039	0.0029	0.0005	0.0052	0.0005	0.0029	0.0032	0.0008	0.0028
0.00086	0.0049	0.015	0.0016	0.0064	0.0032	0.0053	0.0005	0.0068	0.0005	0.0045	0.0005	0.00092	0.0047
0.0027	0.0005	0.13	0.0005	0.004	0.006	0.0005	0.043	0.00025	0.0005	0.0063	0.0032	0.00085	0.0018
0.0005	0.0013	0.013	0.02	0.0057	0.0026	0.0005	0.0035	0.0066	0.0005	0.005	0.0005	0.00098	0.0035
0.0012	0.0005	0.42	0.0054	0.0053	0.0035	0.0005	0.0031	0.0052	0.0005	0.0026	0.0005	0.0005	0.0005
0.0012	0.0005	0.31	0.02	0.0055	0.0033	0.0091	0.0005	0.0067	0.0005	0.0048	0.0005	0.0005	0.0016
0.00084	0.0005	0.21	0.0019	0.0052	0.0026	0.0058	0.0064	0.0024	0.0005	0.0043	0.0005	0.00085	0.0005
0.0011	0.0005	0.0092	0.0038	0.0055	0.0027	0.0005	0.0005	0.0056	0.0005	0.0044	0.0005	0.00077	0.005
0.0005	0.0005	0.036	0.0051	0.085	0.0013	0.0005	0.0043	0.0037	0.0005	0.01	0.0034	0.00092	0.0005
0.0005	0.0005	0.4	0.0005	0.0052	0.0022	0.0028	0.0035	0.0035	0.0005	0.0038	0.0005	0.00081	0.0033
0.0011	0.00017	0.52	0.0025	0.0052	0.0023	0.0041	0.0005	0.0062	0.0005	0.0038	0.0005	0.00079	0.0028
0.00077	0.0005	0.027	0.011	0.0049	0.0019	0.0045	0.0005	0.0042	0.0005	0.0042	0.0005	0.00079	0.0046
0.0005	0.0005	0.05	0.0038	0.0041	0.00077	0.0045	0.0005	0.0043	0.0005	0.0029	0.0005	0.0005	0.0037
0.00095	0.0005	0.093	0.0018	0.0085	0.00083	0.0054	0.0005	0.0042	0.0005	0.0048	0.0032	0.0008	0.0036
0.00066	0.00042	0.0005	0.0005	0.0064	0.0061	0.0053	0.0005	0.0063	0.0055	0.0042	0.0032	0.0005	0.011
0.0005	0.00065	0.027	0.0005	0.0053	0.0012	0.0005	0.11	0.0048	0.0059	0.0061	0.0005	0.0005	0.0094
0.0005	0.0005	0.018	0.028	0.0078	0.0055	0.0021	0.0026	0.0041	0.0054	0.0069	0.0032	0.0005	0.014
0.0005	0.00042	0.022	0.0005	0.0034	0.0005	0.0019	0.0032	0.00025	0.014	0.0035	0.0034	0.0005	0.0005
0.0005	0.00087	0.0005	0.0005	0.01	0.00062	0.0048	0.0005	0.00025	0.0005	0.0029	0.0044	0.0005	0.011
0.0005	0.00021	0.015	0.0005	0.0005	0.0005	0.011	0.0005	0.0031	0.0005	0.56	1.4	0.0005	0.013
0.0005	0.00016	0.0005	0.0005	0.0005	0.0005	0.013	0.0005	0.0029	0.0047	0.64	1.2	0.00072	0.0089
0.00082	0.0002	0.0094	0.0014	0.0045	0.00049	0.0076	0.0005	0.00025	0.0016	0.0042	0.0032	0.0005	0.0031
0.00081	0.00013	0.0039	0.0016	0.0046	0.0033	0.003	0.0034	0.0046	0.0017	0.0024	0.0005	0.0005	0.0011
0.0011	4.90E-05	0.0018	0.0015	0.013	0.0014	0.0017	0.0005	0.00025	0.0011	0.028	0.0005	0.00083	0.0031
0.00064	0.00032	0.0005	0.0016	0.0046	0.0031	0.0012	0.0028	0.0065	0.0013	0.0005	0.0005	0.0005	0.0022
0.0011	0.0016	0.0005	0.0017	0.015	0.017	0.02	0.0041	0.011	0.004	0.0024	0.0005	0.0005	0.014
0.00066	0.00045	0.0005	0.02	0.0045	0.0036	0.0019	0.0005	0.0023	0.0011	0.0023	0.0005	0.0005	0.0008
0.00066	0.0016	0.0005	0.0019	0.0042	0.0028	0.0023	0.0029	0.0043	0.0005	0.0005	0.0005	0.0005	0.001
0.00072	0.00012	0.0005	0.0005	0.005	0.0028	0.0032	0.037	0.0019	0.0005	0.0005	0.0005	0.0005	0.0012
0.0007	0.00049	0.0005	0.0005	0.0048	0.0025	0.0015	0.0066	0.0025	0.0005	0.0005	0.0034	0.0005	0.0017
0.00085	0.0012	0.0005	0.0036	0.0038	0.00058	0.0005	0.0005	0.0028	0.0005	0.0081	0.0005	0.0005	0.001
0.00082	0.0005	0.0005	0.013	0.0035	0.0011	0.0019	0.0005	0.00025	0.0005	0.014	0.0005	0.0005	0.0005
0.00077	0.0005	0.0005	0.003	0.0044	0.0025	0.0014	0.0005	0.0041	0.0005	0.0023	0.0031	0.0005	0.0007
0.00069	0.00045	0.0005	0.0016	0.004	0.0024	0.0022	0.059	0.0035	0.0005	0.0005	0.004	0.0005	0.001
0.00068	0.0005	0.0005	0.0017	0.0045	0.0025	0.0026	0.032	0.0028	0.0005	0.0005	0.0005	0.0005	0.0005
0.0005	0.00023	0.0005	0.0015	0.0042	0.0026	0.0021	0.043	0.0045	0.0005	0.0005	0.0005	0.0005	0.0005

Pentazocine	Pentobarbital	Pentoxifylline	Phenacetin	Phenazone	Phencyclidine (PCP)	Phentermine	Phenytoin	Pipamperone	Prazepam	Pregabalin	Primidone	Promazine	Promethazine
0.0005	0.0005	0.1	0.003	0.005	0.0059	0.0012	0.0005	0.0005	0.028	0.003	0.7	0.0018	0.0067
0.0005	0.0005	0.1	0.003	0.004	0.0037	0.00097	0.0027	0.0005	0.028	0.008	0.047	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.003	0.0049	0.00096	0.0005	0.01	0.068	0.003	1.7	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.004	0.0032	0.0005	0.0022	0.0005	0.04	0.003	1	0.0026	0.0077
0.0005	0.0005	0.1	0.003	0.008	0.0042	0.0005	0.0038	0.0005	0.038	0.003	0.8	0.0005	0.0005
0.0005	0.0005	0.1	0.01	0.008	0.0082	0.0005	0.0013	0.017	0.047	0.003	0.62	0.0005	0.0005
0.0005	0.0005	0.1	0.006	0.01	0.0055	0.0005	0.0012	0.012	0.05	0.003	0.69	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0036	0.0005	0.00094	0.0033	0.05	0.003	0.61	0.002	0.0069
0.03	0.0005	0.1	0.003	0.005	0.11	0.0005	0.015	0.037	0.006	0.003	1.5	0.094	0.12
0.0005	0.0005	0.1	0.003	0.008	0.0038	0.0005	0.0005	0.0037	0.0021	0.003	0.81	0.0021	0.007
0.0005	0.0005	0.1	0.003	0.01	0.0035	0.0005	0.0005	0.0005	0.0022	0.003	0.78	0.0024	0.0074
0.0005	0.0005	0.1	0.02	0.001	0.0047	0.012	0.0018	0.0047	0.0006	0.003	0.79	0.002	0.007
0.0005	0.0005	0.1	0.003	0.01	0.0012	0.0005	0.0043	0.0005	0.0015	0.003	1.1	0.0005	0.0005
0.00026	0.0005	0.1	0.003	0.01	0.0049	0.0019	0.0022	0.0039	0.0021	0.003	1	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.02	0.0039	0.0005	0.0005	0.0005	0.0009	0.003	0.83	0.0027	0.0078
0.0005	0.0005	0.1	0.003	0.008	0.0095	0.0028	0.00061	0.0028	0.036	0.003	0.95	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.02	0.0091	0.0005	0.0005	0.0034	0.03	0.003	0.83	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.001	0.0016	0.0005	0.00069	0.0037	0.036	0.003	0.95	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.02	0.0088	0.0005	0.0005	0.0016	0.029	0.003	0.67	0.0019	0.0068
0.00014	0.0005	0.1	0.003	0.02	0.021	0.0015	0.0005	0.0012	0.0039	0.008	0.69	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0085	0.0005	0.00092	0.0074	0.035	0.003	1.1	0.0005	0.0005
0.0005	0.0046	0.1	0.003	0.01	0.0093	0.0005	0.0012	0.003	0.007	0.003	0.76	0.0026	0.0077
0.0005	0.0005	0.1	0.003	0.02	0.0034	0.00091	0.0005	0.0034	0.0066	0.003	0.77	0.0027	0.0078
0.0005	0.0005	0.1	0.003	0.01	0.0005	0.0011	0.0005	0.0032	0.008	0.003	1	0.0005	0.0005
0.0005	0.12	0.1	0.003	0.01	0.0058	0.0005	0.0005	0.0015	0.017	0.007	0.8	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0049	0.00098	0.0005	0.00075	0.019	0.003	0.8	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0044	0.0005	0.0005	0.0005	0.0051	0.003	0.27	0.0076	0.014
0.0005	0.0005	0.1	0.003	0.01	0.0012	0.0014	0.0005	0.0005	0.0053	0.003	0.89	0.0028	0.008
0.0005	0.0005	0.1	0.003	0.001	0.0054	0.0014	0.0005	0.00076	0.0071	0.003	0.72	0.0029	0.008
0.0005	0.0005	0.1	0.003	0.01	0.0057	0.0005	0.0005	0.0015	0.013	0.007	0.46	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0029	0.0033	0.0005	0.008	0.011	0.003	0.69	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0005	0.0005	0.0005	0.0018	0.018	0.003	0.62	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0022	0.0005	0.0005	0.0005	0.016	0.008	0.61	0.0023	0.0073
0.0005	0.0005	0.1	0.003	0.01	0.0033	0.0005	0.0005	0.0005	0.013	0.003	0.54	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.01	0.0055	0.00072	0.0005	0.0005	0.012	0.003	0.98	0.0019	0.0068
0.0005	0.0005	0.1	0.003	0.007	0.0023	0.0005	0.0005	0.0019	0.011	0.006	0.56	0.0019	0.0068
0.0005	0.0005	0.1	0.003	0.002	0.0043	0.00091	0.0005	0.0005	0.0094	0.003	0.6	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.002	0.0023	0.0005	0.0005	0.021	0.003	0.66	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.001	0.0037	0.0012	0.0005	0.0005	0.0028	0.003	0.59	0.0025	0.0075
0.0011	0.0005	0.1	0.003	0.006	0.0038	0.0023	0.0005	0.0005	0.012	0.003	0.74	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.02	0.0052	0.0029	0.0005	0.0047	0.014	0.003	0.6	0.0054	0.011
0.00038	0.0005	0.1	0.003	0.001	0.017	0.0011	0.0005	0.0005	0.011	0.003	0.59	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.0031	0.0005	0.0005	0.0005	0.023	0.007	0.48	0.0005	0.0005
0.0003	0.0005	0.1	0.003	0.007	0.015	0.0011	0.0005	0.0005	0.022	0.003	0.61	0.002	0.007
0.0011	0.0005	0.1	0.003	0.009	0.02	0.00056	0.0005	0.0005	0.021	0.003	0.64	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.007	0.0022	0.00064	0.0005	0.0005	0.021	0.003	0.53	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.0018	0.0005	0.0055	0.0005	0.033	0.003	0.0005	0.0024	0.0074
0.0005	0.0005	0.1	0.003	0.05	0.0045	0.0005	0.0059	0.0005	0.034	0.003	0.11	0.0021	0.0071
0.0005	0.0005	0.1	0.003	0.008	0.0041	0.0005	0.0053	0.0005	0.036	0.003	0.018	0.0031	0.0083
0.0005	0.0005	0.1	0.003	0.006	0.0054	0.0005	0.014	0.013	0.03	0.003	0.32	0.002	0.0069
0.0005	0.0005	0.1	0.003	0.2	0.0022	0.0005	0.0005	0.0062	0.021	0.003	0.0005	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.0027	0.0005	0.0005	0.0068	0.011	0.003	0.019	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.0012	0.0005	0.0046	0.0005	0.011	0.003	0.0005	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.02	0.0017	0.0005	0.0014	0.0096	0.011	0.003	0.0025	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.0016	0.0013	0.0016	0.0052	0.0066	0.003	0.0026	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.02	0.0017	0.0005	0.00099	0.014	0.02	0.003	0.0028	0.0024	0.0074
0.0005	0.0005	0.1	0.003	0.005	0.0017	0.0005	0.0012	0.0061	0.017	0.003	0.0022	0.0023	0.0074
0.0005	0.0005	0.2	0.003	0.07	0.0005	0.0005	0.0039	0.0031	0.036	0.02	0.0023	0.0034	0.0086
0.0005	0.0005	0.1	0.003	0.006	0.0005	0.0005	0.00091	0.005	0.014	0.003	0.21	0.0027	0.0078
0.0005	0.0005	0.1	0.003	0.009	0.0012	0.0005	0.0005	0.0042	0.014	0.003	0.0018	0.0043	0.0098
0.0005	0.0005	0.1	0.003	0.008	0.0005	0.0005	0.0005	0.0066	0.014	0.003	0.43	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.009	0.0005	0.0012	0.0005	0.0073	0.012	0.003	0.28	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.006	0.0005	0.0005	0.0005	0.021	0.01	0.003	0.36	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.001	0.0009	0.0005	0.0005	0.0047	0.01	0.003	0.4	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.008	0.0005	0.0005	0.0005	0.0036	0.006	0.003	0.25	0.0005	0.0005
0.0005	0.0005	0.1	0.003	0.007	0.0005	0.0005	0.0005	0.0089	0.01	0.003	0.47	0.0022	0.0072
0.0005	0.0005	0.1	0.003	0.007	0.0014	0.0005	0.0005	0.0052	0.008	0.003	0.16	0.0021	0.0071
0.0005	0.0005	0.1	0.003	0.008	0.0005	0.0005	0.0005	0.0049	0.01	0.003	0.029	0.008	0.014

Propafenone	Propoxyphene (Dextropropoxyphene)	Propranolol	Propyphenazone	Protriptyline	Quetiapine	Risperidone	Ritalinic acid	Secobarbital	Sertraline	Sotalol	Strophanthidin	Sulfadimidin / Sulfamethazin	Sulfamethoxazole
0.0037	0.0005	0.01	0.0005	0.0005	0.0005	0.0005	0.0005	0.011	0.0049	0.02	0.0005	0.025	0.04
0.0035	0.0005	0.0025	0.0005	0.0005	0.00064	0.015	0.0019	0.0052	0.005	0.02	0.0035	0.025	0.036
0.0062	0.0005	0.0025	0.0005	0.0024	0.0005	0.011	0.0005	0.0005	0.0084	0.02	0.0005	0.025	0.034
0.0021	0.0005	0.0025	0.0005	0.0005	0.0005	0.0005	0.0005	0.02	0.0005	0.02	0.0005	0.025	0.043
0.0023	3.20E-05	0.0025	0.0005	0.00033	0.0005	0.0018	0.0005	0.015	0.0049	0.02	0.0005	0.025	0.043
0.0005	0.00083	0.0025	0.003	0.0005	0.00048	0.0005	0.001	0.0005	0.0084	0.02	0.0005	0.025	0.021
0.003	0.0005	0.0025	0.003	0.0005	0.0005	0.0005	0.0005	0.0005	0.0088	0.02	0.0027	0.025	0.024
0.0041	0.0005	0.0025	0.0005	0.0005	0.00061	0.0005	0.0005	0.0054	0.006	0.02	0.0005	0.025	0.018
0.021	0.0091	0.0025	0.001	0.037	0.0005	0.0005	0.00062	0.0052	0.05	0.02	0.0005	0.025	0.031
0.0005	0.0005	0.0025	0.001	0.0012	0.001	0.0005	0.0022	0.12	0.029	0.02	0.0005	0.025	0.021
0.0036	0.0005	0.0025	0.001	0.0017	0.0005	0.0005	0.0049	0.0071	0.0005	0.02	0.0005	0.025	0.025
0.0005	0.0005	0.0025	0.0005	0.011	0.00086	0.0005	0.0096	0.0051	0.0005	0.02	0.0038	0.025	0.047
0.003	0.0005	0.0025	0.001	0.0005	0.00046	0.0018	0.00052	0.0005	0.0005	0.02	0.0029	0.025	0.015
0.0005	0.0005	0.0025	0.002	0.0005	0.00018	0.007	0.001	0.0005	0.0005	0.02	0.0005	0.025	0.02
0.0032	0.0005	0.0025	0.002	0.011	0.00038	0.0005	0.0019	0.015	0.0082	0.02	0.0037	0.025	0.025
0.0005	0.0005	0.0025	0.0005	0.0005	0.00033	0.0005	0.0045	0.0005	0.0091	0.02	0.0005	0.025	0.032
0.0005	0.0005	0.0025	0.002	0.00072	0.00039	0.0005	0.0005	0.0052	0.0005	0.02	0.0005	0.025	0.029
0.0022	0.0005	0.0025	0.0005	0.0014	0.0005	0.0017	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.023
0.0005	0.0005	0.0025	0.003	0.00035	0.0019	0.0028	0.0005	0.018	0.0005	0.02	0.0005	0.025	0.024
0.002	0.0005	0.0025	0.003	0.0005	0.00012	0.0038	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.025
0.0019	0.0005	0.0025	0.002	0.0062	0.0005	0.0005	0.0029	0.0005	0.0005	0.02	0.0005	0.025	0.026
0.0005	0.0005	0.0025	0.002	0.0057	0.00035	0.0005	0.0005	0.016	0.0005	0.02	0.0005	0.025	0.027
0.0023	0.0005	0.0025	0.0005	0.0005	0.0013	0.0044	0.0005	0.007	0.0005	0.02	0.0005	0.025	0.011
0.0023	0.00064	0.0025	0.003	0.0005	0.00017	0.0005	0.0047	0.0005	0.0005	0.02	0.0005	0.025	0.023
0.0005	0.0005	0.0025	0.003	0.0022	0.00038	0.0005	0.00084	0.0093	0.0005	0.02	0.003	0.025	0.019
0.0005	0.0005	0.0025	0.003	0.041	0.0005	0.0005	0.0005	0.0005	0.0005	0.02	0.0025	0.025	0.017
0.0005	0.017	0.0025	0.003	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.02	0.0031	0.025	0.024
0.002	0.0005	0.0025	0.003	0.016	0.0005	0.0005	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.02
0.0022	0.0005	0.0025	0.0005	0.014	0.00091	0.0005	0.00029	0.0005	0.0043	0.02	0.003	0.025	0.0037
0.0005	0.0005	0.0025	0.002	0.0041	0.0005	0.0021	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.016
0.0023	0.0005	0.0025	0.003	0.026	0.0005	0.0005	0.00067	0.0005	0.0005	0.02	0.0024	0.025	0.012
0.0005	0.0005	0.0025	0.003	0.0033	0.0005	0.0005	0.0016	0.0005	0.0005	0.02	0.0005	0.025	0.016
0.0019	0.0005	0.0025	0.002	0.002	0.0005	0.0005	0.0014	0.0005	0.0005	0.02	0.0028	0.025	0.013
0.0017	0.0005	0.0025	0.002	0.0005	0.0002	0.0022	0.0006	0.0005	0.0005	0.02	0.0028	0.025	0.015
0.002	0.0005	0.0025	0.0005	0.0005	0.0005	0.0018	0.0005	0.0005	0.0005	0.02	0.0029	0.025	0.018
0.0018	5.90E-05	0.0025	0.0005	0.019	0.0005	0.0005	0.002	0.0005	0.0005	0.02	0.0035	0.025	0.011
0.0005	4.60E-05	0.0025	0.002	0.0039	0.0005	0.0005	0.00025	0.0005	0.0005	0.02	0.0005	0.025	0.016
0.0005	0.0005	0.0025	0.002	0.019	0.0005	0.0032	0.00081	0.0005	0.0005	0.02	0.0029	0.025	0.012
0.0005	0.0005	0.0025	0.003	0.00026	0.0005	0.002	0.00013	0.0005	0.0005	0.02	0.003	0.025	0.013
0.0019	0.0022	0.0025	0.002	0.0022	0.0005	0.0005	0.0047	0.0005	0.0005	0.02	0.0028	0.025	0.013
0.0005	0.0005	0.0025	0.007	0.0036	0.0005	0.014	0.0005	0.0005	0.0005	0.02	0.0033	0.025	0.051
0.0005	0.0029	0.0025	0.003	0.0005	0.00024	0.0021	0.0015	0.0005	0.0005	0.02	0.0005	0.025	0.012
0.0005	0.0005	0.0025	0.002	0.00093	0.0005	0.0005	0.0021	0.0005	0.0005	0.02	0.0025	0.025	0.015
0.0005	0.0027	0.0025	0.003	0.0096	0.0005	0.0015	0.0034	0.0005	0.0005	0.02	0.0029	0.025	0.011
0.0018	0.00088	0.0025	0.002	0.0023	0.00018	0.0005	0.001	0.0005	0.0049	0.02	0.0005	0.025	0.016
0.0019	0.0005	0.0025	0.002	0.00024	0.00021	0.002	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.017
0.0005	0.0005	0.0025	0.002	0.0005	0.0005	0.0016	0.00029	0.0005	0.0005	0.02	0.0005	0.025	0.017
0.0005	0.0005	0.005	0.006	0.0005	0.0005	0.0017	0.00022	0.0005	0.0005	0.04	0.0005	0.025	0.04
0.002	0.0005	0.0025	0.003	0.027	0.0005	0.0017	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.018
0.0005	0.0096	0.0025	0.002	0.0005	0.0005	0.0005	0.00031	0.0005	0.0005	0.02	0.0005	0.025	0.015
0.0021	0.0005	0.0025	0.0005	0.0005	0.00019	0.0081	0.00071	0.0005	0.0005	0.02	0.0005	0.025	0.065
0.003	0.00066	0.0025	0.001	0.0005	0.00053	0.0014	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.015
0.002	0.0005	0.0025	0.0005	0.0005	0.0005	0.0025	0.00042	0.0005	0.0005	0.02	0.0029	0.025	0.014
0.0005	0.0005	0.0025	0.0005	0.0005	0.0002	0.002	0.00016	0.0005	0.005	0.02	0.0028	0.025	0.017
0.0005	0.0005	0.0025	0.002	1.10E-05	0.00024	0.0005	0.0002	0.0005	0.0005	0.02	0.0005	0.025	0.013
0.0005	0.0005	0.0025	0.0005	0.0005	0.00016	0.0005	0.00039	0.0005	0.0044	0.02	0.0029	0.025	0.047
0.0005	0.0005	0.0025	0.001	0.0005	0.00017	0.0005	9.10E-05	0.0005	0.0005	0.02	0.0005	0.025	0.016
0.0005	0.0005	0.06	0.0005	9.20E-05	0.00018	0.025	0.0027	0.0005	0.0005	0.09	0.0005	0.073	0.14
0.0005	0.0005	0.0025	0.002	0.019	0.00018	0.0005	0.00071	0.0005	0.0069	0.02	0.0005	0.025	0.018
0.0005	0.0005	0.0025	0.001	0.00028	0.0002	0.0005	0.0038	0.0005	0.0005	0.02	0.0005	0.025	0.02
0.0005	0.0005	0.0025	0.001	0.0005	0.00016	0.0005	0.0015	0.0005	0.0005	0.02	0.0005	0.025	0.016
0.0005	0.0005	0.0025	0.0005	0.0005	0.0005	0.0016	0.0005	0.0005	0.0005	0.02	0.0005	0.025	0.015
0.0021	0.0005	0.0025	0.001	0.0021	0.0005	0.002	0.0019	0.0005	0.0075	0.02	0.0005	0.025	0.0088
0.0005	0.0005	0.0025	0.0005	0.012	0.00021	0.0017	0.0027	0.0005	0.0005	0.02	0.0005	0.025	0.013
0.0005	0.0005	0.0025	0.001	0.0014	0.00021	0.0005	0.0017	0.0005	0.0005	0.02	0.0005	0.025	0.015
0.0005	0.0005	0.0025	0.0005	2.60E-05	0.00016	0.0005	0.0025	0.0005	0.0005	0.02	0.0005	0.025	0.016
0.0033	0.0005	0.0025	0.002	0.00015	0.00017	0.0005	0.0022	0.0005	0.0005	0.02	0.0005	0.025	0.021
0.0005	0.0005	0.0025	0.002	0.0005	0.0005	0.0005	0.0027	0.0005	0.0044	0.02	0.0005	0.025	0.015

Sulpirid	Telmisartan	Temazepam	Topiramate	Tramadol	Trazodone	Triazolam	Trimethoprim	Trimipramine	Valsartan	Valsartan acid	Venlafaxine	Verapamil	Zolpidem
0.02	0.03	0.0034	0.00064	0.0094	0.0005	0.0027	0.0045	0.011	0.02	0.05	0.0047	0.0005	0.0017
0.02	0.03	0.0034	0.00098	0.014	0.0016	0.0038	0.0045	0.17	0.02	0.06	0.0061	0.041	0.0017
0.02	0.03	0.0005	0.0012	0.014	0.0005	0.0035	0.0045	0.015	0.02	0.06	0.007	0.0005	0.0017
0.02	0.03	0.0035	0.00098	0.015	0.0005	0.0034	0.0045	0.15	0.02	0.065	0.0067	0.0005	0.0018
0.02	0.02	0.0029	0.0005	0.015	0.0005	0.0038	0.0045	0.18	0.015	0.055	0.0072	0.0099	0.0005
0.01	0.02	0.0035	0.0005	0.011	0.0018	0.0049	0.0045	0.041	0.005	0.04	0.0044	0.0069	0.0018
0.01	0.02	0.0039	0.0005	0.008	0.0016	0.0055	0.0045	0.16	0.005	0.04	0.0022	0.0005	0.0017
0.009	0.02	0.0037	0.0005	0.0066	0.0016	0.0048	0.0045	0.027	0.005	0.035	0.0019	0.0005	0.0017
0.009	0.02	0.012	0.0005	0.0038	0.0051	0.0077	0.0045	0.69	0.005	0.045	0.078	0.15	0.0005
0.01	0.02	0.0039	0.0005	0.0065	0.0016	0.0033	0.0045	0.13	0.0045	0.04	0.0022	0.0056	0.0005
0.01	0.02	0.0034	0.0005	0.01	0.0016	0.0037	0.0045	0.11	0.01	0.045	0.0033	0.008	0.0017
0.04	0.2	0.0005	0.0005	0.0048	0.0016	0.0019	0.0045	0.16	0.0095	0.1	0.0015	0.0005	0.0005
0.01	0.02	0.0035	0.0005	0.0069	0.0017	0.0028	0.0045	0.063	0.0095	0.04	0.0026	0.0056	0.0019
0.01	0.03	0.0033	0.0005	0.0096	0.0015	0.0011	0.0045	0.1	0.01	0.05	0.0026	0.0054	0.0005
0.02	0.04	0.0005	0.0005	0.0074	0.0016	0.0016	0.0045	0.1	0.015	0.08	0.0024	0.0005	0.0005
0.02	0.05	0.0035	0.00059	0.013	0.0005	0.0032	0.0045	0.36	0.035	0.2	0.0037	0.0074	0.0005
0.02	0.02	0.0005	0.0005	0.0075	0.0005	0.0021	0.0045	0.32	0.015	0.075	0.0026	0.0043	0.0017
0.03	0.1	0.01	0.00067	0.0077	0.0005	0.0024	0.0045	0.27	0.025	0.2	0.0027	0.0005	0.0017
0.0045	0.04	0.0035	0.0005	0.0068	0.0017	0.0026	0.0045	0.22	0.02	0.08	0.0023	0.0054	0.0018
0.02	0.05	0.0034	0.0005	0.0055	0.0016	0.0018	0.0045	0.079	0.015	0.095	0.0021	0.0005	0.0005
0.02	0.03	0.0032	0.00094	0.0051	0.0017	0.0022	0.0045	0.024	0.015	0.08	0.0022	0.0005	0.0018
0.02	0.04	0.0038	0.0005	0.0071	0.0015	0.0017	0.0045	0.028	0.02	0.085	0.003	0.0005	0.0005
0.0045	0.06	0.0032	0.0019	0.0006	0.0005	0.0023	0.0045	0.053	0.025	0.2	0.0004	0.0047	0.0005
0.02	0.05	0.0031	0.0005	0.006	0.0017	0.0017	0.0045	0.06	0.02	0.085	0.0026	0.0005	0.0005
0.01	0.04	0.0033	0.0005	0.0062	0.0016	0.00023	0.0045	0.053	0.02	0.09	0.0026	0.0005	0.0005
0.02	0.05	0.0033	0.0005	0.0054	0.0016	0.0015	0.0045	0.18	0.02	0.1	0.0023	0.0005	0.0017
0.02	0.04	0.0033	0.0005	0.0055	0.0017	0.00076	0.0045	0.079	0.02	0.095	0.0023	0.0005	0.0005
0.01	0.05	0.0005	0.00065	0.0047	0.0016	0.00053	0.0045	0.085	0.02	0.1	0.0022	0.0005	0.0005
0.0045	0.02	0.0031	0.0005	0.0031	0.0016	0.00092	0.0045	0.032	0.0095	0.055	0.0014	0.0005	0.0005
0.01	0.04	0.0034	0.0005	0.0039	0.0016	0.0013	0.0045	0.24	0.015	0.095	0.0017	0.0005	0.0005
0.01	0.04	0.0005	0.0005	0.0035	0.0016	0.0015	0.0045	0.24	0.02	0.095	0.0015	0.0005	0.0005
0.02	0.05	0.0005	0.0005	0.0035	0.0017	0.0016	0.0045	0.022	0.02	0.095	0.0014	0.0005	0.0018
0.02	0.04	0.0005	0.0005	0.0036	0.0016	0.0012	0.0045	0.33	0.02	0.095	0.0016	0.0005	0.0019
0.02	0.04	0.0005	0.0005	0.0029	0.0015	0.0005	0.0045	0.27	0.015	0.095	0.0014	0.0005	0.0005
0.0045	0.04	0.0031	0.0005	0.0056	0.0016	0.0015	0.0045	0.33	0.008	0.095	0.0004	0.0005	0.0018
0.01	0.03	0.0005	0.0005	0.0023	0.0016	0.00094	0.0045	0.033	0.015	0.085	0.0014	0.0005	0.0005
0.0045	0.01	0.0031	0.0005	0.0032	0.0016	0.00092	0.0045	0.31	0.004	0.01	0.0016	0.0005	0.0017
0.02	0.03	0.0005	0.0005	0.003	0.0017	0.0002	0.0045	0.019	0.01	0.065	0.0029	0.0005	0.0005
0.02	0.04	0.0005	0.00063	0.0023	0.0016	0.0005	0.0045	0.0005	0.015	0.08	0.0014	0.0054	0.0005
0.02	0.03	0.0005	0.0005	0.0024	0.0016	0.0005	0.0045	0.0073	0.015	0.09	0.002	0.0005	0.0017
0.04	0.01	0.0005	0.0005	0.001	0.0016	0.0005	0.0045	0.091	0.025	0.02	0.0006	0.0005	0.0005
0.02	0.04	0.0005	0.0005	0.0019	0.0015	0.0005	0.0045	0.13	0.01	0.095	0.0014	0.0005	0.0018
0.02	0.03	0.0005	0.0005	0.002	0.0005	0.0005	0.0045	0.17	0.015	0.085	0.0016	0.0005	0.0019
0.02	0.03	0.0005	0.0005	0.0016	0.0005	0.0005	0.0045	0.14	0.009	0.09	0.0018	0.0005	0.0005
0.02	0.03	0.0005	0.0005	0.0005	0.0005	0.0005	0.0045	0.011	0.004	0.095	0.0009	0.0005	0.0017
0.02	0.03	0.0005	0.0005	0.0005	0.0005	0.0005	0.0045	0.034	0.004	0.095	0.0013	0.0005	0.0017
0.02	0.03	0.0005	0.0005	0.0058	0.0016	0.0005	0.0045	0.019	0.0045	0.09	0.0013	0.0005	0.0005
0.08	0.01	0.0005	0.0005	0.0009	0.0016	0.0005	0.0045	0.15	0.00175	0.02	0.0004	0.0005	0.0017
0.02	0.02	0.003	0.0005	0.0052	0.0016	0.0005	0.0045	0.0005	0.0045	0.085	0.0014	0.0005	0.0005
0.01	0.03	0.0005	0.0005	0.0005	0.0005	0.0005	0.0045	0.0094	0.0035	0.07	0.0004	0.0005	0.0017
0.0045	0.3	0.0005	0.0005	0.0003	0.0016	0.0005	0.0045	0.0005	0.1	0.4	0.0005	0.0005	0.0005
0.01	0.02	0.0033	0.0005	0.0005	0.0017	0.0005	0.0045	0.0005	0.00175	0.06	0.0005	0.0005	0.0005
0.01	0.02	0.0032	0.0005	0.0005	0.0016	0.0005	0.0045	0.0005	0.0035	0.075	0.0005	0.0005	0.0005
0.0045	0.05	0.0005	0.0005	0.0002	0.0016	0.0005	0.0045	0.27	0.035	0.2	0.0005	0.0005	0.0017
0.01	0.02	0.0005	0.0005	0.003	0.0005	0.0005	0.0045	0.096	0.005	0.065	0.0008	0.0005	0.0005
0.0045	0.07	0.0032	0.0005	0.0011	0.0026	0.0005	0.009	0.28	0.07	0.15	0.0006	0.0005	0.0017
0.01	0.02	0.0005	0.0005	0.0028	0.0005	0.0005	0.0045	0.24	0.00175	0.06	0.0007	0.0005	0.0017
0.02	0.3	0.0063	0.00088	0.016	0.0005	0.0005	0.0045	0.23	0.1	0.05	0.0028	0.0052	0.0005
0.01	0.02	0.0005	0.0005	0.0033	0.0005	0.0005	0.0045	0.26	0.0035	0.055	0.0007	0.0005	0.0017
0.01	0.03	0.0005	0.0005	0.0025	0.0005	0.0005	0.0045	0.18	0.009	0.065	0.0006	0.0005	0.0017
0.01	0.02	0.0005	0.0005	0.0025	0.0005	0.0005	0.0045	0.2	0.01	0.06	0.0005	0.0005	0.0017
0.0045	0.02	0.0005	0.0005	0.0022	0.0005	0.0005	0.0045	0.27	0.0095	0.07	0.0006	0.0005	0.0005
0.0045	0.02	0.0005	0.0005	0.0003	0.0016	0.0005	0.0045	0.37	0.00175	0.02	0.0005	0.0005	0.0017
0.0045	0.01	0.0005	0.0005	0.0008	0.0029	0.0005	0.0045	0.35	0.00175	0.02	0.0005	0.0005	0.0005
0.0045	0.02	0.0005	0.0005	0.0022	0.0005	0.0005	0.0045	0.38	0.00175	0.055	0.0006	0.0005	0.0017
0.009	0.02	0.0005	0.0005	0.0021	0.0005	0.0005	0.0045	0.3	0.00175	0.055	0.0005	0.0005	0.0017
0.0045	0.02	0.0005	0.0005	0.0022	0.0005	0.0005	0.0045	0.28	0.005	0.065	0.0006	0.0005	0.0005
0.01	0.02	0.0005	0.0005	0.0023	0.0005	0.0005	0.0045	0.29	0.0095	0.07	0.0005	0.0005	0.0017

Zopiclone	1H-Benzotriazole	2-(Methylthio)benzothiazole	2-Ethylhexyl diphenyl phosphate (EHDP)	5,6-Dimethylbenzotriazole	5-Methyl-1H-benzotriazole	Benzothiazole-6-carboxylic acid	Nonylphenol (4-Nonylphenol)	Tolyltriazol (mix of isomers)	Triisobutyl phosphate (TIBP)	Tri-n-butyl phosphate (TnBP)	Tri-n-propyl phosphate (TnPP)	Triphenyl phosphate (TPT)	Tris(1-chloro-2-propyl)phosphate (TCPP)
0.0036	0.23	0.015	0.00006	0.0025	0.052	0.005	0.005	0.2	0.011	0.004	0.000035	0.0014	0.11
0.0033	0.46	0.03	0.0014	0.0025	0.097	0.005	0.005	0.25	0.048	0.0038	0.00074	0.0056	0.095
0.0005	0.32	0.015	0.00006	0.0025	0.07	0.005	0.005	0.2	0.023	0.0018	0.000035	0.0042	0.17
0.0063	0.34	0.04	0.00006	0.0025	0.057	0.005	0.005	0.2	0.024	0.0038	0.000035	0.0015	0.18
0.0062	0.48	0.03	0.0016	0.0025	0.092	0.005	0.005	0.1	0.02	0.0051	0.000035	0.0031	0.12
0.0032	0.28	0.03	0.0059	0.0025	0.049	0.005	0.005	0.045	0.017	0.0018	0.00085	0.0034	0.064
0.0022	0.26	0.04	0.00006	0.0025	0.02	0.005	0.005	0.045	0.015	0.0033	0.000035	0.001	0.09
0.00074	0.21	0.04	0.00006	0.0025	0.029	0.005	0.005	0.05	0.013	0.0028	0.000035	0.00001	0.24
0.019	0.31	0.015	0.00006	0.0025	0.052	0.005	0.005	0.05	0.0085	0.0039	0.000035	0.0012	0.056
0.003	0.29	0.03	0.00006	0.0025	0.055	0.005	0.005	0.2	0.022	0.0035	0.000035	0.0012	0.092
0.0054	0.32	0.04	0.00056	0.0025	0.061	0.005	0.005	0.15	0.016	0.0041	0.000035	0.001	0.058
0.0005	0.38	0.015	0.0018	0.0025	0.15	0.005	0.005	0.25	0.012	0.0051	0.000035	0.0076	0.13
0.0023	0.21	0.04	0.00006	0.0025	0.038	0.005	0.005	0.15	0.014	0.0031	0.000035	0.0017	0.045
0.0024	0.27	0.015	0.00006	0.0025	0.039	0.005	0.005	0.15	0.015	0.0039	0.000035	0.0011	0.11
0.0024	0.35	0.04	0.00052	0.0025	0.074	0.005	0.005	0.3	0.015	0.004	0.000035	0.0012	0.059
0.036	0.54	0.015	0.0015	0.007	0.14	0.005	0.005	0.4	0.017	0.0045	0.000035	0.00099	0.095
0.0005	0.36	0.05	0.00054	0.0025	0.097	0.005	0.005	0.3	0.017	0.0062	0.00081	0.001	0.058
0.019	1.6	0.015	0.00093	0.0025	0.1	0.005	0.005	0.35	0.049	0.07	0.00089	0.0012	0.086
0.0005	0.36	0.015	0.00068	0.0025	0.099	0.005	0.005	0.25	0.016	0.0039	0.000035	0.0031	0.052
0.0005	0.55	0.04	0.00006	0.0025	0.1	0.005	0.005	0.2	0.018	0.0094	0.000035	0.0021	0.099
0.0005	0.45	0.015	0.00056	0.0025	0.088	0.005	0.005	0.25	0.017	0.006	0.00071	0.0013	0.073
0.0005	0.47	0.015	0.0034	0.0025	0.093	0.005	0.005	0.25	0.018	0.0072	0.000035	0.0014	0.077
0.0005	0.4	0.015	0.004	0.02	0.051	0.005	0.005	0.2	0.026	0.0057	0.000035	0.00095	0.15
0.0005	0.47	0.015	0.0042	0.0025	0.19	0.005	0.00866667	0.3	0.015	0.005	0.000035	0.002	0.079
0.0005	0.39	0.015	0.00006	0.0025	0.054	0.005	0.005	0.2	0.017	0.0034	0.000035	0.0009	0.11
0.0005	0.38	0.03	0.00006	0.0025	0.06	0.005	0.005	0.4	0.018	0.0035	0.000035	0.0013	0.12
0.0005	0.5	0.015	0.002	0.0025	0.12	0.005	0.005	0.3	0.015	0.0058	0.000035	0.0022	0.079
0.0095	0.36	0.015	0.0003	0.0025	0.1	0.005	0.005	0.3	0.016	0.005	0.000035	0.00085	0.092
0.0005	0.13	0.015	0.00006	0.0025	0.033	0.005	0.005	0.05	0.021	0.0000021	0.000035	0.001	0.036
0.0005	0.3	0.03	0.00006	0.0025	0.087	0.005	0.005	0.25	0.017	0.0031	0.000035	0.00093	0.074
0.0065	0.3	0.015	0.00006	0.0025	0.036	0.005	0.005	0.25	0.019	0.0046	0.000035	0.00074	0.084
0.0072	0.35	0.04	0.00006	0.0025	0.043	0.005	0.005	0.25	0.0095	0.0033	0.000035	0.00001	0.58
0.0063	0.3	0.04	0.00006	0.0025	0.071	0.005	0.005	0.25	0.03	0.00042	0.000035	0.00074	0.082
0.0005	0.28	0.04	0.00006	0.0025	0.077	0.005	0.005	0.2	0.023	0.0035	0.000035	0.0014	0.081
0.0064	0.061	0.05	0.00069	0.02	0.08	0.005	0.005	0.3	0.013	0.0028	0.000035	0.0052	0.072
0.0071	0.28	0.04	0.00006	0.007	0.037	0.005	0.005	0.3	0.023	0.0024	0.000035	0.00001	0.066
0.0011	0.063	0.015	0.00006	0.0025	0.018	0.005	0.005	0.04	0.0047	0.0045	0.000035	0.00001	0.028
0.0036	0.21	0.015	0.00006	0.0025	0.027	0.005	0.005	0.15	0.016	0.0041	0.000035	0.00001	0.057
0.0022	0.21	0.05	0.00006	0.0025	0.043	0.005	0.005	0.25	0.015	0.005	0.000035	0.0009	0.059
0.0027	0.23	0.015	0.00006	0.0025	0.043	0.005	0.005	0.2	0.018	0.0044	0.000035	0.00001	0.065
0.0026	0.14	0.04	0.00006	0.0025	0.065	0.005	0.005	0.3	0.024	0.0029	0.000035	0.0012	0.084
0.0005	0.23	0.015	0.00006	0.0025	0.041	0.005	0.005	0.2	0.015	0.0041	0.000035	0.00062	0.061
0.0005	0.25	0.04	0.00006	0.0025	0.05	0.005	0.005	0.25	0.015	0.0042	0.0021	0.0018	0.12
0.0005	0.25	0.015	0.00006	0.0025	0.036	0.005	0.005	0.25	0.015	0.002	0.000035	0.00058	0.1
0.00072	0.25	0.03	0.00006	0.0025	0.068	0.005	0.005	0.25	0.014	0.0038	0.000035	0.00067	0.11
0.0022	0.25	0.03	0.00006	0.007	0.074	0.005	0.00466667	0.35	0.015	0.0042	0.000035	0.00001	0.12
0.0022	0.21	0.015	0.00006	0.005	0.05	0.005	0.005	0.3	0.019	0.0037	0.000035	0.00063	0.067
0.0045	0.0015	0.03	0.00006	0.0025	0.0095	0.01	0.02	0.0025	0.0025	0.0029	0.000035	0.00001	0.6
0.0005	0.26	0.015	0.00006	0.0025	0.093	0.005	0.005	0.3	0.019	0.0051	0.000035	0.00064	0.074
0.0005	0.26	0.015	0.00006	0.005	0.031	0.005	0.005	0.2	0.022	0.0037	0.000035	0.0012	0.11
0.0022	0.16	0.015	0.00006	0.0025	0.11	0.005	0.005	0.2	0.037	0.019	0.000035	0.00001	0.28
0.0037	0.27	0.06	0.00006	0.0025	0.12	0.005	0.00433333	0.05	0.025	0.0042	0.000035	0.00058	0.069
0.0035	0.25	0.03	0.00006	0.0025	0.072	0.005	0.005	0.2	0.021	0.0066	0.000035	0.00076	0.11
0.0005	0.024	0.05	0.00006	0.0025	0.021	0.005	0.005	0.0025	0.015	0.0024	0.000035	0.0058	0.074
0.0023	0.23	0.015	0.00006	0.0025	0.073	0.005	0.005	0.2	0.021	0.0041	0.000035	0.00001	0.086
0.0018	0.11	0.04	0.00038	0.0025	0.025	0.005	0.018	0.0025	0.0085	0.0073	0.000035	0.0016	0.11
0.0005	0.24	0.06	0.00006	0.0025	0.12	0.04	0.005	0.2	0.021	0.0044	0.000035	0.00074	0.085
0.0005	0.26	0.09	0.00006	0.01	0.29	0.005	0.012	0.25	0.097	0.012	0.001	0.0073	0.3
0.0019	0.28	0.015	0.00006	0.0025	0.083	0.005	0.005	0.2	0.023	0.0046	0.00073	0.00091	0.11
0.0005	0.27	0.04	0.0012	0.0025	0.08	0.005	0.005	0.2	0.025	0.0014	0.000035	0.00074	0.1
0.0019	0.22	0.015	0.00006	0.0025	0.019	0.005	0.005	0.15	0.019	0.0052	0.000035	0.00001	0.12
0.0019	0.24	0.04	0.00006	0.005	0.071	0.005	0.005	0.15	0.022	0.0042	0.000035	0.00064	0.12
0.0005	0.027	0.015	0.00006	0.0025	0.046	0.005	0.009	0.035	0.021	0.0066	0.000035	0.00001	0.096
0.0019	0.0073	0.03	0.00068	0.0025	0.024	0.005	0.005	0.005	0.0074	0.011	0.000035	0.00055	0.035
0.002	0.25	0.03	0.00006	0.0025	0.057	0.005	0.005	0.05	0.0068	0.0059	0.000035	0.00001	0.29
0.0005	0.24	0.05	0.00006	0.0025	0.052	0.005	0.005	0.15	0.027	0.0068	0.000035	0.0038	0.079
0.0024	0.26	0.015	0.00006	0.005	0.077	0.005	0.005	0.2	0.027	0.0082	0.000035	0.0017	0.12
0.0005	0.18	0.05	0.00006	0.0025	0.027	0.005	0.005	0.2	0.019	0.0046	0.000035	0.00001	0.054

Tris(2-butoxyethyl) phosphate (TBEP)	Tris(2-chloroethyl) phosphate (TCEP)	Tris(3,5-dimethylphenyl)phosphate (T35DMPP)	Tris(methylphenyl)phosphate (TMPP)	Dibutyltin-cation	Dioctyltin-cation	Diphenyltin-cation	Tetrabutyltin	Tributyltin-cation	Triphenyltin-cation	2,4-Dinitrophenol (DNP)	Acesulfame	Bisphenol A	Bisphenol S
0.025	0.011	0.000115	0.000042	0.0025	0.00005	0.00005	3.00E-07	2.00E-07	0.00005	0.02	0.43	0.05	0.05
0.049	0.018	0.01	0.0013	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.51333333	0.013	0.05
0.034	0.023	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.62	0.03	0.05
0.04	0.023	0.000115	0.000042	0.00053	0.00005	0.00005	0.00000005	5.00E-07	0.00005	0.02	0.64666667	0.55	0.05
0.042	0.017	0.014	0.000042	0.00056	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.01	0.70666667	0.065	0.05
0.023	0.0068	0.024	0.0093	0.00077	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.01	0.47	0.0083	0.05
0.018	0.011	0.000115	0.000042	0.00005	0.00005	0.00005	2.00E-07	7.00E-07	0.00005	0.02	0.46333333	0.0095	0.05
0.054	0.028	0.000115	0.000042	0.00059	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.43	0.24	0.05
0.024	0.0096	0.000115	0.000042	0.00046	0.00005	0.00005	0.00000005	3.00E-07	0.00005	0.01	0.48666667	0.14	0.05
0.02	0.012	0.000115	0.000042	0.00036	0.00005	0.00005	0.00000005	4.00E-07	0.00005	0.01	0.41	1.3	0.05
0.022	0.0081	0.000115	0.0032	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.45666667	0.039	0.21
0.007	0.012	0.000115	0.013	0.00023	0.00005	0.00034	0.00000005	7.00E-07	0.00021	0.02	0.69	0.014	0.05
0.02	0.004	0.000115	0.000042	0.00021	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.4	0.039	0.05
0.018	0.011	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.385	0.021	0.05
0.019	0.0094	0.008	0.00086	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.49	0.14	0.05
0.02	0.013	0.054	0.0088	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.53	0.017	0.05
0.018	0.0099	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.51333333	0.049	0.05
0.011	0.012	0.000115	0.000042	0.00086	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.59	0.032	0.05
0.016	0.0086	0.000115	0.0022	0.00005	0.00005	0.00005	0.00000005	3.00E-07	0.00005	0.02	0.46666667	0.17	0.05
0.015	0.011	0.000115	0.000042	0.00062	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.49	0.08	0.05
0.019	0.0097	0.000115	0.00082	0.00037	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.46	0.024	0.05
0.018	0.0087	0.011	0.0088	0.00028	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.50666667	0.65	0.05
0.0093	0.0093	0.017	0.0079	0.00025	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.58	0.064	0.05
0.018	0.0092	0.042	0.011	0.00031	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.49	0.0028	0.05
0.0097	0.01	0.000115	0.000042	0.00022	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.45	0.055	0.05
0.0096	0.011	0.000115	0.000042	0.00027	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.49666667	0.0056	0.05
0.017	0.009	0.016	0.000042	0.00028	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.45666667	0.0093	0.27
0.015	0.012	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.54333333	0.0028	0.05
0.0095	0.0034	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.04	0.20666667	0.0028	0.05
0.0077	0.0077	0.000115	0.000042	0.00038	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.4	0.0028	0.05
0.000565	0.0096	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.36666667	0.0028	0.05
0.000565	0.012	0.000115	0.000042	0.00034	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.04	0.47333333	0.0028	0.05
0.0076	0.0081	0.000115	0.000042	0.00044	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.04	0.41333333	0.0028	0.05
0.0061	0.0082	0.000115	0.000042	0.00021	0.00027	0.00005	0.00000005	0.00000005	0.00005	0.04	0.47	0.0028	0.05
0.000565	0.01	0.000115	0.000042	0.00024	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.44	0.0028	0.05
0.000565	0.0069	0.000115	0.000042	0.00023	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.43333333	0.0028	0.05
0.000565	0.0024	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.19666667	0.0028	0.05
0.000565	0.0059	0.000115	0.000042	0.00027	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.41	0.0028	0.05
0.000565	0.0058	0.000115	0.000042	0.00053	0.00023	0.00005	0.00000005	0.00000005	0.00005	0.03	0.48666667	0.0028	0.05
0.000565	0.0059	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.04	0.43	0.0028	0.05
0.000565	0.013	0.000115	0.000042	0.00051	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.58	0.0028	0.05
0.000565	0.0063	0.000115	0.000042	0.00035	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.40333333	0.0028	0.05
0.051	0.033	0.000115	0.000042	0.00027	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.45666667	0.0028	0.05
0.011	0.015	0.000115	0.000042	0.00045	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.44	0.0028	0.05
0.011	0.011	0.000115	0.000042	0.00022	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.44333333	0.0028	0.05
0.0086	0.0096	0.000115	0.000042	0.00024	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.46	0.0028	0.05
0.000565	0.0049	0.000115	0.000042	0.00062	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.49	0.0028	0.05
0.000565	0.01	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.06	0.69	0.0028	0.05
0.000565	0.0091	0.000115	0.00087	0.00022	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.03	0.45	0.0028	0.05
0.0057	0.01	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.47333333	0.0028	0.05
0.000565	0.041	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	1	0.0028	0.05
0.000565	0.0062	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.42666667	0.0028	0.05
0.000565	0.011	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.45666667	0.0028	0.05
0.000565	0.015	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.98	0.0028	0.05
0.000565	0.0079	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.48	0.0028	0.05
0.012	0.017	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.01	1.2	0.0028	0.05
0.000565	0.0098	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.42333333	0.0028	0.05
0.093	0.029	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.01	1.1	0.0028	0.05
0.000565	0.007	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.46666667	0.0028	0.05
0.0052	0.0081	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.52	0.0028	0.05
0.0084	0.0087	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.4	0.0028	0.05
0.000565	0.0048	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.50333333	0.0028	0.05
0.000565	0.0083	0.000115	0.000042	0.00027	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.04	0.25333333	0.0028	0.05
0.0089	0.01	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.04	0.23	0.0028	0.05
0.006	0.0094	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.46333333	0.0028	0.05
0.0053	0.0081	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.37666667	0.0028	0.14
0.01	0.021	0.000115	0.000042	0.00005	0.00005	0.00005	0.00000005	0.00000005	0.00005	0.02	0.43666667	0.0028	0.05
0.000565	0.0054	0.000115	0.000042	0.00021	0.00028	0.00005	0.00000005	0.00000005	0.00005	0.02	0.51	0.0028	0.05

Caffeine	Cotinine	Di(2-ethylhexyl)phthalate (DEHP)	N,N-Diethyl-m-toluamid (DEET)	Nicotine	Perfluorobutanesulfonate (PFBS)	Perfluoroheptanoic acid (PFHpA)	Perfluorohexane sulfonate (PFHxS) (anion)	Perfluorohexanoic acid (PFHxA)	Perfluorononanoate (PFNA)	Perfluorooctanesulfonic acid (PFOS)	Perfluorooctanoic acid (PFOA)	Saccharin	Sucralose
0.1	0.041	0.1	0.015	0.2	0.0022	0.00075	0.002	0.0021	0.00085	0.0069	0.0019	0.07	0.05
0.16	0.046	0.21	0.022	0.29	0.0021	0.00075	0.003	0.0042	0.0014	0.023	0.0034	0.07	0.05
0.2	0.14	0.28	0.018	0.3	0.0022	0.00075	0.001	0.0031	0.0019	0.011	0.003	0.05	0.05
0.14	0.036	0.22	0.022	0.26	0.0023	0.00075	0.001	0.0034	0.0018	0.013	0.0041	0.07	0.05
0.14	0.034	0.1	0.023	0.27	0.0018	0.00075	0.001	0.0049	0.0018	0.015	0.0047	0.04	0.05
0.1	0.039	0.1	0.016	0.24	0.0011	0.00075	0.001	0.006	0.0027	0.016	0.0091	0.1	0.05
0.12	0.031	0.1	0.013	0.27	0.0016	0.0035	0.001	0.0066	0.0013	0.0056	0.007	0.04	0.05
0.092	0.042	0.22	0.011	0.61	0.0013	0.00075	0.001	0.0054	0.0015	0.0054	0.0063	0.04	0.05
0.19	0.036	0.1	0.016	0.0005	0.0021	0.0066	0.001	0.0067	0.002	0.01	0.02	0.06	0.05
0.11	0.079	0.1	0.012	0.38	0.0013	0.00075	0.001	0.005	0.0016	0.0058	0.006	0.04	0.05
0.2	0.052	0.28	0.017	0.33	0.002	0.0062	0.001	0.0079	0.0025	0.0069	0.018	0.04	0.05
0.09	0.079	0.24	0.081	0.28	0.0028	0.0042	0.001	0.0032	0.000145	0.011	0.0047	0.04	0.2
0.12	0.037	0.24	0.012	0.38	0.0016	0.0067	0.001	0.0047	0.002	0.0089	0.032	0.04	0.05
0.15	0.053	0.28	0.015	0.29	0.0014	0.0041	0.001	0.006	0.0013	0.0061	0.0063	0.05	0.05
0.22	0.12	0.55	0.02	0.36	0.000095	0.00075	0.001	0.0067	0.000145	0.000265	0.021	0.07	0.1
0.27	0.041	0.41	0.023	0.1	0.000095	0.00075	0.001	0.0056	0.000145	0.0053	0.017	0.1	0.3
0.073	0.03	0.1	0.017	0.14	0.0021	0.00075	0.001	0.0074	0.001	0.0089	0.008	0.06	0.1
0.12	0.041	0.48	0.028	0.091	0.0015	0.00075	0.001	0.0034	0.00079	0.0095	0.0043	0.1	0.3
0.069	0.021	0.23	0.02	0.21	0.0021	0.0081	0.001	0.0085	0.0017	0.02	0.025	0.06	0.1
0.098	0.026	0.23	0.023	0.28	0.0021	0.00075	0.001	0.0078	0.000145	0.026	0.011	0.07	0.1
0.093	0.025	0.1	0.019	0.056	0.002	0.0074	0.001	0.0068	0.0014	0.0058	0.026	0.07	0.1
0.095	0.022	0.1	0.019	0.16	0.0033	0.01	0.001	0.0077	0.000145	0.0024	0.037	0.06	0.05
0.067	0.03	0.1	0.038	0.2	0.0037	0.0057	0.001	0.0052	0.0007	0.013	0.015	0.04	0.5
0.069	0.023	0.24	0.018	0.25	0.0021	0.0055	0.001	0.0071	0.00095	0.0082	0.018	0.06	0.2
0.052	0.02	0.39	0.013	0.2	0.0016	0.0052	0.001	0.0052	0.0014	0.0078	0.0071	0.07	0.1
0.072	0.018	0.26	0.011	0.1	0.0016	0.004	0.001	0.0055	0.001	0.0071	0.0057	0.1	0.2
0.078	0.015	0.1	0.018	0.19	0.0022	0.0058	0.001	0.0065	0.0008	0.0084	0.017	0.08	0.2
0.08	0.016	0.28	0.005	0.074	0.003	0.0065	0.001	0.0049	0.000145	0.0082	0.018	0.08	0.2
0.085	0.022	0.1	0.00076	0.011	0.0025	0.00075	0.001	0.0016	0.00093	0.005	0.012	0.04	0.1
0.09	0.031	0.1	0.0028	0.14	0.0028	0.0054	0.001	0.0044	0.000145	0.0075	0.019	0.06	0.2
0.056	0.018	0.1	0.0095	0.13	0.0016	0.019	0.001	0.0059	0.0013	0.0063	0.0052	0.08	0.2
0.11	0.025	0.84	0.012	0.15	0.0022	0.0079	0.001	0.0052	0.0014	0.0076	0.0061	0.09	0.2
0.06	0.023	0.1	0.002	0.14	0.003	0.0052	0.001	0.0042	0.00073	0.013	0.012	0.08	0.2
0.11	0.011	0.1	0.002	0.11	0.0021	0.0059	0.001	0.0039	0.0011	0.0097	0.014	0.07	0.2
0.075	0.024	0.1	0.0032	0.091	0.0012	0.00075	0.001	0.0014	0.001	0.000265	0.0082	0.1	0.2
0.094	0.031	0.1	0.0088	0.1	0.003	0.0068	0.001	0.0031	0.00095	0.0052	0.012	0.06	0.2
0.11	0.027	0.1	0.0039	0.1	0.00074	0.0065	0.001	0.00055	0.000145	0.0036	0.00023	0.07	0.05
0.19	0.038	0.26	0.0079	0.19	0.00076	0.0046	0.001	0.0029	0.0008	0.0037	0.0033	0.06	0.2
0.16	0.036	0.2	0.0089	0.2	0.00087	0.0052	0.001	0.0031	0.00074	0.0048	0.0043	0.08	0.1
0.16	0.035	0.1	0.0093	0.14	0.0012	0.0065	0.001	0.003	0.0027	0.0056	0.0037	0.09	0.2
0.25	0.046	0.26	0.018	0.15	0.00063	0.0046	0.001	0.0015	0.000145	0.0047	0.0049	0.6	0.3
0.14	0.034	0.35	0.0014	0.19	0.00094	0.00075	0.001	0.0043	0.00072	0.0049	0.0042	0.1	0.2
0.2	0.037	0.26	0.0098	0.15	0.0014	0.00075	0.001	0.0031	0.0013	0.006	0.0044	0.1	0.2
0.12	0.039	0.1	0.0087	0.17	0.0015	0.00075	0.001	0.0033	0.0015	0.0055	0.0037	0.1	0.2
0.11	0.034	0.1	0.0099	0.13	0.0014	0.00075	0.001	0.0038	0.0016	0.0062	0.0043	0.1	0.2
0.12	0.035	0.1	0.0099	0.16	0.0011	0.00075	0.001	0.0033	0.0015	0.0061	0.0041	0.08	0.2
0.021	0.0001	0.1	0.0072	0.0005	0.0012	0.00075	0.001	0.0035	0.000145	0.0041	0.0039	0.09	0.2
0.066	0.012	0.1	0.014	0.0005	0.000095	0.00075	0.001	0.00055	0.000145	0.0037	0.0018	0.02	0.2
0.027	0.002	0.1	0.012	0.0016	0.0014	0.00075	0.001	0.0038	0.000145	0.0055	0.0051	0.08	0.2
0.013	0.013	0.1	0.02	0.0005	0.0011	0.00075	0.001	0.0036	0.0017	0.0064	0.0046	0.07	0.1
0.026	0.015	0.2	0.025	0.0005	0.00073	0.00075	0.001	0.00055	0.00088	0.0024	0.0048	0.2	0.4
0.023	0.0005	0.1	0.0094	0.0005	0.0014	0.00075	0.001	0.004	0.00075	0.0054	0.0051	0.05	0.1
0.024	0.0005	0.1	0.0094	0.0005	0.0013	0.00075	0.001	0.0038	0.00097	0.0047	0.0044	0.05	0.2
0.036	0.028	0.35	0.0066	0.021	0.0019	0.00075	0.001	0.0031	0.00093	0.008	0.0029	0.3	0.05
0.048	0.017	0.21	0.0077	0.091	0.0011	0.00075	0.001	0.004	0.00081	0.0048	0.0032	0.06	0.2
0.32	0.055	0.46	0.0076	0.051	0.000095	0.00075	0.001	0.00055	0.000145	0.000265	0.0032	0.6	0.05
0.059	0.0092	0.37	0.0085	0.089	0.0014	0.00075	0.001	0.0038	0.000145	0.0047	0.0038	0.05	0.2
1.3	0.34	0.48	0.037	0.075	0.0018	0.00075	0.001	0.0018	0.0011	0.0059	0.0026	1.7	0.4
0.14	0.019	0.1	0.0092	0.015	0.0011	0.00075	0.001	0.005	0.0033	0.0063	0.0057	0.04	0.1
0.049	0.024	0.26	0.0093	0.038	0.0013	0.00075	0.001	0.0042	0.003	0.0054	0.0044	0.09	0.2
0.042	0.021	0.1	0.0051	0.082	0.0013	0.00075	0.001	0.0032	0.0014	0.0057	0.0038	0.07	0.1
0.031	0.023	0.1	0.0082	0.065	0.00084	0.00075	0.001	0.0044	0.0029	0.005	0.0051	0.06	0.2
0.027	0.028	0.1	0.0023	0.077	0.000095	0.00075	0.001	0.00055	0.0016	0.0043	0.0012	0.05	0.05
0.029	0.022	0.1	0.0015	0.089	0.000095	0.00075	0.001	0.00055	0.0011	0.000265	0.0015	0.04	0.05
0.039	0.02	0.1	0.0093	0.063	0.0013	0.00075	0.001	0.004	0.0031	0.0057	0.005	0.06	0.1
0.03	0.023	0.1	0.0095	0.11	0.00093	0.00075	0.001	0.0024	0.003	0.0069	0.0043	0.08	0.1
0.044	0.012	0.23	0.017	0.073	0.0014	0.00075	0.001	0.004	0.0033	0.0069	0.0064	0.07	0.2
0.04	0.021	0.1	0.0048	0.11	0.001	0.00075	0.001	0.0023	0.000145	0.0052	0.0033	0.1	0.1

Concentration with LoD

JDS3 site	Arsenic (As) - dissolved	Cadmium (Cd) - dissolved	Chromium (Cr) - dissolved	Copper (Cu) - dissolved	Lead (Pb) - dissolved	Mercury (Hg) - dissolved	Nickel (Ni) - dissolved	Zinc (Zn) - dissolved	Anthracene	Benzo(a)pyrene	Benzo(b)fluoranthene	Benzo(g,h,i)perylene	Benzo(k)fluoranthene
JDS01	1.1	0.003	0.48	1.2	0.4	0.0006	0.93	6	0.0027	0.002	0.002	0.0015	0.002
JDS02	1.4	0.003	0.68	1.1	0.5	0.0006	0.78	4.2	0.002	0.002	0.002	0.001	0.002
JDS03	1.3	0.024	1.2	2	0.63	0.0027	1.8	13	0.0025	0.002	0.002	0.0021	0.002
JDS04	1.4	0.003	0.5	1.6	0.73	0.0039	0.8	6.4	0.002	0.002	0.002	0.0013	0.002
JDS05	1.4	0.014	0.31	1.5	0.7	0.0028	0.81	10	0.002	0.002	0.002	0.0014	0.002
JDS06	1.5	0.013	0.7	1.6	0.56	0.0006	1.1	8.6	0.002	0.002	0.002	0.001	0.002
JDS07	1.6	0.038	0.5	1.7	1.4	0.0006	1.1	11	0.0024	0.0024	0.002	0.0026	0.0022
JDS08	1.4	0.003	0.97	2.1	0.7	0.0006	1	5.5	0.002	0.002	0.002	0.0016	0.002
JDS09	1.5	0.066	5.3	1.2	1.6	0.0006	19	6.6	0.002	0.002	0.002	0.0005	0.002
JDS10	1.5	0.081	0.84	1.2	1.4	0.0006	1.7	5.7	0.0021	0.002	0.002	0.0022	0.002
JDS11	1.5	0.057	6.7	1.3	0.86	0.0006	25	7	0.002	0.002	0.002	0.0015	0.002
JDS12	3.3	0.073	0.36	1.5	1.2	0.0006	2.8	9.9	0.002	0.002	0.002	0.0014	0.002
JDS13	1.6	0.048	0.91	1.3	1.3	0.0006	0.95	5.4	0.002	0.002	0.002	0.0011	0.002
JDS14	1.6	0.015	0.29	1.4	0.26	0.0006	1	8	0.002	0.002	0.002	0.0014	0.002
JDS15	1.6	0.02	0.5	1.2	0.2	0.0006	1	6.3	0.002	0.002	0.002	0.0019	0.002
JDS16	2.4	0.096	0.58	1.1	1.8	0.0006	1.2	7.3	0.002	0.002	0.002	0.0023	0.002
JDS17	1.7	0.034	0.54	1.3	0.38	0.0046	1	5.5	0.002	0.002	0.002	0.0013	0.002
JDS18	3.6	0.057	0.45	1.4	1	0.0044	1.2	5.7	0.002	0.002	0.002	0.0014	0.002
JDS19	1.7	0.15	0.62	1.5	8.1	0.0006	1.4	6.6	0.002	0.002	0.002	0.0015	0.002
JDS20	1.9	0.07	0.42	1.6	4.2	0.0037	1.2	8.6	0.002	0.002	0.002	1.30E-06	0.002
JDS21	2.3	0.029	2.1	1.3	0.63	0.0056	7.3	6	0.002	0.002	0.002	0.0005	0.002
JDS22	2	0.024	0.63	1.4	0.66	0.0034	1.9	7	2.50E-06	0.002	2.10E-06	2.40E-06	0.002
JDS23	3.5	0.011	0.29	1	0.49	0.0023	1.3	12	2.20E-06	0.002	0.002	2.10E-06	0.002
JDS24	2	0.022	0.34	1.3	0.4	0.0037	1.6	8.5	9.80E-06	2.40E-06	2.70E-06	2.60E-06	0.002
JDS25	2	0.028	0.47	1.4	0.45	0.0046	1.1	7.7	2.40E-06	0.002	0.002	2.10E-06	0.002
JDS26	2.1	0.033	0.56	1.5	0.97	0.005	1.3	7.7	2.10E-06	0.002	0.002	2.40E-06	0.002
JDS27	2.2	0.025	0.67	1.4	0.72	0.0043	1.2	6.8	2.50E-06	0.002	0.002	2.00E-06	0.002
JDS28	2.2	0.022	0.33	1.3	0.23	0.0006	1.1	5.7	2.50E-06	0.002	2.30E-06	2.20E-06	0.002
JDS29	2.4	0.027	0.59	0.74	0.51	0.0045	0.76	5.1	2.10E-06	0.002	0.002	1.80E-06	0.002
JDS30	2.2	0.026	0.52	1.1	0.24	0.0046	0.93	5.7	2.30E-06	0.002	0.002	2.20E-06	0.002
JDS31	2.3	0.028	2.6	1.1	0.49	0.0028	9	6.3	0.002	0.002	0.002	0.002	0.002
JDS32	2.3	0.028	0.67	1.2	0.35	0.0057	1.3	7.1	0.003	0.0023	0.0024	0.029	0.002
JDS33	2.3	0.03	0.68	1.2	0.52	0.0025	1.4	7.4	0.0029	0.002	0.0024	0.0031	0.002
JDS34	2.3	0.029	1.1	1.1	0.27	0.0057	2.2	7.1	0.002	0.002	0.002	0.0015	0.002
JDS35	4.3	0.033	0.56	1.8	0.4	0.0039	1.3	13	0.002	0.002	0.002	0.0012	0.002
JDS36	2.4	0.033	0.86	1.3	0.87	0.0006	2.3	8.7	0.002	0.002	0.002	0.0018	0.002
JDS37	2.5	0.03	1	1.4	0.67	0.0021	1.5	7.1	0.002	0.002	0.002	0.0013	0.002
JDS38	2.2	0.075	0.88	2	1.6	0.0042	1.2	2.3	0.002	0.002	0.002	0.0014	0.002
JDS39	2.2	0.048	0.82	2.1	0.59	0.0051	1.1	2.1	0.002	0.002	0.002	0.0013	0.002
JDS40	2.2	0.044	0.76	1.9	0.29	0.0051	1	1.6	0.002	0.002	0.002	0.0016	0.002
JDS41	5	0.3	67	2.3	2.6	0.0006	230	3.4	0.002	0.002	0.002	0.0017	0.002
JDS42	2.2	0.051	0.84	2	0.8	0.0028	1.4	2.2	0.002	0.002	0.002	0.0013	0.002
JDS43	2.5	0.084	1.6	2	0.38	0.0041	4.7	3.9	0.002	0.002	0.002	0.0014	0.002
JDS44	2.3	0.04	0.76	2.1	0.47	0.0006	1.3	2.1	0.002	0.002	0.002	0.0017	0.002
JDS45	2.5	0.043	0.71	2	0.26	0.0056	1.2	1.5	0.002	0.002	0.002	0.0007	0.002
JDS46	2.4	0.037	0.59	2.1	0.3	0.0047	1.3	1.8	0.002	0.002	0.002	0.0011	0.002
JDS47	2.4	0.045	0.72	2.2	0.36	0.007	1.3	2.1	0.002	0.002	0.002	0.0013	0.002
JDS48	1.5	1.1	0.63	283	0.45	0.0023	36	61	0.002	0.002	0.002	0.0012	0.002
JDS49	2.3	0.04	0.81	9.9	0.29	0.0056	1.2	1.9	0.002	0.002	0.002	0.0013	0.002
JDS50	2.3	0.041	2.2	5.2	0.25	0.0038	8.7	8.3	0.002	0.002	0.002	0.0013	0.002
JDS51	5.3	0.11	1.9	13	1	0.0047	6.4	1.8	0.002	0.002	0.002	0.0017	0.002
JDS52	2.2	0.046	0.71	3.7	0.27	0.0048	1.3	1.7	0.002	0.002	0.002	0.001	0.002
JDS53	2.4	0.043	0.72	3.5	0.32	0.0054	2.2	4.9	0.002	0.002	0.002	0.0012	0.002
JDS54	2	0.041	0.61	2.9	0.23	0.0051	1.5	1	0.002	0.002	0.002	0.0015	0.002
JDS55	2.4	0.039	0.47	3.2	0.35	0.0056	1.2	2.5	0.002	0.002	0.002	0.0012	0.002
JDS56	3.2	0.025	1.5	4.1	0.41	0.0063	1.6	2.9	0.002	0.002	0.002	0.0012	0.002
JDS57	2.4	0.037	0.37	3.1	0.41	0.0032	1.4	5.6	0.002	0.002	0.002	0.0012	0.002
JDS58	2.5	0.024	0.44	5.8	0.43	0.0061	3.3	3.9	0.002	0.002	0.002	0.002	0.002
JDS59	2.4	0.04	0.5	2.6	0.39	0.0027	1.8	1.3	0.002	0.002	0.002	0.0011	0.002
JDS60	2.4	0.038	2.2	2.5	0.32	0.0052	8	2.4	0.002	0.002	0.002	0.0011	0.002
JDS61	2.4	0.046	0.58	2.8	0.33	0.0032	2.8	2.5	0.002	0.002	0.002	0.001	0.002
JDS62	2.3	0.04	0.67	2.7	0.33	0.0026	1.4	1.5	0.002	0.002	0.002	0.0012	0.002
JDS63	1.7	0.03	0.23	2.6	0.36	0.0022	1.6	2.7	0.002	0.002	0.002	0.0027	0.002
JDS64	1.7	0.023	0.71	2.8	0.27	0.0058	2.3	1.4	0.002	0.002	0.002	0.0037	0.002
JDS65	2.4	0.042	0.33	2.8	0.71	0.0041	1.7	2.9	0.002	0.002	0.002	0.0018	0.002
JDS66	2.3	0.038	0.39	3.1	0.41	0.0064	1.4	3.6	0.002	0.002	0.002	0.0029	0.002
JDS67	2.4	0.039	0.7	2.6	0.38	0.0046	1.3	2.5	0.002	0.002	0.002	0.0025	0.002
JDS68	2.4	0.043	0.73	2.7	0.22	0.0032	1.3	1.1	0.002	0.002	0.002	0.0037	0.002

Fluoranthene	Indeno(1,2,3-c,d)pyrene	Naphthalene	2,4-D	2-Methyl-4-chlorphenoxy acetic acid (MCPA)	Ametryn	Aminomethylphosphonic acid (AMPA)	Atrazine	Atrazine-2-hydroxy	Atrazine-desethyl	Atrazine-desisopropyl	Bentazone	Bromacil	Carbetamide
0.004	0.0005	0.022	0.00021	0.0057	0.004	0.03	0.006	0.002	0.0098	0.00033	0.004	0.18	0.031
0.0021	0.0024	0.002	0.0038	0.0056	0.004	0.26	0.00866667	0.002	0.01	0.00033	0.004	0.048	0.0078
0.0047	0.0005	0.035	0.0034	0.0061	0.004	0.27	0.01266667	0.002	0.014	0.00033	0.003	0.084	0.0017
0.0024	0.0005	0.024	0.0021	0.0063	0.004	0.3	0.01133333	0.002	0.016	0.0008	0.005	0.05	0.0015
0.0029	0.0005	0.021	0.0018	0.004	0.004	0.24	0.01266667	0.002	0.012	0.00033	0.003	0.03	0.0022
0.0027	0.0005	0.014	0.00051	0.0024	0.004	0.16	0.006	0.002	0.01	0.00033	0.003	0.083	0.00025
0.005	0.0005	0.018	0.001	0.0028	0.004	0.16	0.005	0.002	0.0077	0.0001	0.003	0.084	0.00025
0.0028	0.0005	0.0087	0.00087	0.0027	0.004	0.17	0.005	0.002	0.0082	0.00033	0.003	0.057	0.0032
0.0025	0.0005	0.0094	0.001	0.0021	0.004	0.18	0.005	0.002	0.007	0.00033	0.003	0.065	0.0028
0.0043	0.0037	0.03	0.00083	0.0026	0.004	0.19	0.005	0.002	0.0072	0.0004	0.003	0.00053	0.00025
0.0028	0.0005	0.01	0.0016	0.0025	0.004	0.17	0.005	0.003	0.013	0.00033	0.003	0.00053	0.0017
0.0041	0.0005	0.017	0.0072	0.012	0.004	0.63	0.014	0.02	0.0079	0.00033	0.01	0.00053	0.011
0.0022	0.0005	0.0072	0.0013	0.0016	0.004	0.2	0.005	0.002	0.0073	0.0003	0.003	0.00053	0.0016
0.0028	0.0005	0.013	0.002	0.0037	0.004	0.21	0.006	0.007	0.0092	0.0006	0.004	0.044	0.00025
0.0032	0.0005	0.013	0.0014	0.0028	0.004	0.21	0.00633333	0.005	0.0099	0.0004	0.005	0.00053	0.0096
0.0035	0.0005	0.015	0.0048	0.0064	0.004	0.33	0.007	0.01	0.011	0.00033	0.008	0.088	0.00025
0.0024	0.0005	0.0057	0.0014	0.0029	0.004	0.21	0.00666667	0.002	0.0088	0.0004	0.004	0.03	0.00025
0.0025	0.0005	0.015	0.0025	0.0036	0.004	0.4	0.006	0.02	0.008	0.00033	0.009	0.035	0.00025
0.0026	0.0005	0.008	0.0019	0.0038	0.004	0.21	0.00566667	0.007	0.0095	0.00033	0.005	0.19	0.00025
0.003	0.0005	0.016	0.0047	0.0051	0.004	0.14	0.00666667	0.01	0.0072	0.00033	0.005	0.077	0.0018
0.002	0.0005	7.20E-06	0.0017	0.003	0.004	0.19	0.00566667	0.006	0.007	0.00033	0.004	0.029	0.0012
4.60E-06	0.0005	1.50E-05	0.0015	0.0029	0.004	0.15	0.00633333	0.005	0.0092	0.00033	0.004	0.068	0.025
4.30E-06	0.0005	1.60E-05	0.0012	0.002	0.004	0.25	0.006	0.01	0.0048	0.00033	0.004	0.056	0.011
2.00E-05	0.0005	4.00E-05	0.0016	0.0028	0.004	0.21	0.00733333	0.006	0.0073	0.0006	0.005	0.044	0.0045
5.50E-06	0.0005	1.90E-05	0.001	0.0029	0.004	0.23	0.00733333	0.007	0.0077	0.00033	0.004	0.048	0.0025
6.10E-06	3.40E-06	1.50E-05	0.0012	0.0029	0.004	0.26	0.00666667	0.01	0.0064	0.00033	0.005	0.00053	0.0023
5.50E-06	0.0005	1.90E-05	0.0017	0.0025	0.004	0.25	0.006	0.008	0.0053	0.00033	0.005	0.00053	0.0038
6.20E-06	4.90E-06	1.60E-05	0.0015	0.0031	0.004	0.27	0.007	0.01	0.0058	0.00033	0.005	0.00053	0.0011
3.10E-06	0.0005	1.50E-05	0.00068	0.00098	0.004	0.16	0.005	0.004	0.0034	0.00033	0.003	0.00053	0.0019
4.10E-06	0.0005	1.50E-05	0.001	0.0022	0.004	0.23	0.005	0.008	0.005	0.00033	0.005	0.067	0.0026
0.0039	0.0031	1.10E-05	0.0013	0.002	0.004	0.24	0.00533333	0.008	0.0038	0.00033	0.005	0.00053	0.0027
0.0055	0.0005	0.019	0.0016	0.002	0.004	0.27	0.00666667	0.009	0.0044	0.00033	0.005	0.039	0.003
0.0057	0.0005	0.02	0.0011	0.0013	0.004	0.27	0.006	0.007	0.0037	0.00033	0.005	0.00053	0.00025
0.0028	0.0005	0.0098	0.00094	0.0017	0.004	0.26	0.00633333	0.009	0.0033	0.00033	0.004	0.00053	0.0021
0.0022	0.0005	0.006	0.0032	0.00066	0.004	0.22	0.00633333	0.002	0.0031	0.00033	0.01	0.051	0.0016
0.003	0.0005	0.0071	0.0013	0.002	0.004	0.25	0.00633333	0.007	0.0034	0.00033	0.004	0.077	0.0057
0.0025	0.0036	0.0058	0.0016	0.00006	0.004	0.21	0.005	0.01	0.0005	0.00033	0.003	0.00053	0.00025
0.0026	0.0005	0.0055	0.0015	0.0017	0.004	0.16	0.005	0.007	0.0005	0.00033	0.004	0.11	0.0016
0.0021	0.0005	0.005	0.0019	0.0014	0.004	0.28	0.006	0.008	0.0035	0.00033	0.005	0.00053	0.0013
0.0024	0.0005	0.0075	0.0013	0.0016	0.004	0.26	0.00533333	0.01	0.0032	0.00033	0.005	0.00053	0.0028
0.0024	0.0005	0.0095	0.0057	0.00006	0.004	0.37	0.005	0.002	0.0033	0.00033	0.008	0.00053	0.0036
0.0029	0.0005	0.0069	0.0014	0.0015	0.004	0.25	0.005	0.01	0.0005	0.00033	0.005	0.00053	0.0011
0.0025	0.0026	0.0065	0.0017	0.0014	0.004	0.24	0.00533333	0.009	0.004	0.0003	0.006	0.00053	0.0014
0.003	0.0005	0.0067	0.0018	0.0015	0.004	0.27	0.00566667	0.008	0.0048	0.0003	0.006	0.00053	0.0016
0.0031	0.0011	0.0034	0.002	0.0016	0.004	0.25	0.005	0.01	0.0034	0.00033	0.005	0.024	0.0019
0.0024	0.0005	0.0067	0.0022	0.0016	0.004	0.29	0.00533333	0.01	0.004	0.00033	0.006	0.00053	0.0019
0.0025	0.0024	0.0064	0.0019	0.0015	0.004	0.28	0.00566667	0.01	0.0005	0.0011	0.005	0.00053	0.00025
0.0023	0.0005	0.0059	0.016	0.00006	0.004	0.03	0.007	0.002	0.0005	0.00033	0.02	0.066	0.00025
0.0023	0.0005	0.0068	0.0018	0.0013	0.004	0.24	0.00533333	0.01	0.0005	0.00033	0.006	0.034	0.00025
0.003	0.0005	0.0057	0.0017	0.0012	0.004	0.25	0.005	0.01	0.0005	0.0015	0.005	0.00053	0.0016
0.003	0.0005	0.0075	0.0017	0.00055	0.004	0.34	0.005	0.002	0.0081	0.0023	0.009	0.00053	0.00025
0.002	0.0025	0.008	0.0014	0.0014	0.004	0.25	0.005	0.009	0.0034	0.0004	0.003	0.023	0.0012
0.0022	0.0005	0.011	0.002	0.0015	0.004	0.25	0.00533333	0.008	0.004	0.0018	0.004	0.00053	0.00025
0.0022	0.0027	0.011	0.004	0.00019	0.004	0.24	0.005	0.01	0.0005	0.00033	0.02	0.00053	0.0014
0.002	0.0005	0.012	0.0031	0.0013	0.004	0.22	0.005	0.01	0.0005	0.00033	0.006	0.00053	0.001
0.0023	0.0005	0.002	0.021	0.00032	0.004	0.96	0.005	0.02	0.0005	0.00033	0.02	0.00053	0.0011
0.002	0.0005	0.011	0.0019	0.0011	0.004	0.25	0.006	0.009	0.0031	0.00033	0.004	0.00053	0.0012
0.0043	0.0005	0.033	0.0084	0.00006	0.004	0.62	0.07	0.045	0.0035	0.00033	0.1	0.00053	0.00025
0.002	0.0005	0.0091	0.00009	0.0026	0.004	0.26	0.006	0.008	0.0005	0.00033	0.005	0.00053	0.00025
0.002	0.002	0.016	0.0027	0.0015	0.004	0.25	0.007	0.01	0.0005	0.00033	0.007	0.00053	0.0087
0.002	0.0021	0.014	0.0018	0.0011	0.004	0.23	0.007	0.01	0.0032	0.00033	0.006	0.00053	0.00025
0.0021	0.0005	0.015	0.00009	0.0013	0.004	0.23	0.007	0.01	0.0014	0.00033	0.007	0.00053	0.00025
0.0027	0.0005	0.016	0.0089	0.00039	0.004	0.13	0.005	0.02	0.0005	0.00033	0.02	0.00053	0.0014
0.002	0.0005	0.0094	0.0044	0.0004	0.004	0.12	0.011	0.03	0.0005	0.00033	0.03	0.00053	0.0011
0.002	0.0005	0.014	0.0023	0.0015	0.004	0.24	0.00533333	0.01	0.0005	0.00033	0.007	0.00053	0.0018
0.0025	0.0025	0.012	0.004	0.0022	0.004	0.24	0.005	0.01	0.0005	0.00033	0.007	0.03	0.0018
0.002	0.0024	0.0097	0.00009	0.0021	0.004	0.26	0.006	0.01	0.0005	0.00033	0.007	0.00053	0.0019
0.0025	0.0005	0.012	0.0013	0.00059	0.004	0.23	0.006	0.01	0.0005	0.00033	0.008	0.032	0.0015

Chloridazon	Chloridazon-desphenyl	Chloridazon-methyl-desphenyl	Chloroxuron	Chlortoluron	Cyanazine (Fortrol)	Cybutryne (Irgarol)	Dimefuron	Dimethachlor CGA 369873	Dimethachlor sulfonic acid CGA 354742	Dimethenamid	Dinoseb	Dinoterb	Diuron
0.027	0.14	0.025	0.012	0.00015	0.001	0.00007	0.014	0.04	0.02	0.004	0.004	0.003	0.02
0.0061	0.18	0.025	0.025	0.00015	0.001	0.00037	0.015	0.02	0.02	0.004	0.004	0.003	0.029
0.0064	0.16	0.025	0.011	0.00015	0.001	0.00007	0.0096	0.02	0.02	0.004	0.004	0.003	0.028
0.0001	0.24	0.025	0.0096	0.00015	0.001	0.00007	0.001	0.02	0.02	0.004	0.004	0.003	0.029
0.0001	0.24	0.025	0.012	0.00015	0.001	0.00022	0.0055	0.02	0.02	0.004	0.004	0.07	0.026
0.0001	0.095	0.025	0.015	0.00015	0.001	0.00043	0.001	0.01	0.02	0.004	0.004	0.03	0.017
0.0001	0.08	0.025	0.014	0.00015	0.001	0.00007	0.0038	0.01	0.02	0.004	0.004	0.08	0.016
0.0001	0.1	0.025	0.013	0.00015	0.001	0.00007	0.001	0.01	0.02	0.004	0.004	0.02	0.013
0.0001	0.13	0.025	0.04	0.00015	0.076	0.00034	0.0066	0.01	0.02	0.004	0.004	0.03	0.0005
0.0001	0.095	0.025	0.023	0.00015	0.001	0.00007	0.026	0.01	0.02	0.004	0.004	0.02	0.0005
0.0001	0.1	0.025	0.026	0.00015	0.001	0.00032	0.014	0.01	0.02	0.004	0.004	0.02	0.012
0.0042	0.25	0.055	0.016	0.00015	0.001	0.00036	0.0086	0.05	0.02	0.004	0.004	0.05	0.0005
0.0001	0.082	0.025	0.019	0.00015	0.001	0.00007	0.014	0.01	0.02	0.004	0.004	0.03	0.0005
0.003	0.098	0.025	0.016	0.00015	0.001	0.00032	0.0075	0.01	0.02	0.004	0.004	0.04	0.0005
0.0001	0.094	0.025	0.017	0.00015	0.001	0.0002	0.013	0.02	0.02	0.004	0.004	0.003	0.0005
0.0001	0.074	0.025	0.0094	0.00015	0.001	0.00007	0.011	0.02	0.02	0.004	0.004	0.003	0.012
0.0001	0.088	0.025	0.012	0.00015	0.001	0.0005	0.001	0.03	0.02	0.004	0.004	0.004	0.016
0.004	0.15	0.025	0.017	0.00015	0.001	0.00066	0.038	0.02	0.02	0.004	0.004	0.004	0.012
0.0001	0.12	0.025	0.011	0.00015	0.001	0.00047	0.032	0.02	0.02	0.004	0.004	0.003	0.0005
0.0001	0.086	0.025	0.015	0.00015	0.001	0.00061	0.041	0.02	0.02	0.004	0.004	0.003	0.012
0.0001	0.089	0.025	0.0099	0.00015	0.001	0.00061	0.011	0.02	0.02	0.004	0.004	0.01	0.0005
0.02	0.1	0.025	0.014	0.00015	0.001	0.00049	0.0097	0.02	0.02	0.004	0.004	0.004	0.0005
0.012	0.025	0.025	0.0096	0.00015	0.001	0.00083	0.041	0.01	0.02	0.004	0.004	0.004	0.0005
0.0032	0.094	0.025	0.0054	0.00015	0.001	0.00031	0.017	0.02	0.02	0.004	0.004	0.004	0.011
0.0026	0.085	0.025	0.0069	0.00015	0.001	0.00007	0.0081	0.02	0.02	0.004	0.004	0.003	0.013
0.0026	0.094	0.025	0.0077	0.00015	0.001	0.00007	0.0033	0.02	0.02	0.004	0.004	0.003	0.0005
0.0033	0.081	0.025	0.0065	0.00015	0.001	0.00054	0.028	0.02	0.02	0.004	0.004	0.004	0.012
0.0027	0.082	0.025	0.009	0.00015	0.001	0.00007	0.028	0.02	0.02	0.004	0.004	0.004	0.0005
0.0026	0.025	0.025	0.0076	0.00015	0.001	0.00007	0.001	0.01	0.02	0.004	0.004	0.003	0.012
0.0026	0.08	0.025	0.0062	0.00015	0.001	0.00007	0.025	0.01	0.02	0.004	0.004	0.004	0.0005
0.0024	0.069	0.025	0.0071	0.00015	0.001	0.00007	0.021	0.01	0.02	0.004	0.004	0.004	0.0005
0.0026	0.079	0.025	0.0086	0.00015	0.001	0.00007	0.009	0.02	0.02	0.004	0.004	0.004	0.0005
0.0026	0.078	0.025	0.0076	0.00015	0.001	0.00007	0.018	0.02	0.02	0.004	0.004	0.003	0.0005
0.0027	0.089	0.025	0.009	0.00015	0.001	0.00007	0.013	0.02	0.02	0.004	0.004	0.003	0.0005
0.0029	0.025	0.025	0.0073	0.00015	0.001	0.00007	0.038	0.01	0.02	0.004	0.004	0.01	0.012
0.0031	0.074	0.025	0.0094	0.00015	0.001	0.00007	0.022	0.01	0.02	0.004	0.004	0.02	0.0005
0.0028	0.025	0.025	0.0065	0.00015	0.001	0.00007	0.0043	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.059	0.025	0.0088	0.00015	0.001	0.00007	0.0066	0.01	0.02	0.004	0.004	0.03	0.0005
0.0023	0.056	0.025	0.007	0.00015	0.001	0.00007	0.00052	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.05	0.025	0.0005	0.00015	0.001	0.00007	0.0088	0.01	0.02	0.004	0.004	0.01	0.0005
0.0024	0.025	0.025	0.0049	0.00015	0.001	0.00007	0.001	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.056	0.025	0.0029	0.00015	0.001	0.00007	0.005	0.01	0.02	0.004	0.004	0.02	0.0005
0.0001	0.06	0.025	0.0036	0.00015	0.001	0.00007	0.001	0.01	0.02	0.004	0.004	0.01	0.012
0.0024	0.025	0.025	0.0037	0.00015	0.001	0.00007	0.0065	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.051	0.025	0.0043	0.00015	0.001	0.00007	0.00072	0.01	0.02	0.004	0.004	0.01	0.0005
0.0025	0.025	0.025	0.0031	0.00015	0.001	0.00007	0.001	0.01	0.02	0.004	0.004	0.02	0.0005
0.0001	0.059	0.025	0.0052	0.00015	0.001	0.00007	0.012	0.01	0.02	0.004	0.004	0.02	0.0005
0.0001	0.025	0.025	0.004	0.00015	0.001	0.00007	0.011	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.025	0.025	0.002	0.00015	0.001	0.00007	0.0064	0.01	0.02	0.004	0.004	0.02	0.0005
0.0001	0.05	0.025	0.0005	0.00015	0.001	0.00007	0.011	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.025	0.025	0.0005	0.00015	0.001	0.00007	0.0054	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.052	0.025	0.0052	0.00015	0.001	0.00007	0.0077	0.01	0.02	0.004	0.004	0.003	0.0005
0.0001	0.025	0.025	0.0031	0.00015	0.001	0.00007	0.001	0.01	0.02	0.004	0.004	0.008	0.0005
0.0001	0.025	0.025	0.0099	0.00015	0.001	0.00007	0.012	0.01	0.02	0.004	0.004	0.005	0.0005
0.0001	0.025	0.025	0.0068	0.00015	0.001	0.00007	0.0099	0.01	0.02	0.004	0.004	0.004	0.0005
0.0001	0.025	0.025	0.0094	0.00015	0.001	0.00007	0.011	0.01	0.02	0.004	0.004	0.006	0.056
0.0001	0.025	0.025	0.0014	0.00015	0.001	0.00007	0.006	0.01	0.02	0.004	0.004	0.004	0.0005
0.0001	0.025	0.025	0.0061	0.00015	0.001	0.00007	0.001	0.01	0.3	0.004	0.004	0.01	0.0005
0.0001	0.025	0.025	0.0076	0.00015	0.001	0.00007	0.0066	0.01	0.02	0.004	0.004	0.007	0.0005
0.0001	0.025	0.025	0.0069	0.00015	0.001	0.00007	0.0055	0.01	0.02	0.004	0.004	0.004	0.0005
0.0001	0.025	0.025	0.0064	0.00015	0.001	0.00007	0.0091	0.01	0.02	0.004	0.004	0.003	0.0005
0.0001	0.05	0.025	0.0069	0.00015	0.001	0.00007	0.0038	0.01	0.02	0.004	0.004	0.003	0.0005
0.0001	0.025	0.025	0.0055	0.00015	0.001	0.00007	0.0083	0.01	0.02	0.004	0.004	0.006	0.0005
0.0001	0.025	0.025	0.0071	0.00015	0.001	0.00007	0.0099	0.01	0.02	0.004	0.004	0.01	0.0005
0.0001	0.025	0.025	0.0066	0.00015	0.001	0.00007	0.0078	0.01	0.02	0.004	0.004	0.004	0.0005
0.0001	0.025	0.025	0.0057	0.00015	0.001	0.00007	0.0076	0.01	0.02	0.004	0.004	0.006	0.0005
0.0001	0.053	0.025	0.0062	0.00015	0.001	0.00007	0.01	0.01	0.02	0.004	0.004	0.003	0.0005
0.0001	0.025	0.025	0.006	0.00015	0.001	0.00007	0.0081	0.01	0.02	0.004	0.004	0.006	0.0005

Ethidimuron (Sulfadiazole)	Ethofumesate	Glyphosate	Hexazinon	Isoproturon	Linuron	Metamitron	Metazachlor	Metazachlor ESA	Metazachlor OA	Methabenzthiazuron	Metobromuron	Metolachlor	Metolachlor ESA
0.0017	0.029	0.03	0.007	0.0052	0.0005	0.0008	0.0009	0.025	0.025	0.0017	0.068	0.00066	0.025
0.0026	0.013	0.03	0.007	0.01	0.0005	0.0008	0.0008	0.025	0.025	0.0023	0.001	0.005	0.054
0.00021	0.08	0.07	0.007	0.0094	1.4	0.0021	0.0005	0.052	0.025	0.0017	0.001	0.0084	0.025
0.0016	0.05	0.03	0.007	0.0073	1.2	0.0008	0.0019	0.063	0.025	0.0018	0.001	0.011	0.057
0.0019	0.001	0.03	0.007	0.0094	0.69	0.0008	0.0011	0.025	0.025	0.001	0.001	0.0062	0.064
0.00021	0.036	0.03	0.007	0.0045	1	0.0008	0.0011	0.025	0.025	0.0016	0.001	0.005	0.025
0.00042	0.031	0.03	0.007	0.0036	0.013	0.0008	0.0006	0.025	0.025	0.0017	0.001	0.007	0.05
0.0022	0.047	0.073	0.007	0.0021	0.93	0.0008	0.0006	0.025	0.025	0.001	0.001	0.0058	0.052
0.00021	0.028	0.065	0.007	0.016	0.083	0.004	0.0026	0.025	0.025	0.0016	0.001	0.0039	0.055
0.00066	0.052	0.03	0.007	0.0001	0.0005	0.025	0.0038	0.025	0.025	0.0017	0.001	0.006	0.06
0.00095	0.027	0.03	0.007	0.0007	0.0005	0.014	0.0006	0.025	0.025	0.001	0.0082	0.0041	0.052
0.00021	0.036	0.03	0.007	0.0052	0.021	0.029	0.0028	0.33	0.17	0.001	0.001	0.01	0.087
0.00078	0.025	0.03	0.007	0.0001	0.0087	0.019	0.0036	0.025	0.025	0.0016	0.001	0.0025	0.054
0.0004	0.015	0.03	0.007	0.0034	0.023	0.025	0.0022	0.025	0.025	0.0017	0.001	0.0063	0.051
0.00025	0.017	0.03	0.007	0.0001	0.038	0.021	0.0013	0.025	0.025	0.001	0.043	0.0035	0.025
0.0035	0.042	0.03	0.007	0.0001	0.0005	0.0021	0.0014	0.025	0.025	0.001	0.001	0.0072	0.072
0.00027	0.043	0.03	0.007	0.0001	0.015	0.0008	0.0005	0.025	0.025	0.001	0.001	0.0039	0.051
0.00025	0.044	0.03	0.007	0.005	0.03	0.0017	0.023	0.025	0.025	0.001	0.001	0.0038	0.025
0.00021	0.041	0.03	0.007	0.0001	0.021	0.0008	0.0013	0.025	0.025	0.001	0.016	0.0044	0.025
6.80E-05	0.028	0.03	0.007	0.0001	0.031	0.0008	0.0009	0.025	0.025	0.001	0.001	0.0038	0.025
0.00021	0.031	0.03	0.007	0.003	0.033	0.0008	0.0005	0.025	0.025	0.001	0.0074	0.0042	0.025
0.00022	0.029	0.03	0.007	0.0051	0.0029	0.0008	0.0006	0.025	0.025	0.001	0.001	0.0031	0.025
0.00019	0.042	0.03	0.007	0.002	0.02	0.0008	0.0011	0.025	0.025	0.001	0.001	0.0024	0.025
0.00021	0.024	0.03	0.007	0.0024	0.018	0.0008	0.0005	0.025	0.025	0.001	0.0087	0.0036	0.025
0.00021	0.036	0.03	0.007	0.0001	0.0093	0.0008	0.0006	0.025	0.025	0.001	0.0066	0.0066	0.025
0.00026	0.022	0.03	0.007	0.0041	0.0081	0.0008	0.0008	0.025	0.025	0.001	0.0086	0.008	0.025
0.00019	0.03	0.03	0.007	0.0001	0.0005	0.0008	0.0006	0.025	0.025	0.001	0.0063	0.0043	0.025
0.00023	0.031	0.03	0.007	0.0076	0.0057	0.0008	0.0011	0.025	0.025	0.001	0.0053	0.0091	0.025
0.00021	0.01	0.03	0.007	0.0019	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0061	0.0046	0.025
0.00021	0.021	0.03	0.007	0.0001	0.0088	0.0019	0.0011	0.025	0.025	0.001	0.0071	0.0078	0.025
0.00021	0.001	0.03	0.007	0.0001	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.01	0.0058	0.025
0.00021	0.02	0.03	0.007	0.027	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0055	0.0087	0.025
0.00021	0.011	0.03	0.007	0.0011	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.006	0.011	0.025
0.00021	0.024	0.03	0.007	0.0015	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0051	0.011	0.025
0.00021	0.029	0.03	0.007	0.0049	0.0005	0.0008	0.0005	0.025	0.025	0.001	0.0047	0.009	0.025
0.00032	0.0098	0.03	0.007	0.0065	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0077	0.0065	0.025
0.00021	0.02	0.03	0.007	0.0001	0.0064	0.0008	0.0005	0.025	0.025	0.001	0.001	0.0026	0.025
0.00021	0.011	0.03	0.007	0.0001	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0089	0.0054	0.025
0.00021	0.015	0.03	0.007	0.0001	0.0005	0.0019	0.0011	0.025	0.025	0.001	0.0047	0.0049	0.025
0.00022	0.001	0.03	0.007	0.0024	0.011	0.0008	0.0011	0.025	0.025	0.001	0.0057	0.0063	0.025
0.00021	0.011	0.03	0.007	0.0001	0.0005	0.0016	0.0011	0.025	0.025	0.001	0.0049	0.0041	0.025
0.00025	0.0059	0.03	0.007	0.0001	0.012	0.0022	0.0011	0.025	0.025	0.001	0.0051	0.0055	0.025
0.00021	0.009	0.03	0.007	0.0001	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0048	0.0057	0.025
0.00021	0.0093	0.03	0.007	0.0042	0.0005	0.0017	0.0011	0.025	0.025	0.001	0.0047	0.0058	0.025
0.00021	0.001	0.03	0.007	0.0001	0.0005	0.0016	0.0011	0.025	0.025	0.001	0.0043	0.0045	0.025
0.00021	0.021	0.03	0.007	0.0011	0.0005	0.0017	0.0011	0.025	0.025	0.001	0.001	0.0049	0.025
0.0014	0.001	0.03	0.007	0.0008	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0051	0.0054	0.025
0.00021	0.001	0.03	0.007	0.0009	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0049	0.004	0.025
0.0015	0.001	0.03	0.007	0.0007	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.001	0.0054	0.025
0.0029	0.001	0.03	0.007	0.0038	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.001	0.0053	0.025
0.00038	0.029	0.03	0.007	0.0016	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.001	0.0046	0.025
0.00037	0.1	0.03	0.007	0.0005	0.0005	0.0008	0.016	0.025	0.025	0.001	0.001	0.0053	0.025
7.50E-05	0.097	0.03	0.007	0.0001	0.0005	0.0008	0.013	0.025	0.025	0.001	0.001	0.0062	0.025
0.0013	0.026	0.062	0.007	0.001	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0058	0.025	0.025
0.0019	0.013	0.03	0.007	0.0007	0.0001	0.0017	0.0011	0.025	0.025	0.001	0.0053	0.0059	0.025
0.00021	0.01	0.069	0.007	0.17	0.0005	0.0025	0.0011	0.025	0.025	0.001	0.001	0.039	0.025
0.00021	0.001	0.03	0.007	0.0005	0.0005	0.0008	0.0011	0.025	0.025	0.001	0.0051	0.0047	0.025
0.00056	0.001	0.03	0.007	0.0018	0.0057	0.0035	0.0011	0.025	0.025	0.001	0.0055	0.0031	0.025
0.00021	0.0094	0.03	0.007	0.0011	0.0005	0.0017	0.0011	0.025	0.025	0.001	0.0023	0.0061	0.025
0.00021	0.001	0.03	0.007	0.0007	0.0005	0.0017	0.0011	0.025	0.025	0.001	0.0052	0.0049	0.025
0.00021	0.015	0.03	0.007	0.0017	0.0086	0.0018	0.0011	0.025	0.025	0.001	0.001	0.004	0.025
0.00092	0.001	0.03	0.007	0.0023	0.0005	0.0017	0.0011	0.025	0.025	0.001	0.001	0.0048	0.025
0.00021	0.0094	0.03	0.007	0.0039	0.0005	0.002	0.0006	0.025	0.025	0.001	0.0052	0.0071	0.025
0.002	0.011	0.03	0.007	0.0037	0.0005	0.0018	0.0097	0.025	0.025	0.001	0.0046	0.0076	0.025
0.00031	0.001	0.03	0.007	0.0013	0.0005	0.0018	0.0011	0.025	0.025	0.001	0.0029	0.0068	0.025
0.00021	0.001	0.03	0.007	0.0017	0.022	0.0017	0.0011	0.025	0.025	0.001	0.0046	0.0056	0.025
0.00021	0.0091	0.03	0.007	0.0017	0.0005	0.0019	0.0011	0.025	0.025	0.001	0.0069	0.0063	0.025
0.00035	0.001	0.03	0.007	0.001	0.0076	0.0019	0.0011	0.025	0.025	0.001	0.0076	0.0043	0.025

Metoxuron	Monolinuron	Prometryn	Propazine	Propazine-2-hydroxy	Simazine	S-Metolachlor CGA 368208	S-Metolachlor NOA 413173	Terbutryn	Terbutylazine	Terbutylazine CGA 324007	Terbutylazine SYN 545666	Terbutylazine-2-hydroxy	Terbutylazine-desethyl
0.0049	0.00036	0.006	0.01	0.01	0.00026	0.01	0.02	0.0047	0.011	0.01	0.0025	0.004	0.00054
0.0056	0.00036	0.0071	0.028	0.01	0.00026	0.01	0.02	0.0044	0.028	0.01	0.0075	0.004	0.00054
0.0013	0.0065	0.0098	0.025	0.01	0.00026	0.01	0.02	0.011	0.025	0.01	0.003	0.004	0.00054
0.005	0.0025	0.0065	0.021	0.01	0.00026	0.01	0.02	0.0092	0.021	0.01	0.004	0.004	0.00054
0.0068	0.00036	0.0081	0.025	0.01	0.004	0.01	0.02	0.0094	0.025	0.01	0.008	0.004	0.0062
0.0049	0.00036	0.0039	0.021	0.01	0.0016	0.01	0.02	0.005	0.021	0.01	0.0035	0.004	0.0038
0.0056	0.0068	0.001	0.0039	0.01	0.00026	0.01	0.02	0.004	0.0046	0.01	0.008	0.004	0.00054
0.0026	0.038	0.0018	0.0038	0.01	0.00026	0.01	0.02	0.0033	0.0045	0.01	0.008	0.004	0.00054
0.0095	0.089	0.0024	0.053	0.01	0.0033	0.01	0.02	0.0039	0.052	0.01	0.0085	0.004	0.0056
0.0098	0.00036	0.0018	0.0059	0.01	0.0073	0.01	0.02	0.0031	0.0066	0.01	0.0065	0.004	0.0098
0.0096	0.00036	0.001	0.012	0.01	0.0063	0.01	0.02	0.0033	0.012	0.01	0.008	0.004	0.0086
0.01	0.00036	0.001	0.044	0.01	0.005	0.03	0.03	0.0075	0.043	0.01	0.01	0.02	0.0073
0.0096	0.00036	0.001	0.0082	0.01	0.0011	0.01	0.02	0.0029	0.0087	0.01	0.0095	0.004	0.0033
0.017	0.0027	0.001	0.019	0.01	0.00026	0.01	0.02	0.0029	0.019	0.01	0.0095	0.004	0.00054
0.011	0.0063	0.0026	0.01	0.01	0.00026	0.01	0.03	0.0042	0.011	0.01	0.0045	0.004	0.00054
0.0026	0.0084	0.002	0.0008	0.01	0.0022	0.01	0.04	0.0034	0.0016	0.01	0.0045	0.004	0.0044
0.0014	0.027	0.0021	0.013	0.01	0.00026	0.01	0.02	0.005	0.014	0.01	0.005	0.004	0.00054
0.00018	0.00036	0.0019	0.0074	0.01	0.0044	0.01	0.02	0.0044	0.0079	0.01	0.0145	0.004	0.0067
0.0031	0.028	0.001	0.008	0.01	0.0055	0.01	0.03	0.0029	0.0086	0.01	0.015	0.004	0.0078
0.00035	0.0039	0.0017	0.0011	0.01	0.0052	0.01	0.02	0.0035	0.0019	0.01	0.014	0.006	0.0075
0.0019	0.012	0.001	0.0075	0.01	0.00026	0.01	0.02	0.0035	0.0081	0.01	0.015	0.004	0.00054
0.0017	0.014	0.001	0.0089	0.01	0.00026	0.01	0.02	0.0034	0.0094	0.01	0.0145	0.004	0.00054
0.0013	0.00036	0.001	0.0048	0.01	0.0014	0.01	0.02	0.0044	0.0055	0.01	0.003	0.004	0.0035
0.00044	0.00036	0.001	0.0058	0.01	0.00026	0.01	0.02	0.0032	0.0065	0.01	0.0095	0.004	0.00054
0.00018	0.00036	0.0014	0.0014	0.01	0.00026	0.01	0.02	0.0035	0.0022	0.01	0.009	0.004	0.00054
0.001	0.00036	0.001	0.004	0.01	0.00026	0.01	0.03	0.0032	0.0047	0.01	0.015	0.004	0.00054
0.001	0.00036	0.0022	0.0025	0.01	0.011	0.01	0.03	0.0041	0.0033	0.01	0.0145	0.005	0.014
0.0023	0.012	0.001	0.005	0.01	0.00026	0.01	0.03	0.0023	0.0057	0.01	0.015	0.004	0.00054
0.00019	0.00036	0.001	0.0017	0.01	0.00026	0.01	0.02	0.002	0.0025	0.01	0.0025	0.004	0.00054
0.00093	0.00036	0.001	0.0024	0.01	0.00026	0.01	0.03	0.0035	0.0031	0.01	0.0135	0.004	0.00054
0.00018	0.00036	0.001	0.0015	0.01	0.00026	0.01	0.02	0.0028	0.0023	0.01	0.0145	0.004	0.00054
0.019	0.00036	0.0017	0.00028	0.01	0.00026	0.01	0.02	0.0026	0.00029	0.01	0.01	0.004	0.00054
0.0032	0.00036	0.001	0.0017	0.01	0.00026	0.01	0.02	0.0041	0.0024	0.01	0.0095	0.004	0.00054
0.0053	0.00036	0.001	0.0008	0.01	0.00026	0.01	0.02	0.0028	0.0016	0.01	0.0145	0.004	0.00054
0.0023	0.00036	0.001	0.0008	0.01	0.00026	0.01	0.02	0.0037	0.0017	0.01	0.0025	0.004	0.00054
0.0048	0.00036	0.001	0.00028	0.01	0.00026	0.01	0.02	0.0032	0.00029	0.01	0.0085	0.004	0.00054
0.0046	0.00036	0.001	0.0017	0.01	0.00026	0.01	0.02	0.0016	0.0024	0.01	0.0025	0.004	0.00054
0.00018	0.00036	0.001	0.0024	0.01	0.00026	0.01	0.02	0.003	0.0031	0.01	0.0075	0.004	0.00054
0.00018	0.00036	0.001	0.0004	0.01	0.00026	0.01	0.02	0.002	0.0013	0.01	0.0085	0.004	0.00054
0.00018	0.00036	0.001	0.0021	0.01	0.00026	0.01	0.03	0.0025	0.0029	0.01	0.003	0.004	0.00054
0.00018	0.00036	0.001	0.0003	0.01	0.00026	0.01	0.04	0.0018	0.0012	0.01	0.0025	0.004	0.00054
0.00018	0.00036	0.001	0.0019	0.01	0.00026	0.01	0.02	0.0026	0.0027	0.01	0.005	0.004	0.00054
0.00018	0.007	0.0015	0.0019	0.01	0.00026	0.01	0.02	0.0021	0.0027	0.01	0.008	0.004	0.00054
0.0025	0.0028	0.001	0.00028	0.01	0.0022	0.01	0.02	0.0021	0.00029	0.01	0.003	0.004	0.0044
0.00018	0.003	0.001	0.00028	0.01	0.00026	0.01	0.02	0.0027	0.00029	0.01	0.008	0.004	0.00054
0.0027	0.0026	0.0017	0.00028	0.01	0.00026	0.01	0.03	0.0025	0.00029	0.01	0.009	0.004	0.00054
0.00031	0.00036	0.001	0.0057	0.01	0.0012	0.01	0.02	0.0028	0.0063	0.01	0.0095	0.007	0.0034
0.0018	0.00036	0.0051	0.0018	0.01	0.00026	0.01	0.02	0.00033	0.0026	0.01	0.0025	0.004	0.00054
0.00018	0.00036	0.001	0.0025	0.01	0.001	0.01	0.02	0.0027	0.0033	0.01	0.0135	0.008	0.0031
0.00039	0.00036	0.0017	0.0041	0.01	0.00026	0.01	0.02	0.0017	0.0048	0.01	0.0085	0.004	0.00054
0.0038	0.00036	0.001	0.00028	0.01	0.00026	0.01	0.02	0.0039	0.00029	0.01	0.0025	0.004	0.00054
0.00018	0.00036	0.0021	0.0083	0.01	0.00026	0.01	0.02	0.0027	0.0086	0.01	0.007	0.005	0.00054
0.00096	0.012	0.0019	0.0042	0.01	0.0013	0.01	0.02	0.0028	0.0082	0.01	0.005	0.005	0.0034
0.0017	0.0028	0.001	0.0014	0.01	0.00026	0.01	0.02	0.00033	0.0022	0.01	0.0025	0.005	0.00054
0.0064	0.0057	0.001	0.0019	0.01	0.00026	0.01	0.02	0.002	0.0027	0.01	0.0045	0.006	0.00054
0.0031	0.0034	0.0029	0.0066	0.01	0.00026	0.01	0.02	0.0018	0.0072	0.01	0.0025	0.004	0.00054
0.00018	0.0005	0.001	0.0011	0.01	0.00026	0.01	0.02	0.0025	0.0019	0.01	0.0065	0.004	0.00054
0.00018	0.0024	0.0038	0.0011	0.01	0.0013	0.01	0.02	0.0029	0.0019	0.01	0.0025	0.01	0.0034
0.00018	0.00036	0.001	0.0011	0.01	0.00026	0.01	0.02	0.002	0.0019	0.01	0.0025	0.006	0.00054
0.00045	0.00036	0.001	0.00028	0.01	0.00026	0.01	0.02	0.0025	0.00029	0.01	0.0025	0.006	0.00054
0.0018	0.0027	0.001	0.00028	0.01	0.00026	0.01	0.02	0.0014	0.00029	0.01	0.0025	0.006	0.00054
0.00018	0.00036	0.001	0.00028	0.01	0.00026	0.01	0.02	0.00033	0.00029	0.01	0.003	0.007	0.00054
0.00018	0.0034	0.0026	0.0068	0.01	0.00026	0.01	0.02	0.00088	0.0074	0.01	0.0025	0.009	0.00054
0.00018	0.0032	0.0092	0.0087	0.01	0.00026	0.01	0.02	0.00077	0.0092	0.01	0.0025	0.01	0.00054
0.0019	0.0027	0.001	0.0022	0.01	0.00026	0.01	0.02	0.0025	0.003	0.01	0.005	0.004	0.00054
0.00018	0.0026	0.001	0.00028	0.01	0.00026	0.01	0.02	0.0016	0.00029	0.01	0.0025	0.005	0.00054
0.0044	0.0027	0.0015	0.00028	0.01	0.0015	0.01	0.02	0.0017	0.00029	0.01	0.0025	0.007	0.0036
0.00018	0.00036	0.001	0.00028	0.01	0.0023	0.01	0.02	0.0014	0.00029	0.01	0.0025	0.004	0.0045

Terbutylazine-desethyl-2-hydroxy	Diazinone	Fipronil	4-Chlorophenol	Azoxystrobin	Carbendazim	Cyproconazol	Flusilazole	Metalaxyl NOA 409045	Picoxystrobin	Propiconazole	Quinoxyfen	Tebuconazol	Trifloxystrobin CGA 321113
0.03	0.004	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.04	0.003	0.01	0.002	0.005
0.03	0.003	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.004	0.008	0.002	0.005
0.03	0.001	0.02	0.0015	0.002	0.005	0.005	0.003	0.006	0.01	0.006	0.005	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.007	0.005	0.003	0.006	0.01	0.004	0.004	0.002	0.005
0.03	0.001	0.02	0.0005	0.002	0.004	0.005	0.003	0.006	0.01	0.004	0.004	0.002	0.005
0.03	0.001	0.02	0.0006	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.0005	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.0005	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.0005	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.005	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.004	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.006	0.005
0.1	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.008	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.005	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.009	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.008	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.008	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.002	0.02	0.001	0.002	0.007	0.005	0.003	0.006	0.01	0.003	0.004	0.004	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.009	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.004	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.008	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.007	0.009	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.005	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.007	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.02	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.007	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.02	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.008	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.02	0.005	0.003	0.006	0.01	0.003	0.004	0.005	0.005
0.03	0.001	0.02	0.001	0.002	0.006	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.007	0.02	0.001	0.004	0.04	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.007	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.003	0.02	0.001	0.002	0.009	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.002	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.005	0.005
0.03	0.001	0.02	0.001	0.002	0.004	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.007	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005
0.03	0.001	0.02	0.001	0.002	0.01	0.005	0.003	0.006	0.01	0.003	0.004	0.003	0.005
0.03	0.001	0.02	0.001	0.002	0.009	0.005	0.003	0.006	0.01	0.003	0.004	0.002	0.005

10,11-Dihydro-10,11-dihydroxycarbamazepine	10,11-Dihydro-10-hydroxycarbamazepine	17-beta Estradiol	1-Adamantylamin	2-Hydroxycarbamazepine	3,4-Methylendioxyamphetamine (MDA)	3,4-Methylenedioxyethamphetamine (MDEA)	6-Acetylmorphine	7-Aminoclonazepam	7-Aminoflunitrazepam	Acetylcodeine	Acetyl-sulfamethoxazole	Alfentanil	alpha-Hydroxyalprazolam
0.029	0.0054	0.0015	0.005	0.01	0.0043	0.0048	0.00095	0.0024	0.00086	0.0035	0.02	0.001	0.055
0.068	0.0045	0.001	0.005	0.01	0.0018	0.0048	0.0041	0.0021	0.001	0.001	0.02	0.00037	0.049
0.045	0.005	0.0052	0.008	0.01	0.0029	0.015	0.0041	0.001	0.0013	0.0037	0.02	0.001	0.08
0.044	0.0024	0.029	0.005	0.01	0.0015	0.0042	0.0043	0.0021	0.00074	0.001	0.02	0.00065	0.065
0.073	0.0044	0.023	0.005	0.01	0.001	0.0074	0.0027	0.0024	0.00087	0.001	0.02	0.00057	0.06
0.05	0.0017	0.0019	0.005	0.01	0.0023	0.005	0.0011	0.0034	0.0016	0.0055	0.02	0.00094	0.099
0.029	0.0012	0.0048	0.005	0.01	0.001	0.005	0.0011	0.0025	0.0015	0.0041	0.02	0.00024	0.089
0.026	0.0017	0.0078	0.005	0.01	0.0079	0.0052	0.00095	0.0038	0.00082	0.003	0.02	0.00028	0.075
0.055	0.0054	0.0032	0.005	0.01	0.0095	0.001	0.0043	0.0032	0.00061	0.001	0.02	0.003	0.021
0.03	0.001	0.001	0.005	0.01	0.011	0.0021	0.00091	0.001	0.0013	0.0033	0.02	0.0003	0.15
0.054	0.0027	0.001	0.005	0.014	0.0023	0.0028	0.001	0.001	0.0015	0.001	0.02	0.00016	0.1
0.11	0.0022	0.001	0.005	0.011	0.024	0.001	0.0015	0.001	0.0012	0.001	0.02	0.0075	0.12
0.035	0.0017	0.001	0.005	0.01	0.016	0.002	0.00091	0.0022	0.0013	0.001	0.02	0.0076	0.11
0.031	0.0015	0.001	0.005	0.01	0.019	0.0017	0.0011	0.002	0.0014	0.001	0.02	0.001	0.11
0.062	0.0031	0.001	0.005	0.01	0.092	0.0022	0.00087	0.0021	0.00094	0.0038	0.02	0.0063	0.1
0.15	0.0024	0.001	0.01	0.01	0.0035	0.001	0.001	0.0029	0.001	0.0045	0.02	0.0011	0.15
0.058	0.001	0.001	0.005	0.01	0.001	0.0028	0.00073	0.002	0.00084	0.001	0.02	0.0019	0.073
0.093	0.0018	0.001	0.03	0.01	0.027	0.0024	0.001	0.0021	0.001	0.001	0.02	0.0019	0.046
0.049	0.0015	0.001	0.005	0.01	0.001	0.00084	0.0011	0.002	0.00097	0.0037	0.02	0.001	0.05
0.021	0.0024	0.001	0.005	0.01	0.0019	0.0054	0.00087	0.0019	0.00096	0.0034	0.02	0.00066	0.069
0.065	0.001	0.001	0.005	0.01	0.054	0.0047	0.00097	0.0034	0.00062	0.0031	0.02	0.001	0.063
0.08	0.0027	0.001	0.005	0.01	0.001	0.0038	0.00097	0.001	0.001	0.0031	0.02	0.001	0.058
0.14	0.0014	0.001	0.009	0.01	0.0058	0.0016	0.001	0.0019	0.00067	0.001	0.02	0.001	0.099
0.08	0.0023	0.001	0.006	0.01	0.001	0.001	0.00095	0.0019	0.00065	0.0035	0.02	0.002	0.053
0.043	0.001	0.001	0.005	0.01	0.00045	0.001	0.00095	0.001	0.00067	0.0033	0.02	0.00012	0.069
0.042	0.0012	0.001	0.005	0.01	0.0033	0.0017	0.00092	0.002	0.00063	0.0029	0.02	0.001	0.098
0.057	0.001	0.001	0.005	0.01	0.003	0.0076	0.00082	0.001	0.00062	0.0031	0.02	0.001	0.066
0.06	0.001	0.001	0.009	0.01	0.011	0.0034	0.00081	0.0021	0.00063	0.0029	0.02	0.0036	0.089
0.037	0.0018	0.001	0.005	0.01	0.091	0.0027	0.0008	0.0024	0.00062	0.003	0.02	0.001	0.058
0.052	0.0029	0.001	0.005	0.01	0.001	0.0031	0.001	0.002	0.0006	0.0029	0.02	0.00045	0.06
0.036	0.001	0.001	0.005	0.01	0.0051	0.0038	0.001	0.0032	0.00066	0.001	0.02	0.001	0.052
0.05	0.001	0.001	0.01	0.01	0.013	0.0022	0.001	0.001	0.0006	0.003	0.02	0.0018	0.047
0.051	0.001	0.001	0.005	0.01	0.072	0.0027	0.001	0.0028	0.00062	0.003	0.02	0.001	0.075
0.045	0.0011	0.001	0.005	0.01	0.001	0.003	0.00083	0.0025	0.00059	0.003	0.02	0.00016	0.076
0.084	0.001	0.001	0.01	0.01	0.19	0.001	0.0009	0.0066	0.0006	0.003	0.02	0.001	0.067
0.039	0.001	0.001	0.008	0.01	0.066	0.0031	0.001	0.0033	0.001	0.001	0.02	0.001	0.052
0.024	0.001	0.001	0.005	0.01	0.01	0.0063	0.001	0.0021	0.00059	0.001	0.02	0.001	0.052
0.034	0.0011	0.001	0.01	0.01	0.001	0.00058	0.001	0.001	0.00059	0.001	0.02	0.00098	0.051
0.039	0.004	0.001	0.01	0.01	0.011	0.0024	0.001	0.002	0.00062	0.001	0.02	0.001	0.057
0.043	0.0009	0.001	0.005	0.01	0.62	0.0045	0.001	0.014	0.00094	0.001	0.02	8.90E-05	0.052
0.11	0.0011	0.001	0.01	0.011	0.05	0.0015	0.00079	0.0025	0.0006	0.0032	0.063	0.0019	0.052
0.04	0.001	0.001	0.009	0.01	0.44	0.0028	0.00096	0.013	0.00062	0.0031	0.02	0.00042	0.052
0.042	0.001	0.001	0.01	0.01	0.11	0.0016	0.001	0.0047	0.001	0.001	0.02	0.001	0.049
0.043	0.001	0.001	0.01	0.01	0.32	0.0046	0.001	0.0081	0.00061	0.001	0.02	0.001	0.048
0.044	0.001	0.001	0.005	0.01	0.58	0.0018	0.001	0.012	0.00071	0.001	0.02	0.00091	0.048
0.045	0.001	0.001	0.005	0.01	0.049	0.0013	0.001	0.0037	0.001	0.001	0.02	0.001	0.051
0.041	0.0035	0.001	0.007	0.01	0.001	0.002	0.23	0.001	0.001	0.0078	0.02	0.00022	0.062
0.075	0.0056	0.001	0.09	0.014	0.00013	0.002	0.22	0.001	0.001	0.0075	0.042	0.001	0.07
0.043	0.0024	0.001	0.005	0.01	7.30E-05	0.002	0.22	0.001	0.001	0.0076	0.02	0.00015	0.056
0.041	0.0054	0.001	0.008	0.01	0.001	0.0016	0.24	0.002	0.001	0.0064	0.02	0.00085	0.045
0.13	0.0025	0.001	0.005	0.012	5.50E-05	0.002	0.0048	0.0055	0.00078	0.0072	0.02	0.001	0.0035
0.04	0.001	0.001	0.005	0.01	0.001	0.001	0.0029	0.0019	0.001	0.018	0.02	0.001	0.005
0.034	0.0009	0.001	0.005	0.01	0.00039	0.001	0.0028	0.0021	0.00072	0.019	0.02	8.60E-05	0.0053
0.032	0.001	0.001	0.01	0.01	0.013	0.0011	0.001	0.002	0.001	0.001	0.02	0.001	0.00024
0.036	0.001	0.001	0.005	0.01	2.90E-06	0.001	0.001	0.001	0.001	0.001	0.02	0.001	0.00042
0.086	0.004	0.001	0.01	0.011	0.0068	0.0014	0.001	0.0019	0.001	0.003	0.045	0.001	0.0018
0.035	0.001	0.001	0.005	0.01	0.001	0.00099	0.001	0.001	0.001	0.001	0.02	0.001	0.00024
0.16	0.0088	0.001	0.04	0.045	0.0036	0.0044	0.001	0.001	0.00069	0.0053	0.023	0.001	0.00086
0.038	0.001	0.001	0.005	0.01	0.024	0.00035	0.001	0.001	0.001	0.001	0.02	0.001	0.12
0.041	0.001	0.001	0.005	0.01	0.001	0.00019	0.001	0.001	0.001	0.001	0.02	0.001	0.00022
0.05	0.001	0.001	0.005	0.01	0.001	0.00036	0.001	0.001	0.001	0.001	0.02	0.001	0.11
0.043	0.001	0.001	0.005	0.01	0.001	0.00069	0.001	0.001	0.001	0.001	0.02	0.00029	0.1
0.013	0.001	0.001	0.005	0.01	0.023	0.00079	0.001	0.001	0.001	0.001	0.02	0.00077	0.15
0.016	0.0024	0.001	0.005	0.01	0.0034	0.0016	0.001	0.001	0.001	0.001	0.02	0.001	0.16
0.037	0.001	0.001	0.005	0.01	0.001	0.001	0.001	0.001	0.001	0.001	0.02	0.001	0.14
0.036	0.001	0.001	0.005	0.01	0.001	0.00032	0.001	0.001	0.001	0.001	0.02	0.001	0.13
0.046	0.0018	0.001	0.005	0.01	0.001	0.00062	0.001	0.001	0.001	0.001	0.02	0.001	0.14
0.034	0.001	0.001	0.007	0.01	0.001	0.0011	0.001	0.001	0.001	0.001	0.02	0.001	0.12

alpha-Hydroxymidazolam	alpha-Hydroxytriazolam	Alprazolam	Amidotrizoic acid	Amisulpride	Amitriptyline	Amoxapine	Amoxicillin	Amphetamine	Atenolol	Atropine	Benzoylecgonine	Betaxolol	Bezafibrate
0.00094	0.0056	0.0045	0.5	0.0093	0.0078	0.00045	0.012	0.001	0.03	0.016	0.0042	0.01	0.005
0.00099	0.0082	0.0067	0.5	0.0098	0.0092	0.00045	0.017	0.001	0.01	0.028	0.005	0.01	0.005
0.002	0.0071	0.012	0.5	0.014	0.012	0.00074	0.035	0.001	0.01	0.033	0.00023	0.01	0.005
0.00077	0.0055	0.01	0.5	0.011	0.012	0.00049	0.048	0.001	0.01	0.037	0.007	0.01	0.005
0.00059	0.0026	0.0066	0.5	0.014	0.011	0.001	0.011	0.001	0.01	0.031	0.00084	0.01	0.005
0.00075	0.0051	0.01	0.5	0.0092	0.0025	0.00084	0.026	0.001	0.01	0.02	0.0051	0.01	0.005
0.0019	0.0054	0.0077	0.5	0.003	0.0047	0.0005	0.0091	0.001	0.01	0.016	0.0062	0.01	0.005
0.00066	0.0061	0.011	0.5	0.00054	0.0073	0.00062	0.0096	0.001	0.01	0.015	0.0089	0.01	0.005
0.0079	0.001	0.0096	0.5	0.0044	0.0023	0.0038	0.13	0.004	0.01	0.16	6.60E-05	0.01	0.005
0.0012	0.0076	0.0023	0.5	0.0034	0.001	0.001	0.0092	0.001	0.01	0.013	0.001	0.01	0.005
0.0023	0.0061	0.002	0.5	0.0071	0.0018	0.001	0.011	0.001	0.01	0.004	0.00022	0.01	0.005
0.00081	0.006	0.0031	0.5	0.002	0.001	0.00047	0.28	0.001	0.01	0.021	0.001	0.01	0.005
0.00044	0.01	0.0027	0.5	0.0048	0.001	0.001	0.0088	0.001	0.01	0.012	0.001	0.01	0.005
0.001	0.013	0.002	0.5	0.0046	0.001	0.00047	0.017	0.001	0.01	0.016	0.001	0.01	0.005
0.001	0.0066	0.0043	0.5	0.002	0.0018	0.001	0.009	0.001	0.01	0.013	0.001	0.01	0.005
0.001	0.0066	0.001	0.5	0.008	0.0048	0.0022	0.034	0.001	0.01	0.038	0.0089	0.01	0.005
0.001	0.0059	0.001	0.5	0.0029	0.0041	0.00064	0.0096	0.001	0.01	0.019	0.0085	0.01	0.005
0.001	0.0075	0.001	0.5	0.0018	0.0041	0.00028	0.011	0.001	0.02	0.0038	0.0003	0.01	0.005
0.00058	0.0029	0.0063	0.5	0.0017	0.004	0.00068	0.0098	0.0018	0.01	0.017	0.00063	0.01	0.005
0.001	0.0065	0.0052	0.5	0.0015	0.0047	0.001	0.0089	0.001	0.01	0.021	0.0066	0.01	0.005
0.001	0.0056	0.001	0.5	0.0024	0.0029	0.0012	0.01	0.0024	0.01	0.0025	0.0089	0.01	0.005
0.001	0.001	0.0048	0.5	0.0035	0.003	0.0009	0.0091	0.0019	0.01	0.021	0.0056	0.01	0.005
0.001	0.001	0.0073	0.5	0.001	0.0025	0.00061	0.01	0.001	0.01	0.011	0.0025	0.01	0.005
0.001	0.001	0.0019	0.5	0.0008	0.0051	0.00075	0.0095	0.0019	0.01	0.018	0.007	0.01	0.005
0.001	0.0057	0.0068	0.5	0.0033	0.0021	0.00036	0.0099	0.00071	0.01	0.0072	0.0033	0.01	0.005
0.001	0.0067	0.0061	0.5	0.0026	0.005	0.00064	0.0094	0.001	0.01	0.02	0.0022	0.01	0.005
0.001	0.0055	0.001	0.5	0.0019	0.0048	0.00057	0.001	0.0027	0.01	0.02	0.0055	0.01	0.005
0.001	0.001	0.001	0.5	0.0022	0.0019	0.0011	0.018	0.00092	0.01	0.0097	0.005	0.01	0.005
0.001	0.001	0.0034	0.5	0.00059	0.0025	0.0005	0.001	0.0012	0.01	0.0081	0.0025	0.01	0.005
0.001	0.001	0.0012	0.5	0.0006	0.0038	0.00054	0.009	0.001	0.01	0.013	0.0051	0.01	0.005
0.001	0.001	0.0022	0.5	0.00064	0.0029	0.00025	0.001	0.0005	0.01	0.015	0.0051	0.01	0.005
0.001	0.001	0.0031	0.5	0.00032	0.0033	0.00053	0.0015	0.00096	0.01	0.028	0.0079	0.01	0.005
0.001	0.001	0.0021	0.5	0.001	0.002	0.00054	0.001	0.0018	0.01	0.012	0.0024	0.01	0.005
0.001	0.001	0.0023	0.5	0.00035	0.0034	0.00084	0.001	0.00077	0.01	0.018	0.0051	0.01	0.005
0.001	0.001	0.0022	0.5	0.0005	0.001	0.0014	0.009	0.001	0.01	0.019	0.0044	0.01	0.005
0.001	0.001	0.0042	0.5	0.0011	0.0036	0.00074	0.001	0.00057	0.01	0.0096	0.0042	0.01	0.005
0.001	0.001	0.0043	0.5	0.00094	0.0034	0.001	0.001	0.001	0.01	0.02	0.0077	0.01	0.005
0.001	0.0099	0.0035	0.5	0.0021	0.0042	0.001	0.001	0.0017	0.01	0.0094	5.20E-05	0.01	0.005
0.001	0.0057	0.0034	0.5	0.00043	0.0035	0.00055	0.001	0.00084	0.01	0.012	0.0007	0.01	0.005
0.001	0.0095	0.001	0.5	0.0021	0.0027	0.001	0.001	0.001	0.01	0.02	0.0014	0.01	0.005
0.001	0.0056	0.0024	0.5	0.0016	0.0019	0.0015	0.001	0.00055	0.02	0.011	0.0004	0.01	0.005
0.001	0.001	0.0016	0.5	0.00047	0.0029	0.00073	0.009	0.00068	0.01	0.021	0.0026	0.01	0.005
0.001	0.0063	0.0016	0.5	0.00091	0.0024	0.00067	0.0091	0.00081	0.01	0.018	0.0043	0.01	0.005
0.001	0.001	0.001	0.5	0.00041	0.0023	0.0005	0.0087	0.00059	0.01	0.019	0.0065	0.01	0.005
0.001	0.001	0.0017	0.5	0.00045	0.0024	0.00052	0.001	0.001	0.01	0.019	0.0036	0.01	0.005
0.001	0.001	0.0016	0.5	0.00028	0.0026	0.001	0.001	0.001	0.01	0.0092	0.00095	0.01	0.005
0.001	0.0071	0.009	0.5	0.0042	0.0059	0.00039	0.001	0.001	0.01	0.0015	0.0041	0.01	0.005
0.001	0.001	0.0068	0.5	0.0042	0.0069	0.00047	0.001	0.001	0.02	0.002	0.0048	0.01	0.005
0.001	0.001	0.0057	0.5	0.0037	0.0098	0.00044	0.001	0.001	0.01	0.0017	0.0059	0.01	0.005
0.001	0.001	0.004	0.5	0.0047	0.0099	0.00046	0.001	0.001	0.01	0.0024	0.0059	0.01	0.005
0.001	0.001	0.004	0.5	0.003	0.013	0.00049	0.001	0.001	0.01	0.0023	0.0025	0.01	0.005
0.00061	0.0075	0.001	0.5	0.004	0.013	0.00084	0.001	0.001	0.01	0.0015	0.0081	0.01	0.005
0.001	0.016	0.001	0.5	0.0038	0.011	0.001	0.001	0.001	0.01	0.0017	0.0046	0.01	0.005
0.001	0.01	0.0053	0.5	0.0011	0.001	0.0011	0.001	0.001	0.01	0.013	0.0036	0.01	0.005
0.001	0.001	0.0037	0.5	0.0005	0.0023	0.001	0.001	0.001	0.01	0.011	0.0043	0.01	0.005
0.001	0.001	0.0017	0.5	0.0083	0.0026	0.00045	0.001	0.001	0.03	0.075	0.0031	0.01	0.005
0.001	0.001	0.0008	0.5	0.001	0.0017	0.00054	0.001	0.001	0.01	0.0015	0.0026	0.01	0.005
0.001	0.001	0.0015	0.5	0.031	0.006	0.001	0.001	0.001	0.2	0.14	0.0012	0.01	0.005
0.001	0.0085	0.0041	0.5	0.00051	0.0022	0.00046	0.001	0.001	0.02	0.0096	0.0032	0.01	0.005
0.001	0.001	0.0021	0.5	0.0003	0.0022	0.001	0.001	0.011	0.02	0.0093	0.0017	0.01	0.005
0.001	0.001	0.0015	0.5	0.001	0.001	0.001	0.001	0.001	0.01	0.01	0.0031	0.01	0.005
0.001	0.001	0.0033	0.5	0.00064	0.001	0.0021	0.001	0.00045	0.01	0.011	0.0036	0.01	0.005
0.001	0.001	0.003	0.5	0.00063	0.002	0.00055	0.001	0.001	0.01	0.0095	0.0033	0.01	0.005
0.001	0.001	0.0035	0.5	0.00033	0.001	0.00046	0.001	0.001	0.01	0.011	0.0039	0.01	0.005
0.001	0.001	0.0025	0.5	0.00033	0.001	0.00075	0.001	0.001	0.01	0.0084	0.0026	0.01	0.005
0.001	0.001	0.002	0.5	0.001	0.0023	0.00049	0.001	0.001	0.01	0.0079	0.0025	0.01	0.005
0.001	0.001	0.0031	0.5	0.001	0.001	0.00052	0.001	0.001	0.01	0.0083	0.0025	0.01	0.005
0.001	0.012	0.0027	0.5	0.001	0.001	0.00067	0.001	0.001	0.01	0.0092	0.0025	0.01	0.005

Bisoprolol	Bromazepam	Buprenorphine	Buprenorphine glucuronide	Candesartan	Carbamazepine	Carbamazepine-10,11-epoxide	Carisoprodol	Cetirizine	Chlorprothixene	Citalopram	Clobazam (Urbadan)	Clonazepam	Clonidine
0.009	0.001	0.025	0.001	0.008	0.02	0.007	0.0025	0.01	0.0012	0.0018	0.001	0.04	0.0013
0.005	0.011	0.034	0.2	0.02	0.032	0.007	0.46	0.01	0.0013	0.0015	0.011	0.034	0.001
0.007	0.001	0.038	0.001	0.008	0.03	0.007	0.02	0.01	0.0039	0.001	0.001	0.001	0.0013
0.008	0.001	0.025	0.001	0.02	0.034	0.007	0.013	0.01	0.0013	0.001	0.001	0.001	0.001
0.006	0.001	0.0062	0.044	0.01	0.033	0.007	0.03	0.01	0.0019	0.001	0.005	0.0038	0.0013
0.007	0.012	0.011	0.001	0.008	0.028	0.007	0.021	0.01	0.0015	0.0011	0.001	0.041	0.0013
0.003	0.001	0.0092	0.001	0.01	0.024	0.007	0.0019	0.01	0.00083	0.001	0.001	0.042	0.0013
0.003	0.001	0.014	0.001	0.009	0.017	0.007	0.012	0.01	0.001	0.001	0.001	0.034	0.001
0.003	0.015	0.062	0.039	0.01	0.023	0.007	0.029	0.01	0.014	0.001	0.001	0.029	0.0013
0.003	0.001	0.025	0.001	0.01	0.019	0.007	0.003	0.01	0.00078	0.001	0.001	0.28	0.001
0.003	0.001	0.018	0.001	0.01	0.023	0.007	0.0026	0.01	0.0014	0.0014	0.001	0.26	0.0014
0.003	0.001	0.02	0.001	0.01	0.047	0.007	0.013	0.018	0.0012	0.0011	0.001	0.25	0.001
0.003	0.001	0.021	0.001	0.01	0.016	0.007	0.0037	0.01	0.001	0.001	0.001	0.24	0.001
0.003	0.001	0.02	0.001	0.01	0.022	0.007	0.0051	0.01	0.0012	0.001	0.001	0.22	0.001
0.003	0.001	0.021	0.001	0.02	0.025	0.007	0.015	0.01	0.001	0.001	0.001	0.21	0.001
0.008	0.012	0.022	0.001	0.025	0.059	0.01	0.019	0.01	0.0015	0.001	0.001	0.05	0.001
0.003	0.001	0.017	0.001	0.02	0.027	0.007	0.0086	0.01	0.0018	0.001	0.001	0.05	0.001
0.003	0.015	0.019	0.001	0.01	0.031	0.007	0.025	0.014	0.001	0.001	0.001	0.0029	0.0013
0.003	0.001	0.022	0.001	0.02	0.032	0.007	0.001	0.011	0.0013	0.001	0.0039	0.042	0.0013
0.003	0.001	0.018	0.001	0.02	0.035	0.007	0.009	0.01	0.001	0.001	0.001	0.021	0.001
0.003	0.018	0.015	0.001	0.02	0.027	0.007	0.017	0.01	0.0012	0.001	0.001	0.0079	0.001
0.003	0.001	0.019	0.001	0.01	0.035	0.007	0.0073	0.01	0.001	0.001	0.001	0.022	0.001
0.003	0.001	0.017	0.001	0.008	0.043	0.007	0.001	0.01	0.001	0.001	0.001	0.0022	0.001
0.003	0.001	0.0055	0.001	0.01	0.035	0.007	0.0063	0.01	0.001	0.001	0.0032	0.018	0.001
0.003	0.001	0.014	0.001	0.02	0.032	0.007	0.08	0.01	0.001	0.001	0.001	0.0055	0.001
0.003	0.014	0.016	0.001	0.02	0.025	0.007	0.0096	0.01	0.0013	0.001	0.001	0.011	0.001
0.005	0.001	0.013	0.001	0.02	0.032	0.007	0.015	0.01	0.0012	0.001	0.001	0.0098	0.001
0.003	0.001	0.014	0.001	0.02	0.047	0.007	0.001	0.01	0.001	0.001	0.001	0.009	0.001
0.003	0.001	0.012	0.001	0.01	0.027	0.007	0.0022	0.01	0.001	0.0017	0.0032	0.001	0.001
0.003	0.001	0.013	0.001	0.01	0.029	0.007	0.034	0.01	0.001	0.001	0.001	0.0068	0.001
0.003	0.001	0.011	0.001	0.02	0.021	0.007	0.0023	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.012	0.001	0.02	0.033	0.009	0.22	0.01	0.0012	0.0057	0.0056	0.001	0.001
0.003	0.001	0.015	0.001	0.02	0.036	0.007	0.0036	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.022	0.012	0.001	0.02	0.031	0.007	0.018	0.01	0.001	0.001	0.001	0.0036	0.001
0.003	0.012	0.011	0.001	0.008	0.034	0.009	0.0075	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.01	0.011	0.001	0.01	0.022	0.007	0.0032	0.01	0.001	0.001	0.001	0.0032	0.001
0.003	0.017	0.0075	0.001	0.01	0.0089	0.007	0.001	0.01	0.001	0.001	0.0036	0.001	0.001
0.004	0.014	0.012	0.001	0.01	0.022	0.007	0.001	0.01	0.001	0.001	0.001	0.0037	0.001
0.003	0.012	0.0094	0.001	0.01	0.02	0.007	0.0069	0.01	0.001	0.0092	0.001	0.001	0.001
0.003	0.011	0.011	0.001	0.01	0.023	0.007	0.0064	0.01	0.001	0.001	0.0026	0.001	0.001
0.009	0.012	0.01	0.001	0.008	0.027	0.01	0.001	0.01	0.001	0.001	0.0051	0.001	0.001
0.003	0.012	0.011	0.001	0.01	0.024	0.007	0.0087	0.01	0.001	0.001	0.0043	0.001	0.001
0.003	0.013	0.0081	0.001	0.01	0.025	0.007	0.0042	0.01	0.001	0.001	0.0041	0.0043	0.001
0.003	0.014	0.0099	0.001	0.01	0.025	0.007	0.015	0.01	0.001	0.0016	0.001	0.001	0.001
0.003	0.012	0.0091	0.001	0.02	0.025	0.007	0.0064	0.01	0.001	0.001	0.01	0.001	0.001
0.003	0.012	0.0078	0.001	0.02	0.024	0.007	0.0038	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.009	0.001	0.02	0.019	0.007	0.25	0.01	0.001	0.001	0.0084	0.001	0.001
0.003	0.001	0.0094	0.001	0.008	0.039	0.007	0.076	0.01	0.001	0.001	0.0096	0.001	0.001
0.003	0.001	0.0092	0.001	0.02	0.023	0.007	0.0032	0.01	0.001	0.001	0.0061	0.001	0.001
0.003	0.011	0.02	0.081	0.01	0.023	0.007	0.0034	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.007	0.001	0.008	0.034	0.01	0.0056	0.053	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.066	0.29	0.01	0.02	0.007	0.0066	0.01	0.0035	0.0047	0.0046	0.001	0.001
0.003	0.001	0.07	0.18	0.01	0.018	0.007	0.0039	0.01	0.0085	0.0036	0.0083	0.001	0.001
0.007	0.011	0.005	0.001	0.008	0.0062	0.007	0.012	0.01	0.001	0.0063	0.001	0.001	0.001
0.003	0.001	0.0043	0.001	0.008	0.019	0.007	0.001	0.01	0.001	0.001	0.01	0.001	0.001
0.01	0.011	0.0029	0.001	0.008	0.038	0.007	0.001	0.01	0.001	0.0014	0.001	0.001	0.001
0.003	0.012	0.001	0.001	0.01	0.018	0.007	0.0033	0.01	0.001	0.001	0.0037	0.001	0.001
0.03	0.011	0.0032	0.001	0.065	0.068	0.04	0.042	0.01	0.001	0.001	0.008	0.001	0.001
0.003	0.012	0.0047	0.001	0.01	0.024	0.007	0.001	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.0045	0.001	0.02	0.023	0.007	0.001	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.011	0.0048	0.001	0.01	0.024	0.007	0.001	0.01	0.001	0.0056	0.001	0.001	0.001
0.003	0.001	0.0043	0.33	0.01	0.02	0.007	0.001	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.001	0.001	0.008	0.0036	0.007	0.001	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.0028	0.001	0.008	0.005	0.007	0.011	0.01	0.001	0.002	0.001	0.001	0.001
0.003	0.001	0.006	0.001	0.01	0.023	0.007	0.001	0.01	0.001	0.001	0.002	0.001	0.001
0.003	0.012	0.0032	0.001	0.009	0.023	0.007	0.001	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.001	0.0037	0.001	0.01	0.028	0.007	0.0068	0.01	0.001	0.001	0.001	0.001	0.001
0.003	0.012	0.001	0.001	0.008	0.017	0.007	0.014	0.01	0.001	0.001	0.001	0.001	0.001

Clozapine	Cocaethylene	Cocaine	Codeine	CP 47,497	CP 47,497-C8 homologue	Crotamiton	Desalkylflurazepam	Desipramine	Dextromethorphan (Methorphan)	Diazepam	Diclofenac	Digitoxin	Digoxin
0.001	0.0032	0.019	0.044	0.0091	0.0025	0.003	0.0052	0.12	0.0029	0.012	0.011	0.042	0.01
0.001	0.0024	0.029	0.042	0.0023	0.018	0.003	0.0053	0.048	0.0039	0.018	0.018	0.03	0.024
0.012	0.002	0.024	0.11	0.0015	0.0077	0.003	0.0087	0.03	0.004	0.016	0.01	0.037	0.001
0.014	0.00054	0.035	0.041	0.0096	0.026	0.003	0.001	0.04	0.0028	0.015	0.0093	0.001	0.001
0.001	0.0012	0.015	0.04	0.011	0.011	0.003	0.0052	0.064	0.003	0.015	0.016	0.035	0.001
0.0055	0.0045	0.0071	0.044	0.0073	0.12	0.003	0.0087	0.058	0.0035	0.022	0.01	0.044	0.01
0.001	0.00037	0.01	0.044	0.015	0.014	0.003	0.0091	0.014	0.0034	0.019	0.0051	0.038	0.001
0.001	0.001	0.024	0.06	0.0092	0.028	0.003	0.0063	0.011	0.0041	0.021	0.0032	0.072	0.013
0.33	0.0016	0.064	0.0016	0.026	0.014	0.003	0.051	0.0086	0.016	0.021	0.00034	0.05	0.0097
0.0033	0.001	0.001	0.0017	0.51	0.001	0.003	0.029	0.0097	0.0033	0.012	0.012	0.001	0.001
0.0042	0.001	0.001	0.001	0.46	0.001	0.003	0.001	0.019	0.0035	0.011	0.011	0.001	0.001
0.0065	0.001	0.001	0.001	0.45	0.001	0.003	0.001	0.026	0.0038	0.0047	0.021	0.001	0.001
0.014	0.00072	0.001	0.001	0.47	0.001	0.003	0.001	0.023	0.0032	0.009	0.0037	0.001	0.001
0.0094	0.001	0.001	0.001	0.46	0.001	0.003	0.001	0.011	0.0033	0.0075	0.0067	0.001	0.001
0.001	0.00071	0.001	0.001	0.46	0.0024	0.003	0.0086	0.015	0.0036	0.0044	0.01	0.094	0.001
0.092	0.0011	0.0065	0.034	0.07	0.0033	0.003	0.0094	0.0077	0.0033	0.026	0.016	0.001	0.014
0.069	0.001	0.002	0.026	0.001	0.014	0.003	0.001	0.011	0.001	0.006	0.01	0.074	0.001
0.005	0.001	0.02	0.039	0.001	0.0006	0.003	0.001	0.015	0.0029	0.0005	0.0097	0.11	0.001
0.011	0.001	0.0061	0.032	0.001	0.0078	0.003	0.001	0.0065	0.003	0.0005	0.0036	0.001	0.001
0.022	0.001	0.005	0.031	0.001	0.0054	0.003	0.001	0.017	0.0029	0.0005	0.051	0.042	0.012
0.019	0.001	0.004	0.02	0.0024	0.0043	0.003	0.001	0.0071	0.0041	0.0005	0.004	0.046	0.011
0.0072	0.00058	0.012	0.021	0.001	0.0039	0.003	0.001	0.0084	0.0029	0.0005	0.015	0.001	0.001
0.01	0.00056	0.0034	0.023	0.001	0.0047	0.003	0.001	0.0066	0.0042	0.0005	0.00034	0.001	0.012
0.013	0.00046	0.0071	0.021	0.001	0.0027	0.003	0.001	0.015	0.001	0.007	0.0071	0.001	0.001
0.054	0.001	0.0066	0.019	0.001	0.0023	0.003	0.001	0.0085	0.0029	0.0005	0.0076	0.001	0.001
0.073	0.001	0.0052	0.017		0.001	0.003	0.001	0.0085	0.001	0.0058	0.0066	0.001	0.001
0.03	0.00066	0.009	0.019	0.001	0.0003	0.003	0.001	0.001	0.001	0.0005	0.0045	0.001	0.001
0.011	0.001	0.0047	0.016	0.001	0.001	0.003	0.001	0.0082	0.0028	0.0053	0.0039	0.001	0.001
0.019	0.001	0.0093	0.017	0.001	0.001	0.003	0.0046	0.017	0.0029	0.0005	0.0039	0.001	0.001
0.028	0.001	0.0063	0.02	0.001	0.001	0.003	0.001	0.013	0.001	0.0005	0.0033	0.001	0.001
0.06	0.001	0.0074	0.019	0.0099	0.001	0.003	0.001	0.096	0.0029	0.0005	0.001	0.001	0.001
0.0095	0.001	0.0046	0.022	0.001	0.001	0.003	0.001	0.012	0.0031	0.0081	0.0036	0.001	0.001
0.013	0.00065	0.0082	0.017	0.001	0.001	0.003	0.001	0.0055	0.001	0.0049	0.0041	0.001	0.001
0.042	0.001	0.0074	0.016	0.001	0.0045	0.003	0.001	0.0055	0.003	0.0005	0.0037	0.001	0.001
0.0056	0.001	0.0094	0.016	0.001	0.001	0.003	0.001	0.001	0.001	0.0005	0.0021	0.001	0.001
0.052	0.001	0.001	0.015	0.001	0.0014	0.003	0.001	0.0047	0.003	0.0005	0.0038	0.001	0.001
0.021	0.001	0.014	0.02	0.001	0.001	0.003	0.001	0.0051	0.0028	0.0048	0.00034	0.001	0.001
0.0044	0.0015	0.0094	0.014	0.001	0.0025	0.003	0.001	0.016	0.001	0.0041	0.0037	0.001	0.001
0.001	0.001	0.0064	0.012	0.001	0.00079	0.003	0.001	0.014	0.001	0.0042	0.00034	0.001	0.001
0.001	0.001	0.0061	0.0095	0.001	0.001	0.003	0.001	0.011	0.0064	0.0005	0.0027	0.001	0.001
0.001	0.001	0.014	0.011	0.0039	0.0013	0.003	0.001	0.014	0.001	0.0047	0.0057	0.001	0.001
0.001	0.001	0.011	0.011	0.001	0.0019	0.003	0.001	0.011	0.0082	0.0005	0.0017	0.001	0.001
0.001	0.0019	0.015	0.015	0.001	0.001	0.003	0.001	0.0099	0.0038	0.0005	0.0017	0.001	0.001
0.001	0.00043	0.011	0.012	0.001	0.0042	0.003	0.001	0.0081	0.003	0.0005	0.0037	0.001	0.001
0.001	0.00063	0.016	0.0096	0.001	0.0025	0.003	0.0052	0.01	0.0084	0.0005	0.00034	0.001	0.001
0.001	0.00052	0.007	0.0087	0.001	0.001	0.003	0.001	0.0092	0.0038	0.0005	0.00034	0.001	0.001
0.001	0.00093	0.038	0.096	0.001	0.00048	0.003	0.001	0.03	0.0055	0.0005	0.00034	0.001	0.001
0.0054	0.0025	0.025	0.1	0.001	0.00011	0.003	0.001	0.004	0.0061	0.0043	0.0021	0.001	0.001
0.001	0.001	0.037	0.098	0.001	0.0013	0.003	0.001	0.006	0.0051	0.0005	0.0014	0.001	0.001
0.001	0.00095	0.0076	0.11	0.00089	0.0017	0.003	0.001	0.0037	0.0047	0.0041	0.00034	0.001	0.001
0.012	0.00098	0.001	0.1	0.025	0.0057	0.003	0.001	0.001	0.0039	0.0005	0.00097	0.001	0.0088
0.0024	0.001	0.011	0.11	0.027	0.0022	0.003	0.001	0.0011	0.0029	0.0047	0.00034	0.037	0.001
0.001	0.001	0.0039	0.11	0.013	0.0026	0.003	0.001	0.001	0.0033	0.0043	0.00034	0.047	0.001
0.001	0.00071	0.0082	0.074	0.0076	0.0064	0.003	0.0053	0.07	0.0031	0.0005	0.0017	0.001	0.001
0.0061	0.00085	0.0066	0.062	0.0014	0.0033	0.003	0.001	0.07	0.0039	0.0005	0.00034	0.001	0.001
0.0042	0.0012	0.0076	0.065	0.013	0.001	0.003	0.0047	0.054	0.0036	0.0005	0.069	0.001	0.001
0.0052	0.0004	0.0014	0.044	0.00092	0.001	0.003	0.001	0.001	0.001	0.0005	0.00034	0.001	0.001
0.0023	0.00078	0.023	0.058	0.0029	0.00026	0.01	0.001	0.036	0.001	0.0041	0.25	0.001	0.001
0.001	0.0006	0.0043	0.058	0.0084	0.00064	0.003	0.0072	0.02	0.001	0.0005	0.00034	0.001	0.001
0.001	0.00068	0.0059	0.057	0.0015	0.00022	0.003	0.001	0.011	0.001	0.0005	0.0049	0.001	0.001
0.001	0.00094	0.0059	0.063	0.017	0.00052	0.003	0.001	0.0053	0.001	0.0005	0.00034	0.001	0.001
0.001	0.0011	0.0033	0.068	0.029	0.00088	0.003	0.001	0.016	0.001	0.0005	0.00089	0.001	0.001
0.023	0.00073	0.002	0.066	0.0068	0.001	0.003	0.0078	0.039	0.001	0.0005	0.0016	0.001	0.001
0.0081	0.001	0.0017	0.061	0.013	0.00072	0.003	0.001	0.031	0.001	0.0005	0.0017	0.001	0.001
0.001	0.00064	0.0058	0.057	0.0033	0.001	0.003	0.001	0.04	0.001	0.0005	0.00034	0.001	0.001
0.0034	0.00068	0.0066	0.057	0.0077	0.001	0.003	0.001	0.0095	0.001	0.0005	0.00034	0.001	0.001
0.0069	0.00069	0.0058	0.056	0.0065	0.001	0.003	0.001	0.0044	0.0028	0.0005	0.003	0.001	0.001
0.001	0.00075	0.0081	0.061	0.0046	0.001	0.003	0.0047	0.0074	0.001	0.0005	0.0015	0.001	0.001

Dihydrocodeine	Diphenhydramine	Dothiepin	Doxepin	EDDP (metabolite of Methadone)	Felbamate	Fenazepam	Fenofibrate	Fentanyl	Flumazenil	Flunitrazepam	Flupentixol	Flurazepam	Gabapentin
0.83	0.0031	0.0059	0.001	0.0087	0.001	0.001	0.02	0.001	0.0015	0.0005	0.53	0.001	0.1
0.76	0.0035	0.0071	0.0012	0.01	0.001	0.11	0.01	0.001	0.001	0.0005	0.41	0.001	0.1
0.63	0.0056	0.011	0.0015	0.013	0.001	0.001	0.006	0.001	0.0014	0.0005	0.63	0.001	0.08
0.59	0.0023	0.0017	0.001	0.013	0.0003	0.001	0.006	0.001	0.001	0.0005	0.43	0.001	0.09
0.78	0.0026	0.0083	0.001	0.012	0.001	0.018	0.006	0.001	0.001	0.0005	0.32	0.001	0.07
0.95	0.0052	0.00058	0.001	0.0033	0.0042	0.016	0.006	0.001	0.001	0.0005	0.53	0.001	0.06
0.39	0.0034	0.0034	0.001	0.0055	0.001	0.031	0.006	0.00027	0.001	0.0005	0.37	0.001	0.05
0.51	0.0034	0.00062	0.001	0.0081	0.001	0.001	0.006	0.00044	0.001	0.0005	0.29	0.001	0.06
0.031	0.001	0.029	0.033	0.003	0.001	0.0099	0.006	0.001	0.001	0.0005	0.052	0.001	0.06
0.001	0.001	0.0021	0.0018	0.001	0.00027	0.01	0.006	0.00057	0.001	0.0005	0.36	0.001	0.1
0.001	0.001	0.0034	0.0013	0.0024	0.00029	0.001	0.006	0.0023	0.001	0.0005	0.25	0.001	0.08
0.0017	0.001	0.0031	0.0012	0.001	0.001	0.001	0.006	0.001	0.001	0.0005	0.23	0.001	0.2
0.0025	0.00034	0.0045	0.001	0.001	4.70E-06	0.001	0.006	0.0075	0.001	0.0005	0.2	0.001	0.07
0.001	0.001	0.0035	0.0012	0.001	0.001	0.01	0.006	0.001	0.001	0.0005	0.2	0.001	0.1
0.001	0.001	0.0035	0.0013	0.0024	0.00031	0.001	0.006	0.001	0.001	0.0005	0.17	0.001	0.1
0.52	0.0092	0.00074	0.001	0.0056	0.001	0.021	0.006	0.001	0.001	0.0005	0.53	0.001	0.2
0.34	0.0043	0.0032	0.001	0.0049	0.001	0.015	0.006	0.00052	0.001	0.0005	0.32	0.001	0.2
0.56	0.001	0.0055	0.001	0.0048	0.0014	0.001	0.006	0.001	0.001	0.0005	0.22	0.001	0.2
0.49	0.0049	0.00045	0.001	0.0048	0.0011	0.011	0.006	0.001	0.001	0.0005	0.2	0.001	0.2
0.84	0.0042	0.0026	0.001	0.0054	0.001	0.014	0.006	0.00097	0.001	0.0005	0.17	0.001	0.2
0.63	0.0042	0.0003	0.001	0.0036	0.0016	0.001	0.006	0.001	0.001	0.0005	0.19	0.001	0.1
0.3	0.0037	0.0041	0.001	0.0038	0.001	0.001	0.006	0.001	0.001	0.0005	0.18	0.001	0.1
0.8	0.0039	0.001	0.0012	0.0032	0.0035	0.001	0.006	0.001	0.001	0.0005	0.17	0.001	0.1
0.67	0.00078	0.0033	0.001	0.0059	0.0077	0.001	0.006	0.001	0.001	0.0005	0.17	0.001	0.1
0.41	0.0066	0.0033	0.00098	0.0028	0.001	0.001	0.006	0.001	0.001	0.0005	0.22	0.001	0.1
0.46	0.0037	0.0035	0.001	0.0058	0.001	0.011	0.006	0.001	0.001	0.0005	0.19	0.001	0.2
0.14	0.0043	0.0035	0.001	0.0055	0.0009	0.001	0.006	0.00052	0.001	0.0005	0.19	0.001	0.2
0.62	0.003	0.0032	0.001	0.0026	0.001	0.001	0.006	0.001	0.001	0.0005	0.18	0.001	0.1
0.23	0.0041	0.00039	0.0013	0.0032	0.00029	0.001	0.006	0.001	0.001	0.0005	0.18	0.001	0.1
0.21	0.0029	0.002	0.001	0.0045	0.001	0.011	0.006	0.0051	0.001	0.0005	0.17	0.001	0.1
0.2	0.004	0.0021	0.001	0.0036	0.0068	0.0099	0.006	0.001	0.001	0.0005	0.16	0.001	0.2
0.19	0.0024	0.0023	0.001	0.004	0.0058	0.001	0.006	0.0021	0.001	0.0005	0.16	0.001	0.1
0.47	0.0043	0.0023	0.001	0.0027	0.001	0.011	0.006	0.001	0.001	0.0005	0.14	0.001	0.1
0.083	0.0039	0.0026	0.001	0.0041	0.001	0.012	0.006	0.041	0.001	0.0005	0.14	0.001	0.1
0.36	0.0031	0.0039	0.001	0.001	0.001	0.01	0.006	0.001	0.001	0.0005	0.16	0.001	0.1
0.35	0.00074	0.0007	0.001	0.0043	0.001	0.012	0.006	0.001	0.001	0.0005	0.15	0.001	0.1
0.33	0.00078	0.00064	0.001	0.0041	0.001	0.001	0.006	0.001	0.001	0.0005	0.1	0.001	0.005
0.19	0.0033	0.0037	0.001	0.005	0.0087	0.001	0.006	0.002	0.001	0.002	0.3	0.001	0.1
0.31	0.0035	0.003	0.001	0.0042	0.0039	0.001	0.006	0.001	0.001	0.0013	0.26	0.001	0.1
0.89	0.0017	0.0032	0.0013	0.0034	0.0062	0.001	0.006	0.001	0.001	0.0012	0.23	0.001	0.1
0.86	0.004	0.004	0.001	0.0026	0.0026	0.001	0.006	0.001	0.001	0.0005	0.19	0.001	0.005
0.17	0.00044	0.0031	0.001	0.0037	0.001	0.001	0.006	0.001	0.001	0.0005	0.12	0.001	0.1
0.36	0.0039	0.0046	0.00094	0.0031	0.001	0.001	0.006	0.001	0.001	0.0005	0.1	0.001	0.1
0.43	0.0032	0.0034	0.0031	0.003	0.001	0.001	0.006	0.001	0.001	0.0005	0.098	0.001	0.1
0.25	0.0034	0.0028	0.00091	0.0031	0.001	0.001	0.006	0.001	0.001	0.0005	0.091	0.001	0.1
0.079	0.00046	0.003	0.001	0.0033	0.003	0.011	0.006	0.001	0.001	0.0005	0.081	0.001	0.1
0.58	0.003	0.0036	0.001	0.0067	0.0043	0.047	0.006	0.00046	0.001	0.0005	0.2	0.001	0.1
0.6	0.002	0.01	0.001	0.0077	0.12	0.001	0.006	0.001	0.001	0.0005	0.15	0.001	0.005
0.87	0.0006	0.0035	0.001	0.011	0.0013	0.014	0.006	0.001	0.001	0.0005	0.093	0.001	0.1
0.67	0.0018	0.001	0.001	0.011	0.001	0.0098	0.006	0.001	0.001	0.0005	0.065	0.001	0.08
0.5	0.001	0.0092	0.001	0.013	0.01	0.001	0.006	0.0005	0.001	0.0005	0.043	0.001	0.1
0.34	0.00061	0.00029	0.001	0.014	0.001	0.0097	0.006	0.001	0.0014	0.0005	0.039	0.001	0.06
0.077	0.001	0.0007	0.0011	0.012	0.001	0.0098	0.006	0.001	0.0014	0.0005	0.044	0.00091	0.08
0.66	0.0017	0.0014	0.0011	0.001	0.0006	0.012	0.006	0.00057	0.001	0.0005	0.12	0.001	0.07
0.55	0.001	0.0021	0.0011	0.003	0.0013	0.001	0.006	0.001	0.001	0.0005	0.093	0.001	0.1
0.39	0.001	0.0055	0.001	0.003	0.00076	0.001	0.006	0.001	0.001	0.0005	0.082	0.001	0.06
0.26	0.0012	0.0022	0.001	0.0025	0.001	0.001	0.006	0.001	0.001	0.0005	0.068	0.001	0.07
0.29	0.001	0.0093	0.001	0.0067	0.001	0.001	0.006	0.001	0.001	0.0005	0.06	0.001	0.4
0.34	0.001	0.0017	0.00097	0.0029	0.001	0.011	0.006	0.001	0.001	0.0005	0.056	0.001	0.06
0.25	0.00046	0.0022	0.00095	0.0029	0.00078	0.001	0.006	0.001	0.001	0.0005	0.053	0.001	0.09
0.21	0.00093	0.0026	0.0018	0.001	0.001	0.001	0.006	0.001	0.001	0.0005	0.051	0.001	0.06
0.49	0.001	0.0022	0.001	0.0028	0.001	0.001	0.006	0.001	0.001	0.0005	0.051	0.001	0.09
0.21	0.0025	0.0014	0.0011	0.0027	0.0045	0.001	0.006	0.0019	0.001	0.0005	0.077	0.001	0.05
0.39	0.001	0.0014	0.00098	0.001	0.001	0.001	0.006	0.001	0.001	0.0005	0.062	0.001	0.06
0.47	0.00085	0.002	0.0012	0.001	0.00052	0.001	0.006	0.00035	0.001	0.0005	0.053	0.001	0.06
0.33	0.0011	0.0016	0.001	0.003	0.001	0.001	0.006	0.001	0.001	0.0005	0.048	0.001	0.07
0.26	0.00092	0.0021	0.001	0.001	0.001	0.001	0.006	0.001	0.001	0.0005	0.047	0.001	0.08
0.18	0.001	0.002	0.0015	0.001	0.0074	0.001	0.006	0.001	0.001	0.0005	0.044	0.001	0.1

Gabapentin-lactam	Haloperidol	Hydrochlorothiazide	Hydrocodone	Hydromorphone	Imipramine	Indometacin	Iohexol	Iomeprol	Iopamidol	Iopromid	Irbesartan	JWH-018 (N-(n-pentanoic acid)	JWH-073 (2-methylnaphthyl analog)
0.03	0.0019	0.05	0.033	0.00092	0.001	0.01	0.1	0.3	2	0.07	0.0065	0.001	0.22
0.02	0.002	0.04	0.031	0.0015	0.001	0.01	0.1	0.3	2	0.07	0.0065	0.001	0.14
0.02	0.001	0.03	0.081	0.001	0.0038	0.01	0.1	0.1	2	0.1	0.0025	0.001	0.48
0.02	0.0021	0.03	0.03	0.00094	0.001	0.01	0.1	0.3	2	0.2	0.0025	0.001	0.26
0.02	0.0021	0.03	0.029	0.0015	0.001	0.01	0.1	0.1	2	0.07	0.0025	0.001	0.74
0.01	0.0023	0.03	0.032	0.00087	0.001	0.01	0.1	0.1	2	0.07	0.00375	6.30E-05	0.018
0.02	0.002	0.03	0.032	0.001	0.014	0.01	0.1	0.1	2	0.07	0.00175	0.001	0.027
0.01	0.001	0.03	0.044	0.00087	0.001	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.12
0.02	0.0032	0.03	0.0021	0.01	0.0073	0.01	0.1	0.1	2	0.07	0.0015	0.0024	0.093
0.02	0.002	0.03	0.0022	0.00094	0.0086	0.01	0.1	0.1	2	0.07	0.00175	0.001	0.0035
0.02	0.0021	0.03	0.001	0.0014	0.003	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.033
0.1	0.001	0.03	0.001	0.002	0.018	0.01	0.1	0.1	2	0.07	0.00475	0.001	0.3
0.02	0.001	0.03	0.001	0.00096	0.014	0.01	0.1	0.1	2	0.09	0.0015	4.70E-05	0.026
0.02	0.001	0.03	0.001	0.00093	0.001	0.01	0.1	0.1	2	0.1	0.0015	0.001	0.06
0.04	0.001	0.03	0.001	0.0029	0.001	0.01	0.1	0.1	2	0.07	0.0025	0.001	0.21
0.08	0.002	0.04	0.025	0.0078	0.042	0.01	0.1	0.1	5	0.07	0.0075	0.001	0.15
0.04	0.002	0.03	0.019	0.0026	0.0022	0.01	0.1	0.1	2	0.07	0.0025	0.001	0.078
0.08	0.002	0.03	0.029	0.0019	0.0028	0.01	0.1	0.1	3	0.1	0.0225	0.001	0.0088
0.04	0.001	0.03	0.024	0.0021	0.0018	0.01	0.1	0.1	2	0.07	0.00425	1.70E-05	0.0043
0.04	0.001	0.03	0.023	0.0019	0.0021	0.01	0.1	0.1	2	0.1	0.005	0.001	0.0023
0.04	0.001	0.03	0.016	0.0009	0.0032	0.01	0.1	0.2	2.2	0.09	0.00725	6.00E-05	0.074
0.04	0.002	0.03	0.016	0.001	0.053	0.01	0.1	0.1	2	0.07	0.007	0.001	0.15
0.03	0.002	0.03	0.018	0.0069	0.001	0.01	0.1	0.1	2	0.07	0.03	0.001	0.085
0.03	0.002	0.03	0.016	0.0008	0.1	0.01	0.1	0.1	2	0.09	0.005	8.00E-06	0.079
0.04	0.001	0.03	0.014	0.0032	0.0068	0.01	0.1	0.1	2.2	0.07	0.005	0.001	0.02
0.04	0.001	0.03	0.013	0.0014	0.0028	0.01	0.1	0.2	2.1	0.08	0.005	0.001	0.09
0.04	0.002	0.03	0.015	0.0033	0.003	0.01	0.1	0.1	2.1	0.07	0.00725	3.60E-05	0.3
0.05	0.001	0.03	0.013	0.001	0.001	0.01	0.1	0.1	2	0.1	0.0075	0.001	0.0038
0.007	0.001	0.03	0.013	0.0014	0.0097	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.001
0.04	0.001	0.03	0.015	0.00089	0.0069	0.01	0.1	0.2	2	0.07	0.007	0.001	0.033
0.04	0.001	0.03	0.015	0.0009	0.003	0.01	0.1	0.1	2.3	0.07	0.00675	0.001	0.001
0.04	0.001	0.03	0.017	0.001	0.019	0.01	0.1	0.2	2	0.07	0.01	3.70E-05	0.0059
0.04	0.001	0.03	0.013	0.00095	0.0014	0.01	0.1	0.1	2.2	0.07	0.00675	0.001	0.048
0.04	0.001	0.03	0.013	0.0017	0.0014	0.01	0.1	0.1	2.2	0.1	0.007	0.001	0.001
0.04	0.001	0.03	0.012	0.0023	0.001	0.01	0.1	0.1	2	0.07	0.01	0.001	0.001
0.03	0.001	0.03	0.011	0.001	0.001	0.01	0.1	0.1	2	0.07	0.00425	0.001	0.0042
0.007	0.001	0.03	0.015	0.001	0.0051	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.012
0.02	0.002	0.03	0.011	0.0017	0.023	0.01	0.1	0.1	2	0.07	0.00425	0.001	0.083
0.007	0.001	0.03	0.0093	0.0009	0.0049	0.01	0.1	0.1	2	0.07	0.005	0.001	0.001
0.03	0.001	0.03	0.0078	0.001	0.0018	0.01	0.1	0.1	2	0.07	0.00475	0.001	0.0055
0.007	0.001	0.03	0.0089	0.00086	0.005	0.01	0.4	0.1	2	0.7	0.0015	0.001	0.037
0.03	0.001	0.03	0.009	0.001	0.001	0.01	0.1	0.1	2	0.1	0.0025	0.001	0.19
0.04	0.001	0.03	0.011	0.0039	0.0035	0.01	0.1	0.1	2	0.09	0.00475	0.001	0.088
0.04	0.001	0.03	0.0097	0.001	0.001	0.01	0.1	0.1	2	0.1	0.009	0.001	0.11
0.03	0.001	0.03	0.0079	0.0014	0.0051	0.01	0.1	0.1	2	0.07	0.007	0.001	0.056
0.03	0.001	0.03	0.0072	0.00098	0.0076	0.01	0.1	0.1	2	0.08	0.0045	0.001	0.0036
0.03	0.001	0.03	0.063	0.001	0.001	0.01	0.2	0.1	2	0.07	0.00725	0.001	0.15
0.007	0.001	0.03	0.065	0.001	0.001	0.01	0.2	0.1	2	0.07	0.0015	0.001	0.62
0.03	0.001	0.03	0.065	0.001	0.031	0.01	0.1	0.1	2	0.08	0.0075	0.001	0.23
0.02	0.001	0.03	0.08	0.001	0.032	0.01	0.1	0.1	2	0.07	0.0025	0.001	0.09
0.03	0.0019	0.03	0.077	0.00091	0.0028	0.01	0.3	1.3	2.5	0.07	0.0095	0.001	0.001
0.02	0.0047	0.03	0.075	0.001	0.0017	0.01	0.1	0.1	2	0.07	0.00225	1.60E-05	0.001
0.01	0.0054	0.03	0.064	0.001	0.001	0.01	0.1	0.1	2	0.07	0.00225	0.001	0.001
0.007	0.001	0.03	0.054	0.001	0.0014	0.01	0.1	0.1	2	0.07	0.0015	0.001	2.1
0.02	0.001	0.03	0.045	0.001	0.0019	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.13
0.02	0.001	0.08	0.047	0.001	0.0026	0.01	0.1	0.1	2	0.07	0.0015	0.00063	0.0048
0.01	0.001	0.03	0.046	0.001	0.0015	0.01	0.1	0.1	2	0.07	0.00175	0.001	0.33
0.03	0.001	0.03	0.042	0.0015	0.0015	0.01	1.1	1.4	11	0.3	0.0575	0.001	1.2
0.02	0.001	0.03	0.042	0.00085	0.001	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.05
0.02	0.001	0.03	0.042	0.001	0.0014	0.01	0.1	0.1	2	0.07	0.00225	0.001	0.11
0.01	0.001	0.03	0.046	0.001	0.019	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.083
0.02	0.001	0.03	0.049	0.0008	0.0063	0.01	0.1	0.1	2	0.07	0.00175	0.001	0.14
0.008	0.001	0.03	0.048	0.001	0.0014	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.0061
0.01	0.001	0.03	0.045	0.0023	0.001	0.01	0.1	0.1	2	0.07	0.0015	0.00085	0.18
0.01	0.001	0.03	0.042	0.00093	0.0019	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.14
0.01	0.001	0.03	0.041	0.001	0.0013	0.01	0.1	0.1	2	0.07	0.00225	0.001	0.1
0.01	0.001	0.03	0.041	0.00069	0.0016	0.01	0.1	0.1	2	0.07	0.002	0.001	0.14
0.02	0.001	0.03	0.045	0.001	0.0014	0.01	0.1	0.1	2	0.07	0.0015	0.001	0.35

Ketamine	Ketoprofen	Lamotrigine	Librium (Chlordiazepoxide)	Lidocaine	Lorazepam	Losartan	Maprotiline	Medazepam	Meperidine (Pethidine)	Methamphetamine	Methylendioxymethamphetamine (MDMA)	Methylphenidate	Metoprolol
0.0021	0.02	0.021	0.001	0.005	0.035	0.006	0.0058	0.00064	0.0018	0.0029	0.0069	0.0024	0.02
0.001	0.02	0.027	0.001	0.0049	0.049	0.006	0.0071	0.00029	0.00091	0.0027	0.0087	0.013	0.028
0.0026	0.02	0.03	0.0028	0.0057	0.045	0.006	0.01	0.0028	0.0058	0.0026	0.0098	0.022	0.041
0.0013	0.02	0.03	0.001	0.006	0.051	0.006	0.0095	0.0012	0.0016	0.001	0.0082	0.012	0.06233333
0.001	0.02	0.034	0.001	0.0069	0.039	0.006	0.0092	0.0012	0.001	0.001	0.0065	0.01	0.04166667
0.001	0.02	0.021	0.001	0.0052	0.07	0.006	0.00054	0.00023	0.00065	0.001	0.0039	0.014	0.04033333
0.001	0.02	0.02	0.0026	0.0037	0.081	0.006	0.0027	0.00096	0.001	0.001	0.0062	0.012	0.01333333
0.001	0.02	0.019	0.001	0.0037	0.056	0.006	0.0052	0.00073	0.001	0.001	0.0053	0.012	0.02
0.0029	0.02	0.013	0.031	0.042	0.001	0.006	0.00026	0.0095	0.022	0.001	0.2	0.034	0.02
0.0015	0.02	0.018	0.023	0.004	0.0023	0.006	0.001	0.0016	0.0018	0.001	0.0039	0.001	0.00666667
0.001	0.02	0.028	0.041	0.0051	0.0006	0.006	0.001	0.0014	0.0014	0.001	0.0049	0.017	0.01533333
0.001	0.02	0.046	0.0065	0.0034	0.001	0.006	0.001	0.0012	0.0014	0.014	0.014	0.02	0.02
0.0014	0.02	0.019	0.034	0.0056	0.0043	0.006	0.001	0.0012	0.001	0.001	0.0064	0.001	0.02
0.001	0.02	0.026	0.046	0.005	0.004	0.006	0.001	0.0012	0.0015	0.0036	0.0053	0.014	0.02
0.0011	0.02	0.026	0.048	0.0049	0.001	0.006	0.001	0.0011	0.0011	0.001	0.0062	0.015	0.02
0.001	0.02	0.046	0.0029	0.007	0.039	0.01	0.0028	0.002	0.002	0.0045	0.03	0.012	0.02
0.0014	0.02	0.024	0.001	0.0048	0.019	0.006	0.0021	0.0003	0.0018	0.001	0.0087	0.0034	0.02
0.0013	0.02	0.029	0.0085	0.0037	0.013	0.006	0.0021	0.00074	0.0017	0.001	0.027	0.001	0.02
0.001	0.02	0.023	0.001	0.0042	0.03	0.006	0.002	0.00052	0.0017	0.001	0.0059	0.001	0.02
0.001	0.02	0.022	0.001	0.0032	0.014	0.006	0.0026	0.00016	0.001	0.0032	0.0095	0.0015	0.02
0.001	0.02	0.021	0.0027	0.0041	0.0029	0.006	0.0009	0.00023	0.0016	0.001	0.01	0.0018	0.02
0.0013	0.02	0.026	0.001	0.0055	0.018	0.007	0.001	0.001	0.0018	0.001	0.0085	0.011	0.02
0.0013	0.02	0.028	0.001	0.0054	0.018	0.01	0.00046	0.00031	0.0018	0.0026	0.28	0.0016	0.02
0.001	0.02	0.022	0.001	0.005	0.011	0.007	0.0031	0.00081	0.0022	0.0028	0.0077	0.0079	0.02466667
0.0014	0.02	0.021	0.001	0.0045	0.0059	0.006	0.00014	0.00041	0.0011	0.001	0.0074	0.001	0.022
0.0012	0.02	0.021	0.001	0.0043	0.0064	0.008	0.003	0.00069	0.0018	0.0027	0.0065	0.0095	0.025
0.0011	0.02	0.021	0.0026	0.0048	0.0064	0.008	0.0027	0.00017	0.0018	0.001	0.0072	0.0053	0.024
0.0011	0.02	0.019	0.001	0.0047	0.013	0.006	0.001	0.001	0.0014	0.0031	0.0077	0.001	0.0105
0.0023	0.02	0.0074	0.001	0.0035	0.0038	0.006	0.00051	0.001	0.0012	0.0031	0.00035	0.0013	0.02
0.001	0.02	0.018	0.001	0.0038	0.0044	0.008	0.0018	0.001	0.001	0.001	0.006	0.0015	0.02
0.001	0.02	0.016	0.001	0.0038	0.0068	0.008	0.00086	0.001	0.0015	0.0049	0.0063	0.001	0.02
0.001	0.02	0.015	0.001	0.0041	0.0033	0.007	0.0012	0.001	0.0017	0.001	0.0068	0.0015	0.02
0.001	0.02	0.016	0.001	0.0039	0.0048	0.007	0.001	0.00021	0.0012	0.001	0.0072	0.0012	0.02
0.001	0.02	0.015	0.001	0.004	0.0023	0.009	0.0013	0.001	0.0012	0.001	0.0064	0.0046	0.02
0.001	0.02	0.009	0.001	0.0043	0.0007	0.006	0.001	0.00069	0.0016	0.0024	0.064	0.001	0.02
0.0012	0.02	0.015	0.001	0.0043	0.0054	0.007	0.0016	0.001	0.001	0.001	0.01	0.0019	0.02
0.001	0.02	0.0054	0.001	0.0039	0.0052	0.006	0.0014	0.00016	0.001	0.0026	0.0056	0.001	0.02
0.001	0.02	0.013	0.001	0.0043	0.016	0.007	0.0022	0.00065	0.0015	0.004	0.013	0.001	0.02
0.001	0.02	0.013	0.001	0.0037	0.0033	0.007	0.0014	0.001	0.0015	0.0029	0.0095	0.001	0.00666667
0.001	0.02	0.012	0.001	0.0043	0.0009	0.008	0.00073	0.0048	0.00038	0.004	0.011	0.001	0.02
0.0014	0.02	0.019	0.001	0.0037	0.0055	0.03	0.001	0.001	0.0031	0.0046	0.049	0.001	0.02
0.001	0.02	0.014	0.001	0.0037	0.001	0.006	0.00094	0.00028	0.0017	0.0027	0.0098	0.001	0.02
0.001	0.02	0.013	0.001	0.0038	0.0006	0.008	0.00041	0.0003	0.00075	0.001	0.01	0.0011	0.02
0.0014	0.02	0.013	0.001	0.0042	0.0021	0.008	0.00034	0.0002	0.00043	0.0028	0.009	0.001	0.02
0.001	0.02	0.013	0.001	0.0037	0.002	0.008	0.00039	0.00038	0.00019	0.0022	0.011	0.001	0.02
0.001	0.02	0.012	0.001	0.0034	0.001	0.006	0.00056	0.00029	0.00031	0.0023	0.01	0.001	0.02
0.001	0.02	0.013	0.001	0.004	0.001	0.006	0.0039	0.00033	0.0014	0.001	0.00054	0.0013	0.02
0.0014	0.02	0.012	0.001	0.0039	0.0021	0.006	0.0048	0.0014	0.001	0.001	0.00011	0.0015	0.02
0.0016	0.02	0.013	0.001	0.0038	0.0009	0.006	0.0077	0.00025	0.00085	0.001	0.001	0.001	0.02
0.001	0.02	0.001	0.0084	0.0036	0.001	0.006	0.0078	0.00077	0.00089	0.001	0.00021	0.0013	0.02
0.001	0.02	0.017	0.001	0.0067	0.001	0.03	0.01	0.00062	1.20E-05	0.001	0.00073	0.0016	0.02
0.001	0.02	0.001	0.003	0.001	0.001	0.006	0.011	0.005	0.001	0.001	0.00014	0.0011	0.02
0.001	0.02	0.001	0.002	0.001	0.001	0.006	0.0091	0.0021	0.001	0.001	8.60E-05	0.0011	0.02
0.001	0.02	0.003	0.001	0.0035	0.001	0.02	0.001	0.001	0.001	0.001	0.011	0.0011	0.02
0.001	0.02	0.008	0.001	0.0035	0.001	0.006	0.00027	0.001	0.001	0.003	0.0059	0.0011	0.02
0.001	0.02	0.0024	0.001	0.0036	0.001	0.02	0.00056	0.00046	0.00096	0.001	0.0042	0.001	0.02
0.00099	0.02	0.0081	0.001	0.0029	0.001	0.006	0.0003	0.001	0.00087	0.001	0.0021	0.0012	0.02
0.001	0.02	0.017	0.001	0.025	0.001	0.02	0.0039	0.00014	0.0022	0.001	0.016	0.0022	0.82
0.0012	0.02	0.0084	0.001	0.0033	0.001	0.006	0.00022	0.001	0.0033	0.001	0.0069	0.0013	0.008
0.0012	0.02	0.0078	0.001	0.0034	0.001	0.006	0.00016	0.001	0.00091	0.001	0.0037	0.0021	0.01466667
0.0012	0.02	0.0073	0.001	0.0033	0.001	0.006	0.001	0.00022	0.00073	0.001	0.0037	0.0011	0.02
0.0014	0.02	0.0081	0.001	0.0034	0.001	0.006	5.90E-05	0.001	0.00087	0.0029	0.0069	0.0013	0.02
0.001	0.02	0.0021	0.001	0.0035	0.001	0.006	2.30E-05	0.0003	0.0011	0.001	0.0016	0.0019	0.02
0.001	0.02	0.0027	0.0025	0.0041	0.001	0.006	0.001	0.0005	0.00079	0.001	0.011	0.001	0.02
0.0012	0.02	0.0077	0.001	0.0036	0.001	0.006	0.001	0.001	0.00081	0.001	0.0041	0.001	0.02
0.001	0.02	0.0072	0.001	0.0034	0.001	0.006	0.00027	0.00039	0.00078	0.001	0.0045	0.0013	0.021
0.0013	0.02	0.0077	0.0027	0.0034	0.001	0.006	0.001	0.001	0.00078	0.001	0.0038	0.001	0.02
0.0013	0.02	0.0071	0.001	0.0033	0.001	0.006	0.001	0.0002	0.00036	0.001	0.0034	0.0011	0.02

Metroprolol acid	Midazolam	Mirtazapine	Morphine	Morphine glucuronide	n-Acetyl-4-aminoantipyrine	Nadolol	Naltrexone	Naproxen	N-Desmethylclozapine	N-Formyl-4-aminoantipyrine	Nitrazepam	Norbuprenorphine	Nordiazepam
0.03	0.0005	0.001	0.0021	0.001	0.091	0.003	0.00098	0.07	0.001	0.1	0.001	0.023	0.02
0.04	0.0005	0.001	0.0026	0.001	0.14333333	0.003	0.001	0.07	0.001	0.1	0.015	0.022	0.0051
0.03	0.0005	0.0074	0.001	0.001	0.18	0.003	0.0012	0.07	0.001	0.1	0.099	0.055	0.0069
0.03	0.0005	0.001	0.0021	0.001	0.19	0.003	0.001	0.07	0.001	0.1	0.022	0.033	0.0034
0.02	0.0005	0.0051	0.0026	0.001	0.19666667	0.003	0.001	0.07	0.001	0.09	0.035	0.0048	0.0043
0.02	0.0014	0.0058	0.002	0.001	0.08033333	0.003	0.0027	0.07	0.0044	0.07	0.06	0.01	0.034
0.01	0.0023	0.0029	0.001	0.001	0.06933333	0.003	0.0015	0.07	0.0025	0.07	0.03	0.0097	0.0086
0.01	0.0005	0.0023	0.002	0.001	0.06233333	0.003	0.00059	0.07	0.0039	0.05	0.034	0.0061	0.021
0.01	0.0005	0.025	0.0099	0.001	0.06933333	0.003	0.001	0.07	0.014	0.07	0.92	0.14	0.0029
0.01	0.0005	0.0028	0.0021	0.001	0.07	0.003	0.00083	0.07	0.017	0.06	0.041	0.01	0.0049
0.02	0.0005	0.0041	0.0025	0.001	0.1	0.003	0.001	0.07	0.001	0.07	0.029	0.012	0.0029
0.04	0.0005	0.001	0.003	0.06	0.18	0.003	0.001	0.07	0.001	0.1	0.041	0.0026	0.0048
0.01	0.0005	0.003	0.0021	0.001	0.058	0.003	0.001	0.07	0.001	0.07	0.036	0.022	0.0028
0.02	0.0005	0.0054	0.0021	0.001	0.05333333	0.003	0.001	0.07	0.001	0.07	0.0089	0.013	0.0046
0.03	0.0005	0.0043	0.0038	0.001	0.07733333	0.003	0.0012	0.07	0.029	0.1	0.016	0.012	0.0031
0.04	0.0005	0.0039	0.008	0.001	0.12	0.003	0.0018	0.07	0.052	0.3	0.031	0.001	0.0043
0.03	0.0005	0.001	0.0035	0.001	0.086	0.003	0.001	0.07	0.001	0.1	0.018	0.001	0.0099
0.04	0.0005	0.001	0.0029	0.001	0.12	0.003	0.001	0.07	0.015	0.3	0.012	0.0084	0.0095
0.03	0.0005	0.0022	0.0031	0.001	0.077	0.003	0.0012	0.07	0.001	0.1	0.012	0.001	0.014
0.03	0.0005	0.001	0.0029	0.001	0.08233333	0.003	0.00094	0.07	0.035	0.2	0.0093	0.001	0.017
0.03	0.0005	0.001	0.002	0.001	0.077	0.003	0.00068	0.07	0.0062	0.1	0.011	0.001	0.026
0.01	0.0005	0.0024	0.0021	0.001	0.08466667	0.003	0.00071	0.07	0.022	0.2	0.019	0.001	0.018
0.04	0.0005	0.0027	0.0073	0.001	0.075	0.003	0.001	0.07	0.015	0.3	0.016	0.0065	0.022
0.03	0.0018	0.001	0.002	0.001	0.08566667	0.003	0.001	0.07	0.001	0.1	0.01	0.01	0.022
0.03	0.0005	0.001	0.0041	0.001	0.06766667	0.003	0.00083	0.07	0.024	0.1	0.017	0.0037	0.025
0.04	0.0005	0.001	0.0025	0.001	0.081	0.003	0.00052	0.07	0.034	0.2	0.011	0.0025	0.021
0.03	0.0005	0.001	0.0041	0.001	0.06866667	0.003	0.00066	0.07	0.001	0.2	0.014	0.0051	0.026
0.03	0.0005	0.0048	0.001	0.001	0.08166667	0.003	0.00053	0.07	0.001	0.2	0.015	0.0024	0.021
0.01	0.0005	0.0022	0.0025	0.001	0.039	0.003	0.00063	0.07	0.18	0.07	0.003	0.002	0.026
0.03	0.0018	0.001	0.002	0.001	0.06266667	0.003	0.00053	0.07	0.011	0.1	0.014	0.0059	0.025
0.03	0.0005	0.0062	0.0021	0.001	0.062	0.003	0.001	0.07	0.001	0.2	0.001	0.0025	0.022
0.03	0.0005	0.0027	0.001	0.001	0.08766667	0.003	0.00062	0.07	0.001	0.2	0.001	0.0022	0.018
0.03	0.0005	0.001	0.0021	0.001	0.062	0.003	0.00058	0.07	0.058	0.2	0.01	0.0025	0.0085
0.03	0.0005	0.001	0.0027	0.001	0.07966667	0.003	0.00061	0.07	0.025	0.2	0.0042	0.0021	0.013
0.03	0.0005	0.0045	0.0033	0.001	0.19	0.003	0.00059	0.07	0.056	0.4	0.0043	0.0027	0.016
0.02	0.0005	0.0027	0.001	0.001	0.086	0.003	0.001	0.07	0.0054	0.1	0.012	0.0023	0.018
0.02	0.0005	0.001	0.001	0.001	0.041	0.003	0.001	0.07	0.029	0.04	0.0047	0.0021	0.015
0.02	0.0005	0.0022	0.0027	0.001	0.077	0.003	0.001	0.07	0.001	0.1	0.044	0.0066	0.024
0.04	0.0005	0.0023	0.002	0.001	0.07866667	0.003	0.001	0.07	0.001	0.1	0.001	0.003	0.013
0.03	0.0005	0.001	0.001	0.001	0.09133333	0.003	0.001	0.07	0.001	0.2	0.001	0.001	0.015
0.3	0.0005	0.0034	0.002	0.001	0.31	0.003	0.00072	0.07	0.0029	0.4	0.0038	0.02	0.019
0.04	0.0005	0.001	0.001	0.001	0.09733333	0.003	0.00066	0.07	0.001	0.2	0.001	0.001	0.0096
0.04	0.0005	0.0062	0.0047	0.001	0.09033333	0.003	0.001	0.07	0.024	0.2	0.004	0.0033	0.0092
0.05	0.0005	0.004	0.001	0.001	0.09	0.003	0.001	0.07	0.091	0.2	0.0044	0.0029	0.015
0.04	0.0005	0.001	0.0024	0.001	0.07933333	0.003	0.001	0.07	0.01	0.2	0.001	0.0026	0.016
0.05	0.0005	0.001	0.0021	0.001	0.08866667	0.003	0.001	0.07	0.016	0.2	0.039	0.001	0.012
0.04	0.0005	0.0031	0.001	0.001	0.086	0.003	0.0045	0.07	0.001	0.2	0.001	0.017	0.018
0.4	0.0005	0.001	0.001	0.001	0.73	0.003	0.0042	0.07	0.012	0.4	0.001	0.014	0.025
0.04	0.0005	0.001	0.001	0.001	0.079	0.003	0.0043	0.07	0.0024	0.1	0.0044	0.015	0.011
0.03	0.0005	0.001	0.001	0.001	0.08966667	0.003	0.0034	0.07	0.001	0.1	0.0039	0.011	0.012
0.1	0.0005	0.001	0.0021	0.001	0.79	0.003	0.004	0.07	0.012	1.5	0.001	0.0028	0.015
0.02	0.0005	0.001	0.001	0.001	0.08733333	0.003	0.013	0.07	0.001	0.09	0.017	0.001	0.015
0.02	0.0005	0.001	0.001	0.001	0.09633333	0.003	0.014	0.07	0.001	0.1	0.013	0.001	0.01
0.05	0.0005	0.001	0.001	0.001	0.44	0.003	0.001	0.07	0.001	0.8	0.001	0.0048	0.039
0.03	0.0005	0.001	0.001	0.001	0.09333333	0.003	0.001	0.07	0.001	0.1	0.001	0.0044	0.038
0.05	0.0005	0.001	0.001	0.001	0.65	0.003	0.00059	0.07	0.001	0.5	0.001	0.001	0.04
0.02	0.0005	0.001	0.001	0.001	0.09566667	0.003	0.001	0.07	0.001	0.1	0.001	0.0028	0.029
0.7	0.0005	0.0022	0.0025	0.001	1.5	0.003	0.0025	0.07	0.0016	1.2	0.0047	0.003	0.031
0.02	0.0005	0.001	0.002	0.001	0.08733333	0.003	0.001	0.07	0.001	0.1	0.001	0.012	0.034
0.04	0.0005	0.0026	0.0021	0.001	0.12666667	0.003	0.001	0.07	0.001	0.2	0.001	0.0028	0.025
0.03	0.0005	0.001	0.001	0.001	0.08366667	0.003	0.001	0.07	0.001	0.1	0.001	0.0093	0.03
0.04	0.0005	0.001	0.002	0.001	0.13	0.003	0.001	0.07	0.001	0.1	0.001	0.0094	0.03
0.03	0.0005	0.001	0.0022	0.001	0.07233333	0.003	0.001	0.07	0.001	0.1	0.001	0.011	0.03
0.01	0.0005	0.0033	0.0033	0.001	0.09	0.003	0.001	0.07	0.001	0.1	0.001	0.01	0.037
0.03	0.002	0.003	0.0021	0.001	0.09133333	0.003	0.001	0.07	0.001	0.1	0.001	0.0021	0.024
0.03	0.0005	0.0036	0.001	0.001	0.07233333	0.003	0.001	0.07	0.0067	0.1	0.001	0.0087	0.029
0.03	0.0005	0.001	0.0019	0.001	0.091	0.003	0.001	0.07	0.001	0.1	0.001	0.0092	0.036
0.03	0.0015	0.029	0.0021	0.001	0.08566667	0.003	0.001	0.07	0.001	0.2	0.001	0.011	0.032

Norfentanyl	Normeperidine (Norpethidine)	Norpropoxyphene (Desmethylpropoxyphene)	Nortriptyline	O-Desmethyltramadol	O-Desmethylvenlafaxine (Desvenlafaxine)	Olanzapine	Opipramol	Oxazepam	Oxcarbazepine	Oxycodone	Oxymorphone	Paliperidone (9-Hydroxyrisperidone)	Paroxetine
0.001	0.0019	0.091	0.001	0.0074	0.0097	0.011	0.0029	0.0005	0.001	0.0072	0.0034	0.001	0.0011
0.0016	0.016	0.094	0.001	0.0089	0.014	0.0067	0.0054	0.0052	0.0028	0.014	0.0054	0.001	0.013
0.0012	0.028	0.049	0.004	0.011	0.015	0.0065	0.001	0.0005	0.001	0.013	0.0048	0.00087	0.016
0.0011	0.015	0.001	0.0014	0.011	0.015	0.0081	0.001	0.0005	0.0024	0.019	0.0056	0.00076	0.017
0.001	0.012	0.059	0.0019	0.01	0.015	0.0071	0.0061	0.0046	0.0039	0.014	0.0056	0.001	0.019
0.00082	0.018	0.018	0.001	0.0075	0.011	0.03	0.0032	0.0032	0.0015	0.012	0.0036	0.001	0.013
0.001	0.015	0.16	0.0016	0.0068	0.0083	0.012	0.0044	0.0041	0.0013	0.0077	0.0033	0.00077	0.0082
0.00076	0.015	0.036	0.001	0.0062	0.0069	0.013	0.0025	0.0062	0.0011	0.015	0.007	0.001	0.0084
0.001	0.045	0.75	0.001	0.014	0.0042	0.19	0.001	0.0044	0.015	0.0031	0.0058	0.0014	0.0021
0.0012	0.001	0.001	0.0027	0.0073	0.0068	0.011	0.001	0.015	0.001	0.0029	0.0035	0.001	0.0053
0.00096	0.022	0.012	0.0032	0.011	0.011	0.02	0.001	0.012	0.001	0.0037	0.0074	0.001	0.0074
0.0017	0.026	0.22	0.013	0.011	0.0051	0.008	0.001	0.0059	0.002	0.001	0.001	0.001	0.0087
0.001	0.001	0.49	0.001	0.0081	0.0072	0.0086	0.0029	0.0059	0.0044	0.0034	0.0056	0.001	0.0046
0.001	0.018	0.21	0.001	0.0089	0.0099	0.013	0.001	0.011	0.0023	0.0088	0.001	0.001	0.0056
0.001	0.019	0.001	0.012	0.0074	0.0077	0.0096	0.001	0.012	0.001	0.0069	0.0066	0.001	0.0037
0.0025	0.014	0.21	0.001	0.012	0.014	0.011	0.023	0.013	0.00078	0.019	0.001	0.00072	0.0009
0.0017	0.0033	0.28	0.0023	0.0077	0.0079	0.012	0.001	0.0092	0.001	0.011	0.0061	0.001	0.017
0.0088	0.001	0.001	0.0029	0.012	0.0081	0.001	0.0052	0.0042	0.00086	0.021	0.001	0.001	0.001
0.0044	0.001	0.13	0.0019	0.0071	0.0071	0.001	0.001	0.0037	0.001	0.015	0.0062	0.001	0.001
0.0049	0.00075	0.15	0.001	0.0074	0.0058	0.0049	0.001	0.0064	0.001	0.01	0.0041	0.001	0.001
0.0026	0.0012	0.093	0.0076	0.0066	0.0054	0.0042	0.001	0.0063	0.0011	0.012	0.0041	0.001	0.001
0.0025	0.013	0.21	0.0071	0.0078	0.0074	0.0078	0.001	0.0072	0.0013	0.013	0.0037	0.001	0.0057
0.0026	0.00091	0.068	0.001	0.004	0.00087	0.0016	0.001	0.0005	0.001	0.0036	0.004	0.0016	0.001
0.0015	0.0095	0.56	0.001	0.0072	0.0063	0.0069	0.001	0.0074	0.001	0.013	0.004	0.001	0.0035
0.001	0.001	0.24	0.0037	0.0072	0.0066	0.0057	0.001	0.0057	0.001	0.011	0.0035	0.00085	0.001
0.0035	0.012	0.15	0.041	0.0066	0.0057	0.0087	0.001	0.0055	0.001	0.0078	0.0033	0.00098	0.001
0.0027	0.0059	0.27	0.001	0.007	0.0058	0.012	0.001	0.0078	0.001	0.0066	0.0034	0.00096	0.0032
0.001	0.001	0.66	0.018	0.0068	0.0051	0.0021	0.001	0.0077	0.001	0.0083	0.0034	0.00084	0.0053
0.001	0.00042	0.11	0.015	0.0077	0.0034	0.001	0.001	0.012	0.001	0.011	0.001	0.0008	0.002
0.0019	0.00074	0.0065	0.0055	0.0071	0.0042	0.0042	0.001	0.0067	0.001	0.007	0.001	0.00078	0.0049
0.001	7.40E-05	0.041	0.026	0.0061	0.0039	0.001	0.001	0.0079	0.001	0.0057	0.001	0.001	0.001
0.0017	0.00067	0.024	0.0048	0.0063	0.0038	0.0093	0.001	0.008	0.001	0.005	0.001	0.0008	0.0028
0.001	0.0003	0.36	0.0036	0.006	0.0039	0.0029	0.001	0.0052	0.001	0.0029	0.0032	0.0008	0.0028
0.00086	0.0049	0.015	0.0016	0.0064	0.0032	0.0053	0.001	0.0068	0.001	0.0045	0.001	0.00092	0.0047
0.0027	0.001	0.13	0.001	0.004	0.006	0.001	0.043	0.0005	0.001	0.0063	0.0032	0.00085	0.0018
0.001	0.0013	0.013	0.02	0.0057	0.0026	0.001	0.0035	0.0066	0.001	0.005	0.001	0.00098	0.0035
0.0012	0.001	0.42	0.0054	0.0053	0.0035	0.001	0.0031	0.0052	0.001	0.0026	0.001	0.001	0.001
0.0012	0.001	0.31	0.02	0.0055	0.0033	0.0091	0.001	0.0067	0.001	0.0048	0.001	0.001	0.0016
0.00084	0.001	0.21	0.0019	0.0052	0.0026	0.0058	0.0064	0.0024	0.001	0.0043	0.001	0.00085	0.001
0.0011	0.001	0.0092	0.0038	0.0055	0.0027	0.001	0.001	0.0056	0.001	0.0044	0.001	0.00077	0.005
0.001	0.001	0.036	0.0051	0.085	0.0013	0.001	0.0043	0.0037	0.001	0.01	0.0034	0.00092	0.001
0.001	0.001	0.4	0.001	0.0052	0.0022	0.0028	0.0035	0.0035	0.001	0.0038	0.001	0.00081	0.0033
0.0011	0.00017	0.52	0.0025	0.0052	0.0023	0.0041	0.001	0.0062	0.001	0.0038	0.001	0.00079	0.0028
0.00077	0.001	0.027	0.011	0.0049	0.0019	0.0045	0.001	0.0042	0.001	0.0042	0.001	0.00079	0.0046
0.001	0.001	0.05	0.0038	0.0041	0.00077	0.0045	0.001	0.0043	0.001	0.0029	0.001	0.001	0.0037
0.00095	0.001	0.093	0.0018	0.0085	0.00083	0.0054	0.001	0.0042	0.001	0.0048	0.0032	0.0008	0.0036
0.00066	0.00042	0.001	0.001	0.0064	0.0061	0.0053	0.001	0.0063	0.0055	0.0042	0.0032	0.001	0.011
0.001	0.00065	0.027	0.001	0.0053	0.0012	0.001	0.11	0.0048	0.0059	0.0061	0.001	0.001	0.0094
0.001	0.001	0.018	0.028	0.0078	0.0055	0.0021	0.0026	0.0041	0.0054	0.0069	0.0032	0.001	0.014
0.001	0.00042	0.022	0.001	0.0034	0.001	0.0019	0.0032	0.0005	0.014	0.0035	0.0034	0.001	0.001
0.001	0.00087	0.001	0.001	0.01	0.00062	0.0048	0.001	0.0005	0.001	0.0029	0.0044	0.001	0.011
0.001	0.00021	0.015	0.001	0.001	0.001	0.011	0.001	0.0031	0.001	0.56	1.4	0.001	0.013
0.001	0.00016	0.001	0.001	0.001	0.001	0.013	0.001	0.0029	0.0047	0.64	1.2	0.00072	0.0089
0.00082	0.0002	0.0094	0.0014	0.0045	0.00049	0.0076	0.001	0.0005	0.0016	0.0042	0.0032	0.001	0.0031
0.00081	0.00013	0.0039	0.0016	0.0046	0.0033	0.003	0.0034	0.0046	0.0017	0.0024	0.001	0.001	0.0011
0.0011	4.90E-05	0.0018	0.0015	0.013	0.0014	0.0017	0.001	0.0005	0.0011	0.028	0.001	0.00083	0.0031
0.00064	0.00032	0.001	0.0016	0.0046	0.0031	0.0012	0.0028	0.0065	0.0013	0.001	0.001	0.001	0.0022
0.0011	0.0016	0.001	0.0017	0.015	0.017	0.02	0.0041	0.011	0.004	0.0024	0.001	0.001	0.014
0.00066	0.00045	0.001	0.02	0.0045	0.0036	0.0019	0.001	0.0023	0.0011	0.0023	0.001	0.001	0.0008
0.00066	0.0016	0.001	0.0019	0.0042	0.0028	0.0023	0.0029	0.0043	0.001	0.001	0.001	0.001	0.001
0.00072	0.00012	0.001	0.001	0.005	0.0028	0.0032	0.037	0.0019	0.001	0.001	0.001	0.001	0.0012
0.0007	0.00049	0.001	0.001	0.0048	0.0025	0.0015	0.0066	0.0025	0.001	0.001	0.0034	0.001	0.0017
0.00085	0.0012	0.001	0.0036	0.0038	0.00058	0.001	0.001	0.0028	0.001	0.0081	0.001	0.001	0.001
0.00082	0.001	0.001	0.013	0.0035	0.0011	0.0019	0.001	0.0005	0.001	0.014	0.001	0.001	0.001
0.00077	0.001	0.001	0.003	0.0044	0.0025	0.0014	0.001	0.0041	0.001	0.0023	0.0031	0.001	0.0007
0.00069	0.00045	0.001	0.0016	0.004	0.0024	0.0022	0.059	0.0035	0.001	0.001	0.004	0.001	0.001
0.00068	0.001	0.001	0.0017	0.0045	0.0025	0.0026	0.032	0.0028	0.001	0.001	0.001	0.001	0.001
0.001	0.00023	0.001	0.0015	0.0042	0.0026	0.0021	0.043	0.0045	0.001	0.001	0.001	0.001	0.001

Pentazocine	Pentobarbital	Pentoxifylline	Phenacetin	Phenazone	Phencyclidine (PCP)	Phentermine	Phenytoin	Pipamperone	Prazepam	Pregabalin	Primidone	Promazine	Promethazine
0.001	0.001	0.2	0.006	0.005	0.0059	0.0012	0.001	0.001	0.028	0.006	0.7	0.0018	0.0067
0.001	0.001	0.2	0.006	0.004	0.0037	0.00097	0.0027	0.001	0.028	0.008	0.047	0.001	0.001
0.001	0.001	0.2	0.006	0.003	0.0049	0.00096	0.001	0.01	0.068	0.006	1.7	0.001	0.001
0.001	0.001	0.2	0.006	0.004	0.0032	0.001	0.0022	0.001	0.04	0.006	1	0.0026	0.0077
0.001	0.001	0.2	0.006	0.008	0.0042	0.001	0.0038	0.001	0.038	0.006	0.8	0.001	0.001
0.001	0.001	0.2	0.01	0.008	0.0082	0.001	0.0013	0.017	0.047	0.006	0.62	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0055	0.001	0.0012	0.012	0.05	0.006	0.69	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0036	0.001	0.00094	0.0033	0.05	0.006	0.61	0.002	0.0069
0.03	0.001	0.2	0.006	0.005	0.11	0.001	0.015	0.037	0.006	0.006	1.5	0.094	0.12
0.001	0.001	0.2	0.006	0.008	0.0038	0.001	0.001	0.0037	0.0021	0.006	0.81	0.0021	0.007
0.001	0.001	0.2	0.006	0.01	0.0035	0.001	0.001	0.001	0.0022	0.006	0.78	0.0024	0.0074
0.001	0.001	0.2	0.02	0.002	0.0047	0.012	0.0018	0.0047	0.0006	0.006	0.79	0.002	0.007
0.001	0.001	0.2	0.006	0.01	0.0012	0.001	0.0043	0.001	0.0015	0.006	1.1	0.001	0.001
0.00026	0.001	0.2	0.006	0.01	0.0049	0.0019	0.0022	0.0039	0.0021	0.006	1	0.001	0.001
0.001	0.001	0.2	0.006	0.02	0.0039	0.001	0.001	0.001	0.0009	0.006	0.83	0.0027	0.0078
0.001	0.001	0.2	0.006	0.008	0.0095	0.0028	0.00061	0.0028	0.036	0.006	0.95	0.001	0.001
0.001	0.001	0.2	0.006	0.02	0.0091	0.001	0.001	0.0034	0.03	0.006	0.83	0.001	0.001
0.001	0.001	0.2	0.006	0.002	0.0016	0.001	0.00069	0.0037	0.036	0.006	0.95	0.001	0.001
0.001	0.001	0.2	0.006	0.02	0.0088	0.001	0.001	0.0016	0.029	0.006	0.67	0.0019	0.0068
0.00014	0.001	0.2	0.006	0.02	0.021	0.0015	0.001	0.0012	0.0039	0.008	0.69	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0085	0.001	0.00092	0.0074	0.035	0.006	1.1	0.001	0.001
0.001	0.0046	0.2	0.006	0.01	0.0093	0.001	0.0012	0.003	0.007	0.006	0.76	0.0026	0.0077
0.001	0.001	0.2	0.006	0.02	0.0034	0.00091	0.001	0.0034	0.0066	0.006	0.77	0.0027	0.0078
0.001	0.001	0.2	0.006	0.01	0.001	0.0011	0.001	0.0032	0.008	0.006	1	0.001	0.001
0.001	0.12	0.2	0.006	0.01	0.0058	0.001	0.001	0.0015	0.017	0.007	0.8	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0049	0.00098	0.001	0.00075	0.019	0.006	0.8	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0044	0.001	0.001	0.001	0.0051	0.006	0.27	0.0076	0.014
0.001	0.001	0.2	0.006	0.01	0.0012	0.0014	0.001	0.001	0.0053	0.006	0.89	0.0028	0.008
0.001	0.001	0.2	0.006	0.002	0.0054	0.0014	0.001	0.00076	0.0071	0.006	0.72	0.0029	0.008
0.001	0.001	0.2	0.006	0.01	0.0057	0.001	0.001	0.0015	0.013	0.007	0.46	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0029	0.0033	0.001	0.008	0.011	0.006	0.69	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.001	0.001	0.001	0.0018	0.018	0.006	0.62	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0022	0.001	0.001	0.001	0.016	0.008	0.61	0.0023	0.0073
0.001	0.001	0.2	0.006	0.01	0.0033	0.001	0.001	0.001	0.013	0.006	0.54	0.001	0.001
0.001	0.001	0.2	0.006	0.01	0.0055	0.00072	0.001	0.001	0.012	0.006	0.98	0.0019	0.0068
0.001	0.001	0.2	0.006	0.007	0.0023	0.001	0.001	0.0019	0.011	0.006	0.56	0.0019	0.0068
0.001	0.001	0.2	0.006	0.002	0.0043	0.00091	0.001	0.001	0.0094	0.006	0.6	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.002	0.0023	0.001	0.001	0.021	0.006	0.66	0.001	0.001
0.001	0.001	0.2	0.006	0.002	0.0037	0.0012	0.001	0.001	0.0028	0.006	0.59	0.0025	0.0075
0.0011	0.001	0.2	0.006	0.006	0.0038	0.0023	0.001	0.001	0.012	0.006	0.74	0.001	0.001
0.001	0.001	0.2	0.006	0.02	0.0052	0.0029	0.001	0.0047	0.014	0.006	0.6	0.0054	0.011
0.00038	0.001	0.2	0.006	0.002	0.017	0.0011	0.001	0.001	0.011	0.006	0.59	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.0031	0.001	0.001	0.001	0.023	0.007	0.48	0.001	0.001
0.0003	0.001	0.2	0.006	0.007	0.015	0.0011	0.001	0.001	0.022	0.006	0.61	0.002	0.007
0.0011	0.001	0.2	0.006	0.009	0.02	0.00056	0.001	0.001	0.021	0.006	0.64	0.001	0.001
0.001	0.001	0.2	0.006	0.007	0.0022	0.00064	0.001	0.001	0.021	0.006	0.53	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.0018	0.001	0.0055	0.001	0.033	0.006	0.001	0.0024	0.0074
0.001	0.001	0.2	0.006	0.05	0.0045	0.001	0.0059	0.001	0.034	0.006	0.11	0.0021	0.0071
0.001	0.001	0.2	0.006	0.008	0.0041	0.001	0.0053	0.001	0.036	0.006	0.018	0.0031	0.0083
0.001	0.001	0.2	0.006	0.006	0.0054	0.001	0.014	0.013	0.03	0.006	0.32	0.002	0.0069
0.001	0.001	0.2	0.006	0.2	0.0022	0.001	0.001	0.0062	0.021	0.006	0.001	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.0027	0.001	0.001	0.0068	0.011	0.006	0.019	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.0012	0.001	0.0046	0.001	0.011	0.006	0.001	0.001	0.001
0.001	0.001	0.2	0.006	0.02	0.0017	0.001	0.0014	0.0096	0.011	0.006	0.0025	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.0016	0.0013	0.0016	0.0052	0.0066	0.006	0.0026	0.001	0.001
0.001	0.001	0.2	0.006	0.02	0.0017	0.001	0.00099	0.014	0.02	0.006	0.0028	0.0024	0.0074
0.001	0.001	0.2	0.006	0.005	0.0017	0.001	0.0012	0.0061	0.017	0.006	0.0022	0.0023	0.0074
0.001	0.001	0.2	0.006	0.07	0.001	0.001	0.0039	0.0031	0.036	0.02	0.0023	0.0034	0.0086
0.001	0.001	0.2	0.006	0.006	0.001	0.001	0.00091	0.005	0.014	0.006	0.21	0.0027	0.0078
0.001	0.001	0.2	0.006	0.009	0.0012	0.001	0.001	0.0042	0.014	0.006	0.0018	0.0043	0.0098
0.001	0.001	0.2	0.006	0.008	0.001	0.001	0.001	0.0066	0.014	0.006	0.43	0.001	0.001
0.001	0.001	0.2	0.006	0.009	0.001	0.0012	0.001	0.0073	0.012	0.006	0.28	0.001	0.001
0.001	0.001	0.2	0.006	0.006	0.001	0.001	0.001	0.021	0.01	0.006	0.36	0.001	0.001
0.001	0.001	0.2	0.006	0.002	0.0009	0.001	0.001	0.0047	0.01	0.006	0.4	0.001	0.001
0.001	0.001	0.2	0.006	0.008	0.001	0.001	0.001	0.0036	0.006	0.006	0.25	0.001	0.001
0.001	0.001	0.2	0.006	0.007	0.001	0.001	0.001	0.0089	0.01	0.006	0.47	0.0022	0.0072
0.001	0.001	0.2	0.006	0.007	0.0014	0.001	0.001	0.0052	0.008	0.006	0.16	0.0021	0.0071
0.001	0.001	0.2	0.006	0.008	0.001	0.001	0.001	0.0049	0.01	0.006	0.029	0.008	0.014

Propafenone	Propoxyphene (Dextropropoxyphene)	Propranolol	Propyphenazone	Protriptyline	Quetiapine	Risperidone	Ritalinic acid	Secobarbital	Sertraline	Sotalol	Strophanthidin	Sulfadimidin / Sulfamethazin	Sulfamethoxazole
0.0037	0.001	0.01	0.001	0.001	0.001	0.001	0.001	0.011	0.0049	0.04	0.001	0.05	0.04
0.0035	0.001	0.005	0.001	0.001	0.00064	0.015	0.0019	0.0052	0.005	0.04	0.0035	0.05	0.036
0.0062	0.001	0.005	0.001	0.0024	0.001	0.011	0.001	0.001	0.0084	0.04	0.001	0.05	0.034
0.0021	0.001	0.005	0.001	0.001	0.001	0.001	0.001	0.02	0.001	0.04	0.001	0.05	0.043
0.0023	3.20E-05	0.005	0.001	0.00033	0.001	0.0018	0.001	0.015	0.0049	0.04	0.001	0.05	0.043
0.001	0.00083	0.005	0.003	0.001	0.00048	0.001	0.001	0.001	0.0084	0.04	0.001	0.05	0.021
0.003	0.001	0.005	0.003	0.001	0.001	0.001	0.001	0.001	0.0088	0.04	0.0027	0.05	0.024
0.0041	0.001	0.005	0.001	0.001	0.00061	0.001	0.001	0.0054	0.006	0.04	0.001	0.05	0.018
0.021	0.0091	0.005	0.001	0.037	0.001	0.001	0.00062	0.0052	0.05	0.04	0.001	0.05	0.031
0.001	0.001	0.005	0.001	0.0012	0.001	0.001	0.0022	0.12	0.029	0.04	0.001	0.05	0.021
0.0036	0.001	0.005	0.001	0.0017	0.001	0.001	0.0049	0.0071	0.001	0.04	0.001	0.05	0.025
0.001	0.001	0.005	0.001	0.011	0.00086	0.001	0.0096	0.0051	0.001	0.04	0.0038	0.05	0.047
0.003	0.001	0.005	0.001	0.001	0.00046	0.0018	0.00052	0.001	0.001	0.04	0.0029	0.05	0.015
0.001	0.001	0.005	0.002	0.001	0.00018	0.007	0.001	0.001	0.001	0.04	0.001	0.05	0.02
0.0032	0.001	0.005	0.002	0.011	0.00038	0.001	0.0019	0.015	0.0082	0.04	0.0037	0.05	0.025
0.001	0.001	0.005	0.001	0.001	0.00033	0.001	0.0045	0.001	0.0091	0.04	0.001	0.05	0.032
0.001	0.001	0.005	0.002	0.00072	0.00039	0.001	0.001	0.0052	0.001	0.04	0.001	0.05	0.029
0.0022	0.001	0.005	0.001	0.0014	0.001	0.0017	0.001	0.001	0.001	0.04	0.001	0.05	0.023
0.001	0.001	0.005	0.003	0.00035	0.0019	0.0028	0.001	0.018	0.001	0.04	0.001	0.05	0.024
0.002	0.001	0.005	0.003	0.001	0.00012	0.0038	0.001	0.001	0.001	0.04	0.001	0.05	0.025
0.0019	0.001	0.005	0.002	0.0062	0.001	0.001	0.0029	0.001	0.001	0.04	0.001	0.05	0.026
0.001	0.001	0.005	0.002	0.0057	0.00035	0.001	0.001	0.016	0.001	0.04	0.001	0.05	0.027
0.0023	0.001	0.005	0.001	0.001	0.0013	0.0044	0.001	0.007	0.001	0.04	0.001	0.05	0.011
0.0023	0.00064	0.005	0.003	0.001	0.00017	0.001	0.0047	0.001	0.001	0.04	0.001	0.05	0.023
0.001	0.001	0.005	0.003	0.0022	0.00038	0.001	0.00084	0.0093	0.001	0.04	0.003	0.05	0.019
0.001	0.001	0.005	0.003	0.041	0.001	0.001	0.001	0.001	0.001	0.04	0.0025	0.05	0.017
0.001	0.017	0.005	0.003	0.001	0.001	0.001	0.001	0.001	0.001	0.04	0.0031	0.05	0.024
0.002	0.001	0.005	0.003	0.016	0.001	0.001	0.001	0.001	0.001	0.04	0.001	0.05	0.02
0.0022	0.001	0.005	0.001	0.014	0.00091	0.001	0.00029	0.001	0.0043	0.04	0.003	0.05	0.0037
0.001	0.001	0.005	0.002	0.0041	0.001	0.0021	0.001	0.001	0.001	0.04	0.001	0.05	0.016
0.0023	0.001	0.005	0.003	0.026	0.001	0.001	0.00067	0.001	0.001	0.04	0.0024	0.05	0.012
0.001	0.001	0.005	0.003	0.0033	0.001	0.001	0.0016	0.001	0.001	0.04	0.001	0.05	0.016
0.0019	0.001	0.005	0.002	0.002	0.001	0.001	0.0014	0.001	0.001	0.04	0.0028	0.05	0.013
0.0017	0.001	0.005	0.002	0.001	0.0002	0.0022	0.0006	0.001	0.001	0.04	0.0028	0.05	0.015
0.002	0.001	0.005	0.001	0.001	0.001	0.0018	0.001	0.001	0.001	0.04	0.0029	0.05	0.018
0.0018	5.90E-05	0.005	0.001	0.019	0.001	0.001	0.002	0.001	0.001	0.04	0.0035	0.05	0.011
0.001	4.60E-05	0.005	0.002	0.0039	0.001	0.001	0.00025	0.001	0.001	0.04	0.001	0.05	0.016
0.001	0.001	0.005	0.002	0.019	0.001	0.0032	0.00081	0.001	0.001	0.04	0.0029	0.05	0.012
0.001	0.001	0.005	0.003	0.00026	0.001	0.002	0.00013	0.001	0.001	0.04	0.003	0.05	0.013
0.0019	0.0022	0.005	0.002	0.0022	0.001	0.001	0.0047	0.001	0.001	0.04	0.0028	0.05	0.013
0.001	0.001	0.005	0.007	0.0036	0.001	0.014	0.001	0.001	0.001	0.04	0.0033	0.05	0.051
0.001	0.0029	0.005	0.003	0.001	0.00024	0.0021	0.0015	0.001	0.001	0.04	0.001	0.05	0.012
0.001	0.001	0.005	0.002	0.00093	0.001	0.001	0.0021	0.001	0.001	0.04	0.0025	0.05	0.015
0.001	0.0027	0.005	0.003	0.0096	0.001	0.0015	0.0034	0.001	0.001	0.04	0.0029	0.05	0.011
0.0018	0.00088	0.005	0.002	0.0023	0.00018	0.001	0.001	0.001	0.0049	0.04	0.001	0.05	0.016
0.0019	0.001	0.005	0.002	0.00024	0.00021	0.002	0.001	0.001	0.001	0.04	0.001	0.05	0.017
0.001	0.001	0.005	0.002	0.001	0.001	0.0016	0.00029	0.001	0.001	0.04	0.001	0.05	0.017
0.001	0.001	0.005	0.006	0.001	0.001	0.0017	0.00022	0.001	0.001	0.04	0.001	0.05	0.04
0.002	0.001	0.005	0.003	0.027	0.001	0.0017	0.001	0.001	0.001	0.04	0.001	0.05	0.018
0.001	0.0096	0.005	0.002	0.001	0.001	0.001	0.00031	0.001	0.001	0.04	0.001	0.05	0.015
0.0021	0.001	0.005	0.001	0.001	0.00019	0.0081	0.00071	0.001	0.001	0.04	0.001	0.05	0.065
0.003	0.00066	0.005	0.001	0.001	0.00053	0.0014	0.001	0.001	0.001	0.04	0.001	0.05	0.015
0.002	0.001	0.005	0.001	0.001	0.001	0.0025	0.00042	0.001	0.001	0.04	0.0029	0.05	0.014
0.001	0.001	0.005	0.001	0.001	0.0002	0.002	0.00016	0.001	0.005	0.04	0.0028	0.05	0.017
0.001	0.001	0.005	0.002	1.10E-05	0.00024	0.001	0.0002	0.001	0.001	0.04	0.001	0.05	0.013
0.001	0.001	0.005	0.001	0.001	0.00016	0.001	0.00039	0.001	0.0044	0.04	0.0029	0.05	0.047
0.001	0.001	0.005	0.001	0.001	0.00017	0.001	9.10E-05	0.001	0.001	0.04	0.001	0.05	0.016
0.001	0.001	0.06	0.001	9.20E-05	0.00018	0.025	0.0027	0.001	0.001	0.09	0.001	0.073	0.14
0.001	0.001	0.005	0.002	0.019	0.00018	0.001	0.00071	0.001	0.0069	0.04	0.001	0.05	0.018
0.001	0.001	0.005	0.001	0.00028	0.0002	0.001	0.0038	0.001	0.001	0.04	0.001	0.05	0.02
0.001	0.001	0.005	0.001	0.001	0.00016	0.001	0.0015	0.001	0.001	0.04	0.001	0.05	0.016
0.001	0.001	0.005	0.001	0.001	0.001	0.0016	0.001	0.001	0.001	0.04	0.001	0.05	0.015
0.0021	0.001	0.005	0.001	0.0021	0.001	0.002	0.0019	0.001	0.0075	0.04	0.001	0.05	0.0088
0.001	0.001	0.005	0.001	0.012	0.00021	0.0017	0.0027	0.001	0.001	0.04	0.001	0.05	0.013
0.001	0.001	0.005	0.001	0.0014	0.00021	0.001	0.0017	0.001	0.001	0.04	0.001	0.05	0.015
0.001	0.001	0.005	0.001	2.60E-05	0.00016	0.001	0.0025	0.001	0.001	0.04	0.001	0.05	0.016
0.0033	0.001	0.005	0.002	0.00015	0.00017	0.001	0.0022	0.001	0.001	0.04	0.001	0.05	0.021
0.001	0.001	0.005	0.002	0.001	0.001	0.001	0.0027	0.001	0.0044	0.04	0.001	0.05	0.015

Sulpirid	Telmisartan	Temazepam	Topiramate	Tramadol	Trazodone	Triazolam	Trimethoprim	Trimipramine	Valsartan	Valsartan acid	Venlafaxine	Verapamil	Zolpidem
0.02	0.03	0.0034	0.00064	0.0094	0.001	0.0027	0.009	0.011	0.02	0.05	0.0047	0.001	0.0017
0.02	0.03	0.0034	0.00098	0.014	0.0016	0.0038	0.009	0.17	0.02	0.06	0.0061	0.041	0.0017
0.02	0.03	0.001	0.0012	0.014	0.001	0.0035	0.009	0.015	0.02	0.06	0.007	0.001	0.0017
0.02	0.03	0.0035	0.00098	0.015	0.001	0.0034	0.009	0.15	0.02	0.065	0.0067	0.001	0.0018
0.02	0.02	0.0029	0.001	0.015	0.001	0.0038	0.009	0.18	0.015	0.055	0.0072	0.0099	0.001
0.01	0.02	0.0035	0.001	0.011	0.0018	0.0049	0.009	0.041	0.005	0.04	0.0044	0.0069	0.0018
0.01	0.02	0.0039	0.001	0.008	0.0016	0.0055	0.009	0.16	0.005	0.04	0.0022	0.001	0.0017
0.009	0.02	0.0037	0.001	0.0066	0.0016	0.0048	0.009	0.027	0.005	0.035	0.0019	0.001	0.0017
0.009	0.02	0.012	0.001	0.0038	0.0051	0.0077	0.009	0.69	0.005	0.045	0.078	0.15	0.001
0.01	0.02	0.0039	0.001	0.0065	0.0016	0.0033	0.009	0.13	0.0045	0.04	0.0022	0.0056	0.001
0.01	0.02	0.0034	0.001	0.01	0.0016	0.0037	0.009	0.11	0.01	0.045	0.0033	0.008	0.0017
0.04	0.2	0.001	0.001	0.0048	0.0016	0.0019	0.009	0.16	0.0095	0.1	0.0015	0.001	0.001
0.01	0.02	0.0035	0.001	0.0069	0.0017	0.0028	0.009	0.063	0.0095	0.04	0.0026	0.0056	0.0019
0.01	0.03	0.0033	0.001	0.0096	0.0015	0.0011	0.009	0.1	0.01	0.05	0.0026	0.0054	0.001
0.02	0.04	0.001	0.001	0.0074	0.0016	0.0016	0.009	0.1	0.015	0.08	0.0024	0.001	0.001
0.02	0.05	0.0035	0.00059	0.013	0.001	0.0032	0.009	0.36	0.035	0.2	0.0037	0.0074	0.001
0.02	0.02	0.001	0.001	0.0075	0.001	0.0021	0.009	0.32	0.015	0.075	0.0026	0.0043	0.0017
0.03	0.1	0.01	0.00067	0.0077	0.001	0.0024	0.009	0.27	0.025	0.2	0.0027	0.001	0.0017
0.009	0.04	0.0035	0.001	0.0068	0.0017	0.0026	0.009	0.22	0.02	0.08	0.0023	0.0054	0.0018
0.02	0.05	0.0034	0.001	0.0055	0.0016	0.0018	0.009	0.079	0.015	0.095	0.0021	0.001	0.001
0.02	0.03	0.0032	0.00094	0.0051	0.0017	0.0022	0.009	0.024	0.015	0.08	0.0022	0.001	0.0018
0.02	0.04	0.0038	0.001	0.0071	0.0015	0.0017	0.009	0.028	0.02	0.085	0.003	0.001	0.001
0.009	0.06	0.0032	0.0019	0.0006	0.001	0.0023	0.009	0.053	0.025	0.2	0.0004	0.0047	0.001
0.02	0.05	0.0031	0.001	0.006	0.0017	0.0017	0.009	0.06	0.02	0.085	0.0026	0.001	0.001
0.01	0.04	0.0033	0.001	0.0062	0.0016	0.00023	0.009	0.053	0.02	0.09	0.0026	0.001	0.001
0.02	0.05	0.0033	0.001	0.0054	0.0016	0.0015	0.009	0.18	0.02	0.1	0.0023	0.001	0.0017
0.02	0.04	0.0033	0.001	0.0055	0.0017	0.00076	0.009	0.079	0.02	0.095	0.0023	0.001	0.001
0.01	0.05	0.001	0.00065	0.0047	0.0016	0.00053	0.009	0.085	0.02	0.1	0.0022	0.001	0.001
0.009	0.02	0.0031	0.001	0.0031	0.0016	0.00092	0.009	0.032	0.0095	0.055	0.0014	0.001	0.001
0.01	0.04	0.0034	0.001	0.0039	0.0016	0.0013	0.009	0.24	0.015	0.095	0.0017	0.001	0.001
0.01	0.04	0.001	0.001	0.0035	0.0016	0.0015	0.009	0.24	0.02	0.095	0.0015	0.001	0.001
0.02	0.05	0.001	0.001	0.0035	0.0017	0.0016	0.009	0.022	0.02	0.095	0.0014	0.001	0.0018
0.02	0.04	0.001	0.001	0.0036	0.0016	0.0012	0.009	0.33	0.02	0.095	0.0016	0.001	0.0019
0.02	0.04	0.001	0.001	0.0029	0.0015	0.001	0.009	0.27	0.015	0.095	0.0014	0.001	0.001
0.009	0.04	0.0031	0.001	0.0056	0.0016	0.0015	0.009	0.33	0.008	0.095	0.0004	0.001	0.0018
0.01	0.03	0.001	0.001	0.0023	0.0016	0.00094	0.009	0.033	0.015	0.085	0.0014	0.001	0.001
0.009	0.02	0.0031	0.001	0.0032	0.0016	0.00092	0.009	0.31	0.004	0.01	0.0016	0.001	0.0017
0.02	0.03	0.001	0.001	0.003	0.0017	0.0002	0.009	0.019	0.01	0.065	0.0029	0.001	0.001
0.02	0.04	0.001	0.00063	0.0023	0.0016	0.001	0.009	0.001	0.015	0.08	0.0014	0.0054	0.001
0.02	0.03	0.001	0.001	0.0024	0.0016	0.001	0.009	0.0073	0.015	0.09	0.002	0.001	0.0017
0.04	0.02	0.001	0.001	0.001	0.0016	0.001	0.009	0.091	0.025	0.04	0.0006	0.001	0.001
0.02	0.04	0.001	0.001	0.0019	0.0015	0.001	0.009	0.13	0.01	0.095	0.0014	0.001	0.0018
0.02	0.03	0.001	0.001	0.002	0.001	0.001	0.009	0.17	0.015	0.085	0.0016	0.001	0.0019
0.02	0.03	0.001	0.001	0.0016	0.001	0.001	0.009	0.14	0.009	0.09	0.0018	0.001	0.001
0.02	0.03	0.001	0.001	0.0005	0.001	0.001	0.009	0.011	0.004	0.095	0.0009	0.001	0.0017
0.02	0.03	0.001	0.001	0.0005	0.001	0.001	0.009	0.034	0.004	0.095	0.0013	0.001	0.0017
0.02	0.03	0.001	0.001	0.0058	0.0016	0.001	0.009	0.019	0.0045	0.09	0.0013	0.001	0.001
0.08	0.02	0.001	0.001	0.0009	0.0016	0.001	0.009	0.15	0.0035	0.04	0.0004	0.001	0.0017
0.02	0.02	0.003	0.001	0.0052	0.0016	0.001	0.009	0.001	0.0045	0.085	0.0014	0.001	0.001
0.01	0.03	0.001	0.001	0.001	0.001	0.001	0.009	0.0094	0.0035	0.07	0.0004	0.001	0.0017
0.009	0.3	0.001	0.001	0.0003	0.0016	0.001	0.009	0.001	0.1	0.4	0.0005	0.001	0.001
0.01	0.02	0.0033	0.001	0.001	0.0017	0.001	0.009	0.001	0.0035	0.06	0.001	0.001	0.001
0.01	0.02	0.0032	0.001	0.001	0.0016	0.001	0.009	0.001	0.0035	0.075	0.001	0.001	0.001
0.009	0.05	0.001	0.001	0.0002	0.0016	0.001	0.009	0.27	0.035	0.2	0.001	0.001	0.0017
0.01	0.02	0.001	0.001	0.003	0.001	0.001	0.009	0.096	0.005	0.065	0.0008	0.001	0.001
0.009	0.07	0.0032	0.001	0.0011	0.0026	0.001	0.009	0.28	0.07	0.15	0.0006	0.001	0.0017
0.01	0.02	0.001	0.001	0.0028	0.001	0.001	0.009	0.24	0.0035	0.06	0.0007	0.001	0.0017
0.02	0.3	0.0063	0.00088	0.016	0.001	0.001	0.009	0.23	0.1	0.05	0.0028	0.0052	0.001
0.01	0.02	0.001	0.001	0.0033	0.001	0.001	0.009	0.26	0.0035	0.055	0.0007	0.001	0.0017
0.01	0.03	0.001	0.001	0.0025	0.001	0.001	0.009	0.18	0.009	0.065	0.0006	0.001	0.0017
0.01	0.02	0.001	0.001	0.0025	0.001	0.001	0.009	0.2	0.01	0.06	0.0005	0.001	0.0017
0.009	0.02	0.001	0.001	0.0022	0.001	0.001	0.009	0.27	0.0095	0.07	0.0006	0.001	0.001
0.009	0.02	0.001	0.001	0.0003	0.0016	0.001	0.009	0.37	0.0035	0.04	0.001	0.001	0.0017
0.009	0.02	0.001	0.001	0.0008	0.0029	0.001	0.009	0.35	0.0035	0.04	0.001	0.001	0.001
0.009	0.02	0.001	0.001	0.0022	0.001	0.001	0.009	0.38	0.0035	0.055	0.0006	0.001	0.0017
0.009	0.02	0.001	0.001	0.0021	0.001	0.001	0.009	0.3	0.0035	0.055	0.0005	0.001	0.0017
0.009	0.02	0.001	0.001	0.0022	0.001	0.001	0.009	0.28	0.005	0.065	0.0006	0.001	0.001
0.01	0.02	0.001	0.001	0.0023	0.001	0.001	0.009	0.29	0.0095	0.07	0.001	0.001	0.0017

Zopiclone	1H-Benzotriazole	2-(Methylthio)benzothiazole	2-Ethylhexyl diphenyl phosphate (EHDP)	5,6-Dimethylbenzotriazole	5-Methyl-1H-benzotriazole	Benzothiazole-6-carboxylic acid	Nonylphenol (4-Nonylphenol)	Tolyltriazol (mix of isomers)	Triisobutyl phosphate (TIBP)	Tri-n-butyl phosphate (TnBP)	Tri-n-propyl phosphate (TnPP)	Triphenyl phosphate (TPT)	Tris(1-chloro-2-propyl)phosphate (TCPP)
0.0036	0.23	0.03	0.00012	0.005	0.052	0.01	0.01	0.2	0.011	0.004	0.00007	0.0014	0.11
0.0033	0.46	0.03	0.0014	0.005	0.097	0.01	0.01	0.25	0.048	0.0038	0.00074	0.0056	0.095
0.001	0.32	0.03	0.00012	0.005	0.07	0.01	0.01	0.2	0.023	0.0018	0.00007	0.0042	0.17
0.0063	0.34	0.04	0.00012	0.005	0.057	0.01	0.01	0.2	0.024	0.0038	0.00007	0.0015	0.18
0.0062	0.48	0.03	0.0016	0.005	0.092	0.01	0.01	0.1	0.02	0.0051	0.00007	0.0031	0.12
0.0032	0.28	0.03	0.0059	0.005	0.049	0.01	0.01	0.045	0.017	0.0018	0.00085	0.0034	0.064
0.0022	0.26	0.04	0.00012	0.005	0.02	0.01	0.01	0.045	0.015	0.0033	0.00007	0.001	0.09
0.00074	0.21	0.04	0.00012	0.005	0.029	0.01	0.01	0.05	0.013	0.0028	0.00007	0.00002	0.24
0.019	0.31	0.03	0.00012	0.005	0.052	0.01	0.01	0.05	0.0085	0.0039	0.00007	0.0012	0.056
0.003	0.29	0.03	0.00012	0.005	0.055	0.01	0.01	0.2	0.022	0.0035	0.00007	0.0012	0.092
0.0054	0.32	0.04	0.00056	0.005	0.061	0.01	0.01	0.15	0.016	0.0041	0.00007	0.001	0.058
0.001	0.38	0.03	0.0018	0.005	0.15	0.01	0.01	0.25	0.012	0.0051	0.00007	0.0076	0.13
0.0023	0.21	0.04	0.00012	0.005	0.038	0.01	0.01	0.15	0.014	0.0031	0.00007	0.0017	0.045
0.0024	0.27	0.03	0.00012	0.005	0.039	0.01	0.01	0.15	0.015	0.0039	0.00007	0.0011	0.11
0.0024	0.35	0.04	0.00052	0.005	0.074	0.01	0.01	0.3	0.015	0.004	0.00007	0.0012	0.059
0.036	0.54	0.03	0.0015	0.007	0.14	0.01	0.01	0.4	0.017	0.0045	0.00007	0.00099	0.095
0.001	0.36	0.05	0.00054	0.005	0.097	0.01	0.01	0.3	0.017	0.0062	0.00081	0.001	0.058
0.019	1.6	0.03	0.00093	0.005	0.1	0.01	0.01	0.35	0.049	0.07	0.00089	0.0012	0.086
0.001	0.36	0.03	0.00068	0.005	0.099	0.01	0.01	0.25	0.016	0.0039	0.00007	0.0031	0.052
0.001	0.55	0.04	0.00012	0.005	0.1	0.01	0.01	0.2	0.018	0.0094	0.00007	0.0021	0.099
0.001	0.45	0.03	0.00056	0.005	0.088	0.01	0.01	0.25	0.017	0.006	0.00071	0.0013	0.073
0.001	0.47	0.03	0.0034	0.005	0.093	0.01	0.01	0.25	0.018	0.0072	0.00007	0.0014	0.077
0.001	0.4	0.03	0.004	0.02	0.051	0.01	0.01	0.2	0.026	0.0057	0.00007	0.00095	0.15
0.001	0.47	0.03	0.0042	0.005	0.19	0.01	0.00866667	0.3	0.015	0.005	0.00007	0.002	0.079
0.001	0.39	0.03	0.00012	0.005	0.054	0.01	0.01	0.2	0.017	0.0034	0.00007	0.0009	0.11
0.001	0.38	0.03	0.00012	0.005	0.06	0.01	0.01	0.4	0.018	0.0035	0.00007	0.0013	0.12
0.001	0.5	0.03	0.002	0.005	0.12	0.01	0.01	0.3	0.015	0.0058	0.00007	0.0022	0.079
0.0095	0.36	0.03	0.0003	0.005	0.1	0.01	0.01	0.3	0.016	0.005	0.00007	0.00085	0.092
0.001	0.13	0.03	0.00012	0.005	0.033	0.01	0.01	0.05	0.021	0.0000042	0.00007	0.001	0.036
0.001	0.3	0.03	0.00012	0.005	0.087	0.01	0.01	0.25	0.017	0.0031	0.00007	0.00093	0.074
0.0065	0.3	0.03	0.00012	0.005	0.036	0.01	0.01	0.25	0.019	0.0046	0.00007	0.00074	0.084
0.0072	0.35	0.04	0.00012	0.005	0.043	0.01	0.01	0.25	0.0095	0.0033	0.00007	0.00002	0.58
0.0063	0.3	0.04	0.00012	0.005	0.071	0.01	0.01	0.25	0.03	0.00042	0.00007	0.00074	0.082
0.001	0.28	0.04	0.00012	0.005	0.077	0.01	0.01	0.2	0.023	0.0035	0.00007	0.0014	0.081
0.0064	0.061	0.05	0.00069	0.02	0.08	0.01	0.01	0.3	0.013	0.0028	0.00007	0.0052	0.072
0.0071	0.28	0.04	0.00012	0.007	0.037	0.01	0.01	0.3	0.023	0.0024	0.00007	0.00002	0.066
0.0011	0.063	0.03	0.00012	0.005	0.018	0.01	0.01	0.04	0.0047	0.0045	0.00007	0.00002	0.028
0.0036	0.21	0.03	0.00012	0.005	0.027	0.01	0.01	0.15	0.016	0.0041	0.00007	0.00002	0.057
0.0022	0.21	0.05	0.00012	0.005	0.043	0.01	0.01	0.25	0.015	0.005	0.00007	0.0009	0.059
0.0027	0.23	0.03	0.00012	0.005	0.043	0.01	0.01	0.2	0.018	0.0044	0.00007	0.00002	0.065
0.0026	0.14	0.04	0.00012	0.005	0.065	0.01	0.01	0.3	0.024	0.0029	0.00007	0.0012	0.084
0.001	0.23	0.03	0.00012	0.005	0.041	0.01	0.01	0.2	0.015	0.0041	0.00007	0.00062	0.061
0.001	0.25	0.04	0.00012	0.005	0.05	0.01	0.01	0.25	0.015	0.0042	0.0021	0.0018	0.12
0.001	0.25	0.03	0.00012	0.005	0.036	0.01	0.01	0.25	0.015	0.002	0.00007	0.00058	0.1
0.00072	0.25	0.03	0.00012	0.005	0.068	0.01	0.01	0.25	0.014	0.0038	0.00007	0.00067	0.11
0.0022	0.25	0.03	0.00012	0.007	0.074	0.01	0.00466667	0.35	0.015	0.0042	0.00007	0.00002	0.12
0.0022	0.21	0.03	0.00012	0.005	0.05	0.01	0.01	0.3	0.019	0.0037	0.00007	0.00063	0.067
0.0045	0.0015	0.03	0.00012	0.005	0.0095	0.01	0.02	0.005	0.0025	0.0029	0.00007	0.00002	0.6
0.001	0.26	0.03	0.00012	0.005	0.093	0.01	0.01	0.3	0.019	0.0051	0.00007	0.00064	0.074
0.001	0.26	0.03	0.00012	0.005	0.031	0.01	0.01	0.2	0.022	0.0037	0.00007	0.0012	0.11
0.0022	0.16	0.03	0.00012	0.005	0.11	0.01	0.01	0.2	0.037	0.019	0.00007	0.00002	0.28
0.0037	0.27	0.06	0.00012	0.005	0.12	0.01	0.00433333	0.05	0.025	0.0042	0.00007	0.00058	0.069
0.0035	0.25	0.03	0.00012	0.005	0.072	0.01	0.01	0.2	0.021	0.0066	0.00007	0.00076	0.11
0.001	0.024	0.05	0.00012	0.005	0.021	0.01	0.01	0.005	0.015	0.0024	0.00007	0.0058	0.074
0.0023	0.23	0.03	0.00012	0.005	0.073	0.01	0.01	0.2	0.021	0.0041	0.00007	0.00002	0.086
0.0018	0.11	0.04	0.00038	0.005	0.025	0.01	0.018	0.005	0.0085	0.0073	0.00007	0.0016	0.11
0.001	0.24	0.06	0.00012	0.005	0.12	0.04	0.01	0.2	0.021	0.0044	0.00007	0.00074	0.085
0.001	0.26	0.09	0.00012	0.01	0.29	0.01	0.012	0.25	0.097	0.012	0.001	0.0073	0.3
0.0019	0.28	0.03	0.00012	0.005	0.083	0.01	0.01	0.2	0.023	0.0046	0.00073	0.00091	0.11
0.001	0.27	0.04	0.0012	0.005	0.08	0.01	0.01	0.2	0.025	0.0014	0.00007	0.00074	0.1
0.0019	0.22	0.03	0.00012	0.005	0.019	0.01	0.01	0.15	0.019	0.0052	0.00007	0.00002	0.12
0.0019	0.24	0.04	0.00012	0.005	0.071	0.01	0.01	0.15	0.022	0.0042	0.00007	0.00064	0.12
0.001	0.027	0.03	0.00012	0.005	0.046	0.01	0.009	0.035	0.021	0.0066	0.00007	0.00002	0.096
0.0019	0.0073	0.03	0.00068	0.005	0.024	0.01	0.01	0.005	0.0074	0.011	0.00007	0.00055	0.035
0.002	0.25	0.03	0.00012	0.005	0.057	0.01	0.01	0.05	0.0068	0.0059	0.00007	0.00002	0.29
0.001	0.24	0.05	0.00012	0.005	0.052	0.01	0.01	0.15	0.027	0.0068	0.00007	0.0038	0.079
0.0024	0.26	0.03	0.00012	0.005	0.077	0.01	0.01	0.2	0.027	0.0082	0.00007	0.0017	0.12
0.001	0.18	0.05	0.00012	0.005	0.027	0.01	0.01	0.2	0.019	0.0046	0.00007	0.00002	0.054

Tris(2-butoxyethyl) phosphate (TBEP)	Tris(2-chloroethyl) phosphate (TCEP)	Tris(3,5-dimethylphenyl)phosphate (T35DMPP)	Tris(methylphenyl)phosphate (TMPP)	Dibutyltin-cation	Dioctyltin-cation	Diphenyltin-cation	Tetrabutyltin	Tributyltin-cation	Triphenyltin-cation	2,4-Dinitrophenol (DNP)	Acesulfame	Bisphenol A	Bisphenol S
0.025	0.011	0.00023	0.000084	0.0025	0.0001	0.0001	3.00E-07	2.00E-07	0.0001	0.02	0.43	0.05	0.1
0.049	0.018	0.01	0.0013	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.51333333	0.013	0.1
0.034	0.023	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.62	0.03	0.1
0.04	0.023	0.00023	0.000084	0.00053	0.0001	0.0001	0.0000001	5.00E-07	0.0001	0.02	0.64666667	0.55	0.1
0.042	0.017	0.014	0.000084	0.00056	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.01	0.70666667	0.065	0.1
0.023	0.0068	0.024	0.0093	0.00077	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.01	0.47	0.0083	0.1
0.018	0.011	0.00023	0.000084	0.0001	0.0001	0.0001	2.00E-07	7.00E-07	0.0001	0.02	0.46333333	0.0095	0.1
0.054	0.028	0.00023	0.000084	0.00059	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.43	0.24	0.1
0.024	0.0096	0.00023	0.000084	0.00046	0.0001	0.0001	0.0000001	3.00E-07	0.0001	0.01	0.48666667	0.14	0.1
0.02	0.012	0.00023	0.000084	0.00036	0.0001	0.0001	0.0000001	4.00E-07	0.0001	0.01	0.41	1.3	0.1
0.022	0.0081	0.00023	0.0032	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.45666667	0.039	0.21
0.007	0.012	0.00023	0.013	0.00023	0.0001	0.00034	0.0000001	7.00E-07	0.00021	0.02	0.69	0.014	0.1
0.02	0.004	0.00023	0.000084	0.00021	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.4	0.039	0.1
0.018	0.011	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.385	0.021	0.1
0.019	0.0094	0.008	0.00086	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.49	0.14	0.1
0.02	0.013	0.054	0.0088	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.53	0.017	0.1
0.018	0.0099	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.51333333	0.049	0.1
0.011	0.012	0.00023	0.000084	0.00086	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.59	0.032	0.1
0.016	0.0086	0.00023	0.0022	0.0001	0.0001	0.0001	0.0000001	3.00E-07	0.0001	0.02	0.46666667	0.17	0.1
0.015	0.011	0.00023	0.000084	0.00062	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.49	0.08	0.1
0.019	0.0097	0.00023	0.00082	0.00037	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.46	0.024	0.1
0.018	0.0087	0.011	0.0088	0.00028	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.50666667	0.65	0.1
0.0093	0.0093	0.017	0.0079	0.00025	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.58	0.064	0.1
0.018	0.0092	0.042	0.011	0.00031	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.49	0.0056	0.1
0.0097	0.01	0.00023	0.000084	0.00022	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.45	0.055	0.1
0.0096	0.011	0.00023	0.000084	0.00027	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.49666667	0.0056	0.1
0.017	0.009	0.016	0.000084	0.00028	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.45666667	0.0093	0.27
0.015	0.012	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.54333333	0.0056	0.1
0.0095	0.0034	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.04	0.20666667	0.0056	0.1
0.0077	0.0077	0.00023	0.000084	0.00038	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.4	0.0056	0.1
0.00113	0.0096	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.36666667	0.0056	0.1
0.00113	0.012	0.00023	0.000084	0.00034	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.04	0.47333333	0.0056	0.1
0.0076	0.0081	0.00023	0.000084	0.00044	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.04	0.41333333	0.0056	0.1
0.0061	0.0082	0.00023	0.000084	0.00021	0.00027	0.0001	0.0000001	0.0000001	0.0001	0.04	0.47	0.0056	0.1
0.00113	0.01	0.00023	0.000084	0.00024	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.44	0.0056	0.1
0.00113	0.0069	0.00023	0.000084	0.00023	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.43333333	0.0056	0.1
0.00113	0.0024	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.19666667	0.0056	0.1
0.00113	0.0059	0.00023	0.000084	0.00027	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.41	0.0056	0.1
0.00113	0.0058	0.00023	0.000084	0.00053	0.00023	0.0001	0.0000001	0.0000001	0.0001	0.03	0.48666667	0.0056	0.1
0.00113	0.0059	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.04	0.43	0.0056	0.1
0.00113	0.013	0.00023	0.000084	0.00051	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.58	0.0056	0.1
0.00113	0.0063	0.00023	0.000084	0.00035	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.40333333	0.0056	0.1
0.051	0.033	0.00023	0.000084	0.00027	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.45666667	0.0056	0.1
0.011	0.015	0.00023	0.000084	0.00045	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.44	0.0056	0.1
0.011	0.011	0.00023	0.000084	0.00022	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.44333333	0.0056	0.1
0.0086	0.0096	0.00023	0.000084	0.00024	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.46	0.0056	0.1
0.00113	0.0049	0.00023	0.000084	0.00062	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.49	0.0056	0.1
0.00113	0.01	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.06	0.69	0.0056	0.1
0.00113	0.0091	0.00023	0.00087	0.00022	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.03	0.45	0.0056	0.1
0.0057	0.01	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.47333333	0.0056	0.1
0.00113	0.041	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	1	0.0056	0.1
0.00113	0.0062	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.42666667	0.0056	0.1
0.00113	0.011	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.45666667	0.0056	0.1
0.00113	0.015	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.98	0.0056	0.1
0.00113	0.0079	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.48	0.0056	0.1
0.012	0.017	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.01	1.2	0.0056	0.1
0.00113	0.0098	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.42333333	0.0056	0.1
0.093	0.029	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.01	1.1	0.0056	0.1
0.00113	0.007	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.46666667	0.0056	0.1
0.0052	0.0081	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.52	0.0056	0.1
0.0084	0.0087	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.4	0.0056	0.1
0.00113	0.0048	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.50333333	0.0056	0.1
0.00113	0.0083	0.00023	0.000084	0.00027	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.04	0.25333333	0.0056	0.1
0.0089	0.01	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.04	0.23	0.0056	0.1
0.006	0.0094	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.46333333	0.0056	0.1
0.0053	0.0081	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.37666667	0.0056	0.14
0.01	0.021	0.00023	0.000084	0.0001	0.0001	0.0001	0.0000001	0.0000001	0.0001	0.02	0.43666667	0.0056	0.1
0.00113	0.0054	0.00023	0.000084	0.00021	0.00028	0.0001	0.0000001	0.0000001	0.0001	0.02	0.51	0.0056	0.1

Caffeine	Cotinine	Di(2-ethylhexyl)phthalate (DEHP)	N,N-Diethyl-m-toluamid (DEET)	Nicotine	Perfluorobutanesulfonate (PFBS)	Perfluoroheptanoic acid (PFHpA)	Perfluorohexane sulfonate (PFHxS) (anion)	Perfluorohexanoic acid (PFHxA)	Perfluorononanoate (PFNA)	Perfluorooctanesulfonic acid (PFOS)	Perfluorooctanoic acid (PFOA)	Saccharin	Sucralose
0.1	0.041	0.2	0.015	0.2	0.0022	0.0015	0.002	0.0021	0.00085	0.0069	0.0019	0.07	0.1
0.16	0.046	0.21	0.022	0.29	0.0021	0.0015	0.003	0.0042	0.0014	0.023	0.0034	0.07	0.1
0.2	0.14	0.28	0.018	0.3	0.0022	0.0015	0.002	0.0031	0.0019	0.011	0.003	0.05	0.1
0.14	0.036	0.22	0.022	0.26	0.0023	0.0015	0.002	0.0034	0.0018	0.013	0.0041	0.07	0.1
0.14	0.034	0.2	0.023	0.27	0.0018	0.0015	0.002	0.0049	0.0018	0.015	0.0047	0.04	0.1
0.1	0.039	0.2	0.016	0.24	0.0011	0.0015	0.002	0.006	0.0027	0.016	0.0091	0.1	0.1
0.12	0.031	0.2	0.013	0.27	0.0016	0.0035	0.002	0.0066	0.0013	0.0056	0.007	0.04	0.1
0.092	0.042	0.22	0.011	0.61	0.0013	0.0015	0.002	0.0054	0.0015	0.0054	0.0063	0.04	0.1
0.19	0.036	0.2	0.016	0.001	0.0021	0.0066	0.002	0.0067	0.002	0.01	0.02	0.06	0.1
0.11	0.079	0.2	0.012	0.38	0.0013	0.0015	0.002	0.005	0.0016	0.0058	0.006	0.04	0.1
0.2	0.052	0.28	0.017	0.33	0.002	0.0062	0.002	0.0079	0.0025	0.0069	0.018	0.04	0.1
0.09	0.079	0.24	0.081	0.28	0.0028	0.0042	0.002	0.0032	0.00029	0.011	0.0047	0.04	0.2
0.12	0.037	0.24	0.012	0.38	0.0016	0.0067	0.002	0.0047	0.002	0.0089	0.032	0.04	0.1
0.15	0.053	0.28	0.015	0.29	0.0014	0.0041	0.002	0.006	0.0013	0.0061	0.0063	0.05	0.1
0.22	0.12	0.55	0.02	0.36	0.00019	0.0015	0.002	0.0067	0.00029	0.00053	0.021	0.07	0.1
0.27	0.041	0.41	0.023	0.1	0.00019	0.0015	0.002	0.0056	0.00029	0.0053	0.017	0.1	0.3
0.073	0.03	0.2	0.017	0.14	0.0021	0.0015	0.002	0.0074	0.001	0.0089	0.008	0.06	0.1
0.12	0.041	0.48	0.028	0.091	0.0015	0.0015	0.002	0.0034	0.00079	0.0095	0.0043	0.1	0.3
0.069	0.021	0.23	0.02	0.21	0.0021	0.0081	0.002	0.0085	0.0017	0.02	0.025	0.06	0.1
0.098	0.026	0.23	0.023	0.28	0.0021	0.0015	0.002	0.0078	0.00029	0.026	0.011	0.07	0.1
0.093	0.025	0.2	0.019	0.056	0.002	0.0074	0.002	0.0068	0.0014	0.0058	0.026	0.07	0.1
0.095	0.022	0.2	0.019	0.16	0.0033	0.01	0.002	0.0077	0.00029	0.0024	0.037	0.06	0.1
0.067	0.03	0.2	0.038	0.2	0.0037	0.0057	0.002	0.0052	0.0007	0.013	0.015	0.04	0.5
0.069	0.023	0.24	0.018	0.25	0.0021	0.0055	0.002	0.0071	0.00095	0.0082	0.018	0.06	0.2
0.052	0.02	0.39	0.013	0.2	0.0016	0.0052	0.002	0.0052	0.0014	0.0078	0.0071	0.07	0.1
0.072	0.018	0.26	0.011	0.1	0.0016	0.004	0.002	0.0055	0.001	0.0071	0.0057	0.1	0.2
0.078	0.015	0.2	0.018	0.19	0.0022	0.0058	0.002	0.0065	0.0008	0.0084	0.017	0.08	0.2
0.08	0.016	0.28	0.005	0.074	0.003	0.0065	0.002	0.0049	0.00029	0.0082	0.018	0.08	0.2
0.085	0.022	0.2	0.00076	0.011	0.0025	0.0015	0.002	0.0016	0.00093	0.005	0.012	0.04	0.1
0.09	0.031	0.2	0.0028	0.14	0.0028	0.0054	0.002	0.0044	0.00029	0.0075	0.019	0.06	0.2
0.056	0.018	0.2	0.0095	0.13	0.0016	0.019	0.002	0.0059	0.0013	0.0063	0.0052	0.08	0.2
0.11	0.025	0.84	0.012	0.15	0.0022	0.0079	0.002	0.0052	0.0014	0.0076	0.0061	0.09	0.2
0.06	0.023	0.2	0.002	0.14	0.003	0.0052	0.002	0.0042	0.00073	0.013	0.012	0.08	0.2
0.11	0.011	0.2	0.002	0.11	0.0021	0.0059	0.002	0.0039	0.0011	0.0097	0.014	0.07	0.2
0.075	0.024	0.2	0.0032	0.091	0.0012	0.0015	0.002	0.0014	0.001	0.00053	0.0082	0.1	0.2
0.094	0.031	0.2	0.0088	0.1	0.003	0.0068	0.002	0.0031	0.00095	0.0052	0.012	0.06	0.2
0.11	0.027	0.2	0.0039	0.1	0.00074	0.0065	0.002	0.0011	0.00029	0.0036	0.00046	0.07	0.1
0.19	0.038	0.26	0.0079	0.19	0.00076	0.0046	0.002	0.0029	0.0008	0.0037	0.0033	0.06	0.2
0.16	0.036	0.2	0.0089	0.2	0.00087	0.0052	0.002	0.0031	0.00074	0.0048	0.0043	0.08	0.1
0.16	0.035	0.2	0.0093	0.14	0.0012	0.0065	0.002	0.003	0.0027	0.0056	0.0037	0.09	0.2
0.25	0.046	0.26	0.018	0.15	0.00063	0.0046	0.002	0.0015	0.00029	0.0047	0.0049	0.6	0.3
0.14	0.034	0.35	0.0014	0.19	0.00094	0.0015	0.002	0.0043	0.00072	0.0049	0.0042	0.1	0.2
0.2	0.037	0.26	0.0098	0.15	0.0014	0.0015	0.002	0.0031	0.0013	0.006	0.0044	0.1	0.2
0.12	0.039	0.2	0.0087	0.17	0.0015	0.0015	0.002	0.0033	0.0015	0.0055	0.0037	0.1	0.2
0.11	0.034	0.2	0.0099	0.13	0.0014	0.0015	0.002	0.0038	0.0016	0.0062	0.0043	0.1	0.2
0.12	0.035	0.2	0.0099	0.16	0.0011	0.0015	0.002	0.0033	0.0015	0.0061	0.0041	0.08	0.2
0.021	0.0001	0.2	0.0072	0.001	0.0012	0.0015	0.002	0.0035	0.00029	0.0041	0.0039	0.09	0.2
0.066	0.012	0.2	0.014	0.001	0.00019	0.0015	0.002	0.0011	0.00029	0.0037	0.0018	0.04	0.2
0.027	0.002	0.2	0.012	0.0016	0.0014	0.0015	0.002	0.0038	0.00029	0.0055	0.0051	0.08	0.2
0.013	0.013	0.2	0.02	0.001	0.0011	0.0015	0.002	0.0036	0.0017	0.0064	0.0046	0.07	0.1
0.026	0.015	0.2	0.025	0.001	0.00073	0.0015	0.002	0.0011	0.00088	0.0024	0.0048	0.2	0.4
0.023	0.001	0.2	0.0094	0.001	0.0014	0.0015	0.002	0.004	0.00075	0.0054	0.0051	0.05	0.1
0.024	0.001	0.2	0.0094	0.001	0.0013	0.0015	0.002	0.0038	0.00097	0.0047	0.0044	0.05	0.2
0.036	0.028	0.35	0.0066	0.021	0.0019	0.0015	0.002	0.0031	0.00093	0.008	0.0029	0.3	0.1
0.048	0.017	0.21	0.0077	0.091	0.0011	0.0015	0.002	0.004	0.00081	0.0048	0.0032	0.06	0.2
0.32	0.055	0.46	0.0076	0.051	0.00019	0.0015	0.002	0.0011	0.00029	0.00053	0.0032	0.6	0.1
0.059	0.0092	0.37	0.0085	0.089	0.0014	0.0015	0.002	0.0038	0.00029	0.0047	0.0038	0.05	0.2
1.3	0.34	0.48	0.037	0.075	0.0018	0.0015	0.002	0.0018	0.0011	0.0059	0.0026	1.7	0.4
0.14	0.019	0.2	0.0092	0.015	0.0011	0.0015	0.002	0.005	0.0033	0.0063	0.0057	0.04	0.1
0.049	0.024	0.26	0.0093	0.038	0.0013	0.0015	0.002	0.0042	0.003	0.0054	0.0044	0.09	0.2
0.042	0.021	0.2	0.0051	0.082	0.0013	0.0015	0.002	0.0032	0.0014	0.0057	0.0038	0.07	0.1
0.031	0.023	0.2	0.0082	0.065	0.00084	0.0015	0.002	0.0044	0.0029	0.005	0.0051	0.06	0.2
0.027	0.028	0.2	0.0023	0.077	0.00019	0.0015	0.002	0.0011	0.0016	0.0043	0.0012	0.05	0.1
0.029	0.022	0.2	0.0015	0.089	0.00019	0.0015	0.002	0.0011	0.0011	0.00053	0.0015	0.04	0.1
0.039	0.02	0.2	0.0093	0.063	0.0013	0.0015	0.002	0.004	0.0031	0.0057	0.005	0.06	0.1
0.03	0.023	0.2	0.0095	0.11	0.00093	0.0015	0.002	0.0024	0.003	0.0069	0.0043	0.08	0.1
0.044	0.012	0.23	0.017	0.073	0.0014	0.0015	0.002	0.004	0.0033	0.0069	0.0064	0.07	0.2
0.04	0.021	0.2	0.0048	0.11	0.001	0.0015	0.002	0.0023	0.00029	0.0052	0.0033	0.1	0.1

Concentration Metals BioMet

JDS3 site	Arsenic (As) - dissolved	Cadmium (Cd) - dissolved	Chromium (Cr) - dissolved	Copper (Cu) - dissolved	Lead (Pb) - dissolved	Mercury (Hg) - dissolved	Nickel (Ni) - dissolved	Zinc (Zn) - dissolved
JDS01				0.12110003	0.04244487		0.63911198	2.05902016
JDS02				0.10782312	0.05305608		0.48508469	0.99373246
JDS03				0.20183339	0.09533964		1.23699092	5.02762963
JDS04				0.11136674	0.08130409		0.42118832	1.76007317
JDS05				0.15781875	0.10593294		0.55664591	3.77072222
JDS06				0.19088686	0.08474635		0.82328338	3.18139002
JDS07				0.35394285	0.3122074		1.1	5.37741817
JDS08				0.47227062	0.1561037		1	2.41983817
JDS09				0.27327669	0.24213243		19	2.20351013
JDS10				0.18876266	0.14855703		1.60146607	1.47206111
JDS11				0.50707423	0.26136095		25	4.01657049
JDS12				0.10041027	0.09019365		1.28056826	2.59689052
JDS13				0.35324421	0.28990687		0.95	2.33069059
JDS14				0.50335705	0.0790161		1	3.70791685
JDS15				0.30038506	0.04460106		1	2.80742276
JDS16				0.01910062	0.04956066		0.18999702	0.55143093
JDS17				0.32541715	0.08474201		1	2.38366083
JDS18				0.16623935	0.10611216		0.91617943	1.4278376
JDS19				0.37548132	1.80634283		1.4	2.96633348
JDS20				0.33312269	0.93662221		1.2	4.08683781
JDS21				0.29235801	0.13397016		7.3	2.68870908
JDS22				0.42181746	0.19138647		1.9	3.2264509
JDS23				0.12835334	0.07415306		1.07935889	4.65104864
JDS24				0.19112986	0.08920212		1.39712862	4.13808614
JDS25				0.21441857	0.10035238		0.96052593	3.69669028
JDS26				0.22973419	0.21631513		1.135167	3.69669028
JDS27				0.167026	0.10895959		0.89812732	2.42790291
JDS28				0.24313796	0.05129122		1.1	2.52738654
JDS29				0.20122874	0.15499312		0.76	2.20474145
JDS30				0.22902185	0.05352127		0.93	2.52738654
JDS31				0.22902185	0.10927259		9	2.85003163
JDS32				0.30038506	0.07805185		1.3	3.23118468
JDS33				0.26986893	0.11596275		1.4	3.44154763
JDS34				0.19143046	0.05836481		2.1212448	3.3250646
JDS35				0.23103602	0.06053311		1.07935889	4.91809767
JDS36				0.16534631	0.2028121		1.82313193	4.29207082
JDS37				0.24363876	0.14483119		1.44630327	3.21742737
JDS38				0.34805537	0.34024166		1.15704262	0.70862033
JDS39				0.46870635	0.17930577		1.1	0.73013837
JDS40				0.29099663	0.06467153		0.87320539	0.33104689
JDS41				0.21381547	0.4128063		145.671386	1.04947965
JDS42				0.2178133	0.20055651		0.9126708	0.6792213
JDS43				0.29404594	0.08474201		4.10406532	1.60005997
JDS44				0.26709788	0.10956516		1.03046587	0.61315297
JDS45				0.29404594	0.05798137		1.04784646	0.27587241
JDS46				0.32162786	0.06690159		1.135167	0.44139585
JDS47				0.32345053	0.0802819		1.135167	0.6069193
JDS48				40.9273227	0.11382141		31.4353939	18.5383341
JDS49				1.45657659	0.07679563		0.43619848	0.50907979
JDS50				0.79641184	0.05404149		7.59688686	4.02773718
JDS51				1.37857656	0.10611216		3.98018209	0.24819487
JDS52				0.39979583	0.04085985		0.89338233	0.29944466
JDS53				0.50086941	0.04842649		1.82660735	1.59838174
JDS54				0.28426094	0.0244058		0.93285518	0
JDS55				0.4107307	0.05296647		0.89812732	0.62790592
JDS56				0.55151584	0.04895498		0.99504552	0.56408376
JDS57				0.84235159	0.08862804		1.4	2.39623887
JDS58				0.56852188	0.04562823		2.05228139	0.87262982
JDS59				0.28093761	0.05901978		1.23699092	0.12833343
JDS60				0.5205042	0.0691731		8	0.75283854
JDS61				0.43315416	0.04993981		2.324773	0.61476221
JDS62				0.50497884	0.07133476		1.34988305	0.27254628
JDS63				0.30873022	0.03820038		1.22157257	0.5164519
JDS64				0.27445884	0.02855596		1.43037794	0.1199302
JDS65				0.43315416	0.10744626		1.41146932	0.7786988
JDS66				0.47956353	0.06204643		1.1623865	1.06558783
JDS67				0.54132436	0.08474201		1.3	0.80661272
JDS68				0.56214453	0.04906116		1.3	0.05377418

ANNEX 3

SOLUTIONS Deliverable D18.1, Common assessment framework for HRA and ERA higher tier assessments including fish and drinking water and multi-species ERA via SSD, population-level ERA via IBM and food web vulnerability ERA

Sheets	***Content***
Information	Information on ecotoxocological data Information on calculations of drinking water guideline values and rules to derive regulatory values
Chemicals	List of chemicals measured and detected at at least one site in the Danube, with CAS numbers
Ecotox data	Ecotoxicological data and (derived) regulatory values used for different tiers in the MRA Values collected from WFD PS dossiers and Dick de Zwarts database Lowest chronic values for Algae, Daphnia and Fish
Human Tox data	Human Toxicity data and regulatory values use for different tiers in the MRA Data includes calculations of (provisional) guideline values for drinking water and human consumption of fish

Information

Ecotoxicity Data:

All data are chronic toxicity

Colour code denotes origin of toxicity data:

Yellow		From EQS dossiers, the lowest NOEC recorded	
Green		From Dick de Zwart's database	
Blue 1 for chemicals with no toxicity data	**"HC50"**	Median of NOEC probability distribution	These probability distributions are based on taxa-specific chronic NOECs
Blue 2 for chemicals with no toxicity data	**"HC5"**	5th percentile of NOEC probability distribution	from Dick de Zwart's database

Human Toxicity Data:

Calculations:

provisional GLV for drinking water (ug/l) pGLV = ADI*bodyweight*P/drinking water consumption

P = fraction of ADI allocated to drinking water (10%)
bodyweight = 70kg
drinking water consumption = 2l

provisional GLV for fish consumptio (ug/l) pGLV = ADI*bodyweight*P/fish consumption

P = fraction of ADI allocated to drinking water (10%)
bodyweight = 70kg
fish consumption = 0.115 kg/d

ADI calculation for pharmaceuticals: ADI = DDD/(UF*bw)

DDD: defined daily dose
UF: uncertainty factor = 100
bw: bodyweight = 70 kg

TTC values:

Cramer classes determined with toxtree 2.6.13

	TTC value (ug/person/day)	TTC value (ug/kg bw/day)	TTC for regulatory values (mg/kg bw/day)	TTC for NOAEL values (mg/kg bw/day)
Cramer class I	1800	30	0.03	3
Cramer class II	540	9	0.009	0.9
Cramer class III	90	1.5	0.0015	0.15
Genotox alert	0.15	0.0025	0.0000025	0.00025
OP/carbamate	18	0.3	0.0003	0.03

Values for compounds not available in toxtree assumed Cramer class III

Chemicals

Group	Substance	CAS_No	Unit	Organisation
Metals	Arsenic (As) - dissolved	7440-38-2	µg/l	CW - Croatian Waters
Metals	Cadmium (Cd) - dissolved	7440-43-9	µg/l	CW - Croatian Waters
Metals	Chromium (Cr) - dissolved	7440-47-3	µg/l	CW - Croatian Waters
Metals	Copper (Cu) - dissolved	7440-50-8	µg/l	CW - Croatian Waters
Metals	Lead (Pb) - dissolved	7439-92-1	µg/l	CW - Croatian Waters
Metals	Mercury (Hg) - dissolved	7439-97-6	µg/l	CW - Croatian Waters
Metals	Nickel (Ni) - dissolved	7440-02-0	µg/l	CW - Croatian Waters
Metals	Zinc (Zn) - dissolved	7440-66-6	µg/l	CW - Croatian Waters
PAHs	Anthracene	120-12-7	µg/l	PM - Povodi Moravy, s.p.
PAHs	Benzo(a)pyrene	50-32-8	µg/l	PM - Povodi Moravy, s.p.
PAHs	Benzo(b)fluoranthene	205-99-2	µg/l	PM - Povodi Moravy, s.p.
PAHs	Benzo(g,h,i)perylene	191-24-2	µg/l	PM - Povodi Moravy, s.p.
PAHs	Benzo(k)fluoranthene	207-08-9	µg/l	PM - Povodi Moravy, s.p.
PAHs	Fluoranthene	206-44-0	µg/l	PM - Povodi Moravy, s.p.
PAHs	Indeno(1,2,3-c,d)pyrene	193-39-5	µg/l	PM - Povodi Moravy, s.p.
PAHs	Naphthalene	91-20-3	µg/l	PM - Povodi Moravy, s.p.
Herbicides	2,4-D	94-75-7	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Herbicides	2-Methyl-4-chlorphenoxy acetic acid (MCPA)	94-74-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Herbicides	Ametryn	834-12-8	µg/l	ZLBF - LW Langenau
Herbicides	Aminomethylphosphonic acid (AMPA)	1066-51-9	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Atrazine	1912-24-9	µg/l	UFZ - Helmholtz Centre for Environmental Research
Herbicides	Atrazine-2-hydroxy	2163-68-0	µg/l	ZLBF - LW Langenau
Herbicides	Atrazine-desethyl	6190-65-4	µg/l	CW - Croatian Waters
Herbicides	Atrazine-desisopropyl	1007-28-9	µg/l	CW - Croatian Waters
Herbicides	Bentazone	25057-89-0	µg/l	ZLBF - LW Langenau
Herbicides	Bromacil	314-40-9	µg/l	CW - Croatian Waters
Herbicides	Carbetamide	16118-49-3	µg/l	CW - Croatian Waters
Herbicides	Chloridazon	1698-60-8	µg/l	CW - Croatian Waters
Herbicides	Chloridazon-desphenyl	6339-19-1	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Chloridazon-methyl-desphenyl	17254-80-7	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Chloroxuron	1982-47-4	µg/l	CW - Croatian Waters
Herbicides	Chlortoluron	15545-48-9	µg/l	CW - Croatian Waters
Herbicides	Cyanazine (Fortrol)	21725-46-2	µg/l	CW - Croatian Waters
Herbicides	Cybutryne (Irgarol)	28159-98-0	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Herbicides	Dimefuron	34205-21-5	µg/l	CW - Croatian Waters
Herbicides	Dimethachlor CGA 369873	1418095-08-5	µg/l	ZLBF - LW Langenau
Herbicides	Dimethachlor sulfonic acid CGA 354742	N/A	µg/l	ZLBF - LW Langenau
Herbicides	Dimethenamid	87674-68-8	µg/l	ZLBF - LW Langenau
Herbicides	Dinoseb	88-85-7	µg/l	ZLBF - LW Langenau
Herbicides	Dinoterb	1420-07-1	µg/l	ZLBF - LW Langenau
Herbicides	Diuron	330-54-1	µg/l	CW - Croatian Waters
Herbicides	Ethidimuron (Sulfadiazole)	30043-49-3	µg/l	CW - Croatian Waters
Herbicides	Ethofumesate	26225-79-6	µg/l	CW - Croatian Waters
Herbicides	Glyphosate	1071-83-6	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Hexazinon	51235-04-2	µg/l	ZLBF - LW Langenau
Herbicides	Isoproturon	34123-59-6	µg/l	CW - Croatian Waters
Herbicides	Linuron	330-55-2	µg/l	CW - Croatian Waters
Herbicides	Metamitron	41394-05-2	µg/l	CW - Croatian Waters
Herbicides	Metazachlor	67129-08-2	µg/l	CW - Croatian Waters
Herbicides	Metazachlor ESA	172960-62-2	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Metazachlor OA	1231244-60-2	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Methabenzthiazuron	18691-97-9	µg/l	CW - Croatian Waters
Herbicides	Metobromuron	3060-89-7	µg/l	CW - Croatian Waters
Herbicides	Metolachlor	51218-45-2	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Herbicides	Metolachlor ESA	171118-09-5	µg/l	UBAAT - Umweltbundesamt GmbH
Herbicides	Metoxuron	19937-59-8	µg/l	CW - Croatian Waters
Herbicides	Monolinuron	1746-81-2	µg/l	CW - Croatian Waters
Herbicides	Prometryn	7287-19-6	µg/l	CW - Croatian Waters
Herbicides	Propazine	139-40-2	µg/l	CW - Croatian Waters
Herbicides	Propazine-2-hydroxy	7374-53-0	µg/l	ZLBF - LW Langenau
Herbicides	Simazine	122-34-9	µg/l	CW - Croatian Waters
Herbicides	S-Metolachlor CGA 368208	1173021-76-5	µg/l	ZLBF - LW Langenau
Herbicides	S-Metolachlor NOA 413173	1418095-19-8	µg/l	ZLBF - LW Langenau
Herbicides	Terbutryn	886-50-0	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Herbicides	Terbutylazine	5915-41-3	µg/l	CW - Croatian Waters
Herbicides	Terbutylazine CGA 324007	309923-18-0	µg/l	ZLBF - LW Langenau
Herbicides	Terbutylazine SYN 545666	N/A	µg/l	ZLBF - LW Langenau
Herbicides	Terbutylazine-2-hydroxy	66753-07-9	µg/l	ZLBF - LW Langenau
Herbicides	Terbutylazine-desethyl	30125-63-4	µg/l	CW - Croatian Waters
Herbicides	Terbutylazine-desethyl-2-hydroxy	66753-06-8	µg/l	ZLBF - LW Langenau
Insecticides	Diazinone	333-41-5	µg/l	ZLBF - LW Langenau
Insecticides	Fipronil	120068-37-3	µg/l	ZLBF - LW Langenau
Fungicides	4-Chlorophenol	106-48-9	µg/l	CW - Croatian Waters
Fungicides	Azoxystrobin	131860-33-8	µg/l	ZLBF - LW Langenau
Fungicides	Carbendazim	10605-21-7	µg/l	ZLBF - LW Langenau
Fungicides	Cyproconazol	94361-06-5	µg/l	ZLBF - LW Langenau
Fungicides	Flusilazole	85509-19-9	µg/l	ZLBF - LW Langenau
Fungicides	Metalaxyl NOA 409045	75596-99-5	µg/l	ZLBF - LW Langenau
Fungicides	Picoxystrobin	117428-22-5	µg/l	ZLBF - LW Langenau
Fungicides	Propiconazole	60207-90-1	µg/l	ZLBF - LW Langenau
Fungicides	Quinoxyfen	124495-18-7	µg/l	ZLBF - LW Langenau
Fungicides	Tebuconazol	107534-96-3	µg/l	ZLBF - LW Langenau
Fungicides	Trifloxystrobin CGA 321113	252913-85-2	µg/l	ZLBF - LW Langenau
Pharmaceuticals	10,11-Dihydro-10,11-dihydroxycarbamazepine	58955-93-4	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Pharmaceuticals	10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	µg/l	CW - Croatian Waters
Pharmaceuticals	17-beta Estradiol	50-28-2	µg/l	CW - Croatian Waters
Pharmaceuticals	1-Adamantylamin	768-94-5	µg/l	ZLBF - LW Langenau
Pharmaceuticals	2-Hydroxycarbamazepine	68011-66-5	µg/l	UFZ - Helmholtz Centre for Environmental Research
Pharmaceuticals	3,4-Methylendioxyamphetamine (MDA)	4764-17-4	µg/l	CW - Croatian Waters
Pharmaceuticals	3,4-Methylenedioxyethamphetamine (MDEA)	14089-52-2	µg/l	CW - Croatian Waters
Pharmaceuticals	6-Acetylmorphine	2784-73-8	µg/l	CW - Croatian Waters
Pharmaceuticals	7-Aminoclonazepam	4959-17-5	µg/l	CW - Croatian Waters
Pharmaceuticals	7-Aminoflunitrazepam	34084-50-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Acetylcodeine	6703-27-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Acetyl-sulfamethoxazole	21312-10-7	µg/l	UFZ - Helmholtz Centre for Environmental Research
Pharmaceuticals	Alfentanil	71195-58-9	µg/l	CW - Croatian Waters
Pharmaceuticals	alpha-Hydroxyalprazolam	37115-43-8	µg/l	CW - Croatian Waters
Pharmaceuticals	alpha-Hydroxymidazolam	59468-90-5	µg/l	CW - Croatian Waters
Pharmaceuticals	alpha-Hydroxytriazolam	37115-45-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Alprazolam	28981-97-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Amidotrizoic acid	117-96-4	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Amisulpride	71675-85-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Amitriptyline	50-48-6	µg/l	CW - Croatian Waters
Pharmaceuticals	Amoxapine	14028-44-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Amoxicillin	26787-78-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Amphetamine	300-62-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Atenolol	29122-68-7	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Atropine	51-55-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Benzoylecgonine	519-09-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Betaxolol	63659-18-7	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Bezafibrate	41859-67-0	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Bisoprolol	66722-44-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Bromazepam	1812-30-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Buprenorphine	52485-79-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Buprenorphine glucuronide	101224-22-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Candesartan	139481-59-7	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Carbamazepine	298-46-4	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Pharmaceuticals	Carbamazepine-10,11-epoxide	36507-30-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Carisoprodol	78-44-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Cetirizine	83881-51-0	µg/l	UFZ - Helmholtz Centre for Environmental Research
Pharmaceuticals	Chlorprothixene	113-59-7	µg/l	CW - Croatian Waters

Pharmaceuticals	Citalopram	59729-33-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Clobazam (Urbadan)	22316-47-8	µg/l	UNI Umea - Umeå University
Pharmaceuticals	Clonazepam	1622-61-3	µg/l	CW - Croatian Waters
Pharmaceuticals	Clonidine	4205-90-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Clozapine	5786-21-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Cocaethylene	529-38-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Cocaine	50-36-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Codeine	76-57-3	µg/l	CW - Croatian Waters
Pharmaceuticals	CP 47,497	70434-82-1	µg/l	CW - Croatian Waters
Pharmaceuticals	CP 47,497-C8 homologue	70434-92-3	µg/l	CW - Croatian Waters
Pharmaceuticals	Crotamiton	483-63-6	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Desalkylflurazepam	2886-65-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Desipramine	50-47-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Dextromethorphan (Methorphan)	125-71-3	µg/l	CW - Croatian Waters
Pharmaceuticals	Diazepam	439-14-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Diclofenac	15307-79-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Pharmaceuticals	Digitoxin	71-63-6	µg/l	CW - Croatian Waters
Pharmaceuticals	Digoxin	20830-75-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Dihydrocodeine	125-28-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Diphenhydramine	58-73-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Dothiepin	113-53-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Doxepin	1668-19-5	µg/l	CW - Croatian Waters
Pharmaceuticals	EDDP (metabolite of Methadone)	30223-73-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Felbamate	25451-15-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Fenazepam	51753-57-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Fenofibrate	49562-28-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Fentanyl	437-38-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Flumazenil	78755-81-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Flunitrazepam	1622-62-4	µg/l	UNI Umea - Umeå University
Pharmaceuticals	Flupentixol	2709-56-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Flurazepam	17617-23-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Gabapentin	60142-96-3	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Gabapentin-lactam	64744-50-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Haloperidol	52-86-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Hydrochlorothiazide	58-93-5	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Hydrocodone	125-29-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Hydromorphone	466-99-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Imipramine	50-49-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Indometacin	53-86-1	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Iohexol	66108-95-0	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Iomeprol	78649-41-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Iopamidol	62883-00-5	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Iopromid	73334-07-3	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Irbesartan	138402-11-6	µg/l	ZLBF - LW Langenau
Pharmaceuticals	JWH-018 (N-(n-pentanoic acid)	209414-07-3	µg/l	CW - Croatian Waters
Pharmaceuticals	JWH-073 (2-methylnaphthyl analog)	1427325-61-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Ketamine	6740-88-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Ketoprofen	22071-15-4	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Lamotrigine	84057-84-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Librium (Chlordiazepoxide)	58-25-3	µg/l	CW - Croatian Waters
Pharmaceuticals	Lidocaine	137-58-6	µg/l	CW - Croatian Waters
Pharmaceuticals	Lorazepam	846-49-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Losartan	114798-26-4	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Maprotiline	10262-69-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Medazepam	364-85-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Meperidine (Pethidine)	57-42-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Methamphetamine	537-46-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Methylendioxymethamphetamine (MDMA)	69610-10-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Methylphenidate	113-45-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Metoprolol	37350-58-6	µg/l	UFZ - Helmholtz Centre for Environmental Research
Pharmaceuticals	Metroprolol acid	56392-14-4	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Midazolam	59467-70-8	µg/l	UNI Umea - Umeå University
Pharmaceuticals	Mirtazapine	61337-67-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Morphine	57-27-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Morphine glucuronide	20290-10-2	µg/l	CW - Croatian Waters
Pharmaceuticals	n-Acetyl-4-aminoantipyrine	83-15-8	µg/l	UFZ - Helmholtz Centre for Environmental Research
Pharmaceuticals	Nadolol	42200-33-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Naltrexone	16590-41-3	µg/l	CW - Croatian Waters
Pharmaceuticals	Naproxen	22204-53-1	µg/l	ZLBF - LW Langenau
Pharmaceuticals	N-Desmethylclozapine	6104-71-8	µg/l	CW - Croatian Waters
Pharmaceuticals	N-Formyl-4-aminoantipyrine	1672-58-8	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Nitrazepam	146-22-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Norbuprenorphine	78715-23-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Nordiazepam	1088-11-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Norfentanyl	1609-66-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Normeperidine (Norpethidine)	77-17-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Norpropoxyphene (Desmethyl propoxyphene)	32504-12-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Nortriptyline	72-69-5	µg/l	CW - Croatian Waters
Pharmaceuticals	O-Desmethyltramadol	73986-53-5	µg/l	CW - Croatian Waters
Pharmaceuticals	O-Desmethylvenlafaxine (Desvenlafaxine)	93413-62-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Olanzapine	132539-06-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Opipramol	315-72-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Oxazepam	604-75-1	µg/l	UNI Umea - Umeå University
Pharmaceuticals	Oxcarbazepine	28721-07-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Oxycodone	76-42-6	µg/l	CW - Croatian Waters
Pharmaceuticals	Oxymorphone	76-41-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Paliperidone (9-Hydroxyrisperidone)	144598-75-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Paroxetine	61869-08-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Pentazocine	359-83-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Pentobarbital	76-74-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Pentoxifylline	6493-05-6	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Phenacetin	62-44-2	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Phenazone	60-80-0	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Phencyclidine (PCP)	77-10-1	µg/l	CW - Croatian Waters
Pharmaceuticals	Phentermine	122-09-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Phenytoin	125-59-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Pipamperone	1893-33-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Prazepam	2955-38-6	µg/l	CW - Croatian Waters
Pharmaceuticals	Pregabalin	148553-50-8	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Primidone	125-33-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Promazine	58-40-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Promethazine	60-87-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Propafenone	54063-53-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Propoxyphene (Dextropropoxyphene)	469-62-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Propranolol	525-66-6	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Propyphenazone	479-92-5	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Protriptyline	438-60-8	µg/l	CW - Croatian Waters
Pharmaceuticals	Quetiapine	111974-69-7	µg/l	CW - Croatian Waters
Pharmaceuticals	Risperidone	106266-06-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Ritalinic acid	19395-41-6	µg/l	CW - Croatian Waters
Pharmaceuticals	Secobarbital	76-73-3	µg/l	CW - Croatian Waters
Pharmaceuticals	Sertraline	79617-96-2	µg/l	CW - Croatian Waters
Pharmaceuticals	Sotalol	3930-20-9	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Strophanthidin	66-28-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Sulfadimidin / Sulfamethazin	57-68-1	µg/l	UFZ - Helmholtz Centre for Environmental Research
Pharmaceuticals	Sulfamethoxazole	723-46-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Pharmaceuticals	Sulpirid	15676-16-1	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Telmisartan	144701-48-4	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Temazepam	846-50-4	µg/l	CW - Croatian Waters

Pharmaceuticals	Topiramate	97240-79-4	µg/l	CW - Croatian Waters
Pharmaceuticals	Tramadol	27203-92-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Trazodone	19794-93-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Triazolam	28911-01-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Trimethoprim	738-70-5	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Trimipramine	739-71-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Valsartan	137862-53-4	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Valsartan acid	164265-78-5	µg/l	ZLBF - LW Langenau
Pharmaceuticals	Venlafaxine	93413-69-5	µg/l	CW - Croatian Waters
Pharmaceuticals	Verapamil	52-53-9	µg/l	CW - Croatian Waters
Pharmaceuticals	Zolpidem	82626-48-0	µg/l	CW - Croatian Waters
Pharmaceuticals	Zopiclone	43200-80-2	µg/l	CW - Croatian Waters
Polar compounds	1H-Benzotriazole	95-14-7	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	2-(Methylthio)benzothiazole	615-22-5	µg/l	ZLBF - LW Langenau
Polar compounds	2-Ethylhexyl diphenyl phosphate (EHDP)	1241-94-7	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	5,6-Dimethylbenzotriazole	4184-79-6	µg/l	ZLBF - LW Langenau
Polar compounds	5-Methyl-1H-benzotriazole	136-85-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Benzothiazole-6-carboxylic acid	3622-35-3	µg/l	ZLBF - LW Langenau
Polar compounds	Nonylphenol (4-Nonylphenol)	104-40-5	µg/l	UFZ - Helmholtz Centre for Environmental Research
Polar compounds	Tolyltriazol (mix of isomers)	29385-43-1	µg/l	ZLBF - LW Langenau
Polar compounds	Triisobutyl phosphate (TIBP)	126-71-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tri-n-butyl phosphate (TnBP)	126-73-8	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tri-n-propyl phosphate (TnPP)	513-08-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Triphenyl phosphate (TPT)	115-86-6	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tris(1-chloro-2-propyl)phosphate (TCPP)	13674-84-5	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tris(2-butoxyethyl)phosphate (TBEP)	78-51-3	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tris(2-chloroethyl)phosphate (TCEP)	115-96-8	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tris(3,5-dimethylphenyl)phosphate (T35DMPP)	25653-16-1	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Polar compounds	Tris(methylphenyl)phosphate (TMPP)	1330-78-5	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Organotin compounds	Dibutyltin-cation	1002-53-5	µg/l	UBAAT - Umweltbundesamt GmbH
Organotin compounds	Dioctyltin-cation	94410-05-6	µg/l	UBAAT - Umweltbundesamt GmbH
Organotin compounds	Diphenyltin-cation	6381-06-2	µg/l	UBAAT - Umweltbundesamt GmbH
Organotin compounds	Tetrabutyltin	1461-25-2	µg/l	UBAAT - Umweltbundesamt GmbH
Organotin compounds	Tributyltin-cation	36643-28-4	µg/l	UBAAT - Umweltbundesamt GmbH
Organotin compounds	Triphenyltin-cation	668-34-8	µg/l	UBAAT - Umweltbundesamt GmbH
Other	2,4-Dinitrophenol (DNP)	51-28-5	µg/l	ZLBF - LW Langenau
Other	Acesulfame	33665-90-6	µg/l	UFZ - Helmholtz Centre for Environmental Research
Other	Bisphenol A	80-05-7	µg/l	CW - Croatian Waters
Other	Bisphenol S	80-09-1	µg/l	UFZ - Helmholtz Centre for Environmental Research
Other	Caffeine	58-08-2	µg/l	CW - Croatian Waters
Other	Cotinine	486-56-6	µg/l	CW - Croatian Waters
Other	Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	µg/l	WRISK - Water Research Institute
Other	N,N-Diethyl-m-toluamid (DEET)	134-62-3	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Nicotine	54-11-5	µg/l	CW - Croatian Waters
Other	Perfluorobutanesulfonate (PFBS)	375-73-5	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Perfluoroheptanoic acid (PFHpA)	375-85-9	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Perfluorohexane sulfonate (PFHxS) (anion)	108427-53-8	µg/l	ZLBF - LW Langenau
Other	Perfluorohexanoic acid (PFHxA)	307-24-4	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Perfluorononanoate (PFNA)	375-95-1	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Perfluorooctanesulfonic acid (PFOS)	1763-23-1	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Perfluorooctanoic acid (PFOA)	335-67-1	µg/l	JRC - European Commission -DG Joint Research Centre - Institute for Environment and Sustainability
Other	Saccharin	81-07-2	µg/l	ZLBF - LW Langenau
Other	Sucralose	56038-13-2	µg/l	ZLBF - LW Langenau

Ecotx data

			Tier 1 input values			Tier 2A input values for "HC50" and "HC5" for bridging data gaps					
			RV	ug/L		Algae (NOEC)	ug/L	Daphnia (NOEC)	ug/L	Fish (NOEC)	ug/L
Group	Substance	CAS #	"HC50"	"HC5"	AF	"HC50"	"HC5"	"HC50"	"HC5"	"HC50"	"HC5"
Metals	Arsenic (As) - dissolved	7440-38-2	1	1	10	12.09	12.09	10.56	10.56	402.99	402.99
Metals	Cadmium (Cd) - dissolved	7440-43-9	0.08	0.08		0.85	0.85	0.12	0.12	0.10	0.10
Metals	Chromium (Cr) - dissolved	7440-47-3	22.3	22.3	10	1050.77	1050.77	229.86	229.86	1868.40	1868.40
Metals	Copper (Cu) - dissolved	7440-50-8	0.02	0.02	10	22.90	22.90	0.19	0.19	2.68	2.68
Metals	Lead (Pb) - dissolved	7439-92-1	1.2	1.2		4.50	4.50	7.40	7.40	5.96	5.96
Metals	Mercury (Hg) - dissolved	7439-97-6	0.047	0.047		0.20	0.20	0.70	0.70	0.29	0.29
Metals	Nickel (Ni) - dissolved	7440-02-0	3.8	3.8		12.30	12.30	1.02	1.02	40.00	40.00
Metals	Zinc (Zn) - dissolved	7440-66-6	2	2	10	479.61	479.61	19.18	19.18	26.60	26.60
PAHs	Anthracene	120-12-7	0.1	0.1		1.50	1.50	1.90	1.90	1.20	1.20
PAHs	Benzo(a)pyrene	50-32-8	0.05	0.05		0.78	0.78	0.02	0.02	2.90	2.90
PAHs	Benzo(b)fluoranthene	205-99-2	0.027	0.027		600.00	1	1.08	1.08	87.00	0.039
PAHs	Benzo(g,h,i)perylene	191-24-2	0.002	0.002		1.20	1.20	0.08	0.08	0.16	0.16
PAHs	Benzo(k)fluoranthene	207-08-9	0.027	0.027		600.00	1	1.08	1.08	0.27	0.27
PAHs	Fluoranthene	206-44-0	0.12	0.12		8.60	8.60	1.20	1.20	4.40	4.40
PAHs	Indeno(1,2,3-c,d)pyrene	193-39-5	0.002	0.002		1.50	1.50	0.27	0.27	87.00	0.039
PAHs	Naphthalene	91-20-3	2.4	2.4		1200.00	1200.00	514.00	514.00	20.00	20.00
Herbicides	2,4-D	94-75-7	16	16	10	220.00	220.00	23300.00	23300.00	160.00	160.00
Herbicides	2-Methyl-4-chlorphenoxy acetic acid (M	94-74-6	0.87	0.00039	100	17000.00	17000.00	100000.00	100000.00	87.00	0.039
Herbicides	Ametryn	834-12-8	0.114	0.114	10	1.14	1.14	240.00	240.00	700.00	700.00
Herbicides	Aminomethylphosphonic acid (AMPA)	1066-51-9	0.87	0.00039	100	600.00	1	15000.00	15000.00	87.00	0.039
Herbicides	Atrazine	1912-24-9	0.6	0.6		1.00	1.00	25.00	25.00	0.5	0.50
Herbicides	Atrazine-2-hydroxy	2163-68-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Atrazine-desethyl	6190-65-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Atrazine-desisopropyl	1007-28-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Bentazone	25057-89-0	0.0567	0.0567	100	5.67	5.67	100.00	0.03	87.00	0.039
Herbicides	Bromacil	314-40-9	0.11	0.11	10	1.10	1.10	8200.00	8200.00	3000.00	3000.00
Herbicides	Carbetamide	16118-49-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Chloridazon	1698-60-8	1.2	1.2	50	60.00	60.00	100.00	0.03	3200.00	3200.00
Herbicides	Chloridazon-desphenyl	6339-19-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Chloridazon-methyl-desphenyl	17254-80-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Chloroxuron	1982-47-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Chlortoluron	15545-48-9	0.1	0.1	100	10.00	10.00	100.00	0.03	87.00	0.039
Herbicides	Cyanazine (Fortrol)	21725-46-2	0.023	0.023	100	2.30	2.30	100.00	0.03	87.00	0.039
Herbicides	Cybutryne (Irgarol)	28159-98-0	0.0025	0.0025		0.02	0.02	560.00	560.00	4.00	4.00
Herbicides	Dimefuron	34205-21-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Dimethachlor CGA 369873	1418095-08-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Dimethachlor sulfonic acid CGA 354742	N/A	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Dimethenamid	87674-68-8	0.4	0.4	10	4.00	4.00	680.00	680.00	120.00	120.00
Herbicides	Dinoseb	88-85-7	0.025	0.025	10	1300.00	1300.00	100.00	0.03	0.25	0.25
Herbicides	Dinoterb	1420-07-1	0.87	0.00039	100	1010.00	1010.00	100.00	0.03	87.00	0.039
Herbicides	Diuron	330-54-1	0.2	0.2		0.44	0.44	6.00	6.00	26.40	26.40
Herbicides	Ethidimuron (Sulfadiazole)	30043-49-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Ethofumesate	26225-79-6	25	25	10	2700.00	2700.00	250.00	250.00	2560.00	2560.00
Herbicides	Glyphosate	1071-83-6	0.2	0.2	50	770.00	770.00	100.00	0.03	10.00	10.00
Herbicides	Hexazinon	51235-04-2	0.4	0.4	10	4.00	4.00	20000.00	20000.00	17000.00	17000.00
Herbicides	Isoproturon	34123-59-6	0.32	0.32		2.00	2.00	120.00	120.00	1000.00	1000.00
Herbicides	Linuron	330-55-2	0.045	0.045	10	0.45	0.45	130.00	130.00	5.95	5.95
Herbicides	Metamitron	41394-05-2	0.87	0.00039	100	100.00	100.00	100.00	0.03	87.00	0.039
Herbicides	Metazachlor	67129-08-2	0.87	0.00039	100	340.00	340.00	100.00	0.03	87.00	0.039
Herbicides	Metazachlor ESA	172960-62-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Metazachlor OA	1231244-60-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Methabenzthiazuron	18691-97-9	0.18	0.18	100	18.00	18.00	100.00	0.03	87.00	0.039
Herbicides	Metobromuron	3060-89-7	0.87	0.00039	100	100.00	100.00	100.00	0.03	87.00	0.039
Herbicides	Metolachlor	51218-45-2	3.1	3.1	10	31.00	31.00	354.00	354.00	100.00	100.00
Herbicides	Metolachlor ESA	171118-09-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Metoxuron	19937-59-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Monolinuron	1746-81-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Prometryn	7287-19-6	0.8	0.8	10	8.00	8.00	1000.00	1000.00	620.00	620.00
Herbicides	Propazine	139-40-2	1	1	50	600.00	1	47.00	47.00	1340.00	1340.00
Herbicides	Propazine-2-hydroxy	7374-53-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Simazine	122-34-9	1	1		5.00	5.00	36.00	36.00	0.06	0.06
Herbicides	S-Metolachlor CGA 368208	1173021-76-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	S-Metolachlor NOA 413173	1418095-19-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Terbutryn	886-50-0	0.065	0.065		0.40	0.40	1300.00	1300.00	9.00	9.00
Herbicides	Terbutylazine	5915-41-3	0.006	0.006	100	0.60	0.60	100.00	0.03	87.00	0.039
Herbicides	Terbutylazine CGA 324007	309923-18-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Terbutylazine SYN 545666	N/A	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Terbutylazine-2-hydroxy	66753-07-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Terbutylazine-desethyl	30125-63-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Herbicides	Terbutylazine-desethyl-2-hydroxy	66753-06-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Insecticides	Diazinone	333-41-5	0.00036	0.00036	10	205.00	205.00	0.10	0.10	0.0036	0.0036
Insecticides	Fipronil	120068-37-3	0.001	0.001	50	600.00	1	9.60	9.60	0.05	0.05
Fungicides	4-Chlorophenol	106-48-9	0.87	0.00039	100	600.00	600.00	200.00	200.00	87.00	0.039
Fungicides	Azoxystrobin	131860-33-8	2.7	2.7	10	27.70	27.70	44.00	44.00	147.00	147.00
Fungicides	Carbendazim	10605-21-7	0.031	0.031	100	600.00	1	3.10	3.10	87.00	0.039
Fungicides	Cyproconazol	94361-06-5	0.38	0.38	50	600.00	1	19.00	19.00	650.00	650.00
Fungicides	Flusilazole	85509-19-9	0.87	0.00039	100	600.00	1	270.00	270.00	87.00	0.039
Fungicides	Metalaxyl NOA 409045	75596-99-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Fungicides	Picoxystrobin	117428-22-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Fungicides	Propiconazole	60207-90-1	0.018	0.018	10	40.00	40.00	310.00	310.00	0.18	0.18
Fungicides	Quinoxyfen	124495-18-7	0.152	0.152		4.63	4.63	27.80	27.80	13.00	13.00
Fungicides	Tebuconazol	107534-96-3	1.2	1.2	10	320.00	320.00	120.00	120.00	12.00	12.00
Fungicides	Trifloxystrobin CGA 321113	252913-85-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	10,11-Dihydro-10,11-dihydroxycarbama	58955-93-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	10,11-Dihydro-10-	29331-92-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	17-beta Estradiol	50-28-2	0.00005	0.00005	10	523.00	523.00	10000.00	10000.00	0.0005	0.0005
Pharmaceuticals	1-Adamantylamin	768-94-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	2-Hydroxycarbamazepine	68011-66-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	3,4-Methylendioxyamphetamine	4764-17-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	3,4-Methylenedioxyethamphetamine (M	14089-52-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	6-Acetylmorphine	2784-73-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	7-Aminoclonazepam	4959-17-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	7-Aminoflunitrazepam	34084-50-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Acetylcodeine	6703-27-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Acetyl-sulfamethoxazole	21312-10-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Alfentanil	71195-58-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	alpha-Hydroxyalprazolam	37115-43-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	alpha-Hydroxymidazolam	59468-90-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	alpha-Hydroxytriazolam	37115-45-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Alprazolam	28981-97-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Amidotrizoic acid	117-96-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Amisulpride	71675-85-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Amitriptyline	50-48-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Amoxapine	14028-44-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Amoxicillin	26787-78-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Amphetamine	300-62-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Atenolol	29122-68-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Atropine	51-55-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Benzoylecgonine	519-09-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Betaxolol	63659-18-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Bezafibrate	41859-67-0	0.0006	0.0006	50	600.00	1	23.00	23.00	0.03	0.03
Pharmaceuticals	Bisoprolol	66722-44-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Bromazepam	1812-30-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Buprenorphine	52485-79-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Buprenorphine glucuronide	101224-22-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Candesartan	139481-59-7	6	0.01	100	600.00	1	10000.00	10000.00	1000.00	1000.00
Pharmaceuticals	Carbamazepine	298-46-4	0.05	0.05	10	10.00	10.00	0.50	0.50	0.50	0.50
Pharmaceuticals	Carbamazepine-10,11-epoxide	36507-30-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Carisoprodol	78-44-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Cetirizine	83881-51-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Chlorprothixene	113-59-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Citalopram	59729-33-8	0.87	0.00039	100	600.00	1	800.00	800.00	87.00	0.039
Pharmaceuticals	Clobazam (Urbadan)	22316-47-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Clonazepam	1622-61-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Clonidine	4205-90-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Clozapine	5786-21-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Cocaethylene	529-38-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039

Pharmaceuticals	Cocaine	50-36-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Codeine	76-57-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	CP 47,497	70434-82-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	CP 47,497-C8 homologue	70434-92-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Crotamiton	483-63-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Desalkylflurazepam	2886-65-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Desipramine	50-47-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Dextromethorphan (Methorphan)	125-71-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Diazepam	439-14-5	1	0.0003	100	600.00	1	100.00	0.03	72000.00	72000.00
Pharmaceuticals	Diclofenac	15307-79-6	0.1	0.1		100.00	100.00	1000.00	1000.00	0.50	0.50
Pharmaceuticals	Digitoxin	71-63-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Digoxin	20830-75-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Dihydrocodeine	125-28-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Diphenhydramine	58-73-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Dothiepin	113-53-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Doxepin	1668-19-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	EDDP (metabolite of Methadone)	30223-73-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Felbamate	25451-15-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Fenazepam	51753-57-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Fenofibrate	49562-28-9	0.87	0.00039	100	600.00	1	39.00	39.00	87.00	0.039
Pharmaceuticals	Fentanyl	437-38-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Flumazenil	78755-81-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Flunitrazepam	1622-62-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Flupentixol	2709-56-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Flurazepam	17617-23-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Gabapentin	60142-96-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Gabapentin-lactam	64744-50-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Haloperidol	52-86-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Hydrochlorothiazide	58-93-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Hydrocodone	125-29-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Hydromorphone	466-99-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Imipramine	50-49-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Indometacin	53-86-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Iohexol	66108-95-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Iomeprol	78649-41-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Iopamidol	62883-00-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Iopromid	73334-07-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Irbesartan	138402-11-6	0.87	0.00039	100	600.00	1	10400.00	10400.00	87.00	0.039
Pharmaceuticals	JWH-018 (N-(n-pentanoic acid)	209414-07-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	JWH-073 (2-methylnaphthyl analog)	1427325-61-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Ketamine	6740-88-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Ketoprofen	22071-15-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Lamotrigine	84057-84-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Librium (Chlordiazepoxide)	58-25-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Lidocaine	137-58-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Lorazepam	846-49-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Losartan	114798-26-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Maprotiline	10262-69-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Medazepam	364-85-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Meperidine (Pethidine)	57-42-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Methamphetamine	537-46-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Methylendioxymethamphetamine (MDI	69610-10-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Methylphenidate	113-45-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Metoprolol	37350-58-6	0.12	0.12	10	13400.00	13400.00	1.20	1.20	5.00	5.00
Pharmaceuticals	Metroprolol acid	56392-14-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Midazolam	59467-70-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Mirtazapine	61337-67-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Morphine	57-27-2	1	0.0003	100	600.00	1	100.00	0.03	1000.00	1000.00
Pharmaceuticals	Morphine glucuronide	20290-10-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	n-Acetyl-4-aminoantipyrine	83-15-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Nadolol	42200-33-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Naltrexone	16590-41-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Naproxen	22204-53-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	N-Desmethylclozapine	6104-71-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	N-Formyl-4-aminoantipyrine	1672-58-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Nitrazepam	146-22-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Norbuprenorphine	78715-23-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Nordiazepam	1088-11-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Norfentanyl	1609-66-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Normeperidine (Norpethidine)	77-17-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Norpropoxyphene (Desmethyl	32504-12-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Nortriptyline	72-69-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	O-Desmethyltramadol	73986-53-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	O-Desmethylvenlafaxine	93413-62-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Olanzapine	132539-06-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Opipramol	315-72-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Oxazepam	604-75-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Oxcarbazepine	28721-07-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Oxycodone	76-42-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Oxymorphone	76-41-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Paliperidone (9-Hydroxyrisperidone)	144598-75-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Paroxetine	61869-08-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Pentazocine	359-83-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Pentobarbital	76-74-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Pentoxifylline	6493-05-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Phenacetin	62-44-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Phenazone	60-80-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Phencyclidine (PCP)	77-10-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Phentermine	122-09-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Phenytoin	125-59-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Pipamperone	1893-33-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Prazepam	2955-38-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Pregabalin	148553-50-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Primidone	125-33-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Promazine	58-40-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Promethazine	60-87-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Propafenone	54063-53-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Propoxyphene (Dextropropoxyphene)	469-62-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Propranolol	525-66-6	0.01	0.01	50	600.00	1	55.00	55.00	0.50	0.50
Pharmaceuticals	Propyphenazone	479-92-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Protriptyline	438-60-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Quetiapine	111974-69-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Risperidone	106266-06-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Ritalinic acid	19395-41-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Secobarbital	76-73-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Sertraline	79617-96-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Sotalol	3930-20-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Strophanthidin	66-28-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Sulfadimidin / Sulfamethazin	57-68-1	1.5	1.5	100	600.00	1	1563.00	1563.00	87.00	0.039
Pharmaceuticals	Sulfamethoxazole	723-46-6	0.5	0.5	100	600.00	1	100.00	0.03	533.00	533.00
Pharmaceuticals	Sulpirid	15676-16-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Telmisartan	144701-48-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Temazepam	846-50-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Topiramate	97240-79-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Tramadol	27203-92-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Trazodone	19794-93-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Triazolam	28911-01-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Trimethoprim	738-70-5	3.2	3.2	50	600.00	1	6000.00	6000.00	157.00	157.00
Pharmaceuticals	Trimipramine	739-71-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Valsartan	137862-53-4	5.6	5.6	100	600.00	1	5600.00	5600.00	87.00	0.039
Pharmaceuticals	Valsartan acid	164265-78-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Venlafaxine	93413-69-5	0.2874	0.2874	100	600.00	1	100.00	0.03	28.74	28.74
Pharmaceuticals	Verapamil	52-53-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Zolpidem	82626-48-0	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Pharmaceuticals	Zopiclone	43200-80-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	1H-Benzotriazole	95-14-7	3	3	100	600.00	1	3000.00	3000.00	87.00	0.039

Polar compounds	2-(Methylthio)benzothiazole	615-22-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	2-Ethylhexyl diphenyl phosphate (EHDP	1241-94-7	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	5,6-Dimethylbenzotriazole	4184-79-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	5-Methyl-1H-benzotriazole	136-85-6	0.1	0.1	100	600.00	1	10.00	10.00	87.00	0.039
Polar compounds	Benzothiazole-6-carboxylic acid	3622-35-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	Nonylphenol (4-Nonylphenol)	104-40-5	0.33	0.33		3.30	3.30	1.00	1.00	1.00	1.00
Polar compounds	Tolyltriazol (mix of isomers)	29385-43-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	Triisobutyl phosphate (TIBP)	126-71-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	Tri-n-butyl phosphate (TnBP)	126-73-8	70	70	10	3200.00	3200.00	730.00	730.00	8300.00	8300.00
Polar compounds	Tri-n-propyl phosphate (TnPP)	513-08-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	Triphenyl phosphate (TPT)	115-86-6	1	1	50	100.00	100.00	100.00	0.03	55.00	55.00
Polar compounds	Tris(1-chloro-2-propyl)phosphate (TCPP	13674-84-5	32	32	100	600.00	1	32000.00	32000.00	87.00	0.039
Polar compounds	Tris(2-butoxyethyl)phosphate (TBEP)	78-51-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	Tris(2-chloroethyl)phosphate (TCEP)	115-96-8	0.1	0.1	100	600.00	1	10.00	10.00	87.00	0.039
Polar compounds	Tris(3,5-dimethylphenyl)phosphate (T3	25653-16-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Polar compounds	Tris(methylphenyl)phosphate (TMPP)	1330-78-5	0.032	0.032	10	320.00	320.00	100.00	100.00	0.32	0.32
ganotin compoun	Dibutyltin-cation	1002-53-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
ganotin compoun	Dioctyltin-cation	94410-05-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
ganotin compoun	Diphenyltin-cation	6381-06-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
ganotin compoun	Tetrabutyltin	1461-25-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
ganotin compoun	Tributyltin-cation	36643-28-4	0.0002	0.0002		0.05	0.05	0.16	0.16	0.01	0.01
ganotin compoun	Triphenyltin-cation	668-34-8	0.001	0.001	50	600.00	1	0.10	0.10	0.05	0.05
Other	2,4-Dinitrophenol (DNP)	51-28-5	50	50	10	1000.00	1000.00	2000.00	2000.00	500.00	500.00
Other	Acesulfame	33665-90-6	10000	10000	10	1000000.00	1000000.00	1000000.00	1000000.00	1000000.00	1000000.00
Other	Bisphenol A	80-05-7	0.02	0.02	50	600.00	1	30.00	30.00	10.00	10.00
Other	Bisphenol S	80-09-1	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Caffeine	58-08-2	0.1	0.1	100	10.00	10.00	100.00	0.03	87.00	0.039
Other	Cotinine	486-56-6	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	1.3	1.3		600.00	1	77.00	77.00	320.00	320.00
Other	N,N-Diethyl-m-toluamid (DEET)	134-62-3	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Nicotine	54-11-5	1.4	1.4	50	600.00	1	70.00	70.00	2900.00	2900.00
Other	Perfluorobutanesulfonate (PFBS)	375-73-5	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Perfluoroheptanoic acid (PFHpA)	375-85-9	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Perfluorohexane sulfonate (PFHxS) (anic	108427-53-8	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Perfluorohexanoic acid (PFHxA)	307-24-4	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Perfluorononanoate (PFNA)	375-95-1	0.01	0.01	100	600.00	1	100.00	0.03	10.00	10.00
Other	Perfluorooctanesulfonic acid (PFOS)	1763-23-1	0.23	0.23		5300.00	5300.00	5300.00	5300.00	10.00	10.00
Other	Perfluorooctanoic acid (PFOA)	335-67-1	1	1	100	600.00	1	100.00	0.03	100.00	100.00
Other	Saccharin	81-07-2	0.87	0.00039	100	600.00	1	100.00	0.03	87.00	0.039
Other	Sucralose	56038-13-2	10000	10000	10	1000000.00	1000000.00	1000000.00	1000000.00	1000000.00	1000000.00

Human Tox data

Group	Substance	CAS_No	TIER 1 drinking water pGLV (ug/l)	TIER 1 fish consumption pGLV (mg/kg)	calculated RV mg/kg bw/day	TIER 2 drinking water NOAEL conversion to ug/l	TIER 2 fish consumption NOAEL conversion to mg/kg	NOAEL or equivalent (mg/kg bw/d)	Which eq	AF	AF provided or assumed	Critical effect	Study	Reference
Metals	Arsenic (As) - dissolved	7440-38-2	0.933333333	0.016231884	0.000266667	2.8	0.048695652	0.0008	NOAEL	3	g	Hyperpigmentation, keratosis and possible vascular complications	Human chronic oral exposure	https://toxnet.nlm.nih.gov/
Metals	Cadmium (Cd) - dissolved	7440-43-9	1.75	0.030434783	0.0005	17.5	0.304347826	0.005	NOAEL	10	g	Significant proteinuria	Human studies involving chronic exposures	https://toxnet.nlm.nih.gov/
Metals	Chromium (Cr) - dissolved	7440-47-3	1050	18.26086957	0.3	1001000	17408.69565	286	NOAEL	1000	g	Effects on bodyweight	Long term rat study	EFSA 2014
Metals	Copper (Cu) - dissolved	7440-50-8	245	4.260869565	0.07	490	8.52173913	0.14	NOAEL	2	g	No effects	Human 12 week supplementations study to determine Upper Limit, used as ADI	EFSA 2015
Metals	Lead (Pb) - dissolved	7439-92-1	1.75	0.030434783	0.0005	1.75	0.030434783	0.0005	BMDL1	1	g	Neurology, developmental	Human volunteer study	EFSA 2012
Metals	Mercury (Hg) - dissolved	7439-97-6	2.1	0.036521739	0.0006	210	3.652173913	0.06	BMDL10	100	a	Increased kidney weight	6 month rat study	EFSA 2012
Metals	Nickel (Ni) - dissolved	7440-02-0	38.5	0.669565217	0.011	3850	66.95652174	1.1	NOAEL	100	g		2 gen rodent study	WFD PS dossier
Metals	Zinc (Zn) - dissolved	7440-66-6	1061.666667	18.46376812	0.303333333	3185	55.39130435	0.91	LOAEL	3	g	Decrease in erythrocute Cu, Zn-superoxide dismutase (ESOD) activity in healthy adult male and femal volunteers	Human exposure	https://toxnet.nlm.nih.gov/
PAHs	Anthracene	120-12-7	1166.666667	20.28985507	0.333333333	3500000	60869.56522	1000	NOAEL	3000	g	No observed effects	Subchronic toxicity study in mice	https://toxnet.nlm.nih.gov/
PAHs	Benzo(a)pyrene	50-32-8	2.45	0.042608696	0.0007	245	4.260869565	0.07	BMDL10 (mg/kg bw/day)	100	a	histopathology, neoplastic	Mouse, chronic	EFSA
PAHs	Benzo(b)fluoranthene	205-99-2	11.9	0.206956522	0.0034	1190	20.69565217	0.34	BMDL10 (mg/kg bw/day)	100	a	histopathology, neoplastic	Mouse, chronic	EFSA
PAHs	Benzo(g,h,i)perylene	191-24-2	17.15	0.29826087	0.0049	1715	29.82608696	0.49	BMDL10 (mg/kg bw/day)	100	a	histopathology, neoplastic	Mouse, chronic	EFSA
PAHs	Benzo(k)fluoranthene	207-08-9	17.15	0.29826087	0.0049	1715	29.82608696	0.49	BMDL10 (mg/kg bw/day)	100	a	histopathology, neoplastic	Mouse, chronic	EFSA
PAHs	Fluoranthene	206-44-0	145.8333333	2.536231884	0.041666667	437500	7608.695652	125	NOAEL	3000	g	Nephropathy, increasd liver weights, hematological alterations and clinical effects	Mouse subchronic study	https://toxnet.nlm.nih.gov/
PAHs	Indeno(1,2,3-c,d)pyrene	193-39-5	17.15	0.29826087	0.0049	1715	29.82608696	0.49	BMDL10 (mg/kg/day)	100	a	histopathology, neoplastic	Mouse, chronic	EFSA
PAHs	Naphthalene	91-20-3	82.83333333	1.44057971	0.023666667	248500	4321.73913	71	NOAEL	3000	g	Decreased mean terminal body weight in males	Subchronic oral rat study	https://toxnet.nlm.nih.gov/
Herbicides	2,4-D	94-75-7	35	0.608695652	0.01	3500	60.86956522	1	NOAEL	100	g	Hematologic, hepatic and renal toxicity	90 day rat oral bioassay and 1 year interim report from a 2 year rat oral bioassay	https://toxnet.nlm.nih.gov/
Herbicides	2-Methyl-4-chlorphenoxy acetic acid (MCPA)	94-74-6	1.75	0.030434783	0.0005	525	9.130434783	0.15	NOAEL	300	g	Kidney and liver toxicity	1 year dog feeding study	https://toxnet.nlm.nih.gov/
Herbicides	Ametryn	834-12-8	30.1	0.523478261	0.0086	30100	523.4782609	8.6	NOAEL	1000	g	Liver toxicity	rat subchronic oral gavage bioassay	https://toxnet.nlm.nih.gov/
Herbicides	Aminomethylphosphonic acid (AMPA)	1066-51-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Atrazine	1912-24-9	17.5	0.304347826	0.005	1750	30.43478261	0.5	NOAEL	100	g	Carcinogenicity	Rat	WFD PS dossier
Herbicides	Atrazine-2-hydroxy	2163-68-0	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Atrazine-desethyl	6190-65-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Atrazine-desisopropyl	1007-28-9	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g			TTC
Herbicides	Bentazone	25057-89-0	112	1.947826087	0.032	11200	194.7826087	3.2	NOAEL	100	g	Blood loss into GI tract (NOAEL), coagulation defect (LOAEL)	1 year dog feeding study	https://toxnet.nlm.nih.gov/
Herbicides	Bromacil	314-40-9	437.5	7.608695652	0.125	43750	760.8695652	12.5	NOAEL	100	a		chronic, rat	US EPA
Herbicides	Carbetamide	16118-49-3	210	3.652173913	0.06	21000	365.2173913	6	NOAEL	100	g	Liver changes	2 year rat study	EFSA 2010
Herbicides	Chloridazon	1698-60-8	350	6.086956522	0.1	45500	791.3043478	13	NOAEL	100	g	Body weight	Long term rat study	EFSA 2007
Herbicides	Chloridazon-desphenyl	6339-19-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Chloridazon-methyl-desphenyl	17254-80-7	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g			TTC
Herbicides	Chloroxuron	1982-47-4	350	6.086956522	0.1	35000	608.6956522	10	NOAEL	100	a	Body weight	2 gen rat study	https://toxnet.nlm.nih.gov/
Herbicides	Chlortoluron	15545-48-9	140	2.434782609	0.04	14000	243.4782609	4	NOAEL	100	g		2 year rat study	EC report 2005
Herbicides	Cyanazine (Fortrol)	21725-46-2	1050	18.26086957	0.3	105000	1826.086957	30	NOAEL	100	a		Oral, rat	https://toxnet.nlm.nih.gov/
Herbicides	Cybutryne (Irgarol)	28159-98-0	81.66666667	1.420289855	0.023333333	24500	426.0869565	7	NOAEL	300	g	Liver changes	Rat, oral	WFD PS dossier
Herbicides	Dimefuron	34205-21-5	245	4.260869565	0.07	24500	426.0869565	7	NOAEL	100	a		NOEAL assumed from ADI	https://sitem.herts.ac.uk/aeru/ppdb/en/index.htm
Herbicides	Dimethachlor CGA 369873	1418095-08-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Dimethachlor sulfonic acid CGA 354742	N/A	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Dimethenamid	87674-68-8	70	1.217391304	0.02	7000	121.7391304	2	NOAEL	100	a	Organ weights, hepatotoxicity	Dog, chronic	EFSA pesticide database
Herbicides	Dinoseb	88-85-7	3.5	0.060869565	0.001	3500	60.86956522	1	LOAEL	1000	g	Decreased fetal weight	3 generation rat reproduction study	https://toxnet.nlm.nih.gov/
Herbicides	Dinoterb	1420-07-1	13.125	0.22826087	0.00375	1312.5	22.82608696	0.375	NOAEL	100	a		2 year rat study	UNEP
Herbicides	Diuron	330-54-1	23.8	0.413913043	0.0068	5950	103.4782609	1.7	LOAEL	250	g	Effects on blood system	2 year rat study	WFD PS dossier
Herbicides	Ethidimuron (Sulfadiazole)	30043-49-3	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Ethofumesate	26225-79-6	3500	60.86956522	1	350000	6086.956522	100	NOAEL	100	g		2 year rat study	EFSA 2016
Herbicides	Glyphosate	1071-83-6	350	6.086956522	0.1	35000	608.6956522	10	NOAEL	100	g	Increased incidence of renal tubular dilation in	3 generation rat reproduction study	https://toxnet.nlm.nih.gov/
Herbicides	Hexazinon	51235-04-2	116.6666667	2.028985507	0.033333333	35000	608.6956522	10	NOAEL	300	g	Decreased body weight	2 year rat feeding study	https://toxnet.nlm.nih.gov/
Herbicides	Isoproturon	34123-59-6	54.25	0.943478261	0.0155	10850	188.6956522	3.1	NOAEL	200	g	histopathology, neoplastic, hepatotoxicity	Rat, chronic	WFD PS dossier
Herbicides	Linuron	330-55-2	7.291666667	0.126811594	0.002083333	2187.5	38.04347826	0.625	LOAEL	300	g	Abnormal blood pigment	2 year dog feeding study	https://toxnet.nlm.nih.gov/
Herbicides	Metamitron	41394-05-2	105	1.826086957	0.03	10500	182.6086957	3	NOAEL	100	g	clinical chemistry	chronic, Dog	EFSA 2008
Herbicides	Metazachlor	67129-08-2	280	4.869565217	0.08	29750	517.3913043	8.5	NOAEL	100	g	Organ weights, hepatotoxicity	chronic, Rat	EFSA 2017
Herbicides	Metazachlor ESA	172960-62-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Metazachlor OA	1231244-60-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Methabenzthiazuron	18691-97-9	14	0.243478261	0.004	26250	456.5217391	7.5	NOAEL	1875	a			Australian Government
Herbicides	Metobromuron	3060-89-7	28	0.486956522	0.008	2800	48.69565217	0.8	NOAEL	100	g	haematology	chronic, Mouse	EFSA 2014
Herbicides	Metolachlor	51218-45-2	525	9.130434783	0.15	52500	913.0434783	15	NOAEL	100	a	Reduced pup weights and parental food consun	2 generation rat reproduction study	https://toxnet.nlm.nih.gov/
Herbicides	Metolachlor ESA	171118-09-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Metoxuron	19937-59-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Monolinuron	1746-81-2	10.5	0.182608696	0.003	5250	91.30434783	1.5	NOAEL	500	g		2 year rat study	EFSA pesticide database
Herbicides	Prometryn	7287-19-6	13.125	0.22826087	0.00375	13125	228.2608696	3.75	NOAEL	1000	g	Liver and kidney degeneration and bown marrow atrophy	106 week dog feeding study	https://toxnet.nlm.nih.gov/
Herbicides	Propazine	139-40-2	58.33333333	1.014492754	0.016666667	17500	304.3478261	5	NOAEL	300	g	Decreased body weight		https://toxnet.nlm.nih.gov/
Herbicides	Propazine-2-hydroxy	7374-53-0	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Simazine	122-34-9	17.5	0.304347826	0.005	1750	30.43478261	0.5	NOAEL	100	g	Carcinogenicity	Rat study	WFD PS dossier
Herbicides	S-Metolachlor CGA 368208	1173021-76-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	S-Metolachlor NOA 413173	1418095-19-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Terbutryn	886-50-0	3.5	0.060869565	0.001	350	6.086956522	0.1	NOAEL	100	g	Hematological effects in females	2 year rat feeding study	WFD PS dossier
Herbicides	Terbutylazine	5915-41-3	12.25	0.213043478	0.0035	1225	21.30434783	0.35	NOAEL	100	a	Body weight	Rat, chronic	EFSA pesticide database
Herbicides	Terbutylazine CGA 324007	309923-18-0	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Terbutylazine SYN 545666	N/A	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Terbutylazine-2-hydroxy	66753-07-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Terbutylazine-desethyl	30125-63-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Herbicides	Terbutylazine-desethyl-2-hydroxy	66753-06-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Insecticides	Diazinone	333-41-5	0.7	0.012173913	0.0002	70	1.217391304	0.02	NOAEL	100	a	Clinical chemistry, neurotoxicity	Dog, chronic	EFSA pesticide database
Insecticides	Fipronil	120068-37-3	0.7	0.012173913	0.0002	70	1.217391304	0.02	NOAEL	100	a	clinical signs, neurotoxicity	Rat, chronic	https://toxnet.nlm.nih.gov/
Fungicides	4-Chlorophenol	106-48-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Fungicides	Azoxystrobin	131860-33-8	630	10.95652174	0.18	63000	1095.652174	18	NOAEL	100	a	Organ weights, hepatotoxicity	Rat, chronic	https://toxnet.nlm.nih.gov/
Fungicides	Carbendazim	10605-21-7	87.5	1.52173913	0.025	8750	152.173913	2.5	NOAEL	100	g		1 year dog study	Schriks et al. 2010
Fungicides	Cyproconazol	94361-06-5	70	1.217391304	0.02	7000	121.7391304	2	NOAEL	100	g	Hepatotoxicity	2 generation rat study	EFSA 2010
Fungicides	Flusilazole	85509-19-9	2.333333333	0.04057971	0.000666667	700	12.17391304	0.2	NOAEL	300	g	Liver cell enlargement	1 year dog feeding study	https://toxnet.nlm.nih.gov/
Fungicides	Metalaxyl NOA 409045	75596-99-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Fungicides	Picoxystrobin	117428-22-5	168	2.92173913	0.048	16800	292.173913	4.8	NOAEL	100	a	not specified	90 days rat subchronic	EFSA pesticide database
Fungicides	Propiconazole	60207-90-1	43.75	0.760869565	0.0125	4375	76.08695652	1.25	NOAEL	100	g	Gastric mucosal irritation	1 year dog feeding study	https://toxnet.nlm.nih.gov/
Fungicides	Quinoxyfen	124495-18-7	700	12.17391304	0.2	70000	1217.391304	20	NOAEL	100	g	Liver hypertrophy and glomerulonephrosis, reduced bw	Rat, oral, 2 year study	WFD PS dossier
Fungicides	Tebuconazol	107534-96-3	105	1.826086957	0.03	10500	182.6086957	3	NOAEL	100	a	Histopathology non-neoplastic, endocrine	Dog, chronic	EFSA pesticide database
Fungicides	Trifloxystrobin CGA 321113	252913-85-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Pharmaceuticals	10,11-Dihydro-10,11-dihydroxycarbamazepine	58955-93-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	17-beta Estradiol	50-28-2	0.175	0.003043478	0.00005	17.5	0.304347826	0.005	NOAEL	100	g	Hormone dependent parameters in postmenopausal women	Human clinical studies	WFD PS dossier
Pharmaceuticals	1-Adamantylamin	768-94-5	100	1.739130435	0.028571429	10000	173.9130435	2.857142857	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	2-Hydroxycarbamazepine	68011-66-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	3,4-Methylendioxyamphetamine (MDA)	4764-17-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA (drug of abuse)		na
Pharmaceuticals	3,4-Methylenedioxyethamphetamine (MDEA)	14089-52-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		na
Pharmaceuticals	6-Acetylmorphine	2784-73-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	7-Aminoclonazepam	4959-17-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	7-Aminoflunitrazepam	34084-50-9	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	metabolite		TTC
Pharmaceuticals	Acetylcodeine	6703-27-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Acetyl-sulfamethoxazole	21312-10-7	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	metabolite		TTC
Pharmaceuticals	Alfentanil	71195-58-9	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	nervous system		no DDD given, therefore TTC
Pharmaceuticals	alpha-Hydroxyalprazolam	37115-43-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	alpha-Hydroxymidazolam	59468-90-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	alpha-Hydroxytriazolam	37115-45-0	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Alprazolam	28981-97-7	0.5	0.008695652	0.000142857	50	0.869565217	0.014285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Amidotrizoic acid	117-96-4	25	0.434782609	0.007142857	2500	43.47826087	0.714285714	DDD	100	g	contrast agent (Schricks et al.)		derived from DDD
Pharmaceuticals	Amisulpride	71675-85-9	200	3.47826087	0.057142857	20000	347.826087	5.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Amitriptyline	50-48-6	37.5	0.652173913	0.010714286	3750	65.2173913	1.071428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Amoxapine	14028-44-5	75	1.304347826	0.021428571	7500	130.4347826	2.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Amoxicillin	26787-78-0	500	8.695652174	0.142857143	50000	869.5652174	14.28571429	DDD	100	g	antibacterial		derived from DDD
Pharmaceuticals	Amphetamine	300-62-9	7.5	0.130434783	0.002142857	750	13.04347826	0.214285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Atenolol	29122-68-7	37.5	0.652173913	0.010714286	3750	65.2173913	1.071428571	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Atropine	51-55-8	0.75	0.013043478	0.000214286	75	1.304347826	0.021428571	DDD	100	g	metabolism		derived from DDD
Pharmaceuticals	Benzoylecgonine	519-09-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite /DOA		TTC
Pharmaceuticals	Betaxolol	63659-18-7	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Bezafibrate	41859-67-0	300	5.217391304	0.085714286	30000	521.7391304	8.571428571	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Bisoprolol	66722-44-9	5	0.086956522	0.001428571	500	8.695652174	0.142857143	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Bromazepam	1812-30-2	5	0.086956522	0.001428571	500	8.695652174	0.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Buprenorphine	52485-79-7	0.6	0.010434783	0.000171429	60	1.043478261	0.017142857	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Buprenorphine glucuronide	101224-22-0	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Candesartan	139481-59-7	4	0.069565217	0.001142857	400	6.956521739	0.114285714	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Carbamazepine	298-46-4	55.61111111	0.967149758	0.015888889	5005	87.04347826	1.43	LOAEL	90	g	teratogenocoty and possible carcinogeixity		RIVM 2014
Pharmaceuticals	Carbamazepine-10,11-epoxide	36507-30-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Carisoprodol	78-44-4	700	12.17391304	0.2	70000	1217.391304	20	DDD	100	g	muscolo-skeletal		derived from DDD
Pharmaceuticals	Cetirizine	83881-51-0	5	0.086956522	0.001428571	500	8.695652174	0.142857143	DDD	100	g	respiratory		derived from DDD
Pharmaceuticals	Chlorprothixene	113-59-7	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Citalopram	59729-33-8	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Clobazam (Urbadan)	22316-47-8	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Clonazepam	1622-61-3	4	0.069565217	0.001142857	400	6.956521739	0.114285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Clonidine	4205-90-7	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Clozapine	5786-21-0	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Cocaethylene	529-38-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite /DOA		TTC
Pharmaceuticals	Cocaine	50-36-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	Codeine	76-57-3	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	respiratory		derived from DDD
Pharmaceuticals	CP 47,497	70434-82-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	CP 47,497-C8 homologue	70434-92-3	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	Crotamiton	483-63-6	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	top		TTC
Pharmaceuticals	Desalkylflurazepam	2886-65-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Desipramine	50-47-5	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Dextromethorphan (Methorphan)	125-71-3	45	0.782608696	0.012857143	4500	78.26086957	1.285714286	DDD	100	g	respiratory		derived from DDD
Pharmaceuticals	Diazepam	439-14-5	1.015	0.017652174	0.00029	101.5	1.765217391	0.029	LOAEL	100	g	Increased prothrombin time	Human clinical studies	https://toxnet.nlm.nih.gov/
Pharmaceuticals	Diclofenac	15307-79-6	175	3.043478261	0.05	17500	304.3478261	5	LOAEL	100	g	not specified	Baboon oral 12 month.	WFD PS dossier
Pharmaceuticals	Digitoxin	71-63-6	0.05	0.000869565	1.42857E-05	5	0.086956522	0.001428571	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Digoxin	20830-75-5	0.125	0.002173913	3.57143E-05	12.5	0.217391304	0.003571429	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Dihydrocodeine	125-28-0	75	1.304347826	0.021428571	7500	130.4347826	2.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Diphenhydramine	58-73-1	100	1.739130435	0.028571429	10000	173.9130435	2.857142857	DDD	100	g	respiratory		derived from DDD
Pharmaceuticals	Dothiepin	113-53-1	75	1.304347826	0.021428571	7500	130.4347826	2.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Doxepin	1668-19-5	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	EDDP (metabolite of Methadone)	30223-73-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite /DOA		TTC
Pharmaceuticals	Felbamate	25451-15-4	1200	20.86956522	0.342857143	120000	2086.956522	34.28571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Fenazepam	51753-57-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA / banned		TTC
Pharmaceuticals	Fenofibrate	49562-28-9	100	1.739130435	0.028571429	10000	173.9130435	2.857142857	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Fentanyl	437-38-7	0.3	0.005217391	8.57143E-05	30	0.52173913	0.008571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Flumazenil	78755-81-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	antidotes		TTC
Pharmaceuticals	Flunitrazepam	1622-62-4	0.5	0.008695652	0.000142857	50	0.869565217	0.014285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Flupentixol	2709-56-0	3	0.052173913	0.000857143	300	5.217391304	0.085714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Flurazepam	17617-23-1	15	0.260869565	0.004285714	1500	26.08695652	0.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Gabapentin	60142-96-3	900	15.65217391	0.257142857	90000	1565.217391	25.71428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Gabapentin-lactam	64744-50-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Haloperidol	52-86-8	4	0.069565217	0.001142857	400	6.956521739	0.114285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Hydrochlorothiazide	58-93-5	12.5	0.217391304	0.003571429	1250	21.73913043	0.357142857	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Hydrocodone	125-29-1	7.5	0.130434783	0.002142857	750	13.04347826	0.214285714	DDD	100	g	respiratory		derived from DDD
Pharmaceuticals	Hydromorphone	466-99-9	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Imipramine	50-49-7	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Indometacin	53-86-1	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	antiinflammatory		derived from DDD
Pharmaceuticals	Iohexol	66108-95-0	37500	652.173913	10.71428571	3750000	65217.3913	1071.428571	DDD	100	g	contrast agent (Schricks et al.)		derived from DDD
Pharmaceuticals	Iomeprol	78649-41-9	6666.666667	115.942029	1.904761905	14000000	243478.2609	4000	NOAEL	2100	g	effects on liver and kidney	Dog study	Schriks et al. 2010
Pharmaceuticals	Iopamidol	62883-00-5	41500	721.7391304	11.85714286	4150000	72173.91304	1185.714286	DDD	100	g	contrast agent (Schricks et al.)		derived from DDD
Pharmaceuticals	Iopromid	73334-07-3	25000	434.7826087	7.142857143	2500000	43478.26087	714.2857143	DDD	100	g	contrast agent (Schricks et al.)		derived from DDD
Pharmaceuticals	Irbesartan	138402-11-6	75	1.304347826	0.021428571	7500	130.4347826	2.142857143	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	JWH-018 (N-(n-pentanoic acid)	209414-07-3	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	JWH-073 (2-methylnaphthyl analog)	1427325-61-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	Ketamine	6740-88-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	nervous system		no DDD given, therefore TTC
Pharmaceuticals	Ketoprofen	22071-15-4	17.5	0.304347826	0.005	175	3.043478261	0.05	NOAEL	10	g	slight analgesic effect	human study	EMEA, 1995
Pharmaceuticals	Lamotrigine	84057-84-1	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Librium (Chlordiazepoxide)	58-25-3	15	0.260869565	0.004285714	1500	26.08695652	0.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Lidocaine	137-58-6	1500	26.08695652	0.428571429	150000	2608.695652	42.85714286	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Lorazepam	846-49-1	1.25	0.02173913	0.000357143	125	2.173913043	0.035714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Losartan	114798-26-4	25	0.434782609	0.007142857	2500	43.47826087	0.714285714	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Maprotiline	10262-69-8	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Medazepam	364-85-4	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Meperidine (Pethidine)	57-42-1	200	3.47826087	0.057142857	20000	347.826087	5.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Methamphetamine	537-46-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	Methylendioxymethamphetamine (MDMA)	69610-10-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	Methylphenidate	113-45-1	15	0.260869565	0.004285714	1500	26.08695652	0.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Metoprolol	37350-58-6	9.8	0.170434783	0.0028	980	17.04347826	0.28	DDD	100	g	cardiovascular		RIVM 2014
Pharmaceuticals	Metroprolol acid	56392-14-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Midazolam	59467-70-8	7.5	0.130434783	0.002142857	750	13.04347826	0.214285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Mirtazapine	61337-67-5	15	0.260869565	0.004285714	1500	26.08695652	0.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Morphine	57-27-2	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Morphine glucuronide	20290-10-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	n-Acetyl-4-aminoantipyrine	83-15-8	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	metabolite		TTC
Pharmaceuticals	Nadolol	42200-33-9	80	1.391304348	0.022857143	8000	139.1304348	2.285714286	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Naltrexone	16590-41-3	25	0.434782609	0.007142857	2500	43.47826087	0.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Naproxen	22204-53-1	1983.333333	34.49275362	0.566666667	595000	10347.82609	170	NOAEL	300	g	no effects	Mouse developmental	Bull et al. 2014
Pharmaceuticals	N-Desmethylclozapine	6104-71-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	N-Formyl-4-aminoantipyrine	1672-58-8	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	metabolite		TTC
Pharmaceuticals	Nitrazepam	146-22-5	2.5	0.043478261	0.000714286	250	4.347826087	0.071428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Norbuprenorphine	78715-23-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Nordiazepam	1088-11-5	7.5	0.130434783	0.002142857	750	13.04347826	0.214285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Norfentanyl	1609-66-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	met		TTC
Pharmaceuticals	Normeperidine (Norpethidine)	77-17-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	met		TTC
Pharmaceuticals	Norpropoxyphene (Desmethyl propoxyphene)	32504-12-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	met		TTC
Pharmaceuticals	Nortriptyline	72-69-5	37.5	0.652173913	0.010714286	3750	65.2173913	1.071428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	O-Desmethyltramadol	73986-53-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	met		TTC
Pharmaceuticals	O-Desmethylvenlafaxine (Desvenlafaxine)	93413-62-8	25	0.434782609	0.007142857	2500	43.47826087	0.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Olanzapine	132539-06-1	5	0.086956522	0.001428571	500	8.695652174	0.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Opipramol	315-72-0	75	1.304347826	0.021428571	7500	130.4347826	2.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Oxazepam	604-75-1	25	0.434782609	0.007142857	2500	43.47826087	0.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Oxcarbazepine	28721-07-5	500	8.695652174	0.142857143	50000	869.5652174	14.28571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Oxycodone	76-42-6	37.5	0.652173913	0.010714286	3750	65.2173913	1.071428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Oxymorphone	76-41-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA / banned		TTC
Pharmaceuticals	Paliperidone (9-Hydroxyrisperidone)	144598-75-4	3	0.052173913	0.000857143	300	5.217391304	0.085714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Paroxetine	61869-08-7	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Pentazocine	359-83-1	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Pentobarbital	76-74-4	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Pentoxifylline	6493-05-6	500	8.695652174	0.142857143	50000	869.5652174	14.28571429	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Phenacetin	62-44-2	900	15.65217391	0.257142857	90000	1565.217391	25.71428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Phenazone	60-80-0	1500	26.08695652	0.428571429	150000	2608.695652	42.85714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Phencyclidine (PCP)	77-10-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	DOA		TTC
Pharmaceuticals	Phentermine	122-09-8	7.5	0.130434783	0.002142857	750	13.04347826	0.214285714	DDD	100	g	metabolism / antiobesity		derived from DDD
Pharmaceuticals	Phenytoin	125-59-7	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Pipamperone	1893-33-0	100	1.739130435	0.028571429	10000	173.9130435	2.857142857	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Prazepam	2955-38-6	15	0.260869565	0.004285714	1500	26.08695652	0.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Pregabalin	148553-50-8	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD

Pharmaceuticals	Primidone	125-33-7	625	10.86956522	0.178571429	62500	1086.956522	17.85714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Promazine	58-40-2	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Promethazine	60-87-7	12.5	0.217391304	0.003571429	1250	21.73913043	0.357142857	DDD	100	g	respiratory		derived from DDD
Pharmaceuticals	Propafenone	54063-53-5	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Propoxyphene (Dextropropoxyphene)	469-62-5	100	1.739130435	0.028571429	10000	173.9130435	2.857142857	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Propranolol	525-66-6	80	1.391304348	0.022857143	8000	139.1304348	2.285714286	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Propyphenazone	479-92-5	1500	26.08695652	0.428571429	150000	2608.695652	42.85714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Protriptyline	438-60-8	15	0.260869565	0.004285714	1500	26.08695652	0.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Quetiapine	111974-69-7	200	3.47826087	0.057142857	20000	347.826087	5.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Risperidone	106266-06-2	2.5	0.043478261	0.000714286	250	4.347826087	0.071428571	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Ritalinic acid	19395-41-6	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	met		TTC
Pharmaceuticals	Secobarbital	76-73-3	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Sertraline	79617-96-2	25	0.434782609	0.007142857	2500	43.47826087	0.714285714	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Sotalol	3930-20-9	80	1.391304348	0.022857143	8000	139.1304348	2.285714286	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Strophanthidin	66-28-4	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g	cardiovascular toxin		TTC
Pharmaceuticals	Sulfadimidin / Sulfamethazin	57-68-1	2000	34.7826087	0.571428571	200000	3478.26087	57.14285714	DDD	100	g	antibacterial		derived from DDD
Pharmaceuticals	Sulfamethoxazole	723-46-6	437.5	7.608695652	0.125	87500	1521.73913	25	NOAEL	200	g	thyroid disruption (?)	60 week rat study	Schriks et al. 2010
Pharmaceuticals	Sulpirid	15676-16-1	400	6.956521739	0.114285714	40000	695.6521739	11.42857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Telmisartan	144701-48-4	20	0.347826087	0.005714286	2000	34.7826087	0.571428571	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Temazepam	846-50-4	10	0.173913043	0.002857143	1000	17.39130435	0.285714286	DDD	100	g	nervous system		Houtman et al. 2014
Pharmaceuticals	Topiramate	97240-79-4	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Tramadol	27203-92-5	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Trazodone	19794-93-5	150	2.608695652	0.042857143	15000	260.8695652	4.285714286	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Triazolam	28911-01-5	0.125	0.002173913	3.57143E-05	12.5	0.217391304	0.003571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Trimethoprim	738-70-5	672	11.68695652	0.192	672000	11686.95652	192	NOAEL	1000	g	developmental effects (cleft palate)	Rat study	Bruce et al. 2010
Pharmaceuticals	Trimipramine	739-71-9	75	1.304347826	0.021428571	7500	130.4347826	2.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Valsartan	137862-53-4	40	0.695652174	0.011428571	4000	69.56521739	1.142857143	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Valsartan acid	164265-78-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g	metabolite		TTC
Pharmaceuticals	Venlafaxine	93413-69-5	50	0.869565217	0.014285714	5000	86.95652174	1.428571429	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Verapamil	52-53-9	120	2.086956522	0.034285714	12000	208.6956522	3.428571429	DDD	100	g	cardiovascular		derived from DDD
Pharmaceuticals	Zolpidem	82626-48-0	5	0.086956522	0.001428571	500	8.695652174	0.142857143	DDD	100	g	nervous system		derived from DDD
Pharmaceuticals	Zopiclone	43200-80-2	3.75	0.065217391	0.001071429	375	6.52173913	0.107142857	DDD	100	g	nervous system		derived from DDD
Polar compounds	1H-Benzotriazole	95-14-7	1032.5	17.95652174	0.295	1032500	17956.52174	295	LOAEL	1000	g	bw, inflammation of uterus/prostate	Rat study	Schriks et al. 2010
Polar compounds	2-(Methylthio)benzothiazole	615-22-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Polar compounds	2-Ethylhexyl diphenyl phosphate (EHDP)	1241-94-7	1.05	0.01826087	0.0003	105	1.826086957	0.03	TTC	100	g			TTC
Polar compounds	5,6-Dimethylbenzotriazole	4184-79-6	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Polar compounds	5-Methyl-1H-benzotriazole	136-85-6	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Polar compounds	Benzothiazole-6-carboxylic acid	3622-35-3	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Polar compounds	Nonylphenol (4-Nonylphenol)	104-40-5	525	9.130434783	0.15	52500	913.0434783	15	NOAEL	100	g	reproductive effects	Rat, reproduction	WFD PS dossier
Polar compounds	Tolyltriazol (mix of isomers)	29385-43-1	875	15.2173913	0.25	525000	9130.434783	150	NOAEL	600	g	observed mild apathy	29 day rat study	Schriks et al. 2010
Polar compounds	Triisobutyl phosphate (TIBP)	126-71-6	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g			TTC
Polar compounds	Tri-n-butyl phosphate (TnBP)	126-73-8	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g			TTC
Polar compounds	Tri-n-propyl phosphate (TnPP)	513-08-6	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g			TTC
Polar compounds	Triphenyl phosphate (TPT)	115-86-6	1.05	0.01826087	0.0003	105	1.826086957	0.03	TTC	100	g			TTC
Polar compounds	Tris(1-chloro-2-propyl)phosphate (TCPP)	13674-84-5	0.00875	0.000152174	0.0000025	0.875	0.015217391	0.00025	TTC	100	g			TTC
Polar compounds	Tris(2-butoxyethyl)phosphate (TBEP)	78-51-3	1.05	0.01826087	0.0003	105	1.826086957	0.03	TTC	100	g			TTC
Polar compounds	Tris(2-chloroethyl)phosphate (TCEP)	115-96-8	77	1.339130435	0.022	77000	1339.130435	22	NOAEL	1000	g	increased liver and kidney weights	16 weeks rat study	Schriks et al. 2010
Polar compounds	Tris(3,5-dimethylphenyl)phosphate (T35DMPP)	25653-16-1	1.05	0.01826087	0.0003	105	1.826086957	0.03	TTC	100	g			TTC
Polar compounds	Tris(methylphenyl)phosphate (TMPP)	1330-78-5	1.05	0.01826087	0.0003	105	1.826086957	0.03	TTC	100	g			TTC
Organotin compounds	Dibutyltin-cation	1002-53-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Organotin compounds	Dioctyltin-cation	94410-05-6	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Organotin compounds	Diphenyltin-cation	6381-06-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Organotin compounds	Tetrabutyltin	1461-25-2	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Organotin compounds	Tributyltin-cation	36643-28-4	0.875	0.015217391	0.00025	87.5	1.52173913	0.025	NOAEL	100	g	immunotoxicity	Rat, 17 month feeding study	WFD PS dossier
Organotin compounds	Triphenyltin-cation	668-34-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	2,4-Dinitrophenol (DNP)	51-28-5	7	0.12173913	0.002	7000	121.7391304	2	LOAEL	1000	g	Cataract formation	Human chronic and subchronic exposures	https://toxnet.nlm.nih.gov/
Other	Acesulfame	33665-90-6	96285	1674.521739	27.51	9628500	167452.1739	2751	NOAEL	100	a	Calculated developmental NOEL	Rat, multigen repro study	Kroes et al.
Other	Bisphenol A	80-05-7	175	3.043478261	0.05	17500	304.3478261	5	NOAEL	100	a	Organ weights, hepatotoxicity	Mouse reproduction toxicity	EFSA db
Other	Bisphenol S	80-09-1	58.33333333	1.014492754	0.016666667	35000	608.6956522	10	NOAEL	600	g	liver effects	Rat study	Schriks et al. 2010
Other	Caffeine	58-08-2	21000	365.2173913	6	21000	365.2173913	6	?	1	g	restlessness anxiety	human	Navrot 2003 Food Add Contam 20, 1-30
Other	Cotinine	486-56-6	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	168	2.92173913	0.048	16800	292.173913	4.8	NOAEL	100	g	developmental toxicity, testicular effects	Rat, reproduction	WFD PS dossier/ EFSA db
Other	N,N-Diethyl-m-toluamid (DEET)	134-62-3	6250	108.6956522	1.785714286	350000	6086.956522	100	NOAEL	56	g	reduced haemoglobin/haematocrit levels and histological changes in liver, lymph nodes and uterus	1 year dog study	Schriks et al. 2010
Other	Nicotine	54-11-5	0.28	0.004869565	0.00008	2.8	0.048695652	0.0008	LOAEL	10	g	increased heart rate	human study	EFSA 2009
Other	Perfluorobutanesulfonate (PFBS)	375-73-5	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	Perfluoroheptanoic acid (PFHpA)	375-85-9	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	Perfluorohexane sulfonate (PFHxS) (anion)	108427-53-8	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	Perfluorohexanoic acid (PFHxA)	307-24-4	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	Perfluorononanoate (PFNA)	375-95-1	5.25	0.091304348	0.0015	525	9.130434783	0.15	TTC	100	g			TTC
Other	Perfluorooctanesulfonic acid (PFOS)	1763-23-1	0.525	0.009130435	0.00015	105	1.826086957	0.03	NOAEL	200	g	hormone	Rhesus money, chronic	WFD PS dossire/ EFSA 2008
Other	Perfluorooctanoic acid (PFOA)	335-67-1	5.425	0.094347826	0.00155	1085	18.86956522	0.31	BMDL10 (mg/kg bw/day)	200	a	Histopathology non-neoplastic, hepatotoxicity	Rat, reproduction	EFSA 2008
Other	Saccharin	81-07-2	13300	231.3043478	3.8	1330000	23130.43478	380	NOAEL	100	g	bladder tumours	Rat	EC - Scientific Committee on Food, value corrected for free acid
Other	Sucralose	56038-13-2	52500	913.0434783	15	5250000	91304.34783	1500	NOAEL	100	g	Reduction in body weight gain	Several animal studies	EC - Scientific Committee on Food

ANNEX 4

30.08.2018	**Martin**	Chemical names cleaned, MW checked for ca. 50% of compounds, SMILES & InChI included (yellow fields are missing or suspicious), Results from ToxTree included
03.09.2018	**Martin**	DDD values from DANUBE assessment added, Descriptors (mean, max) from all modelled RHINE water concentrations addded (for guidance of compound importance)
05.09.2018	**Martin**	Chronic human tox data for all pesticides added (only from mammalians, oral route), very few missing values with acute ED50s replaced
10.09.2018	**Sibylle**	Pharmaceuticals: human tox data and DDD values
11.09.2018	**Martin**	Chronic human tox data for all REACH compounds with high modelled water concentrations in Rhine added (only from mammalians, oral route), very few missing values with acute ED50s replaced
11.09.2018	**Martin**	Sheet "ECOTOX-FINAL" included, with link to control parameter (extrapolation factor, TTC)
16.09.2018	**Martin**	Added MW as basic data to all relevant sheets and added unit conversion from ug/l to mol/m3 (HINT: not anymore relvant)
20.09.2018	**Martin**	Added indicator variables in Human tox, for purposes of robust coding the sheets TOXTREE and DD are merged into HUMAN TOX
21.09.2018	**Martin**	Dinking water intake and fish consumption uptake equivalents included
24.09.2018	**Sibylle**	Update control parameters

ECOTOX control parameter

Daphnia acute

EC50 to NOEC extrapolation:	3		Factor
Missing value:	0.3	[ug/l]	5% percentile from all acute tox values

Daphnia chronic

EC50 to NOEC extrapolation:	3		Factor
Missing value:	0.03	[ug/l]	5% percentile from all chronic tox values
Missing value:	0.03	[ug/l]	5% percentile from all chronic reproduction tox values

Fish acute

EC50 to NOEC extrapolation:	3		Factor
Missing value:	0.39	[ug/l]	5% percentile from all acute tox values

Fish chronic

EC50 to NOEC extrapolation:	3		Factor
Missing value:	0.039	[ug/l]	5% percentile from all chronic tox values
Missing value:	0.039	[ug/l]	5% percentile from all chronic reproduction tox values

Algae (acute & chronic)

EC50 to NOEC extrapolation:	3		Factor
Missing value:	1	[ug/l]	5% percentile from all tox values

HUMAN TOX control parameter

Body weight, adult:	70	[kg]		
LOEL to NOEL extrapolation:	3		Factor	
Human to animal extrapolation:	100		Factor	NOELs derived from Human studies require not the standard AF=100 in the MRA, thus these value are multiplied by this factor to achieve a better assessment comparability in the final HRA assesment (whit PODIs>(1/AF), AF=100, are considered as benchmark for concern)

Cramer classes (derived from TOXTREE)

I	3	[mg/kg/day]	These are TTC estimations for compounds with unreported toxicity, with a Genotox alert ranked above the Cramer class estimation . If TOXTREE failed to provide an estimation, compound was set to class III. (EFSA 2011, Draft EFSA opinion on TTC concept for predicting human health risks)
II	0.91	[mg/kg/day]	
III	0.15	[mg/kg/day]	
Genotox alert	0.0003	[mg/kg/day]	

Drinking-water abstraction

Daily uptake of drinking water	2	[Ltr]		Technical guidance value for deriving EQS-WFD 27 EC 2011
intake of the substance via drinking water does not exceed X% of the NOEL	10	%	Factor	Technical guidance value for deriving EQS-WFD 27 EC 2011

Fish consumption

daily fish consumption	0.115	[kd/day]		Technical guidance value for deriving EQS-WFD 27 EC 2011
uptake of the substance from fishery products does not exceed X% of the NOEL	10	%	Factor	Technical guidance value for deriving EQS-WFD 27 EC 2011

CAS	CAS_NR	ID	Compound	Emissions	Compound (NIST)	Compound (ECOTOX)	Formula (NIST)	Formula_EINECS	MW	Canonical_Smiles	InChI	ALogP	LogD	ValidDanube	ValidRhine	ValidScarce
100986-85-4	100986854	139	**Levofloxacin**	1_Pharma		(3S)-9-Fluoro-2,3-dihydro-3-methyl-10-(4-methyl-1-piperazinyl)-7-oxo-7H-pyrido[1,2,3-			361.38	CC1COC2=C3N1C=C(C(=O)C3=CC(=C2N4CCN(CC4)C)F)C(=O)O	InChI=1S/C18H20FN3O4/c1-10-9-26-17-14-11(16(23)12(18(24)25)8-22(10)14)7-13(19)15(17)21-5-3-20(2)4-6-21/h7-8,10H			1	1	1
10238-21-8	10238218	152	**Glibenklamid**	1_Pharma	Glyburide	Glibenclamide	C23H28ClN3O5S	C23H27ClN3O5S	494.01	COc1ccc(Cl)cc1C(=O)NCCc2ccc(cc2)S(=O)(=O)[N-]C(=O)NC3CCCCC3	InChI=1/C23H28ClN3O5S/c1-32-21-12-9-17(24)15-20(21)22(28)25-14-13-16-7-10-19(11-8-16)33(30,31)27-23(29)26-18-5-3-2-4-6-18/h7-12,15,18H,2-6,13-14H2,1H3,(H3,25,26,27,28,29)/p-1	4.243	4.236	1	1	1
103-90-2	103902	165	**paracetamol**	1_Pharma	Acetaminophen	N-(4-Hydroxyphenyl)acetamide	C8H9NO2	C8H9NO2	151.17	CC(=O)Nc1ccc(O)cc1	InChI=1/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)	0.708	0.708	1	1	1
114-07-8	114078	336	**erythromycin**	1_Pharma		Erythromycin		C37H68NO13	733.94	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@	InChI=1/C37H67NO13/c1-14-25-37(10,45)30(41)20(4)27(39)18(2)16-35(8,44)32(51-34-28(40)24(38(11)12)15-19(3)47-34)21(5)29(22(6)33(43)49-25)50-26-17-36(9,46-13)31(42)23(7)48-26/h18-26,28-32,34,40-42,44-45H,14-17H2,1-13H3/p+1/t18-,19-,20+,21+,22-,23+,24+,25-,26+,28-,29+,30-,31+,32-,34+,35-,36-,37-/m1/s1	0.231	0.586	1	1	1
114798-26-4	114798264	1626	**Losartan**	1_Pharma		1H-Imidazole-5-methanol, 2-butyl-4-chloro-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-			422.93	CCCCC1=NC(=C(N1CC2=CC=C(C=C2)C3=CC=CC=C3C4=NNN=N4)CO)Cl	InChI=1S/C22H23ClN6O/c1-2-3-8-20-24-21(23)19(14-30)29(20)13-15-9-11-16(12-10-15)17-6-4-5-7-18(17)22-25-27-28-26			1	1	1
120-51-4	120514	359	**benzyl benzoate**	1_Pharma	Benzyl Benzoate	Benzoic acid, Phenylmethyl ester	C14H12O2	C14H12O2	212.25	O=C(OCc1ccccc1)c2ccccc2	InChI=1/C14H12O2/c15-14(13-9-5-2-6-10-13)16-11-12-7-3-1-4-8-12/h1-10H,11H2	3.268	3.268	1	1	1
121-75-5	121755	374	**Malathion**	1_Pharma	Malathion	Malathion	C10H19O6PS2	C10H19O6PS2	330.36	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC	InChI=1/C10H19O6PS2/c1-5-15-9(11)7-8(10(12)16-6-2)19-17(18,13-3)14-4/h8H,5-7H2,1-4H3	1.787	1.787	1	1	1
123-99-9	123999	1782	**azelaic acid**	1_Pharma	Nonanedioic acid	azelaic acid	C9H16O4	C9H14O4	188.22	[O-]C(=O)CCCCCCCC(=O)[O-]	InChI=1/C9H16O4/c10-8(11)6-4-2-1-3-5-7-9(12)13/h1-7H2,(H,10,11)(H,12,13)/p-2	-1.027	-0.976	1	1	1
126-07-8	126078	1144	**Griseofulvin**	1_Pharma	Griseofulvin	Griseofulvin	C17H17ClO6	C17H17ClO6	352.77	COC1=CC(=O)C[C@@H](C)[C@]12Oc3c(Cl)c(OC)cc(OC)c3C2=O	InChI=1/C17H17ClO6/c1-8-5-9(19)6-12(23-4)17(8)16(20)13-10(21-2)7-11(22-3)14(18)15(13)24-17/h5,7-8H,6H2,1-4H3/t8-,17+/m1/s1	2.495	2.495	1	1	1
127-07-1	127071	411	**Hydroxikarbamid**	1_Pharma		Hydroxyurea		CH4N2O2	76.057	NC(=O)NO	InChI=1/CH4N2O2/c2-1(4)3-5/h5H,(H3,2,3,4)	-1.03	-1.039	1	1	1
128-13-2	128132	1816	**Ursodiol**	1_Pharma		ursodeoxycholic acid		C24H39O4	392.58	C[C@H](CCC(=O)[O-])[C@H]1CC[C@H]2[C@@H]3[C@@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C	InChI=1/C24H40O4/c1-14(4-7-21(27)28)17-5-6-18-22-19(9-11-24(17,18)3)23(2)10-8-16(25)12-	2.54	2.736	1	1	1
130-26-7	130267	1834	**Clioquinol**	1_Pharma	5-Chloro-7-iodo-8-quinolinol	clioquinol	C9H5ClINO	C9H5ClINO	305.5	Oc1c(I)cc(Cl)c2cccnc12	InChI=1/C9H5ClINO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H	3.016	2.981	1	1	1
13311-84-7	13311847	427	**Flutamid**	1_Pharma		Flutamide		C11H11F3N2O3	276.22	CC(C)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]	InChI=1/C11H11F3N2O3/c1-6(2)10(17)15-7-3-4-9(16(18)19)8(5-7)11(12,13)14/h3-6H,1-	2.916	2.916	1	1	1
134523-00-5	134523005	431	**Atorvastatin**	1_Pharma		(betaR,deltaR)-2-(4-Fluorophenyl)-beta,delta-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-1H-pyrrole-1-heptanoic acid			558.65	CC(C)C1=C(C(=C(N1CCC(CC(CC(=O)O)O)O)C2=CC=C(C=C2)F)C3=CC=CC=C3)C(=O)NC4=CC=CC=C4	InChI=1S/C33H35FN2O5/c1-21(2)31-30(33(41)35-25-11-7-4-8-12-25)29(22-9-5-3-6-10-22)32(23-13-15-24(34)16-14-23)3			1	1	1
137862-53-4	137862534	442	**Valsartan**	1_Pharma		Valsartan			435.53	CCCCC(=O)N(CC1=CC=C(C=C1)C2=CC=CC=C2C3=NNN=N3)C(C(C)C)C(=O)O	InChI=1S/C24H29N5O3/c1-4-5-10-21(30)29(22(16(2)3)24(31)32)15-17-11-13-18(14-12-17)19-8-6-7-9-20(19)23-25-27-28-			1	1	1
138402-11-6	138402116	444	**Irbesartan**	1_Pharma		Irbesartan			428.55	CCCCC1=NC2(CCCC2)C(=O)N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NNN=N5	InChI=1S/C25H28N6O/c1-2-3-10-22-26-25(15-6-7-16-25)24(32)31(22)17-18-11-13-19(14-12-18)20-8-4-5-9-21(20)23-27-2			1	1	1
139481-59-7	139481597	447	**Candesartan**	1_Pharma		Candesartan			440.47	CCOC1=NC2=CC=CC(=C2N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NNN=N5)C(=O)O	nChI=1S/C24H20N6O3/c1-2-33-24-25-20-9-5-8-19(23(31)32)21(20)30(24)14-15-10-12-16(13-11-15)17-6-3-4-7-18(17)22-			1	1	1
15307-86-5	15307865	31	**diclofenac**	1_Pharma	Diclofenac	Diclofenac	C14H11Cl2NO2	C14H10Cl2NO2	296.15	[O-]C(=O)Cc1ccccc1Nc2c(Cl)cccc2Cl	InChI=1/C14H11Cl2NO2/c15-10-5-3-6-11(16)14(10)17-12-7-2-1-4-9(12)8-13(18)19/h1-7,17H,8H2,(H,18,19)/p-1	2.899	3.368	1	1	1
15687-27-1	15687271	493	**Ibuprofen**	1_Pharma	2-(4-Isobutylphenyl)propanoic acid	Ibuprofen	C13H18O2	C13H17O2	206.29	CC(C)Cc1ccc(cc1)C(C)C(=O)[O-]	InChI=1/C13H18O2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(14)15/h4-7,9-10H,8H2,1-3H3,(H,14,15)/p-1	2.133	2.15	1	1	1
20830-75-5	20830755	529	**Digoxin**	1_Pharma		(3 beta, 5 beta, 12 beta)-3[O-2,6-Dideoxy-beta-D-ribo-hexapyranosyl-(14)-O-2,6-dideoxy-beta-D-ribo-hexapyranosyl-(14)-2,6-dideoxy-beta-D-ribo-hexapyranosyl)oxy]-12,14-dihydroxycard-20(22)-enolide		C41H64O14	780.95	C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)O[C@H]2[C@@H](O)C[C@H](O[C@H]3[C@@H](O)C[C@H](O[C@H]4CC[	InChI=1/C41H64O14/c1-19-36(47)28(42)15-34(50-19)54-38-21(3)52-35(17-30(38)44)55-37-20(2)51-33(16-29(37)43)53-24-8-10-39(4)23(13-24)6-7-26-27(39)14-31(45)40(5)25(9-11-41(26,40)48)22-12-32(46)49-18-22/h12,19-21,23-31,33-38,42-45,47-48H,6-11,13-18H2,1-5H3/t19-,20-,21-,23-,24+,25-,26-,27+,28+,29+,30+,31-,33+,34+,35+,36-,37-,38-,39+,40+,41+/m1/s1	1.999	1.999	1	1	1
22204-53-1	22204531	539	**Naproxen**	1_Pharma	Naproxen	Naproxen	C14H14O3	C14H13O3	230.26	COc1ccc2cc(ccc2c1)[C@H](C)C(=O)[O-]	InChI=1/C14H14O3/c1-9(14(15)16)10-3-4-12-8-13(17-2)6-5-11(12)7-10/h3-9H,1-2H3,(H,15,16)/p-1/t9-/m0/s1	1.375	1.394	1	1	1
23593-75-1	23593751	553	**Klotrimazol**	1_Pharma	Clotrimazole	1-[(2-Chlorophenyl)diphenylmethyl]-1H-imidazole	C22H17ClN2	C22H17ClN2	344.85	Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4	InChI=1/C22H17ClN2/c23-21-14-8-7-13-20(21)22(25-16-15-24-17-25,18-9-3-1-4-10-18)19-11-5-2-6-12-19/h1-17H	5.222	5.423	1	1	1
25812-30-0	25812300	570	**Gemfibrozil**	1_Pharma		Gemfibrozil		C15H21O3	250.34	Cc1ccc(C)c(OCCCC(C)(C)C(=O)[O-])c1	InChI=1/C15H22O3/c1-11-6-7-12(2)13(10-11)18-9-5-8-15(3,4)14(16)17/h6-7,10H,5,8-9H2,1-4H3,(H,16,17)/p-1	2.698	2.745	1	1	1
26787-78-0	26787780	574	**amoxicillin**	1_Pharma		Amoxicillin		C16H18N3O5S	365.41	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3ccc(O)cc3)C(=O)N2[C@H]1C(=O)[O-]	InChI=1/C16H19N3O5S/c1-16(2)11(15(23)24)19-13(22)10(14(19)25-16)18-12(21)9(17)7-3-5-8(20)6-4-7/h3-6,9-11,14,20H,17H2,1-2H3,(H,18,21)(H,23,24)/p-1/t9-,10-,11+,14-/m1/s1	-1.534	-1.73	1	1	1
29122-68-7	29122687	44	**Atenolol**	1_Pharma		4-[2-Hydroxy-3-[(1-methylethyl)amino]propoxy]benzeneacetamide		C14H23N2O3	266.34	CC(C)[NH2+]CC(O)COc1ccc(CC(=O)N)cc1	InChI=1/C14H22N2O3/c1-10(2)16-8-12(17)9-19-13-5-3-11(4-6-13)7-14(15)18/h3-6,10,12,16-17H,7-9H2,1-2H3,(H2,15,18)/p+1	-0.562	-0.521	1	1	1
298-46-4	298464	45	**Carbamazepine**	1_Pharma	Carbamazepine	Carbamazepine	C15H12N2O	C15H12N2O	236.28	NC(=O)N1c2ccccc2C=Cc3ccccc13	InChI=1/C15H12N2O/c16-15(18)17-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)17/h1-10H,(H2,16,18)	2.679	2.679	1	1	1
3380-34-5	3380345	48	**triclosan**	1_Pharma		Triclosan		C12H7Cl3O2	289.55	Oc1cc(Cl)ccc1Oc2ccc(Cl)cc2Cl	InChI=1/C12H7Cl3O2/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6,16H	5.141	5.132	1	1	1
37350-58-6	37350586	50	**Metoprolol**	1_Pharma	Metoprolol	Metoprolol	C15H25NO3	C15H26NO3	267.37	COCCc1ccc(OCC(O)C[NH2+]C(C)C)cc1	InChI=1/C15H25NO3/c1-12(2)16-10-14(17)11-19-15-6-4-13(5-7-15)8-9-18-3/h4-7,12,14,16-17H,8-11H2,1-3H3/p+1	0.526	0.568	1	1	1
3930-20-9	3930209	51	**Sotalol**	1_Pharma	Sotalol	Sotalol	C12H20N2O3S		272.37	CC(C)NCC(C1=CC=C(C=C1)NS(=O)(=O)C)O	InChI=1S/C12H20N2O3S/c1-9(2)13-8-12(15)10-4-6-11(7-5-10)14-18(3,16)17/h4-7,9,12-15H,8H2,1-3H3			1	1	1
41859-67-0	41859670	53	**Bezafibrat**	1_Pharma		Bezafibrate		C19H19ClNO4	361.83	CC(C)(Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1)C(=O)[O-]	InChI=1/C19H20ClNO4/c1-19(2,18(23)24)25-16-9-3-13(4-10-16)11-12-21-17(22)14-5-7-15(20)8-6-14/h3-10H,11-12H2,1-2H3,(H,21,22)(H,23,24)/p-1	2.394	2.397	1	1	1
42200-33-9	42200339	1154	**Nadolol**	1_Pharma	Nadolol	Nadolol	C17H27NO4	C17H28NO4	309.41	CC(C)(C)[NH2+]CC(O)COc1cccc2C[C@@H](O)[C@@H](O)Cc12	InChI=1/C17H27NO4/c1-17(2,3)18-9-12(19)10-22-16-6-4-5-11-7-14(20)15(21)8-13(11)16/h4-6,12,14-15,18-21H,7-10H2,1-3H3/p+1/t12?,14-,15+/m1/s1	-0.085	0.014	1	1	1
439-14-5	439145	640	**Diazepam**	1_Pharma	2H-1,4-benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-	Diazepam	C16H13ClN2O	C16H13ClN2O	284.75	CN1C(=O)CN=C(c2ccccc2)c3cc(Cl)ccc13	InChI=1/C16H13ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)20)11-5-3-2-4-6-11/h2-9H,10H2,1H3	3.171	3.171	1	1	1
443-48-1	443481	642	**Metronidazol**	1_Pharma	Metronidazole	2-Methyl-5-nitro-1H-imidazole-1-ethanol	C6H9N3O3	C6H9N3O3	171.16	Cc1ncc([N+](=O)[O-])n1CCO	InChI=1/C6H9N3O3/c1-5-7-4-6(9(11)12)8(5)2-3-10/h4,10H,2-3H2,1H3	-0.337	-0.337	1	1	1
49562-28-9	49562289	649	**fenofibrate**	1_Pharma		Fenofibrate		C20H21ClO4	360.84	CC(C)OC(=O)C(C)(C)Oc1ccc(cc1)C(=O)c2ccc(Cl)cc2	InChI=1/C20H21ClO4/c1-13(2)24-19(23)20(3,4)25-17-11-7-15(8-12-17)18(22)14-5-9-16(21)10-6-14/h5-13H,1-4H3	5.111	5.111	1	1	1
50-02-2	50022	652	**Dexametason**	1_Pharma	Prednisolone, 9alpha-fluoro-16alpha-methyl-	11beta,16alpha-9-Fluoro-11,17,21-Trihydroxy-16-methyl-pregna-1,4-diene-3,20-dione	C22H29FO5	C22H29FO5	392.47	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO	InChI=1/C22H29FO5/c1-12-8-16-15-5-4-13-9-14(25)6-7-19(13,2)21(15,23)17(26)10-20(16,3)22(12,28)18(27)11-24/h6-7,9,12,15-17,24,26,28H,4-5,8,10-11H2,1-3H3/t12-,15+,16+,17+,19+,20+,21+,22+/m1/s1	1.708	1.708	1	1	1
50-06-6	50066	4945	**phenobarbital**	1_Pharma	Barbituric acid, 5-ethyl-5-phenyl-,	Phenobarbital	C12H12N2O3	C12H11N2O3	232.24	CCC1(C(=O)NC(=O)[N-]C1=O)c2ccccc2	InChI=1/C12H12N2O3/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(12)16/h3-7H,2H2,1H3,(H2,13,14,15,16,17)/p-1	1.424	1.381	1	1	1
50-18-0	50180	1131	**Cyclophosphamid**	1_Pharma	2-[Bis(2-chloroethylamino)]-tetrahydro-2H-1,3,2-oxazaphosphorine-2-oxide	N,N-Bis(2-chloroethyl)tetrahydro-2H-1,3,2-oxazaphosphorin-2-amine 2-oxide	C7H15Cl2N2O2P	C7H15Cl2N2O2P	261.09	ClCCN(CCCl)P1(=O)NCCCO1	InChI=1/C7H15Cl2N2O2P/c8-2-5-11(6-3-9)14(12)10-4-1-7-13-14/h1-7H2,(H,10,12)	0.144	0.144	1	1	1
50-24-8	50248	656	**prednisolone**	1_Pharma		(11beta)-11,17,21-Trihydroxypregna-1,4-diene-3,20-dione		C21H28O5	360.45	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO	InChI=1/C21H28O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2)10-16(24)18(14)19/h5,7,9,14-16,18,22,24,26H,3-4,6,8,10-11H2,1-2H3/t14-,15-,16-,18+,19-,20-,21-/m0/	1.26	1.26	1	1	1
50-28-2	50282	55	**estradiol**	1_Pharma	Estra-1,3,5(10)-triene-3,17beta-diol	(17beta)Estra-1,3,5(10)triene-3,17-diol	C18H24O2	C18H24O2	272.39	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O	InChI=1/C18H24O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h3,5,10,14-17,19-20H,2,4,6-9H2,1H3/t14-,15-,16+,17+,18+/m1/s1	3.838	3.838	1	1	1
50-78-2	50782	666	**O-acetylsalicylic acid**	1_Pharma	Benzoic acid, 2-(acetyloxy)-	Acetyl salicylic acid	C9H8O4	C9H7O4	180.16	CC(=O)Oc1ccccc1C(=O)[O-]	InChI=1/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)/p-1	-0.247	-0.245	1	1	1
51-21-8	51218	668	**fluorouracil**	1_Pharma	2,4-Pyrimidinedione, 5-fluoro-	Fluoruracil	C4H3FN2O2	C4H2FN2O2	130.08	Oc1ncc(F)c([O-])n1	InChI=1/C4H3FN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9)/p-1	0.129	0.132	1	1	1
51481-61-9	51481619	1129	**Cimetidin**	1_Pharma	Cimetidine	Cimetidine	C10H16N6S	C10H17N6S	252.35	C\N=C(\NCCSCc1[nH]c[nH+]c1C)/NC#N	InChI=1/C10H16N6S/c1-8-9(16-7-15-8)5-17-4-3-13-10(12-2)14-6-11/h7H,3-5H2,1-2H3,(H,15,16)(H2,12,13,14)/p+1	1.007	0.97	1	1	1
51-52-5	51525	5108	**propylthiouracil**	1_Pharma	Tegretol	Propylthiouracil	C15H12N2O	C7H9N2OS	170.24	CCCc1cc(O)nc([S-])n1	InChI=1/C7H10N2OS/c1-2-3-5-4-6(10)9-7(11)8-5/h4H,2-3H2,1H3,(H2,8,9,10,11)/p-1	2.714	2.7	1	1	1
525-66-6	525666	59	**Propranolol**	1_Pharma	Propanolol	Propranolol	C16H21NO2	C16H22NO2	259.35	CC(C)[NH2+]CC(O)COc1cccc2ccccc12	InChI=1/C16H21NO2/c1-12(2)17-10-14(18)11-19-16-9-5-7-13-6-3-4-8-15(13)16/h3-9,12,14,17-18H,10-11H2,1-2H3/p+1	1.309	1.405	1	1	1
52645-53-1	52645531	676	**Permethrin**	1_Pharma	Permethrin	3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid, (3-Phenoxyphenyl)methyl ester	C21H20Cl2O3	C21H20Cl2O3	391.29	CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc2cccc(Oc3ccccc3)c2	InChI=1/C21H20Cl2O3/c1-21(2)17(12-18(22)23)19(21)20(24)25-13-14-7-6-10-16(11-14)26-15-8-4-3-5-9-15/h3-12,17,19H,13H2,1-2H3	5.438	5.438	1	1	1
53-86-1	53861	1101	**Indometacin**	1_Pharma	Indomethacin	1-(4-Chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetic acid	C19H16ClNO4	C19H15ClNO4	357.79	COc1ccc2c(c1)c(CC(=O)[O-])c(C)n2C(=O)c3ccc(Cl)cc3	InChI=1/C19H16ClNO4/c1-11-15(10-18(22)23)16-9-14(25-2)7-8-17(16)21(11)19(24)12-3-5-13(20)6-4-12/h3-9H,10H2,1-2H3,(H,22,23)/p-1	2.761	3.648	1	1	1
54-11-5	54115	5067	**nicotine**	1_Pharma	3-(2-(N-methylpyrrolidinyl))pyridine	Nicotine	C10H14N2	C10H15N2	162.24	C[NH+]1CCC[C@H]1c2cccnc2	InChI=1/C10H14N2/c1-12-7-3-5-10(12)9-4-2-6-11-8-9/h2,4,6,8,10H,3,5,7H2,1H3/p+1/t10-/m0/s1	-0.319	-0.08	1	1	1
54-31-9	54319	62	**Furosemid**	1_Pharma		5-(Aminosulfonyl)-4-chloro-2-[(2-furanylmethyl)amino]benzoic acid		C12H10ClN2O5S	330.75	NS(=O)(=O)c1cc(C(=O)[O-])c(NCc2occc2)cc1Cl	InChI=1/C12H11ClN2O5S/c13-9-5-10(15-6-7-2-1-3-20-7)8(12(16)17)4-11(9)21(14,18)19/h1-5,15H,6H2,(H,16,17)(H2,14,18,19)/p-1	-0.071	-0.063	1	1	1
54739-18-3	54739183	689	**Fluvoxamin**	1_Pharma		(1E)-5-Methoxy-1-[4-(trifluoromethyl)phenyl]-1-pentanone O-(2-aminoethyl)oxime			318.34	COCCCCC(=NOCCN)C1=CC=C(C=C1)C(F)(F)F	InChI=1S/C15H21F3N2O2/c1-21-10-3-2-4-14(20-22-11-9-19)12-5-7-13(8-6-12)15(16,17)18/h5-8H,2-4,9-11,19H2,1H3/b20			1	1	1
54-85-3	54853	691	**Isoniazid**	1_Pharma	Isoniazid	Isoniazid	C6H7N3O	C6H6N3O	137.15	N[N-]C(=O)c1ccncc1	InChI=1/C6H7N3O/c7-9-6(10)5-1-3-8-4-2-5/h1-4H,(H3,7,8,9,10)/p-1	-0.707	-0.707	1	1	1
54910-89-3	54910893	692	**Fluoxetin**	1_Pharma		Fluoxetine			309.33	CNCCC(C1=CC=CC=C1)OC2=CC=C(C=C2)C(F)(F)F	InChI=1S/C17H18F3NO/c1-21-12-11-16(13-5-3-2-4-6-13)22-15-9-7-14(8-10-15)17(18,19)20/h2-10,16,21H,11-12H2,1H3			1	1	1
55-56-1	55561	3175	**chlorhexidine**	1_Pharma		chlorhexidine		C22H32Cl2N10	505.47	Clc1ccc([NH2+]C(=N)NC(=N)NCCCCCCNC(=N)NC(=N)[NH2+]c2ccc(Cl)cc2)cc1	InChI=1/C22H30Cl2N10/c23-15-5-9-17(10-6-15)31-21(27)33-19(25)29-13-3-1-2-4-14-30-20(26)34-22(28)32-18-11-7-16(24)8-12-18/h5-12H,1-4,13-14H2,(H5,25,27,29,31,33)(H5,26,28,30,32,34)/p+2	4.412	4.411	1	1	1
55-63-0	55630	702	**glycerol trinitrate**	1_Pharma	1,2,3-Propanetriol, trinitrate	Nitroglycerin	C3H5N3O9	C3H5N3O9	227.09	[O-][N+](=O)OCC(CO[N+](=O)[O-])O[N+](=O)[O-]	InChI=1/C3H5N3O9/c7-4(8)13-1-3(15-6(11)12)2-14-5(9)10/h3H,1-2H2	5.822	5.822	1	1	1
56-75-7	56757	64	**Chloramphenicol**	1_Pharma	Chloramphenicol	2,2-Dichloro-N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]acetamide	C11H12Cl2N2O5	C11H12Cl2N2O5	323.13	OC[C@@H](NC(=O)C(Cl)Cl)[C@H](O)c1ccc(cc1)[N+](=O)[O-]	InChI=1/C11H12Cl2N2O5/c12-10(13)11(18)14-8(5-16)9(17)6-1-3-7(4-2-6)15(19)20/h1-4,8-10,16-17H,5H2,(H,14,18)/t8-,9-/m1/s1	1.025	1.025	1	1	1
56-81-5	56815	716	**glycerol**	1_Pharma	1,2,3-Propanetriol	1,2,3-Propanetriol	C3H8O3	C3H8O3	92.094	OCC(O)CO	InChI=1/C3H8O3/c4-1-3(6)2-5/h3-6H,1-2H2	-1.409	-1.409	1	1	1
56-86-0	56860	3214	**glutamic acid**	1_Pharma	L-Glutamic acid	glutamic acid	C5H9NO4	C5H8NO4	147.13	[NH3+]C(CCC(=O)[O-])C(=O)[O-]	InChI=1/C5H9NO4/c6-3(5(9)10)1-2-4(7)8/h3H,1-2,6H2,(H,7,8)(H,9,10)/p-1	-4.933	-4.92	1	1	1
57-13-6	57136	719	**urea**	1_Pharma	Urea	Urea	CH4N2O	CH4N2O	60.058	NC(=O)N	InChI=1/CH4N2O/c2-1(3)4/h(H4,2,3,4)	-1.043	-1.043	1	1	1
57-63-6	57636	724	**Etinylestradiol**	1_Pharma	Ethinyl Estradiol	Ethinylestradiol	C20H24O2	C20H24O2	296.41	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#C	InChI=1/C20H24O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(18,20)2/h1,5,7,12,16-18,21-22H,4,6,8-11H2,2H3/t16-,17-,18+,19+,20+/m1/s1	4.886	4.886	1	1	1
58-08-2	58082	66	**caffeine**	1_Pharma	Caffeine	Caffeine	C8H10N4O2	C8H10N4O2	194.2	CN1C(=O)N(C)c2ncn(C)c2C1=O	InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3	-0.1	-0.1	1	1	1
58-22-0	58220	67	**testosterone**	1_Pharma	Testosterone	Testosterone	C19H28O2	C19H28O2	288.43	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O	InChI=1/C19H28O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)18/h11,14-17,21H,3-10H2,1-2H3/t14-,15-,16-,17-,18-,19-/m0/s1	3.473	3.473	1	1	1
58-55-9	58559	730	**theophylline**	1_Pharma	1,3-Dimethylxanthine	Theophylline	C7H8N4O2	C7H8N4O2	180.17	CN1C(=O)N(C)c2[nH]cnc2C1=O	InChI=1/C7H8N4O2/c1-10-5-4(8-3-9-5)6(12)11(2)7(10)13/h3H,1-2H3,(H,8,9)	-0.584	-0.461	1	1	1
59-05-2	59052	732	**Metotrexat**	1_Pharma	Methotrexate	Methotrexate	C20H22N8O5	C20H20N8O5	454.45	CN(Cc1cnc2nc(N)nc(N)c2n1)c3ccc(cc3)C(=O)N[C@@H](CCC(=O)[O-])C(=O)[O-]	InChI=1/C20H22N8O5/c1-28(9-11-8-23-17-15(24-11)16(21)26-20(22)27-17)12-4-2-10(3-5-12)18(31)25-13(19(32)33)6-7-14(29)30/h2-5,8,13H,6-7,9H2,1H3,(H,25,31)(H,29,30)(H,32,33)(H4,21,22,23,26,27)/p-2/t13-/m0/s1	-2.834	-2.253	1	1	1
59277-89-3	59277893	735	**Aciklovir**	1_Pharma		Acyclovir		C8H11N5O3	225.21	Nc1nc([O-])c2[nH+]cn(COCCO)c2n1	InChI=1/C8H11N5O3/c9-8-11-6-5(7(15)12-8)10-3-13(6)4-16-2-1-14/h3,14H,1-2,4H2,(H3,9,11,12,15)	-0.349	-0.306	1	1	1
59467-70-8	59467708	736	**Midazolam**	1_Pharma	4H-Imidazo[1,5-a][1,4]benzodiazepine, 8-chloro-6-(2-fluorophenyl)-1-methyl-	Midazolam (base)	C18H13ClFN3	C18H13ClFN3	325.78	Cc1ncc2CN=C(c3ccccc3F)c4cc(Cl)ccc4n12	InChI=1/C18H13ClFN3/c1-11-21-9-13-10-22-18(14-4-2-3-5-16(14)20)15-8-12(19)6-7-17(15)23(11)13/h2-9H,10H2,1H3	4.126	4.494	1	1	1
59-67-6	59676	739	**Niacin**	1_Pharma	Niacin	Nicotinic Acid/Niacin	C6H5NO2	C6H4NO2	123.11	[O-]C(=O)c1cccnc1	InChI=1/C6H5NO2/c8-6(9)5-2-1-3-7-4-5/h1-4H,(H,8,9)/p-1	-1.165	-1.151	1	1	1
59-92-7	59927	745	**Levodopa**	1_Pharma	Levodopa	3-Hydroxy-1-tyrosine	C9H11NO4	C9H11NO4	197.19	[NH3+][C@@H](Cc1ccc(O)c(O)c1)C(=O)[O-]	InChI=1/C9H11NO4/c10-6(9(13)14)3-5-1-2-7(11)8(12)4-5/h1-2,4,6,11-12H,3,10H2,(H,13,14)/t6-/m0/s1	-2.089	-2.009	1	1	1
60-54-8	60548	754	**Tetracycline**	1_Pharma		Tetracycline		C22H24N2O8	444.44	C[NH+](C)[C@@H]1[C@@H]2C[C@H]3C(=C(O)[C@]2(O)C(=C(C(=O)N)C1=O)[O-])C(=O)c4c(O)cccc4[C@@]3(C)O	InChI=1/C22H24N2O8/c1-21(31)8-5-4-6-11(25)12(8)16(26)13-9(21)7-10-15(24(2)3)17(27)14(20(23)30)19(29)22(10,32)18(13)28/h4-6,9-10,15,25,28-29,31-32H,7H2,1-3H3,(H2,23,30)/t9-,10-,15-,21+,22-/m0/s1	-3.265	-1.834	1	1	1
61-68-7	61687	1150	**Mefenamic acid**	1_Pharma	Mefenamic Acid	2-[(2,3-Dimethylphenyl)amino]benzoic acid	C15H15NO2	C15H14NO2	241.29	Cc1cccc(Nc2ccccc2C(=O)[O-])c1C	InChI=1/C15H15NO2/c1-10-6-5-9-13(11(10)2)16-14-8-4-3-7-12(14)15(17)18/h3-9,16H,1-2H3,(H,17,18)/p-1	2.508	3.122	1	1	1
61869-08-7	61869087	760	**Paroxetin**	1_Pharma		Paroxetine			329.37	C1CNCC(C1C2=CC=C(C=C2)F)COC3=CC4=C(C=C3)OCO4	InChI=1S/C19H20FNO3/c20-15-3-1-13(2-4-15)17-7-8-21-10-14(17)11-22-16-5-6-18-19(9-16)24-12-23-18/h1-6,9,14,17,21			1	1	1
62571-86-2	62571862	1103	**Captopril**	1_Pharma		1-[(2S)-3-Mercapto-2-methyl-1-oxopropyl]-L-proline		C9H14NO3S	217.29	C[C@H](CS)C(=O)N1CCC[C@H]1C(=O)[O-]	InChI=1/C9H15NO3S/c1-6(5-14)8(11)10-4-2-3-7(10)9(12)13/h6-7,14H,2-5H2,1H3,(H,12,13)/p-1/t6-,7+/m1/s1	-0.807	-0.804	1	1	1
657-24-9	657249	79	**Metformin**	1_Pharma		N,N-Dimethylimidodicarbonimidic diamide		C4H12N5	129.17	CN(C)C(=[NH2+])N=C(N)N	InChI=1/C4H11N5/c1-9(2)4(7)8-3(5)6/h1-2H3,(H5,5,6,7,8)/p+1	-1.491	-1.491	1	1	1
66357-35-5	66357355	789	**ranitidine**	1_Pharma	Ranitidine	Ranitidine	C13H22N4O3S	C13H25N4O3S	314.41	C[NH2+]\C(=C\[N+](=O)[O-])\[NH2+]CCSCc1oc(C[NH+](C)C)cc1	InChI=1/C13H22N4O3S/c1-14-13(9-17(18)19)15-6-7-21-10-12-5-4-11(20-12)8-16(2)3/h4-5,9,14-15H,6-8,10H2,1-3H3/p+3/b13-9-	-2.983	-1.134	1	1	1
67-20-9	67209	791	**Nitrofurantoin**	1_Pharma	Hydantoin, n-(5-nitro-2-furfurylidene)-1-amino-	Nitrofurantion	C8H6N4O5	C8H5N4O5	238.16	[O-][N+](=O)c1oc(\C=N\N2CC(=O)[N-]C2=O)cc1	InChI=1/C8H6N4O5/c13-6-4-11(8(14)10-6)9-3-5-1-2-7(17-5)12(15)16/h1-3H,4H2,(H,10,13,14)/p-1/b9-3+	0.208	0.174	1	1	1
68-35-9	68359	1165	**Sulfadiazin**	1_Pharma	Sulfadiazine	Sulfadiazine	C10H10N4O2S	C10H10N4O2S	250.28	Nc1ccc(cc1)S(=O)(=O)Nc2ncccn2	InChI=1/C10H10N4O2S/c11-8-2-4-9(5-3-8)17(15,16)14-10-12-6-1-7-13-10/h1-7H,11H2,(H,12,13,14)	0.313	0.313	1	1	1
69-53-4	69534	808	**ampicillin**	1_Pharma		(2S,5R,6R)-6-[[(2R)-2-Amino-2-phenylacetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid		C16H18N3O4S	349.41	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3ccccc3)C(=O)N2[C@H]1C(=O)[O-]	InChI=1/C16H19N3O4S/c1-16(2)11(15(22)23)19-13(21)10(14(19)24-16)18-12(20)9(17)8-6-4-3-5-7-8/h3-7,9-11,14H,17H2,1-2H3,(H,18,20)(H,22,23)/p-1/t9-,10-,11+,14-/m1/s1	-1.292	-2.283	1	1	1
69-72-7	69727	84	**salicylic acid**	1_Pharma	Benzoic acid, 2-hydroxy-	Salicylic acid	C7H6O3	C7H5O3	138.12	Oc1ccccc1C(=O)[O-]	InChI=1/C7H6O3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H,(H,9,10)/p-1	-0.257	-0.256	1	1	1
70458-96-7	70458967	812	**Norfloxacin**	1_Pharma		1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinoline carboxylic acid		C16H18FN3O3	319.34	CCN1C=C(C(=O)[O-])C(=O)c2cc(F)c(cc12)N3CC[NH2+]CC3	InChI=1/C16H18FN3O3/c1-2-19-9-11(16(22)23)15(21)10-7-12(17)14(8-13(10)19)20-5-3-18-4-6-20/h7-9,18H,2-6H2,1H3,(H,22,23)	-1.411	-0.104	1	1	1
723-46-6	723466	86	**Sulfametoxazol**	1_Pharma	Sulfanilamide, n¹-(5-methyl-3-isoxazolyl)-	4-Amino-N-(5-methyl-3-isoxazolyl)benzenesulfonamide	C10H11N3O3S	C10H10N3O3S	253.28	Cc1onc([N-]S(=O)(=O)c2ccc(N)cc2)c1	InChI=1/C10H11N3O3S/c1-7-6-10(12-16-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2,1H3,(H,12,13)/q-1	0.813	0.803	1	1	1
72956-09-3	72956093	826	**Carvedilol**	1_Pharma		Carvedilol			406.48	COC1=CC=CC=C1OCCNCC(COC2=CC=CC3=C2C4=CC=CC=C4N3)O	InChI=1S/C24H26N2O4/c1-28-21-10-4-5-11-22(21)29-14-13-25-15-17(27)16-30-23-12-6-9-20-24(23)18-7-2-3-8-19(18)26-			1	1	1
73334-07-3	73334073	4988	**Iopromide**	1_Pharma		Iopromide		C18H24I3N3O8	791.11	COCC(=O)Nc1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)N(C)CC(O)CO)c1I	InChI=1/C18H24I3N3O8/c1-24(4-9(28)6-26)18(31)12-13(19)11(17(30)22-3-8(27)5-25)14(20)16(15(12)21)23-10(29)7-32-2/h8-9,25-28H,3-7H2,1-2H3,(H,22,30)(H,23,29)	-1.057	-1.057	1	1	1
738-70-5	738705	89	**Trimetoprim**	1_Pharma	Trimethoprim	Trimethoprim	C14H18N4O3	C14H18N4O3	290.33	COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC	InChI=1/C14H18N4O3/c1-19-10-5-8(6-11(20-2)12(10)21-3)4-9-7-17-14(16)18-13(9)15/h5-7H,4H2,1-3H3,(H4,15,16,17,18)	1.543	1.438	1	1	1
76824-35-6	76824356	1100	**Famotidine**	1_Pharma		Famotidine			337.45	C1=C(N=C(S1)N=C(N)N)CSCCC(=NS(=O)(=O)N)N	InChI=1S/C8H15N7O2S3/c9-6(15-20(12,16)17)1-2-18-3-5-4-19-8(13-5)14-7(10)11/h4H,1-3H2,(H2,9,15)(H2,12,16,17)(H4,			1	1	1
78439-06-2	78439062	896	**Ceftazidim**	1_Pharma		Ceftazidime pentahydrate			546.59	CC(C)(C(=O)O)ON=C(C1=CSC(=N1)N)C(=O)NC2C3N(C2=O)C(=C(CS3)C[N+]4=CC=CC=C4)C(=O)[O-]	InChI=1S/C22H22N6O7S2/c1-22(2,20(33)34)35-26-13(12-10-37-21(23)24-12)16(29)25-14-17(30)28-15(19(31)32)11(9-36			1	1	1
79-57-2	79572	923	**Oxitetracyklin**	1_Pharma		Oxytetracycline (anhydrous)		C22H24N2O9	460.44	C[NH+](C)[C@H]1[C@@H]2[C@@H](O)[C@H]3C(=C(O)[C@]2(O)C(=C(C(=O)N)C1=O)[O-])C(=O)c4c(O)cccc4[C@@]3	InChI=1/C22H24N2O9/c1-21(32)7-5-4-6-8(25)9(7)15(26)10-12(21)17(28)13-14(24(2)3)16(27)11(20(23)31)19(30)22(13,33)18(10)29/h4-6,12-14,17,25-26,28,30,32-33H,1-3H3,(H2,23,31)/t12-,13-,14+,17-,21-,22+/m1/s1	-4.265	-2.956	1	1	1
79617-96-2	79617962	924	**Sertraline**	1_Pharma		(1S,4S)-4-(3,4-Dichlorphenyl)-1,2,3,4-tetrahydro-N-methyl-1-naphthalenamine			306.24	CNC1CCC(C2=CC=CC=C12)C3=CC(=C(C=C3)Cl)Cl	InChI=1S/C17H17Cl2N/c1-20-17-9-7-12(13-4-2-3-5-14(13)17)11-6-8-15(18)16(19)10-11/h2-6,8,10,12,17,20H,7,9H2,1H3/t			1	1	1
80-08-0	80080	3787	**dapsone**	1_Pharma	Dapsone	dapsone	C12H12N2O2S	C12H12N2O2S	248.31	Nc1ccc(cc1)S(=O)(=O)c2ccc(N)cc2	InChI=1/C12H12N2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H,13-14H2	1.439	1.439	1	1	1
81103-11-9	81103119	99	**Claritromycin**	1_Pharma		6-O-Methylerythromycin			747.97	CCC1C(C(C(C(=O)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)C)(C)OC)C)C)O)(C	InChI=1S/C38H69NO13/c1-15-26-38(10,45)31(42)21(4)28(40)19(2)17-37(9,47-14)33(52-35-29(41)25(39(11)12)16-20(3)4			1	1	1
81-13-0	81130	3802	**dexpanthenol**	1_Pharma	Dexpanthelol	dexpanthenol	C9H19NO4	C9H19NO4	205.26	CC(C)(CO)[C@@H](O)C(=O)NCCCO	InChI=1/C9H19NO4/c1-9(2,6-12)7(13)8(14)10-4-3-5-11/h7,11-13H,3-6H2,1-2H3,(H,10,14)/t7-/m0/s1	-1.265	-1.265	1	1	1
81-81-2	81812	942	**warfarin**	1_Pharma	3-(Alpha-acetonylbenzyl)-4-hydroxycoumarin	4-Hydroxy-3-(3-oxo-1-phenylbutyl)-2H-1-benzopyran-2-one	C19H16O4	C19H15O4	308.33	CC(=O)CC(C1=C([O-])Oc2ccccc2C1=O)c3ccccc3	InChI=1/C19H16O4/c1-12(20)11-15(13-7-3-2-4-8-13)17-18(21)14-9-5-6-10-16(14)23-19(17)22/h2-10,15,22H,11H2,1H3/p-1	2.589	3.029	1	1	1
82419-36-1	82419361	945	**Ofloxacin**	1_Pharma		9-Fluoro-2,3-dihydro-3-methyl-10-(4-methyl-1-piperazinyl)-7-oxo-7H-pyrido[1,2,3-de]-1,4-benzoxazine-6-carboxylic acid			361.38	CC1COC2=C3N1C=C(C(=O)C3=CC(=C2N4CCN(CC4)C)F)C(=O)O	InChI=1S/C18H20FN3O4/c1-10-9-26-17-14-11(16(23)12(18(24)25)8-22(10)14)7-13(19)15(17)21-5-3-20(2)4-6-21/h7-8,10H			1	1	1
83799-24-0	83799240	956	**Fexofenadine**	1_Pharma		Fexofenadin			501.67	CC(C)(C1=CC=C(C=C1)C(CCCN2CCC(CC2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)O)C(=O)O	InChI=1S/C32H39NO4/c1-31(2,30(35)36)25-17-15-24(16-18-25)29(34)14-9-21-33-22-19-28(20-23-33)32(37,26-10-5-3-6-1			1	1	1
83905-01-5	83905015	957	**Azithromycin**	1_Pharma		azitromycine			749	CCC1C(C(C(N(CC(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C)C)C)O)(C)O	InChI=1S/C38H72N2O12/c1-15-27-38(10,46)31(42)24(6)40(13)19-20(2)17-36(8,45)33(52-35-29(41)26(39(11)12)16-21(3)			1	1	1
84057-84-1	84057841	102	**Lamotrigin**	1_Pharma		Lamotrigin		C9H7Cl2N5	256.1	Nc1nnc(c(N)n1)c2cccc(Cl)c2Cl	InChI=1/C9H7Cl2N5/c10-5-3-1-2-4(6(5)11)7-8(12)14-9(13)16-15-7/h1-3H,(H4,12,13,14,16)	2.426	2.422	1	1	1
85721-33-1	85721331	969	**Ciprofloxacin**	1_Pharma		Ciprofloxacin			331.35	C1CC1N2C=C(C(=O)C3=CC(=C(C=C32)N4CCNCC4)F)C(=O)O	InChI=1S/C17H18FN3O3/c18-13-7-11-14(8-15(13)20-5-3-19-4-6-20)21(10-1-2-10)9-12(16(11)22)17(23)24/h7-10,19H,1-6			1	1	1
86386-73-4	86386734	970	**Fluconazole**	1_Pharma		fluconazol			306.28	C1=CC(=C(C=C1F)F)C(CN2C=NC=N2)(CN3C=NC=N3)O	InChI=1S/C13H12F2N6O/c14-10-1-2-11(12(15)3-10)13(22,4-20-8-16-6-18-20)5-21-9-17-7-19-21/h1-3,6-9,22H,4-5H2			1	1	1
88150-42-9	88150429	982	**Amlodipine**	1_Pharma		2-[(2-Aminoethoxy)methyl]-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-3,5-pyridinedicarboxylic acid 3-ethyl 5-methyl ester			408.88	CCOC(=O)C1=C(NC(=C(C1C2=CC=CC=C2Cl)C(=O)OC)C)COCCN	InChI=1S/C20H25ClN2O5/c1-4-28-20(25)18-15(11-27-10-9-22)23-12(2)16(19(24)26-3)17(18)13-7-5-6-8-14(13)21/h5-8,17			1	1	1
89-57-6	89576	3980	**Mesalamine**	1_Pharma	Mesalamine	5-aminosalicylic acid	C7H7NO3	C7H6NO3	153.14	Nc1ccc(O)c(c1)C(=O)[O-]	InChI=1/C7H7NO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,8H2,(H,10,11)/p-1	-1.003	-1.003	1	1	1
89-78-1	89781	994	**menthol**	1_Pharma	DL-Menthol	(1R,2S,5R)-rel-5-Methyl-2-(1-methylethyl)cyclohexanol	C10H20O	C10H20O	156.27	CC(C)C1CCC(C)CC1O	InChI=1/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H,4-6H2,1-3H3	2.779	2.779	1	1	1
90-82-4	90824	4008	**pseudoephedrine**	1_Pharma	Pseudoephedrine, (+)-	pseudoephedrine	C10H15NO	C10H16NO	165.24	C[NH2+][C@@H](C)[C@@H](O)c1ccccc1	InChI=1/C10H15NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,10-12H,1-2H3/p+1/t8-,10+/m0/s1	0.003	0.055	1	1	1
93413-69-5	93413695	1019	**Venlafaxine**	1_Pharma		1-[2-(Dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol			277.41	CN(C)CC(C1=CC=C(C=C1)OC)C2(CCCCC2)O	InChI=1S/C17H27NO2/c1-18(2)13-16(17(19)11-5-4-6-12-17)14-7-9-15(20-3)10-8-14/h7-10,16,19H,4-6,11-13H2,1-3H3			1	1	1
94-09-7	94097	1020	**Bensokain**	1_Pharma	Benzoic acid, 4-amino-, ethyl ester	4-Aminobenzoic acid ethyl ester	C9H11NO2	C9H11NO2	165.19	CCOC(=O)c1ccc(N)cc1	InChI=1/C9H11NO2/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6H,2,10H2,1H3	1.287	1.287	1	1	1
94-36-0	94360	4103	**dibenzoyl peroxide**	1_Pharma	Benzoyl peroxide	dibenzoyl peroxide	C14H10O4	C14H10O4	242.23	O=C(OOC(=O)c1ccccc1)c2ccccc2	InChI=1/C14H10O4/c15-13(11-7-3-1-4-8-11)17-18-14(16)12-9-5-2-6-10-12/h1-10H	2.793	2.793	1	1	1
97-77-8	97778	1060	**disulfiram**	1_Pharma	Disulfiram	bis(Diethylthiocarbamoyl)disulfide	C10H20N2S4	C10H20N2S4	296.54	CCN(CC)C(=S)SSC(=S)N(CC)CC	InChI=1/C10H20N2S4/c1-5-11(6-2)9(13)15-16-10(14)12(7-3)8-4/h5-8H2,1-4H3	5.599	5.599	1	1	1
98-92-0	98920	1079	**nicotinamide**	1_Pharma	Niacinamide	3-Pyridinecarboxamide	C6H6N2O	C6H6N2O	122.13	NC(=O)c1cccnc1	InChI=1/C6H6N2O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)	-0.319	-0.319	1	1	1
99-66-1	99661	1091	**Valproic acid**	1_Pharma	Valproic Acid	2-Propylpentanoic acid	C8H16O2	C8H15O2	144.21	CCCC(CCC)C(=O)[O-]	InChI=1/C8H16O2/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)/p-1	1.275	1.317	1	1	1
2164-08-1	2164081	114	**Lenacil**	2_Pest	Lenacil	lenacil	C13H18N2O2	C13H18N2O2	234.3	O=C1NC2=C(CCC2)C(=O)N1C3CCCCC3	InChI=1/C13H18N2O2/c16-12-10-7-4-8-11(10)14-13(17)15(12)9-5-2-1-3-6-9/h9H,1-8H2,(H,14,17)	2.164	2.164	1	1	1
2439-01-2	2439012	5114	**Quinomethionate**	2_Pest	Quinomethionate	6-Methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one	C10H6N2OS2	C10H6N2OS2	234.3	Cc1ccc2nc3SC(=O)Sc3nc2c1	InChI=1/C10H6N2OS2/c1-5-2-3-6-7(4-5)12-9-8(11-6)14-10(13)15-9/h2-4H,1H3	4.132	4.132	1	1	1
3813-05-6	3813056	116	**Benazolin**	2_Pest		benazolin		C9H5ClNO3S	243.67	[O-]C(=O)CN1C(=O)Sc2cccc(Cl)c12	InChI=1/C9H6ClNO3S/c10-5-2-1-3-6-8(5)11(4-7(12)13)9(14)15-6/h1-3H,4H2,(H,12,13)/p-1	0.776	1.044	1	1	1
10004-44-1	10004441	121	**Hymexazol**	2_Pest		5-Methyl-3(2H)-isoxazolone		C4H4NO2	99.09	Cc1onc([O-])c1	InChI=1/C4H5NO2/c1-3-2-4(6)5-7-3/h2H,1H3,(H,5,6)/p-1	0.023	0.726	1	1	1
100646-51-3	100646513	5117	**Quizalofop-P-ethyl**	2_Pest		Quizalofop-P-ethyl			372.81	CCOC(=O)C(C)OC1=CC=C(C=C1)OC2=CN=C3C=C(C=CC3=N2)Cl	InChI=1S/C19H17ClN2O4/c1-3-24-19(23)12(2)25-14-5-7-15(8-6-14)26-18-11-21-17-10-13(20)4-9-16(17)22-18/h4-12H,3H			1	1	1
101-05-3	101053	141	**Anilazine**	2_Pest	4,6-Dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	4,6-Dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine	C9H5Cl3N4	C9H5Cl3N4	275.53	Clc1ccccc1Nc2nc(Cl)nc(Cl)n2	InChI=1/C9H5Cl3N4/c10-5-3-1-2-4-6(5)13-9-15-7(11)14-8(12)16-9/h1-4H,(H,13,14,15,16)	3.755	3.754	1	1	1
101200-48-0	101200480	142	**Tribenuron-methyl**	2_Pest		2-[[[[(4-Methoxy-6-methyl-1,3,5-triazin-2-yl)methylamino]carbonyl]amino]sulfonyl]benzoic acid methyl ester			395.4	CC1=NC(=NC(=N1)OC)N(C)C(=O)NS(=O)(=O)C2=CC=CC=C2C(=O)OC	InChI=1S/C15H17N5O6S/c1-9-16-13(18-14(17-9)26-4)20(2)15(22)19-27(23,24)11-8-6-5-7-10(11)12(21)25-3/h5-8H,1-4H3			1	1	1
101205-02-1	101205021	144	**Cycloxydim**	2_Pest		cycloxydim			325.47	CCCC(=C1C(=O)CC(CC1=O)C2CCCSC2)NOCC	InChI=1S/C17H27NO3S/c1-3-6-14(18-21-4-2)17-15(19)9-13(10-16(17)20)12-7-5-8-22-11-12/h12-13,18H,3-11H2,1-2H3			1	1	1
101-21-3	101213	145	**Chlorpropham**	2_Pest	Chlorpropham	(3-Chlorophenyl)carbamic acid, 1-Methylethyl ester	C10H12ClNO2	C10H12ClNO2	213.66	CC(C)OC(=O)Nc1cccc(Cl)c1	InChI=1/C10H12ClNO2/c1-7(2)14-10(13)12-9-5-3-4-8(11)6-9/h3-7H,1-2H3,(H,12,13)	2.984	2.984	1	1	1
101-42-8	101428	147	**Fenuron**	2_Pest	Urea, N,N-dimethyl-N'-phenyl-	Fenuron	C9H12N2O	C9H12N2O	164.21	CN(C)C(=O)Nc1ccccc1	InChI=1/C9H12N2O/c1-11(2)9(12)10-8-6-4-3-5-7-8/h3-7H,1-2H3,(H,10,12)	1.152	1.152	1	1	1
101463-69-8	101463698	148	**Flufenoxuron**	2_Pest		Flufenoxuron			488.77	C1=CC(=C(C=C1F)C(=O)NC(=O)NC2=C(C=C(C=C2)OC3=C(C=C(C=C3)C(F)(F)F)Cl)F)F	InChI=1S/C21H11ClF6N2O3/c22-12-8-10(21(26,27)28)4-7-17(12)33-11-5-6-16(15(25)9-11)29-20(32)30-19(31)18-13(23)2			1	1	1
1014-69-3	1014693	149	**Desmetryn**	2_Pest	2-Methylthio-4-methylamino-6-isopropyl-1,3,5-triazine	N-Methyl-N'-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine	C8H15N5S	C8H15N5S	213.31	CNc1nc(NC(C)C)nc(SC)n1	InChI=1/C8H15N5S/c1-5(2)10-7-11-6(9-3)12-8(13-7)14-4/h5H,1-4H3,(H2,9,10,11,12,13)	1.449	1.428	1	1	1
10265-92-6	10265926	153	**Methamidophos**	2_Pest	Phosphoramidothioic acid, O,S-dimethyl ester	Phosphoramidothioic acid, O,S-Dimethyl ester	C2H8NO2PS	C2H8NO2PS	141.13	COP(=O)(N)SC	InChI=1/C2H8NO2PS/c1-5-6(3,4)7-2/h1-2H3,(H2,3,4)	-0.274	-0.274	1	1	1
102851-06-9	102851069	157	**Tau-fluvalinate**	2_Pest		N-[2-Chloro-4-(trifluoromethyl)phenyl]-D-valine cyano(3-phenoxyphenyl)methyl ester			502.92	CC(C)C(C(=O)OC(C#N)C1=CC(=CC=C1)OC2=CC=CC=C2)NC3=C(C=C(C=C3)C(F)(F)F)Cl	InChI=1S/C26H22ClF3N2O3/c1-16(2)24(32-22-12-11-18(14-21(22)27)26(28,29)30)25(33)35-23(15-31)17-7-6-10-20(13-17			1	1	1
103055-07-8	103055078	158	**Lufenuron**	2_Pest		N-[[[2,5-Dichloro-4-(1,1,2,3,3,3-hexafluoropropoxy)phenyl]amino]carbonyl]-2,6-difluorobenzamide			511.15	C1=CC(=C(C(=C1)F)C(=O)NC(=O)NC2=CC(=C(C=C2Cl)OC(C(C(F)(F)F)F)(F)F)Cl)F	InChI=1S/C17H8Cl2F8N2O3/c18-6-5-11(32-17(26,27)14(22)16(23,24)25)7(19)4-10(6)28-15(31)29-13(30)12-8(20)2-1-3-9(			1	1	1
10311-84-9	10311849	4894	**Dialifos**	2_Pest	Dialifor	S-[2-Chloro-1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl], O,O-diethyl ester phosphorodithioic acid	C14H17ClNO4PS2	C14H17ClNO4PS2	393.85	CCOP(=S)(OCC)SC(CCl)N1C(=O)c2ccccc2C1=O	InChI=1/C14H17ClNO4PS2/c1-3-19-21(22,20-4-2)23-12(9-15)16-13(17)10-7-5-6-8-11(10)14(16)18/h5-8,12H,3-4,9H2,1-2H3	3.535	3.535	1	1	1
104040-78-0	104040780	166	**Flazasulfuron**	2_Pest		N-[[4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]-3-(trifluoromethyl)-2-pyridinesulfonamide			407.33	COC1=CC(=NC(=N1)NC(=O)NS(=O)(=O)C2=C(C=CC=N2)C(F)(F)F)OC	InChI=1S/C13H12F3N5O5S/c1-25-8-6-9(26-2)19-11(18-8)20-12(22)21-27(23,24)10-7(13(14,15)16)4-3-5-17-10/h3-6H,1-2			1	1	1
104206-82-8	104206828	167	**Mesotrione**	2_Pest		2-[4-(Methylsulfonyl)-2-nitrobenzoyl]-1,3-cyclohexanedione			339.32	CS(=O)(=O)C1=CC(=C(C=C1)C(=O)C2C(=O)CCCC2=O)[N+](=O)[O-]	InChI=1S/C14H13NO7S/c1-23(21,22)8-5-6-9(10(7-8)15(19)20)14(18)13-11(16)3-2-4-12(13)17/h5-7,13H,2-4H2,1H3			1	1	1
10453-86-8	10453868	1114	**Resmethrin**	2_Pest	Resmethrin	2,2-Dimethyl-3-(2-methyl-1-propen-1-yl)cyclopropanecarboxylic acid [5-(phenylmethyl)-3-furanyl]methyl ester	C22H26O3	C22H26O3	338.45	CC(=CC1C(C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C)C	InChI=1/C22H26O3/c1-15(2)10-19-20(22(19,3)4)21(23)25-14-17-12-18(24-13-17)11-16-8-6-5-7-9-16/h5-10,12-13,19-20H,11,14H2,1-4H3	4.934	4.934	1	1	1
10552-74-6	10552746	176	**Nitrothal-isopropyl**	2_Pest		nitrothal-isopropyl		C14H17NO6	295.29	CC(C)OC(=O)c1cc(cc(c1)[N+](=O)[O-])C(=O)OC(C)C	InChI=1/C14H17NO6/c1-8(2)20-13(16)10-5-11(14(17)21-9(3)4)7-12(6-10)15(18)19/h5-9H,1-4H3	2.887	2.887	1	1	1
10605-21-7	10605217	3	**Carbendazim**	2_Pest		N-1H-Benzimidazol-2-yl carbamic acid methyl ester		C9H9N3O2	191.19	COC(=O)Nc1nc2ccccc2[nH]1	InChI=1/C9H9N3O2/c1-14-9(13)12-8-10-6-4-2-3-5-7(6)11-8/h2-5H,1H3,(H2,10,11,12,13)	1.65	1.65	1	1	1
1071-83-6	1071836	212	**Glyphosate**	2_Pest		N-(Phosphonomethyl)glycine		C3H7NO5P	169.07	OP(=O)([O-])C[NH2+]CC(=O)[O-]	InChI=1/C3H8NO5P/c5-3(6)1-4-2-10(7,8)9/h4H,1-2H2,(H,5,6)(H2,7,8,9)/p-1	-5.696	-5.626	0	1	1
107534-96-3	107534963	221	**Tebuconazole**	2_Pest		Tebuconazole			307.83	CC(C)(C)C(CCC1=CC=C(C=C1)Cl)(CN2C=NC=N2)O	InChI=1S/C16H22ClN3O/c1-15(2,3)16(21,10-20-12-18-11-19-20)9-8-13-4-6-14(17)7-5-13/h4-7,11-12,21H,8-10H2,1-3H3			1	1	1
1085-98-9	1085989	241	**Dichlofluanid**	2_Pest	Dichlofluanid	Dichlofluanid	C9H11Cl2FN2O2S2	C9H11Cl2FN2O2S2	333.23	CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccccc1	InChI=1/C9H11Cl2FN2O2S2/c1-13(2)18(15,16)14(17-9(10,11)12)8-6-4-3-5-7-8/h3-7H,1-2H3	3.838	3.838	1	1	1
110488-70-5	110488705	4906	**Dimethomorph**	2_Pest		dimethomorf			387.86	COC1=C(C=C(C=C1)C(=CC(=O)N2CCOCC2)C3=CC=C(C=C3)Cl)OC	InChI=1S/C21H22ClNO4/c1-25-19-8-5-16(13-20(19)26-2)18(15-3-6-17(22)7-4-15)14-21(24)23-9-11-27-12-10-23/h3-8,13-			1	1	1
1113-02-6	1113026	295	**Omethoate**	2_Pest	Omethoate	O,O-Dimethyl S-[2-(methylamino)-2-oxoethyl ester phosphorothioic acid	C5H12NO4PS	C5H12NO4PS	213.19	CNC(=O)CSP(=O)(OC)OC	InChI=1/C5H12NO4PS/c1-6-5(7)4-12-11(8,9-2)10-3/h4H2,1-3H3,(H,6,7)	-0.547	-0.547	1	1	1
111479-05-1	111479051	303	**Propaquizafop**	2_Pest		propaquizafop			443.89	CC(C(=O)OCCON=C(C)C)OC1=CC=C(C=C1)OC2=CN=C3C=C(C=CC3=N2)Cl	InChI=1S/C22H22ClN3O5/c1-14(2)26-29-11-10-28-22(27)15(3)30-17-5-7-18(8-6-17)31-21-13-24-20-12-16(23)4-9-19(20)2			1	1	1
111988-49-9	111988499	6	**Thiacloprid**	2_Pest		Thiacloprid			252.73	C1CSC(=NC#N)N1CC2=CN=C(C=C2)Cl	InChI=1S/C10H9ClN4S/c11-9-2-1-8(5-13-9)6-15-3-4-16-10(15)14-7-12/h1-2,5H,3-4,6H2			1	1	1
111991-09-4	111991094	319	**Nicosulfuron**	2_Pest		Nicosulfuron			410.42	CN(C)C(=O)C1=C(N=CC=C1)S(=O)(=O)NC(=O)NC2=NC(=CC(=N2)OC)OC	InChI=1S/C15H18N6O6S/c1-21(2)13(22)9-6-5-7-16-12(9)28(24,25)20-15(23)19-14-17-10(26-3)8-11(18-14)27-4/h5-8H,1-4			1	1	1
112281-77-3	112281773	323	**Tetraconazole**	2_Pest		1-[2-(2,4-Dichlorophenyl)-3-(1,1,2,2-tetrafluoroethoxy)propyl]-1H-1,2,4-triazole			372.15	C1=CC(=C(C=C1Cl)Cl)C(CN2C=NC=N2)COC(C(F)F)(F)F	InChI=1S/C13H11Cl2F4N3O/c14-9-1-2-10(11(15)3-9)8(4-22-7-20-6-21-22)5-23-13(18,19)12(16)17/h1-3,6-8,12H,4-5H2			1	1	1
112410-23-8	112410238	328	**Tebufenozide**	2_Pest		1-(1,1-Dimethylethyl)-2-(4-ethylbenzoyl)hydrazide-3,5-dimethylbenzoic acid			352.48	CCC1=CC=C(C=C1)C(=O)NN(C(=O)C2=CC(=CC(=C2)C)C)C(C)(C)C	InChI=1S/C22H28N2O2/c1-7-17-8-10-18(11-9-17)20(25)23-24(22(4,5)6)21(26)19-13-15(2)12-16(3)14-19/h8-14H,7H2,1-6			1	1	1
113136-77-9	113136779	334	**Cyclanilide**	2_Pest		1-[[(2,4-Dichlorophenyl)amino]carbonyl]cyclopropanecarboxylic acid			274.1	C1CC1(C(=O)NC2=C(C=C(C=C2)Cl)Cl)C(=O)O	InChI=1S/C11H9Cl2NO3/c12-6-1-2-8(7(13)5-6)14-9(15)11(3-4-11)10(16)17/h1-2,5H,3-4H2,(H,14,15)(H,16,17)			1	1	1
113158-40-0	113158400	335	**Fenoxaprop-P**	2_Pest		(2R)-2-[4-[(6-Chloro-2-			333.73	CC(C(=O)O)OC1=CC=C(C=C1)OC2=NC3=C(O2)C=C(C=C3)Cl	InChI=1S/C16H12ClNO5/c1-9(15(19)20)21-11-3-5-12(6-4-11)22-16-18-13-7-2-10(17)8-14(13)23-16/h2-9H,1H3,(H,19,20)/			1	1	1
1134-23-2	1134232	4878	**Cycloate**	2_Pest	Cycloate	Cyclohexylethylcarbamothioic acid S-ethyl	C11H21NOS	C9H17NOS	215.36	CCSC(=O)NC1CCCCC1	InChI=1/C9H17NOS/c1-2-12-9(11)10-8-6-4-3-5-7-8/h8H,2-7H2,1H3,(H,10,11)	2.782	2.782	1	1	1
114-26-1	114261	337	**Propoxur**	2_Pest	2-Isopropoxyphenyl N-methylcarbamate	Propoxur	C11H19NO3	C11H15NO3	209.25	CNC(=O)Oc1ccccc1OC(C)C	InChI=1/C11H15NO3/c1-8(2)14-9-6-4-5-7-10(9)15-11(13)12-3/h4-8H,1-3H3,(H,12,13)	2.303	2.303	1	1	1
114369-43-6	114369436	338	**Fenbuconazole**	2_Pest		Fenbuconazole			336.83	C1=CC=C(C=C1)C(CCC2=CC=C(C=C2)Cl)(CN3C=NC=N3)C#N	InChI=1S/C19H17ClN4/c20-18-8-6-16(7-9-18)10-11-19(12-21,13-24-15-22-14-23-24)17-4-2-1-3-5-17/h1-9,14-15H,10-11,1			1	1	1
115-29-7	115297	4921	**Endosulfan**	2_Pest	Endosulfan	Endosulfan	C9H6Cl6O3S	C9H6Cl6O3S	406.93	ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)C2(Cl)Cl	InChI=1/C9H6Cl6O3S/c10-5-6(11)8(13)4-2-18-19(16)17-1-3(4)7(5,12)9(8,14)15/h3-4H,1-2H2	2.641	2.641	1	1	1
115-32-2	115322	340	**Dicofol**	2_Pest	Acetic acid, [3,5-diiodo-4-(4-hydroxy-3-iodophenoxy) phenyl]-, 2-[diethylamino]ethyl ester, hydrochloride	4-Chloro-alpha-(4-chlorophenyl)-alpha-(trichloromethyl)benzenemethanol	C14H9Cl5O	C14H9Cl5O	370.49	OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(Cl)(Cl)Cl	InChI=1/C14H9Cl5O/c15-11-5-1-9(2-6-11)13(20,14(17,18)19)10-3-7-12(16)8-4-10/h1-8,20H	5.62	5.62	1	1	1
116-06-3	116063	342	**Aldicarb**	2_Pest	Aldicarb	2-Methyl-2-(methylthio)propionaldehyde, O-(Methylcarbamoyl)oxime	C7H14N2O2S	C7H14N2O2S	190.27	CNC(=O)O\N=C\C(C)(C)SC	InChI=1/C7H14N2O2S/c1-7(2,12-4)5-9-11-6(10)8-3/h5H,1-4H3,(H,8,10)/b9-5+	0.98	0.98	1	1	1
116255-48-2	116255482	343	**Bromuconazole**	2_Pest		Bromuconazole			377.08	C1C(COC1(CN2C=NC=N2)C3=C(C=C(C=C3)Cl)Cl)Br	InChI=1S/C13H12BrCl2N3O/c14-9-4-13(20-5-9,6-19-8-17-7-18-19)11-2-1-10(15)3-12(11)16/h1-3,7-9H,4-6H2			1	1	1
116-29-0	116290	344	**Tetradifon**	2_Pest	P-chlorophenyl, 2,4,5-trichlorophenyl sulfone	p-Chlorophenyl, 2,4,5-Trichlorophenyl sulfone	C12H6Cl4O2S	C12H6Cl4O2S	356.05	Clc1ccc(cc1)S(=O)(=O)c2cc(Cl)c(Cl)cc2Cl	InChI=1/C12H6Cl4O2S/c13-7-1-3-8(4-2-7)19(17,18)12-6-10(15)9(14)5-11(12)16/h1-6H	5.59	5.59	1	1	1
118134-30-8	118134308	347	**Spiroxamine**	2_Pest		8-(1,1-Dimethylethyl)-N-ethyl-N-propyl-1,4-dioxaspiro[4.5]decane-2-methanamine			297.48	CCCN(CC)CC1COC2(O1)CCC(CC2)C(C)(C)C	InChI=1S/C18H35NO2/c1-6-12-19(7-2)13-16-14-20-18(21-16)10-8-15(9-11-18)17(3,4)5/h15-16H,6-14H2,1-5H3			1	1	1
119168-77-3	119168773	350	**Tebufenpyrad**	2_Pest		4-Chloro-N-[[4-(1,1-dimethylethyl)phenyl]methyl]-3-ethyl-1-methyl-1H-pyrazole-5-carboxamide			333.87	CCC1=NN(C(=C1Cl)C(=O)NCC2=CC=C(C=C2)C(C)(C)C)C	InChI=1S/C18H24ClN3O/c1-6-14-15(19)16(22(5)21-14)17(23)20-11-12-7-9-13(10-8-12)18(2,3)4/h7-10H,6,11H2,1-5H3,(H			1	1	1
119446-68-3	119446683	351	**Difenoconazole**	2_Pest		Difenoconazole			406.27	CC1COC(O1)(CN2C=NC=N2)C3=C(C=C(C=C3)OC4=CC=C(C=C4)Cl)Cl	InChI=1S/C19H17Cl2N3O3/c1-13-9-25-19(27-13,10-24-12-22-11-23-24)17-7-6-16(8-18(17)21)26-15-4-2-14(20)3-5-15/h2-			1	1	1
1194-65-6	1194656	352	**dichlobenil**	2_Pest	2,6-Dichlorobenzoic acid nitrile	Dichlobenil	C7H3Cl2N	C7H3Cl2N	172.01	Clc1cccc(Cl)c1C#N	InChI=1/C7H3Cl2N/c8-6-2-1-3-7(9)5(6)4-10/h1-3H	3.037	3.037	1	1	1
120068-37-3	120068373	11	**Fipronil**	2_Pest		Fipronil			437.15	C1=C(C=C(C(=C1Cl)N2C(=C(C(=N2)C#N)S(=O)C(F)(F)F)N)Cl)C(F)(F)F	InChI=1S/C12H4Cl2F6N4OS/c13-5-1-4(11(15,16)17)2-6(14)8(5)24-10(22)9(7(3-21)23-24)26(25)12(18,19)20/h1-2H,22H2			1	1	1
120-36-5	120365	4895	**Dichlorprop**	2_Pest	Alpha-(2,4-dichlorophenoxy)propionic acid	2-(2,4-Dichlorophenoxy)propanoic acid	C9H8Cl2O3	C9H7Cl2O3	235.07	CC(Oc1ccc(Cl)cc1Cl)C(=O)[O-]	InChI=1/C9H8Cl2O3/c1-5(9(12)13)14-8-3-2-6(10)4-7(8)11/h2-5H,1H3,(H,12,13)/p-1	1.634	1.634	1	1	1
120928-09-8	120928098	366	**Fenazaquin**	2_Pest		Fenazaquin			306.41	CC(C)(C)C1=CC=C(C=C1)CCOC2=NC=NC3=CC=CC=C32	InChI=1S/C20H22N2O/c1-20(2,3)16-10-8-15(9-11-16)12-13-23-19-17-6-4-5-7-18(17)21-14-22-19/h4-11,14H,12-13H2,1-3H3			1	1	1
121552-61-2	121552612	371	**Cyprodinil**	2_Pest		Cyprodinil			225.3	CC1=NC(=NC(=C1)C2CC2)NC3=CC=CC=C3	InChI=1S/C14H15N3/c1-10-9-13(11-7-8-11)17-14(15-10)16-12-5-3-2-4-6-12/h2-6,9,11H,7-8H2,1H3,(H,15,16,17)			1	1	1
122-14-5	122145	378	**Fenitrothion**	2_Pest	Fenitrothion	O,O-Dimethyl O-(3-methyl-4-nitrophenyl ester phosphorothioic acid	C9H12NO5PS	C9H12NO5PS	277.24	COP(=S)(OC)Oc1ccc(c(C)c1)[N+](=O)[O-]	InChI=1/C9H12NO5PS/c1-7-6-8(4-5-9(7)10(11)12)15-16(17,13-2)14-3/h4-6H,1-3H3	2.691	2.691	1	1	1
122-34-9	122349	15	**Simazine**	2_Pest	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-diethyl-	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	C7H12ClN5	C7H12ClN5	201.67	CCNc1nc(Cl)nc(NCC)n1	InChI=1/C7H12ClN5/c1-3-9-5-11-6(8)12-7(13-5)10-4-2/h3-4H2,1-2H3,(H2,9,10,11,12,13)	1.213	1.213	1	1	1

122-42-9	122429	5107	**Propham**	2_Pest	Carbamic acid, phenyl-, 1-methylethyl ester	1-Methylethylphenylcarbamic acid	C10H13NO2	C10H13NO2	179.22	CC(C)OC(=O)Nc1ccccc1	InChI=1/C10H13NO2/c1-8(2)13-10(12)11-9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)	2.319	2.319	1	1	1
122453-73-0	122453730	380	**Chlorfenapyr**	2_Pest		chlorfenapyr			407.63	CCOCN1C(=C(C(=C1C(F)(F)F)Br)C#N)C2=CC=C(C=C2)Cl	InChI=1S/C15H11BrClF3N2O/c1-2-23-8-22-13(9-3-5-10(17)6-4-9)11(7-21)12(16)14(22)15(18,19)20/h3-6H,2,8H2,1H3			1	1	1
122931-48-0	122931480	383	**Rimsulfuron**	2_Pest		Rimsulfuron			431.45	CCS(=O)(=O)C1=C(N=CC=C1)S(=O)(=O)NC(=O)NC2=NC(=CC(=N2)OC)OC	InChI=1S/C14H17N5O7S2/c1-4-27(21,22)9-6-5-7-15-12(9)28(23,24)19-14(20)18-13-16-10(25-2)8-11(17-13)26-3/h5-8H,4			1	1	1
123312-89-0	123312890	387	**Pymetrozine**	2_Pest		4,5-Dihydro-6-methyl-4-[(E)-(3-pyridinylmethylene)amino]-1,2,4-triazin-3(2H)-one			217.24	CC1=NNC(=O)N(C1)N=CC2=CN=CC=C2	InChI=1S/C10H11N5O/c1-8-7-15(10(16)14-13-8)12-6-9-3-2-4-11-5-9/h2-6H,7H2,1H3,(H,14,16)/b12-6+			1	1	1
123-33-1	123331	389	**Maleic hydrazide**	2_Pest	Maleic hydrazide	1,2-Dihydro-3,6-pyridazinedione	C4H4N2O2	C4H3N2O2	112.09	Oc1ccc([O-])nn1	InChI=1/C4H4N2O2/c7-3-1-2-4(8)6-5-3/h1-2H,(H,5,7)(H,6,8)/p-1	0.102	0.118	1	1	1
125116-23-6	125116236	405	**Metconazole**	2_Pest		5-[(4-Chlorophenyl)methyl]-2,2-dimethyl-1-(1H-1,2,4-triazol-1-ylmethyl)cyclopentanol			319.84	CC1(CCC(C1(CN2C=NC=N2)O)CC3=CC=C(C=C3)Cl)C	InChI=1S/C17H22ClN3O/c1-16(2)8-7-14(9-13-3-5-15(18)6-4-13)17(16,22)10-21-12-19-11-20-21/h3-6,11-12,14,22H,7-10H			1	1	1
126833-17-8	126833178	409	**Fenhexamid**	2_Pest		N-(2,3-Dichloro-4-hydroxyphenyl)-1-			302.2	CC1(CCCCC1)C(=O)NC2=C(C(=C(C=C2)O)Cl)Cl	InChI=1S/C14H17Cl2NO2/c1-14(7-3-2-4-8-14)13(19)17-9-5-6-10(18)12(16)11(9)15/h5-6,18H,2-4,7-8H2,1H3,(H,17,19)			1	1	1
13071-79-9	13071799	416	**Terbufos**	2_Pest	Phosphorodithioic acid, S-[(tert-butylthio)methyl] O,O-diethyl ester	Phosphorodithioic acid S-[[(1,1-dimethylethyl)thio]O,O-diethylmethyl]ester	C9H21O2PS3	C9H21O2PS3	288.43	CCOP(=S)(OCC)SCSC(C)(C)C	InChI=1/C9H21O2PS3/c1-6-10-12(13,11-7-2)15-8-14-9(3,4)5/h6-8H2,1-5H3	3.517	3.517	1	1	1
13121-70-5	13121705	419	**Cyhexatin**	2_Pest		Tricyclohexylhydroxystannane		C18H34OSn	385.16	O[Sn](C1CCCCC1)(C2CCCCC2)C3CCCCC3	InChI=1/3C6H11.H2O.Sn/c3*1-2-4-6-5-3-1;;/h3*1H,2-6H2;1H2;/q;;;+1/p-1	6.543	6.543	1	1	1
131341-86-1	131341861	420	**Fludioxonil**	2_Pest		4-(2,2-Difluoro-1,3-benzodioxol-4-yl)-1H-pyrrole-3-carbonitrile			248.19	C1=CC(=C2C(=C1)OC(O2)(F)F)C3=CNC=C3C#N	InChI=1S/C12H6F2N2O2/c13-12(14)17-10-3-1-2-8(11(10)18-12)9-6-16-5-7(9)4-15/h1-3,5-6,16H			1	1	1
13171-21-6	13171216	5093	**Phosphamidon**	2_Pest	Phosphamidon	Phosphoric acid, 2-Chloro-3-(diethylamino)-1-methyl-3-oxo-1-propen-1-yl dimethyl ester	C10H19ClNO5P	C10H19ClNO5P	299.69	CCN(CC)C(=O)\C(=C(/C)OP(=O)(OC)OC)\Cl	InChI=1/C10H19ClNO5P/c1-6-12(7-2)10(13)9(11)8(3)17-18(14,15-4)16-5/h6-7H2,1-5H3/b9-8-	0.643	0.643	1	1	1
131807-57-3	131807573	421	**Famoxadone**	2_Pest		Famoxadone			374.4	CC1(C(=O)N(C(=O)O1)NC2=CC=CC=C2)C3=CC=C(C=C3)OC4=CC=CC=C4	InChI=1S/C22H18N2O4/c1-22(16-12-14-19(15-13-16)27-18-10-6-3-7-11-18)20(25)24(21(26)28-22)23-17-8-4-2-5-9-17/h2-			1	1	1
13181-17-4	13181174	422	**Bromofenoxim**	2_Pest		Bromofenoxim		C13H6Br2N3O6	461.04	[O-]c1c(Br)cc(\C=N\Oc2ccc(cc2[N+](=O)[O-])[N+](=O)[O-])cc1Br	InChI=1/C13H7Br2N3O6/c14-9-3-7(4-10(15)13(9)19)6-16-24-12-2-1-8(17(20)21)5-11(12)18(22)23/h 6,19H/p-1/b16-6+	3.799	4.48	1	1	1
131860-33-8	131860338	423	**Azoxystrobin**	2_Pest		Azoxystrobin			403.4	COC=C(C1=CC=CC=C1OC2=NC=NC(=C2)OC3=CC=CC=C3C#N)C(=O)OC	InChI=1S/C22H17N3O5/c1-27-13-17(22(26)28-2)16-8-4-6-10-19(16)30-21-11-20(24-14-25-21)29-18-9-5-3-7-15(18)12-23/			1	1	1
13194-48-4	13194484	4930	**Ethoprophos**	2_Pest	Ethoprophos	Phosphorodithioic acid O-ethyl S,S-dipropyl ester	C8H19O2PS2	C8H19O2PS2	242.34	CCCSP(=O)(OCC)SCCC	InChI=1/C8H19O2PS2/c1-4-7-12-11(9,10-6-3)13-8-5-2/h4-8H2,1-3H3	3.231	3.231	1	1	1
131983-72-7	131983727	424	**Triticonazole**	2_Pest		5-[(4-Chlorophenyl)methylene]-2,2-dimethyl-1-(1H-1,2,4-triazol-1-ylmethyl)cyclopentanol			317.82	CC1(CCC(=CC2=CC=C(C=C2)Cl)C1(CN3C=NC=N3)O)C	InChI=1S/C17H20ClN3O/c1-16(2)8-7-14(9-13-3-5-15(18)6-4-13)17(16,22)10-21-12-19-11-20-21/h3-6,9,11-12,22H,7-8,10H			1	1	1
132-66-1	132661	5059	**Naptalam**	2_Pest		2-[(1-Naphthalenylamino)carbonyl]benzoic acid			291.31	C1=CC=C2C(=C1)C=CC=C2NC(=O)C3=CC=CC=C3C(=O)O	InChI=1S/C18H13NO3/c20-17(14-9-3-4-10-15(14)18(21)22)19-16-11-5-7-12-6-1-2-8-13(12)16/h1-11H,(H,19,20)(H,21,22)			1	1	1
133-06-2	133062	425	**Captan**	2_Pest	Captan	3a,4,7,7a-Tetrahydro-2-[(trichloromethyl)thio]-1H-isoindole-1,3-(2H)-dione	C9H8Cl3NO2S	C9H8Cl3NO2S	300.59	ClC(Cl)(Cl)SN1C(=O)C2CC=CCC2C1=O	InChI=1/C9H8Cl3NO2S/c10-9(11,12)16-13-7(14)5-3-1-2-4-6(5)8(13)15/h1-2,5-6H,3-4H2	4.022	4.022	1	1	1
133-07-3	133073	426	**Folpet**	2_Pest	Folpet	2-[(Trichloromethyl)thio]-1H-isoindole-1,3(2H)dione	C9H4Cl3NO2S	C9H4Cl3NO2S	296.56	ClC(Cl)(Cl)SN1C(=O)c2ccccc2C1=O	InChI=1/C9H4Cl3NO2S/c10-9(11,12)16-13-7(14)5-3-1-2-4-6(5)8(13)15/h1-4H	4.449	4.449	1	1	1
13360-45-7	13360457	428	**Chlorbromuron**	2_Pest	3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methylurea	3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methyl urea	C9H10BrClN2O2	C9H10BrClN2O2	293.56	CON(C)C(=O)Nc1ccc(Br)c(Cl)c1	InChI=1/C9H10BrClN2O2/c1-13(15-2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	2.41	2.817	1	1	1
134098-61-6	134098616	429	**Fenpyroximate**	2_Pest		Fenpyroximaat			421.5	CC1=NN(C(=C1C=NOCC2=CC=C(C=C2)C(=O)OC(C)(C)C)OC3=CC=CC=C3)C	InChI=1S/C24H27N3O4/c1-17-21(22(27(5)26-17)30-20-9-7-6-8-10-20)15-25-29-16-18-11-13-19(14-12-18)23(28)31-24(2,3			1	1	1
13457-18-6	13457186	432	**Pyrazophos**	2_Pest	Pyrazophos	Afugan	C14H20N3O5PS	C14H20N3O5PS	373.37	CCOC(=O)c1cn2nc(OP(=S)(OCC)OCC)cc2nc1C	InChI=1/C14H20N3O5PS/c1-5-19-14(18)11-9-17-12(15-10(11)4)8-13(16-17)22-23(24,20-6-2)21-7-3/h8-9H,5-7H2,1-4H3	2.307	2.307	1	1	1
13593-03-8	13593038	437	**Quinalphos**	2_Pest	Quinalphos	O,O-Diethyl O-2-quinoxalinylester, Phosphorothioic acid	C12H15N2O3PS	C12H15N2O3PS	298.3	CCOP(=S)(OCC)Oc1cnc2ccccc2n1	InChI=1/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-12-9-13-10-7-5-6-8-11(10)14-12/h5-9H,3-4H2,1-2H3	3.011	3.011	1	1	1
136426-54-5	136426545	438	**Fluquinconazole**	2_Pest		Fluquinconazool			376.18	C1=CC2=C(C=C1F)C(=O)N(C(=N2)N3C=NC=N3)C4=C(C=C(C=C4)Cl)Cl	InChI=1S/C16H8Cl2FN5O/c17-9-1-4-14(12(18)5-9)24-15(25)11-6-10(19)2-3-13(11)22-16(24)23-8-20-7-21-23/h1-8H			1	1	1
13684-56-5	13684565	439	**Desmedipham**	2_Pest	Desmedipham	Desmedipham	C16H16N2O4	C16H16N2O4	300.32	CCOC(=O)Nc1cccc(OC(=O)Nc2ccccc2)c1	InChI=1/C16H16N2O4/c1-2-21-15(19)18-13-9-6-10-14(11-13)22-16(20)17-12-7-4-3-5-8-12/h3-11H,2H2,1H3,(H,17,20)(H,18,19)	3.282	3.282	1	1	1
13684-63-4	13684634	440	**Phenmedipham**	2_Pest	Methyl 3-m-tolylcarbamoyloxyphenylcarbamate	(3-Methylphenyl)carbamic acid 3-[(methoxycarbonyl)amino]phenyl ester	C16H16N2O4	C16H16N2O4	300.32	COC(=O)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1	InChI=1/C16H16N2O4/c1-11-5-3-6-12(9-11)18-16(20)22-14-8-4-7-13(10-14)17-15(19)21-2/h3-10H,1-2H3,(H,17,19)(H,18,20)	3.42	3.42	1	1	1
137-26-8	137268	441	**thiram**	2_Pest	Thiram	Thiram	C6H12N2S4	C6H12N2S4	240.43	CN(C)C(=S)SSC(=S)N(C)C	InChI=1/C6H12N2S4/c1-7(2)5(9)11-12-6(10)8(3)4/h1-4H3	4.204	4.204	1	1	1
138261-41-3	138261413	443	**imidacloprid**	2_Pest		imidacloprid			255.67	C1CN(C(=N1)N[N+](=O)[O-])CC2=CN=C(C=C2)Cl	InChI=1S/C9H10ClN5O2/c10-8-2-1-7(5-12-8)6-14-4-3-11-9(14)13-15(16)17/h1-2,5H,3-4,6H2,(H,11,13)			1	1	1
139-40-2	139402	446	**propazine**	2_Pest	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-bis(1-methylethyl)-	Propazine	C9H16ClN5	C9H16ClN5	229.72	CC(C)Nc1nc(Cl)nc(NC(C)C)n1	InChI=1/C9H16ClN5/c1-5(2)11-8-13-7(10)14-9(15-8)12-6(3)4/h5-6H,1-4H3,(H2,11,12,13,14,15)	1.968	1.968	1	1	1
139528-85-1	139528851	1922	**Metosulam**	2_Pest		2',6'-dichloro-5,7-dimethoxy-3'-methyl[1,2,4]triazolo[1,5-a]pyrimidine-2-sulfonanilide			419.27	CC1=C(C(=C(C=C1)Cl)NS(=O)(=O)C2=NN3C(=CC(=NC3=N2)OC)OC)Cl	InChI=1S/C14H13Cl2N5O4S/c1-7-4-5-8(15)12(11(7)16)20-26(22,23)14-18-13-17-9(24-2)6-10(25-3)21(13)19-14/h4-6,20H			1	1	1
140923-17-7	140923177	453	**Iprovalicarb**	2_Pest		iprovalicarb			320.44	CC1=CC=C(C=C1)C(C)NC(=O)C(C(C)C)NC(=O)OC(C)C	InChI=1S/C18H28N2O3/c1-11(2)16(20-18(22)23-12(3)4)17(21)19-14(6)15-9-7-13(5)8-10-15/h7-12,14,16H,1-6H3,(H,19,21			1	1	1
141517-21-7	141517217	5178	**Trifloxystrobine**	2_Pest		(alphaE)-alpha-(Methoxyimino)-2-[[[(E)-[1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetic acid methyl ester			408.38	CC(=NOCC1=CC=CC=C1C(=NOC)C(=O)OC)C2=CC(=CC=C2)C(F)(F)F	InChI=1S/C20H19F3N2O4/c1-13(14-8-6-9-16(11-14)20(21,22)23)24-29-12-15-7-4-5-10-17(15)18(25-28-3)19(26)27-2/h4-			1	1	1
141776-32-1	141776321	457	**Sulfosulfuron**	2_Pest		N-[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]-2-(ethylsulfonyl)imidazo[1,2-a]pyridine-3-sulfonamide			470.49	CCS(=O)(=O)C1=C(N2C=CC=CC2=N1)S(=O)(=O)NC(=O)NC3=NC(=CC(=N3)OC)OC	InChI=1S/C16H18N6O7S2/c1-4-30(24,25)13-14(22-8-6-5-7-10(22)17-13)31(26,27)21-16(23)20-15-18-11(28-2)9-12(19-15			1	1	1
1420-07-1	1420071	4911	**Dinoterb**	2_Pest	2-Tert-butyl-4,6-dinitrophenol	dinoterb	C10H12N2O5	C10H11N2O5	240.22	CC(C)(C)c1cc(cc(c1[O-])[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C10H12N2O5/c1-10(2,3)7-4-6(11(14)15)5-8(9(7)13)12(16)17/h4-5,13H,1-3H3/p-1	2.073	2.078	1	1	1
14214-32-5	14214325	4902	**Difenoxuron**	2_Pest		difenoxuron		C16H18N2O3	286.33	COc1ccc(Oc2ccc(NC(=O)N(C)C)cc2)cc1	InChI=1/C16H18N2O3/c1-18(2)16(19)17-12-4-6-14(7-5-12)21-15-10-8-13(20-3)9-11-15/h4-11H,1-3H3,(H,17,19)	2.695	2.696	1	1	1
142459-58-3	142459583	461	**Flufenacet**	2_Pest		N-(4-Fluorophenyl)-N-(1-methylethyl)-2-[[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]oxy]acetamide			363.34	CC(C)N(C1=CC=C(C=C1)F)C(=O)COC2=NN=C(S2)C(F)(F)F	InChI=1S/C14H13F4N3O2S/c1-8(2)21(10-5-3-9(15)4-6-10)11(22)7-23-13-20-19-12(24-13)14(16,17)18/h3-6,8H,7H2,1-2H3			1	1	1
143390-89-0	143390890	470	**Kresoxim-Methyl**	2_Pest		(alphaE)-alpha-(Methoxyimino)-2-[(2-methylphenoxy)methyl]benzeneacetic acid methyl ester			313.35	CC1=CC=CC=C1OCC2=CC=CC=C2C(=NOC)C(=O)OC	InChI=1S/C18H19NO4/c1-13-8-4-7-11-16(13)23-12-14-9-5-6-10-15(14)17(19-22-3)18(20)21-2/h4-11H,12H2,1-3H3/b19-17+			1	1	1
145701-23-1	145701231	473	**Florasulam**	2_Pest		N-(2,6-Difluorophenyl)-8-fluoro-5-methoxy-[1,2,4]triazolo[1,5-c]pyrimidine-2-sulfonamide			**359.283**	COC1=NC=C(C2=NC(=NN21)S(=O)(=O)NC3=C(C=CC=C3F)F)F	InChI=1S/C12H8F3N5O3S/c1-23-12-16-5-8(15)10-17-11(18-20(10)12)24(21,22)19-9-6(13)3-2-4-7(9)14/h2-5,19H,1H3			1	1	1
14816-18-3	14816183	475	**Phoxim**	2_Pest	phoxim	O,O-Diethyl phosphorothioate, Phenyl-glyoxylonitrile oxime	C12H15N2O3PS	C12H15N2O3PS	298.3	CCOP(=S)(OCC)O\N=C(/C#N)\c1ccccc1	InChI=1/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-14-12(10-13)11-8-6-5-7-9-11/h5-9H,3-4H2,1-2H3/b14-12+	3.05	3.049	1	1	1
148-79-8	148798	476	**Thiabendazole**	2_Pest	Thiabendazole	2-(4-Thiazolyl)-1H-benzimidazole	C10H7N3S	C10H7N3S	201.25	c1ccc2[nH]c(nc2c1)c3cscn3	InChI=1/C10H7N3S/c1-2-4-8-7(3-1)12-10(13-8)9-5-14-6-11-9/h1-6H,(H,12,13)	2.154	2.374	1	1	1
149961-52-4	149961524	481	**Dimoxystrobin**	2_Pest		Dimoxystrobine			326.4	CC1=CC(=C(C=C1)C)OCC2=CC=CC=C2C(=NOC)C(=O)NC	InChI=1S/C19H22N2O3/c1-13-9-10-14(2)17(11-13)24-12-15-7-5-6-8-16(15)18(21-23-4)19(22)20-3/h5-11H,12H2,1-4H3,(H			1	1	1
149979-41-9	149979419	5148	**Tepraloxydim**	2_Pest		2-[1-[[[(2E)-3-Chloro-2-propen-1-yl]oxy]imino]propyl]-3-hydroxy-5-(tetrahydro-2H-pyran-4-yl)-2-cyclohexen-1-one			341.84	CCC(=C1C(=O)CC(CC1=O)C2CCOCC2)NOCC=CCl	InChI=1S/C17H24ClNO4/c1-2-14(19-23-7-3-6-18)17-15(20)10-13(11-16(17)21)12-4-8-22-9-5-12/h3,6,12-13,19H,2,4-5,7-1			1	1	1
150-68-5	150685	482	**Monuron**	2_Pest	Urea, N'-(4-chlorophenyl)-N,N-dimethyl-	Monuron	C9H11ClN2O	C9H11ClN2O	198.66	CN(C)C(=O)Nc1ccc(Cl)cc1	InChI=1/C9H11ClN2O/c1-12(2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	1.816	1.816	1	1	1
15165-67-0	15165670	4896	**Dichlorprop-P**	2_Pest		dichloorprop-p			235.07	CC(C(=O)O)OC1=C(C=C(C=C1)Cl)Cl	InChI=1S/C9H8Cl2O3/c1-5(9(12)13)14-8-3-2-6(10)4-7(8)11/h2-5H,1H3,(H,12,13)/t5-/m1/s1			1	1	1
15299-99-7	15299997	5058	**Napropamide**	2_Pest	Napropamide	N,N-Diethyl-2-(1-naphthalenyloxy)propanamide	C17H21NO2	C17H21NO2	271.36	CCN(CC)C(=O)C(C)Oc1cccc2ccccc12	InChI=1/C17H21NO2/c1-4-18(5-2)17(19)13(3)20-16-12-8-10-14-9-6-7-11-15(14)16/h6-13H,4-5H2,1-3H3	3.169	3.169	1	1	1
153719-23-4	153719234	487	**Thiamethoxam**	2_Pest		Thiamethoxam			291.72	CN1COCN(C1=N[N+](=O)[O-])CC2=CN=C(S2)Cl	InChI=1S/C8H10ClN5O3S/c1-12-4-17-5-13(8(12)11-14(15)16)3-6-2-10-7(9)18-6/h2H,3-5H2,1H3			1	1	1
15457-05-3	15457053	4958	**Fluorodifen**	2_Pest	2-Nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	2-Nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene	C13H7F3N2O5	C13H7F3N2O5	328.2	[O-][N+](=O)c1ccc(Oc2ccc(cc2[N+](=O)[O-])C(F)(F)F)cc1	InChI=1/C13H7F3N2O5/c14-13(15,16)8-1-6-12(11(7-8)18(21)22)23-10-4-2-9(3-5-10)17(19)20/h1-7H	4.121	4.121	1	1	1
15545-48-9	15545489	32	**Chlorotoluron**	2_Pest		Chlorotoluron		C10H13ClN2O	212.68	CN(C)C(=O)Nc1ccc(C)c(Cl)c1	InChI=1/C10H13ClN2O/c1-7-4-5-8(6-9(7)11)12-10(14)13(2)3/h4-6H,1-3H3,(H,12,14)	2.302	2.302	1	1	1
156052-68-5	156052685	490	**Zoxamide**	2_Pest		3,5-Dichloro-N-(3-chloro-1-ethyl-1-methyl-2-oxopropyl)-4-methylbenzamide			336.65	CCC(C)(C(=O)CCl)NC(=O)C1=CC(=C(C(=C1)Cl)C)Cl	InChI=1S/C14H16Cl3NO2/c1-4-14(3,12(19)7-15)18-13(20)9-5-10(16)8(2)11(17)6-9/h5-6H,4,7H2,1-3H3,(H,18,20)			1	1	1
1563-66-2	1563662	491	**Carbofuran**	2_Pest	Carbofuran	2,3-Dihydro-2,2-dimethyl-7-benzofuranol, Methylcarbamate	C12H15NO3	C12H15NO3	221.26	CNC(=O)Oc1cccc2CC(C)(C)Oc12	InChI=1/C12H15NO3/c1-12(2)7-8-5-4-6-9(10(8)16-12)15-11(14)13-3/h4-6H,7H2,1-3H3,(H,13,14)	2.234	2.234	1	1	1
1582-09-8	1582098	496	**Trifluralin**	2_Pest	Trifluralin	2,6-Dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	C13H16F3N3O4	C13H17F3N3O4	335.29	CCC[NH+](CCC)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	InChI=1/C13H16F3N3O4/c1-3-5-17(6-4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(22)23/h7-8H 6H2,1-2H3/p+1	2.812	2.997	1	1	1
15972-60-8	15972608	497	**Alachlor**	2_Pest	Alachlor	2-Chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide	C14H20ClNO2	C14H20ClNO2	269.77	CCc1cccc(CC)c1N(COC)C(=O)CCl	InChI=1/C14H20ClNO2/c1-4-11-7-6-8-12(5-2)14(11)16(10-18-3)13(17)9-15/h6-8H,4-5,9-10H2,1-3H3	3.425	3.425	1	1	1
161050-58-4	161050584	5021	**Methoxyfenozide**	2_Pest		3-Methoxymethylbenzoic acid 2-(3,5-dimethylbenzoyl)-2-(1,1-dimethylethyl)hydrazide			368.48	CC1=CC(=CC(=C1)C(=O)N(C(C)(C)C)NC(=O)C2=C(C(=CC=C2)OC)C)C	InChI=1S/C22H28N2O3/c1-14-11-15(2)13-17(12-14)21(26)24(22(4,5)6)23-20(25)18-9-8-10-19(27-7)16(18)3/h8-13H,1-7H			1	1	1
161326-34-7	161326347	499	**Fenamidone**	2_Pest		(5S)-3,5-Dihydro-5-methyl-2-(methylthio)-5-phenyl-3-(phenylamino)-4H-imidazol-4-one			311.41	CC1(C(=O)N(C(=N1)SC)NC2=CC=CC=C2)C3=CC=CC=C3	InChI=1S/C17H17N3OS/c1-17(13-9-5-3-6-10-13)15(21)20(16(18-17)22-2)19-14-11-7-4-8-12-14/h3-12,19H,1-2H3/t17-/m0			1	1	1
163515-14-8	163515148	502	**Dimethenamid-P**	2_Pest		2-Chloro-N-(2,4-dimethyl-3-thienyl)-N-[(1S)-2-methoxy-1-methylethyl]acetamide			275.8	CC1=CSC(=C1N(C(C)COC)C(=O)CCl)C	InChI=1S/C12H18ClNO2S/c1-8-7-17-10(3)12(8)14(11(15)5-13)9(2)6-16-4/h7,9H,5-6H2,1-4H3/t9-/m0/s1			1	1	1
16672-87-0	16672870	505	**Ethephon**	2_Pest	Phosphonic acid, (2-chloroethyl)-	Ethephon	C2H6ClO3P	C2H4ClO3P	144.49	[O-]P(=O)([O-])CCCl	InChI=1/C2H6ClO3P/c3-1-2-7(4,5)6/h1-2H2,(H2,4,5,6)/p-2	-2.095	-1.531	1	1	1
16752-77-5	16752775	506	**Methomyl**	2_Pest	Methomyl	N-[[(Methylamino)carbonyl]oxy]ethanimidothioic acid methyl ester	C5H10N2O2S	C5H10N2O2S	162.21	CNC(=O)O\N=C(/C)\SC	InChI=1/C5H10N2O2S/c1-4(10-3)7-9-5(8)6-2/h1-3H3,(H,6,8)/b7-4+	0.465	0.465	1	1	1
1689-83-4	1689834	507	**Ioxynil**	2_Pest	Benzonitrile, 4-hydroxy-3,5-diiodo-	4-Hydroxy-3,5-diiodobenzonitrile	C7H3I2NO	C7H2I2NO	370.91	[O-]c1c(I)cc(cc1I)C#N	InChI=1/C7H3I2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H/p-1	1.92	1.92	1	1	1
1689-84-5	1689845	34	**Bromoxynil**	2_Pest	Benzonitrile, 3,5-dibromo-4-hydroxy-	3,5-Dibromo-4-hydroxybenzonitrile	C7H3Br2NO	C7H2Br2NO	276.93	[O-]c1c(Br)cc(cc1Br)C#N	InChI=1/C7H3Br2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H/p-1	2.26	2.261	1	1	1
1698-60-8	1698608	35	**Chloridazon**	2_Pest	Pyrazon	5-Amino-4-chloro-2-phenyl-3(2H)-pyridazinone	C10H8ClN3O	C10H8ClN3O	221.65	NC1=C(Cl)C(=O)N(N=C1)c2ccccc2	InChI=1/C10H8ClN3O/c11-9-8(12)6-13-14(10(9)15)7-4-2-1-3-5-7/h1-6H,12H2	0.649	0.364	1	1	1
1702-17-6	1702176	509	**Clopyralid**	2_Pest		3,6-Dichloro-2-pyridinecarboxylic acid		C6H2Cl2NO2	192	[O-]C(=O)c1nc(Cl)ccc1Cl	InChI=1/C6H3Cl2NO2/c7-3-1-2-4(8)9-5(3)6(10)11/h1-2H,(H,10,11)/p-1	0.801	1.854	1	1	1
173159-57-4	173159574	510	**Foramsulfuron**	2_Pest		foramsulfuron			452.45	CN(C)C(=O)C1=C(C=C(C=C1)NC=O)S(=O)(=O)NC(=O)NC2=NC(=CC(=N2)OC)OC	InChI=1S/C17H20N6O7S/c1-23(2)15(25)11-6-5-10(18-9-24)7-12(11)31(27,28)22-17(26)21-16-19-13(29-3)8-14(20-16)30-			1	1	1
1746-81-2	1746812	511	**Monolinuron**	2_Pest	Urea, N'-(4-chlorophenyl)-N-methoxy-N-methyl-	N'-(4-Chlorophenyl)-N-methoxy-N-methylurea	C9H11ClN2O2	C9H11ClN2O2	214.65	CON(C)C(=O)Nc1ccc(Cl)cc1	InChI=1/C9H11ClN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	1.662	1.674	1	1	1
175013-18-0	175013180	512	**Pyraclostrobin**	2_Pest		[2-[[[1-(4-Chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]methoxycarbamic acid methyl ester			387.83	COC(=O)N(C1=CC=CC=C1COC2=NN(C=C2)C3=CC=C(C=C3)Cl)OC	InChI=1S/C19H18ClN3O4/c1-25-19(24)23(26-2)17-6-4-3-5-14(17)13-27-18-11-12-22(21-18)16-9-7-15(20)8-10-16/h3-12H			1	1	1
17804-35-2	17804352	513	**Benomyl**	2_Pest		[1-[(Butylamino)carbonyl]-1H-benzimidazol-2-yl]carbamic acid, Methyl ester		C14H18N4O3	290.33	CCCCNC(=O)n1c(NC(=O)OC)nc2ccccc12	InChI=1/C14H18N4O3/c1-3-4-9-15-13(19)18-11-8-6-5-7-10(11)16-12(18)17-14(20)21-2/h5-8H,3-4,9H2,1-2H3,(H,15,19)(H,16,17,20)	2.965	2.965	1	1	1
18181-80-1	18181801	4865	**Bromopropylate**	2_Pest	Bromopropylate	4-Bromo-.alpha.-(4-bromophenyl)-.alpha.-hydroxybenzeneacetic acid, 1-Methylethyl ester	C17H16Br2O3	C17H16Br2O3	428.13	CC(C)OC(=O)C(O)(c1ccc(Br)cc1)c2ccc(Br)cc2	InChI=1/C17H16Br2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6-13/h3-11,21H,1-2H3	4.837	4.837	1	1	1
1861-40-1	1861401	514	**Benfluralin**	2_Pest	Benfluralin	N-Butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)benzenamine	C13H16F3N3O4	C13H17F3N3O4	335.29	CCCC[NH+](CC)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	InChI=1/C13H16F3N3O4/c1-3-5-6-17(4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(22)23/h7-8H 6H2,1-2H3/p+1	2.744	3.729	1	1	1
18691-97-9	18691979	515	**Methabenzthiazuron**	2_Pest		1-(2-Benzothiazolyl)-1,3-dimethylurea		C10H11N3OS	221.29	CNC(=O)N(C)c1nc2ccccc2s1	InChI=1/C10H11N3OS/c1-11-9(14)13(2)10-12-7-5-3-4-6-8(7)15-10/h3-6H,1-2H3,(H,11,14)	1.777	1.824	1	1	1
188425-85-6	188425856	36	**Boscalid**	2_Pest		2-Chloro-N-(4'-chloro[1,1'-biphenyl]-2-yl)-3-pyridinecarboxamide			343.21	C1=CC=C(C(=C1)C2=CC=C(C=C2)Cl)NC(=O)C3=C(N=CC=C3)Cl	InChI=1S/C18H12Cl2N2O/c19-13-9-7-12(8-10-13)14-4-1-2-6-16(14)22-18(23)15-5-3-11-21-17(15)20/h1-11H,(H,22,23)			1	1	1
1897-45-6	1897456	516	**Chlorothalonil**	2_Pest	Tetrachloroisophthalonitrile	chloorthalonil	C8Cl4N2	C8Cl4N2	265.92	Clc1c(Cl)c(C#N)c(Cl)c(C#N)c1Cl	InChI=1/C8Cl4N2/c9-5-3(1-13)6(10)8(12)7(11)4(5)2-14	4.245	4.245	1	1	1
19044-88-3	19044883	517	**Oryzalin**	2_Pest	Oryzalin	4-(Dipropylamino)-3,5-dinitrobenzenesulfonamide	C12H18N4O6S	C12H18N4O6S	346.37	CCC[NH+](CCC)c1c(cc(cc1[N+](=O)[O-])S(=O)(=O)[NH-])[N+](=O)[O-]	InChI=1/C12H17N4O6S/c1-3-5-14(6-4-2)12-10(15(17)18)7-9(23(13,21)22)8-11(12)16(19)20/h7-8H, 6H2,1-2H3,(H-,13,21,22)/q-1/p+1	0.678	0.678	1	1	1
1912-24-9	1912249	37	**atrazine**	2_Pest	Atrazine	Atrazine	C8H14ClN5	C8H14ClN5	215.69	CCNc1nc(Cl)nc(NC(C)C)n1	InChI=1/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12,13,14)	1.59	1.59	1	1	1
1918-00-9	1918009	519	**Dicamba**	2_Pest	Benzoic acid, 3,6-dichloro-2-methoxy-	3,6-Dichloro-2-methyoxybenzoic acid	C8H6Cl2O3	C8H5Cl2O3	221.04	COc1c(Cl)ccc(Cl)c1C(=O)[O-]	InChI=1/C8H6Cl2O3/c1-13-7-5(10)3-2-4(9)6(7)8(11)12/h2-3H,1H3,(H,11,12)/p-1	1.298	1.298	1	1	1
1918-16-7	1918167	520	**Propachlor**	2_Pest	Acetamide, 2-chloro-N-(1-methylethyl)-N-phenyl-	2-Chloro-N-(1-methylethyl)-N-phenylacetamide	C11H14ClNO	C11H14ClNO	211.69	CC(C)N(C(=O)CCl)c1ccccc1	InChI=1/C11H14ClNO/c1-9(2)13(11(14)8-12)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3	2.415	2.415	1	1	1
1929-77-7	1929777	521	**Vernolate**	2_Pest	Carbamothioic acid, dipropyl-, S-propyl ester	Dipropylcarbamothioic acid S-propyl ester	C10H21NOS	C10H21NOS	203.35	CCCSC(=O)N(CCC)CCC	InChI=1/C10H21NOS/c1-4-7-11(8-5-2)10(12)13-9-6-3/h4-9H2,1-3H3	3.398	3.398	1	1	1
19666-30-9	19666309	526	**Oxadiazon**	2_Pest	Oxadiazon	3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one	C15H18Cl2N2O3	C15H18Cl2N2O3	345.23	CC(C)Oc1cc(N2N=C(OC2=O)C(C)(C)C)c(Cl)cc1Cl	InChI=1/C15H18Cl2N2O3/c1-8(2)21-12-7-11(9(16)6-10(12)17)19-14(20)22-13(18-19)15(3,4)5/h6-8H,1-5H3	5.224	5.224	1	1	1
1967-16-4	1967164	4870	**Chlorbufam**	2_Pest		Chlorbufam		C11H10ClNO2	223.66	CC(OC(=O)Nc1cccc(Cl)c1)C#C	InChI=1/C11H10ClNO2/c1-3-8(2)15-11(14)13-10-6-4-5-9(12)7-10/h1,4-8H,2H3,(H,13,14)	3.827	3.827	1	1	1
19937-59-8	19937598	527	**Metoxuron**	2_Pest	Metoxuron	N'-(3-Chloro-4-methoxyphenyl)-N,N-Dimethyl urea	C10H13ClN2O2	C10H13ClN2O2	228.68	COc1ccc(NC(=O)N(C)C)cc1Cl	InChI=1/C10H13ClN2O2/c1-13(2)10(14)12-7-4-5-9(15-3)8(11)6-7/h4-6H,1-3H3,(H,12,14)	1.8	1.8	1	1	1
2032-65-7	2032657	528	**Methiocarb**	2_Pest	4-Methylthio-3,5-xylyl methylcarbamate	3,5-Dimethyl-4-(methylthio)phenol, Methylcarbamate	C11H15NO2	C11H15NO2S	225.31	CNC(=O)Oc1cc(C)c(SC)c(C)c1	InChI=1/C11H15NO2S/c1-7-5-9(14-11(13)12-3)6-8(2)10(7)15-4/h5-6H,1-4H3,(H,12,13)	3.107	3.107	1	1	1
208465-21-8	208465218	5020	**Mesosulfuron-methyl**	2_Pest		2-[[[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-4-[[(methylsulfonyl)amino]methyl]benzoic acid, Methyl ester			503.51	COC1=CC(=NC(=N1)NC(=O)NS(=O)(=O)C2=C(C=CC(=C2)CNS(=O)(=O)C)C(=O)OC)OC	InChI=1S/C17H21N5O9S2/c1-29-13-8-14(30-2)20-16(19-13)21-17(24)22-33(27,28)12-7-10(9-18-32(4,25)26)5-6-11(12)15			1	1	1
21087-64-9	21087649	531	**Metribuzin**	2_Pest	Metribuzin	4-Amino-6-(1,1-dimethylethyl)-3-methylthio)-1,2,4-triazin-5(4H)-one	C8H14N4OS	C8H14N4OS	214.29	CSC1=NN=C(C(=O)N1N)C(C)(C)C	InChI=1/C8H14N4OS/c1-8(2,3)5-6(13)12(9)7(14-4)11-10-5/h9H2,1-4H3	1.606	1.606	1	1	1
2164-17-2	2164172	534	**Fluometuron**	2_Pest	Urea, N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]-	Fluometuron	C10H11F3N2O	C10H11F3N2O	232.21	CN(C)C(=O)Nc1cccc(c1)C(F)(F)F	InChI=1/C10H11F3N2O/c1-15(2)9(16)14-8-5-3-4-7(6-8)10(11,12)13/h3-6H,1-2H3,(H,14,16)	2.094	2.094	1	1	1
21725-46-2	21725462	535	**Cyanazine**	2_Pest	Cyanazine	2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	C9H13ClN6	C9H13ClN6	240.7	CCNc1nc(Cl)nc(NC(C)(C)C#N)n1	InChI=1/C9H13ClN6/c1-4-12-7-13-6(10)14-8(15-7)16-9(2,3)5-11/h4H2,1-3H3,(H2,12,13,14,15,16)	1.391	1.391	1	1	1
2212-67-1	2212671	537	**Molinate**	2_Pest	Molinate	Hexahydro-1H-azepine-1-carbothioic acid, S-Ethyl ester	C9H17NOS	C9H17NOS	187.31	CCSC(=O)N1CCCCCC1	InChI=1/C9H17NOS/c1-2-12-9(11)10-7-5-3-4-6-8-10/h2-8H2,1H3	2.503	2.503	1	1	1
22224-92-6	22224926	540	**Fenamiphos**	2_Pest	Fenamiphos	Ethyl-3-methyl-4-(methylthio)phenyl ester, (1-Methylethyl) phosphoramidic acid	C13H22NO3PS	C13H22NO3PS	303.36	CCOP(=O)(NC(C)C)Oc1ccc(SC)c(C)c1	InChI=1/C13H22NO3PS/c1-6-16-18(15,14-10(2)3)17-12-7-8-13(19-5)11(4)9-12/h7-10H,6H2,1-5H3,(H,14,15)	3.054	3.054	1	1	1
2275-23-2	2275232	543	**Vamidothion**	2_Pest		vamidothion		C8H18NO4PS2	287.34	CNC(=O)C(C)SCCSP(=O)(OC)OC	InChI=1/C8H18NO4PS2/c1-7(8(10)9-2)15-5-6-16-14(11,12-3)13-4/h7H,5-6H2,1-4H3,(H,9,10)	0.551	0.551	1	1	1
22781-23-3	22781233	544	**Bendiocarb**	2_Pest	Bendiocarb	2,2-Dimethyl-1,3-benzodioxol-4-ol 4-(N-methylcarbamate)	C11H13NO4	C11H13NO4	223.23	CNC(=O)Oc1cccc2OC(C)(C)Oc12	InChI=1/C11H13NO4/c1-11(2)15-8-6-4-5-7(9(8)16-11)14-10(13)12-3/h4-6H,1-3H3,(H,12,13)	1.478	1.478	1	1	1
2303-17-5	2303175	545	**Tri-allate**	2_Pest	Triallate	N,N-Bis(1-methylethyl)carbamothioic acid, S-(2,3,3-trichloro-2-propen-1-yl) ester	C10H16Cl3NOS	C10H16Cl3NOS	304.67	CC(C)N(C(C)C)C(=O)SCC(=C(Cl)Cl)Cl	InChI=1/C10H16Cl3NOS/c1-6(2)14(7(3)4)10(15)16-5-8(11)9(12)13/h6-7H,5H2,1-4H3	3.96	3.96	1	1	1
2310-17-0	2310170	546	**Phosalone**	2_Pest	Phosalone	S-[(6-Chloro-2-oxo-3(2H)-benzoxazolyl)methyl]O,O-diethyl ester phosphorodithioic acid	C12H15ClNO4PS2	C12H15ClNO4PS2	367.81	CCOP(=S)(OCC)SCN1C(=O)Oc2cc(Cl)ccc12	InChI=1/C12H15ClNO4PS2/c1-3-16-19(20,17-4-2)21-8-14-10-6-5-9(13)7-11(10)18-12(14)15/h5-7H, 4,8H2,1-2H3	4.001	4.001	1	1	1
23103-98-2	23103982	547	**Pirimicarb**	2_Pest	Pirimicarb	Dimethylcarbamic acid, 2-(Dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester	C11H18N4O2	C11H18N4O2	238.29	CN(C)C(=O)Oc1nc(nc(C)c1C)N(C)C	InChI=1/C11H18N4O2/c1-7-8(2)12-10(14(3)4)13-9(7)17-11(16)15(5)6/h1-6H3	1.391	1.391	1	1	1
23135-22-0	23135220	549	**Oxamyl**	2_Pest	Oxamyl	2-(Dimethylamino)-N-[[methylaminocarboxy]oxy]-2-oxo, Methyl ester ethanimidothioic acid	C7H13N3O3S	C7H13N3O3S	219.27	CNC(=O)O\N=C(/SC)\C(=O)N(C)C	InChI=1/C7H13N3O3S/c1-8-7(12)13-9-5(14-4)6(11)10(2)3/h1-4H3,(H,8,12)/b9-5-	0.025	0.025	1	1	1
23560-59-0	23560590	551	**Heptenophos**	2_Pest	Heptenophos	heptenophos	C9H12ClO4P	C9H12ClO4P	250.62	COP(=O)(OC)OC1=C(Cl)C2C=CCC12	InChI=1/C9H12ClO4P/c1-12-15(11,13-2)14-9-7-5-3-4-6(7)8(9)10/h3-4,6-7H,5H2,1-2H3	0.857	0.857	1	1	1
23564-05-8	23564058	552	**Thiophanate-methyl**	2_Pest		N,N'-[1,2-Phenylenebis(iminocarbonothioyl)]bis C,C'- Dimethyl ester carbamic acid		C12H16N4O4S2	342.4	COC(=O)NC(=S)[NH2+]c1ccccc1[NH2+]C(=S)NC(=O)OC	InChI=1/C12H14N4O4S2/c1-19-11(17)15-9(21)13-7-5-3-4-6-8(7)14-10(22)16-12(18)20-2/h3-6H,1-2H3,(H2,13,15,17,21)(H2,14,16,18,22)/p+2	2.754	3.354	1	1	1
23947-60-6	23947606	555	**Ethirimol**	2_Pest	Ethirimol	ethirimol	C11H19N3O	C11H19N3O	209.3	CCCCc1c(C)nc(NCC)nc1O	InChI=1/C11H19N3O/c1-4-6-7-9-8(3)13-11(12-5-2)14-10(9)15/h4-7H2,1-3H3,(H2,12,13,14,15)	2.691	2.69	1	1	1
23950-58-5	23950585	556	**Propyzamide**	2_Pest	Propyzamide	3,5-Dichloro-N-(1,1-dimethyl-2-propynyl)benzamide	C12H11Cl2NO	C12H11Cl2NO	256.13	CC(C)(NC(=O)c1cc(Cl)cc(Cl)c1)C#C	InChI=1/C12H11Cl2NO/c1-4-12(2,3)15-11(16)8-5-9(13)7-10(14)6-8/h1,5-7H,2-3H3,(H,15,16)	4.141	4.141	1	1	1
24017-47-8	24017478	557	**Triazophos**	2_Pest	Triazophos	triazophos	C12H16N3O3PS	C12H16N3O3PS	313.32	CCOP(=S)(OCC)Oc1ncn(n1)c2ccccc2	InChI=1/C12H16N3O3PS/c1-3-16-19(20,17-4-2)18-12-13-10-15(14-12)11-8-6-5-7-9-11/h5-10H,3-4H2,1-2H3	3.072	3.072	1	1	1
														1	1	1
24579-73-5	24579735	5105	**Propamocarb**	2_Pest		Propamocarb			188.27							
24934-91-6	24934916	564	**Chlormephos**	2_Pest	Chlormephos	chloormefos	C5H12ClO2PS2	C5H12ClO2PS2	234.7	CCOP(=S)(OCC)SCCl	InChI=1/C5H12ClO2PS2/c1-3-7-9(10,8-4-2)11-5-6/h3-5H2,1-2H3	2.426	2.426	1	1	1
25057-89-0	25057890	39	**Bentazone**	2_Pest	Bentazone	3-(1-Methylethyl)-1H-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide	C10H12N2O3S	C10H12N2O3S	240.28	CC(C)N1C(=O)c2ccccc2NS1(=O)=O	InChI=1/C10H12N2O3S/c1-7(2)12-10(13)8-5-3-4-6-9(8)11-16(12,14)15/h3-7,11H,1-2H3	0.676	0.676	1	1	1
25311-71-1	25311711	567	**Isofenphos**	2_Pest	Benzoic acid, 2-[[ethoxy[(1-methylethyl)amino]phosphinothioyl]oxy]-, 1-methylethyl ester	2-[[Ethoxy[(1-methylethyl)amino]phosphinothioyl]oxy]benzoic acid 1-methylethyl ester	C15H24NO4PS	C15H24NO4PS	345.4	CCOP(=S)(NC(C)C)Oc1ccccc1C(=O)OC(C)C	InChI=1/C15H24NO4PS/c1-6-18-21(22,16-11(2)3)20-14-10-8-7-9-13(14)15(17)19-12(4)5/h7-12H,6H2,1-5H3,(H,16,22)	3.506	3.506	1	1	1
2540-82-1	2540821	569	**Formothion**	2_Pest	Phosphorodithioic acid, o,o-dimethyl ester, s-ester with n-formyl-n-methylglycolamide	S-[2-(Formylmethylamino)-2-oxoethyl]phosphorodithioic acid, O,O-dimethyl ester	C6H12NO4PS2	C6H12NO4PS2	257.27	COP(=S)(OC)SCC(=O)N(C)C=O	InChI=1/C6H12NO4PS2/c1-7(5-8)6(9)4-14-12(13,10-2)11-3/h5H,4H2,1-3H3	0.263	0.263	1	1	1
2593-15-9	2593159	571	**Etridiazole**	2_Pest	1,2,4-Thiadiazole, 5-ethoxy-3-(trichloromethyl)-	Etridiazool	C5H5Cl3N2OS	C5H5Cl3N2OS	247.53	CCOc1nc(ns1)C(Cl)(Cl)Cl	InChI=1/C5H5Cl3N2OS/c1-2-11-4-9-3(10-12-4)5(6,7)8/h2H2,1H3	2.666	2.666	1	1	1
26225-79-6	26225796	573	**Ethofumesate**	2_Pest	Ethofumesate	2-Ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranol 5-methanesulfonate	C13H18O5S	C13H18O5S	286.35	CCOC1Oc2ccc(OS(=O)(=O)C)cc2C1(C)C	InChI=1/C13H18O5S/c1-5-16-12-13(2,3)10-8-9(18-19(4,14)15)6-7-11(10)17-12/h6-8,12H,5H2,1-4H3	2.457	2.457	1	1	1
2642-71-9	2642719	40	**Azinphos-ethyl**	2_Pest	Azinphos-ethyl	Azinphosethyl	C12H16N3O3PS2	C12H16N3O3PS2	345.38	CCOP(=S)(OCC)SCN1N=Nc2ccccc2C1=O	InChI=1/C12H16N3O3PS2/c1-3-17-19(20,18-4-2)21-9-15-12(16)10-7-5-6-8-11(10)13-14-15/h5-8H,3 4,9H2,1-2H3	3.623	3.623	1	1	1
26644-46-2	26644462	5180	**Triforine**	2_Pest		N,N'-[(2-Methyl-1,4-piperazinediyl)bis(2,2,2-trichloroethylidene)]bisformamide		C10H15Cl6N4O2	434.97	ClC(Cl)(Cl)C(NC=O)N1CC[NH+](CC1)C(NC=O)C(Cl)(Cl)Cl	InChI=1/C10H14Cl6N4O2/c11-9(12,13)7(17-5-21)19-1-2-20(4-3-19)8(18-6-22)10(14,15)16/h5-8H,1-4H2,(H,17,21)(H,18,22)/p+1	0.538	0.543	1	1	1
27314-13-2	27314132	5073	**Norflurazon**	2_Pest	Norflurazon	4-Chloro-5-(methylamino)-2-[3-(trifluoromethyl)phenyl]-3(2H)-pyridazinone	C12H9ClF3N3O	C12H9ClF3N3O	303.67	CNC1=C(Cl)C(=O)N(N=C1)c2cccc(c2)C(F)(F)F	InChI=1/C12H9ClF3N3O/c1-17-9-6-18-19(11(20)10(9)13)8-4-2-3-7(5-8)12(14,15)16/h2-6,17H,1H3	2.023	1.156	1	1	1
2764-72-9	2764729	4912	**Diquat**	2_Pest		6,7-Dihydrodipyrido (1,2-a:2',1'-c)pyrazinediium			184.24	C1C[N+]2=CC=CC=C2C3=CC=CC=[N+]31	InChI=1S/C12H12N2/c1-3-7-13-9-10-14-8-4-2-6-12(14)11(13)5-1/h1-8H,9-10H2/q+2			1	1	1
2797-51-5	2797515	5113	**Quinoclamine**	2_Pest	1,4-Naphthalenedione, 2-amino-3-chloro-	2-Amino-3-chloro-1,4-naphthoquinone	C10H6ClNO2	C10H6ClNO2	207.62	NC1=C(Cl)C(=O)c2ccccc2C1=O	InChI=1/C10H6ClNO2/c11-7-8(12)10(14)6-4-2-1-3-5(6)9(7)13/h1-4H,12H2	0.929	0.929	1	1	1
28249-77-6	28249776	580	**Thiobencarb**	2_Pest	Benthiocarb	N,N-Diethylcarbamothioic acid S-[(4-chlorophenyl)methyl] ester	C12H16ClNOS	C12H16ClNOS	257.78	CCN(CC)C(=O)SCc1ccc(Cl)cc1	InChI=1/C12H16ClNOS/c1-3-14(4-2)12(15)16-9-10-5-7-11(13)8-6-10/h5-8H,3-4,9H2,1-2H3	3.726	3.726	1	1	1
28434-01-7	28434017	581	**Bioresmethrin**	2_Pest		2,2-Dimethyl-3-(2-methyl-1-propen-1-yl)cyclopropanecarboxylic acid, (1R,3R)-[5-(Phenylmethyl)-3-furanyl]methyl ester		C22H26O3	338.45	CC(=C[C@@H]1[C@@H](C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C	InChI=1/C22H26O3/c1-15(2)10-19-20(22(19,3)4)21(23)25-14-17-12-18(24-13-17)11-16-8-6-5-7-9-16/h5-10,12-13,19-20H,11,14H2,1-4H3/t19-,20+/m1/s1	4.934	4.934	1	1	1
29091-05-2	29091052	4910	**Dinitramine**	2_Pest		N1,N1-Diethyl-2,6-dinitro-4-(trifluoromethyl)-1,3-benzenediamine		C11H14F3N4O4	322.25	CC[NH+](CC)c1c(cc(c(N)c1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	InChI=1/C11H13F3N4O4/c1-3-16(4-2)9-7(17(19)20)5-6(11(12,13)14)8(15)10(9)18(21)22/h5H,3-4,15H2,1-2H3/p+1	1.018	1.018	1	1	1
29104-30-1	29104301	4847	**Benzoximate**	2_Pest		Benzomate		C18H18ClNO5	363.8	CCO\N=C(/OC(=O)c1ccccc1)\c2c(OC)ccc(Cl)c2OC	InChI=1/C18H18ClNO5/c1-4-24-20-17(25-18(21)12-8-6-5-7-9-12)15-14(22-2)11-10-13(19)16(15)23-3/h5-11H,4H2,1-3H3/b20-17-	4.22	4.22	1	1	1
2921-88-2	2921882	585	**Chlorpyrifos**	2_Pest	o,o-Diethyl-o-(3,5,6-trichloro-2-pyridyl)phosphorothioate	Chlorpyrifos	C9H11Cl3NO3PS	C9H11Cl3NO3PS	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl	InChI=1/C9H11Cl3NO3PS/c1-3-14-17(18,15-4-2)16-9-7(11)5-6(10)8(12)13-9/h5H,3-4H2,1-2H3	4.599	4.599	1	1	1
29232-93-7	29232937	586	**Pirimiphos-Methyl**	2_Pest	Pirimiphos methyl	O-[2-(Dimethylamino)-6-methyl-4-pyrimidinyl]O,O-dimethyl ester phosphorothioic acid	C11H20N3O3PS	C11H20N3O3PS	305.34	CCN(CC)c1nc(C)cc(OP(=S)(OC)OC)n1	InChI=1/C11H20N3O3PS/c1-6-14(7-2)11-12-9(3)8-10(13-11)17-18(19,15-4)16-5/h8H,6-7H2,1-5H3	2.114	2.114	1	1	1
298-00-0	298000	5086	**Parathion-Methyl**	2_Pest	Phosphorothioic acid, o,o-dimethyl o-p-nitrophenyl ester	O,O-Dimethyl O-(4-nitrophenyl) ester phosphorothioic acid	C8H10NO5PS	C8H10NO5PS	263.21	COP(=S)(OC)Oc1ccc(cc1)[N+](=O)[O-]	InChI=1/C8H10NO5PS/c1-12-15(16,13-2)14-8-5-3-7(4-6-8)9(10)11/h3-6H,1-2H3	2.205	2.205	1	1	1
298-02-2	298022	589	**Phorate**	2_Pest	Phorate	O,O-Diethyl S-[(ethylthio)methyl])ester, Phosphorodithioic acid	C7H17O2PS3	C7H17O2PS3	260.38	CCOP(=S)(OCC)SCSCC	InChI=1/C7H17O2PS3/c1-4-8-10(11,9-5-2)13-7-12-6-3/h4-7H2,1-3H3	2.934	2.934	1	1	1
298-04-4	298044	590	**Disulfoton**	2_Pest	Disulfoton	Disulfoton	C8H19O2PS3	C8H19O2PS3	274.4	CCOP(=S)(OCC)SCCSCC	InChI=1/C8H19O2PS3/c1-4-9-11(12,10-5-2)14-8-7-13-6-3/h4-8H2,1-3H3	2.952	2.952	1	1	1
29973-13-5	29973135	593	**Ethiofencarb**	2_Pest		ethiofencarb		C11H15NO2S	225.31	CCSCc1ccccc1OC(=O)NC	InChI=1/C11H15NO2S/c1-3-15-8-9-6-4-5-7-10(9)14-11(13)12-2/h4-7H,3,8H2,1-2H3,(H,12,13)	2.491	2.491	1	1	1
300-76-5	300765	594	**Naled**	2_Pest	O-(1,2-dibromo-2,2-dichloroethyl)-o,o-dimethyl phosphate	1,2-Dibromo-2,2-dichloroethyldimethyl ester phosphoric acid	C4H7Br2Cl2O4P	C4H7Br2Cl2O4P	380.8	COP(=O)(OC)OC(Br)C(Cl)(Cl)Br	InChI=1/C4H7Br2Cl2O4P/c1-10-13(9,11-2)12-3(5)4(6,7)8/h3H,1-2H3	2.315	2.315	1	1	1
301-12-2	301122	595	**Oxydemeton-methyl**	2_Pest	Oxydemeton-methyl	Phosphorothioic acid, S-[2-(Ethylsulfinyl)ethyl] O,O-dimethyl ester	C6H15O4PS2	C6H15O4PS2	246.28	CCS(=O)CCSP(=O)(OC)OC	InChI=1/C6H15O4PS2/c1-4-13(8)6-5-12-11(7,9-2)10-3/h4-6H2,1-3H3	0.244	0.244	1	1	1
30560-19-1	30560191	596	**Acephate**	2_Pest	Acephate	N-Acetylphosphoramidothioic acid O,S-dimethyl ester	C4H10NO3PS	C4H10NO3PS	183.17	COP(=O)(NC(=O)C)SC	InChI=1/C4H10NO3PS/c1-4(6)5-9(7,8-2)10-3/h1-3H3,(H,5,6,7)	-0.284	-0.283	1	1	1
3060-89-7	3060897	598	**Metobromuron**	2_Pest	N'-(4-Bromophenyl)-N-methoxy-N-methylurea	N'-(4-Bromophenyl)-N-methoxy-N-methylurea	C9H11BrN2O	C9H11BrN2O2	259.11	CON(C)C(=O)Nc1ccc(Br)cc1	InChI=1/C9H11BrN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	1.746	2.149	1	1	1
314-40-9	314409	4864	**Bromacil**	2_Pest	Bromacil	Bromacil	C9H13BrN2O2	C9H13BrN2O2	261.13	CCC(C)N1C(=O)NC(=C(Br)C1=O)C	InChI=1/C9H13BrN2O2/c1-4-5(2)12-8(13)7(10)6(3)11-9(12)14/h5H,4H2,1-3H3,(H,11,14)	1.41	1.41	1	1	1
330-54-1	330541	46	**diuron**	2_Pest	Urea, 3-(3,4-dichlorophenyl)-1,1-dimethyl-	N'-(3,4-Dichlorophenyl)-N,N-dimethylurea	C9H10Cl2N2O	C9H10Cl2N2O	233.1	CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1	InChI=1/C9H10Cl2N2O/c1-13(2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	2.481	2.481	1	1	1
330-55-2	330552	602	**Linuron**	2_Pest	N'-(3,4-Dichlorophenyl)-N-methoxy N-methylurea	Linuron	C9H10Cl2N2O2	C9H10Cl2N2O2	249.1	CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1	InChI=1/C9H10Cl2N2O2/c1-13(15-2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	2.326	2.327	1	1	1
33089-61-1	33089611	603	**Amitraz**	2_Pest		N'-(2,4-Dimethylphenyl)-N-[(2,4-dimethylphenyl)imino]methyl]-N-methyl methanimidamide		C19H23N3	293.42	CN(\C=N\c1ccc(C)cc1C)\C=N\c2ccc(C)cc2C	InChI=1/C19H23N3/c1-14-6-8-18(16(3)10-14)20-12-22(5)13-21-19-9-7-15(2)11-17(19)4/h6-13H,1-5H3/b20-12+,21-13+	4.825	4.721	1	1	1
333-41-5	333415	47	**Diazinon**	2_Pest	Dimpylate	Diazinon	C12H21N2O3PS	C12H21N2O3PS	304.35	CCOP(=S)(OCC)Oc1cc(C)nc(n1)C(C)C	InChI=1/C12H21N2O3PS/c1-6-15-18(19,16-7-2)17-11-8-10(5)13-12(14-11)9(3)4/h8-9H,6-7H2,1-5H3	3.136	3.136	1	1	1
3347-22-6	3347226	604	**Dithianon**	2_Pest		5,10-Dihydro-5,10-dioxo-naphtho(2,3-b)-p-dithiin-2,3-dicarbonitrile		C14H4N2O2S2	296.33	O=C1C2=C(SC(=C(S2)C#N)C#N)C(=O)c3ccccc13	InChI=1/C14H4N2O2S2/c15-5-9-10(6-16)20-14-12(18)8-4-2-1-3-7(8)11(17)13(14)19-9/h1-4H	1.688	1.688	1	1	1
33629-47-9	33629479	605	**Butralin**	2_Pest	Butralin	4-(1,1-Dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzenamine	C14H21N3O4	C14H21N3O4	295.34	CCC(C)Nc1c(cc(cc1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-]	InChI=1/C14H21N3O4/c1-6-9(2)15-13-11(16(18)19)7-10(14(3,4)5)8-12(13)17(20)21/h7-9,15H,6H2, 5H3	4.077	4.077	1	1	1
33693-04-8	33693048	606	**Terbumeton**	2_Pest		N-(1,1-Dimethylethyl)-N'-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine		C10H19N5O	225.3	CCNc1nc(NC(C)(C)C)nc(OC)n1	InChI=1/C10H19N5O/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,12,13,14,15)	1.445	1.444	1	1	1
33820-53-0	33820530	4982	**Isopropalin**	2_Pest	Isopropalin	4-(1-Methylethyl)-2,6-dinitro-N,N-dipropylbenzenamine	C15H23N3O4	C15H24N3O4	309.37	CCC[NH+](CCC)c1c(cc(cc1[N+](=O)[O-])C(C)C)[N+](=O)[O-]	InChI=1/C15H23N3O4/c1-5-7-16(8-6-2)15-13(17(19)20)9-12(11(3)4)10-14(15)18(21)22/h9-11H,5-8H2,1-4H3/p+1	3.064	3.067	1	1	1
34014-18-1	34014181	607	**Tebuthiuron**	2_Pest	Tebuthiuron	Tebuthiuron	C9H16N4OS	C9H16N4OS	228.32	CNC(=O)N(C)c1nnc(s1)C(C)(C)C	InChI=1/C9H16N4OS/c1-9(2,3)6-11-12-8(15-6)13(5)7(14)10-4/h1-5H3,(H,10,14)	1.433	1.433	1	1	1
34123-59-6	34123596	49	**Isoproturon**	2_Pest	Urea, N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]-	N,N-Dimethyl-N'-[4-(1-methylethyl)phenyl]urea	C12H18N2O	C12H18N2O	206.29	CC(C)c1ccc(NC(=O)N(C)C)cc1	InChI=1/C12H18N2O/c1-9(2)10-5-7-11(8-6-10)13-12(15)14(3)4/h5-9H,1-4H3,(H,13,15)	2.346	2.346	1	1	1
34256-82-1	34256821	608	**Acetochlor**	2_Pest	Acetochlor	Acetochlor	C14H20ClNO2	C14H20ClNO2	269.77	CCOCN(C(=O)CCl)c1c(C)cccc1CC	InChI=1/C14H20ClNO2/c1-4-12-8-6-7-11(3)14(12)16(10-18-5-2)13(17)9-15/h6-8H,4-5,9-10H2,1-3H3	3.317	3.317	1	1	1
34681-10-2	34681102	610	**Butocarboxim**	2_Pest	Butocarboxim	3-(Methylthio)-O-[(methylamino)carbonyl]oxime 2-butanone	C7H14N2O2S	C7H14N2O2S	190.27	CNC(=O)O\N=C(/C)\C(C)SC	InChI=1/C7H14N2O2S/c1-5(6(2)12-4)9-11-7(10)8-3/h6H,1-4H3,(H,8,10)/b9-5+	0.747	0.747	1	1	1
35367-38-5	35367385	612	**Diflubenzuron**	2_Pest	Difluron	N-[[(4-Chlorophenyl)amino]carbonyl]-2,6-difluorobenzamide	C14H9ClF2N2O2	C14H9ClF2N2O2	310.69	Fc1cccc(F)c1C(=O)NC(=O)Nc2ccc(Cl)cc2	InChI=1/C14H9ClF2N2O2/c15-8-4-6-9(7-5-8)18-14(21)19-13(20)12-10(16)2-1-3-11(12)17/h1-7H,(H2,18,19,20,21)	3.47	3.47	1	1	1
35554-44-0	35554440	614	**Imazalil**	2_Pest	Imazalil	Imazalil	C14H14Cl2N2O	C14H14Cl2N2O	297.19	Clc1ccc(C(Cn2ccnc2)OCC=C)c(Cl)c1	InChI=1/C14H14Cl2N2O/c1-2-7-19-14(9-18-6-5-17-10-18)12-4-3-11(15)8-13(12)16/h2-6,8,10,14H,1,7,9H2	3.349	3.749	1	1	1
36734-19-7	36734197	616	**Iprodione**	2_Pest	Iprodione	Iprodione	C13H13Cl2N3O3	C13H13Cl2N3O3	330.17	CC(C)NC(=O)N1CC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2	InChI=1/C13H13Cl2N3O3/c1-7(2)16-12(20)17-6-11(19)18(13(17)21)10-4-8(14)3-9(15)5-10/h3-5,7H,6H2,1-2H3,(H,16,20)	2.663	2.663	1	1	1
3689-24-5	3689245	5137	**Sulfotep**	2_Pest	Sulfotep	Triodiphosphoric acid, Tetraethyl ester	C8H20O5P2S2	C8H20O5P2S2	322.32	CCOP(=S)(OCC)OP(=S)(OCC)OCC	InChI=1/C8H20O5P2S2/c1-5-9-14(16,10-6-2)13-15(17,11-7-3)12-8-4/h5-8H2,1-4H3	2.594	2.594	1	1	1
3878-19-1	3878191	622	**Fuberidazole**	2_Pest	Fuberidazole	fuberidazol	C11H8N2O	C11H8N2O	184.2	o1cccc1c2nc3ccccc3[nH]2	InChI=1/C11H8N2O/c1-2-5-9-8(4-1)12-11(13-9)10-6-3-7-14-10/h1-7H,(H,12,13)	2.665	2.67	1	1	1
39515-41-8	39515418	624	**Fenpropathrin**	2_Pest	Cyclopropanecarboxylic acid, 2,2,3,3-tetramethyl-, cyano(3-phenoxyphenyl)methyl ester	2,2,3,3-Tetramethylcyclopropanecarboxylic acid cyano(3-phenoxyphenyl)methyl ester	C22H23NO3	C22H23NO3	349.43	CC1(C)C(C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2)C1(C)C	InChI=1/C22H23NO3/c1-21(2)19(22(21,3)4)20(24)26-18(14-23)15-9-8-12-17(13-15)25-16-10-6-5-7-11-16/h5-13,18-19H,1-4H3	4.704	4.704	1	1	1
39807-15-3	39807153	626	**Oxadiargyl**	2_Pest		3-[2,4-Dichloro-5-(2-propynyloxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one		C15H14Cl2N2O3	341.2	CC(C)(C)C1=NN(C(=O)O1)c2cc(OCC#C)c(Cl)cc2Cl	InChI=1/C15H14Cl2N2O3/c1-5-6-21-12-8-11(9(16)7-10(12)17)19-14(20)22-13(18-19)15(2,3)4/h1,7-8H,6H2,2-4H3	5.69	5.69	1	1	1
40487-42-1	40487421	628	**Pendimethalin**	2_Pest	Penoxaline	Pendimethalin	C13H19N3O4	C13H19N3O4	281.32	CCC(CC)Nc1c(cc(C)c(C)c1[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C13H19N3O4/c1-5-10(6-2)14-12-11(15(17)18)7-8(3)9(4)13(12)16(19)20/h7,10,14H,5-6H2, 4H3	4.173	4.173	1	1	1
41083-11-8	41083118	630	**Azocyclotin**	2_Pest		azocyclotin		C20H35N3Sn	436.21	C1CCC(CC1)[Sn](C2CCCCC2)(C3CCCCC3)n4cncn4	InChI=1/3C6H11.C2H2N3.Sn/c3*1-2-4-6-5-3-1;1-3-2-5-4-1;/h3*1H,2-6H2;1-2H;/q;;;-1;+1	6.697	6.706	1	1	1
41394-05-2	41394052	632	**Metamitron**	2_Pest	1,2,4-Triazin-5(4H)-one, 4-amino-3-methyl-6-phenyl-	metamitron	C10H10N4O	C10H10N4O	202.22	CC1=NN=C(C(=O)N1N)c2ccccc2	InChI=1/C10H10N4O/c1-7-12-13-9(10(15)14(7)11)8-5-3-2-4-6-8/h2-6H,11H2,1H3	0.532	0.532	1	1	1
41483-43-6	41483436	633	**Bupirimate**	2_Pest		bupirimaat		C13H24N4O3S	316.43	CCCCc1c(C)nc(NCC)nc1OS(=O)(=O)N(C)C	InChI=1/C13H24N4O3S/c1-6-8-9-11-10(3)15-13(14-7-2)16-12(11)20-21(18,19)17(4)5/h6-9H2,1-5H3,(H,14,15,16)	2.083	2.081	1	1	1

42576-02-3	42576023	4851	**Bifenox**	2_Pest	Methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	bifenox	C14H9Cl2NO3	C14H9Cl2NO5	342.13	COC(=O)c1cc(Oc2ccc(Cl)cc2Cl)ccc1[N+](=O)[O-]	InChI=1/C14H9Cl2NO5/c1-21-14(18)10-7-9(3-4-12(10)17(19)20)22-13-5-2-8(15)6-11(13)16/h2-7H,1H3	4.468	4.468	1	1	1
42874-03-3	42874033	638	**Oxyfluorfen**	2_Pest	Benzene, 2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)-	Oxyfluorfen	C15H11ClF3NO4	C15H11ClF3NO4	361.7	CCOc1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	InChI=1/C15H11ClF3NO4/c1-2-23-14-8-10(4-5-12(14)20(21)22)24-13-6-3-9(7-11(13)16)15(17,18)19/h3-8H,2H2,1H3	5.223	5.223	1	1	1
43121-43-3	43121433	639	**Triadimefon**	2_Pest	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-	1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone	C14H16ClN3O2	C14H16ClN3O2	293.76	CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n2cncn2	InChI=1/C14H16ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h4-9,13H,1-3H3	3.639	3.639	1	1	1
4685-14-7	4685147	5085	**Paraquat**	2_Pest	Paraquat	1,1'-Dimethyl-4,4'-bipyridinium	C12H14N2	C12H14N2	186.26	C[n+]1ccc(cc1)c2cc[n+](C)cc2	InChI=1/C12H14N2/c1-13-7-3-11(4-8-13)12-5-9-14(2)10-6-12/h3-10H,1-2H3/q+2	2.557	2.557	1	1	1
470-90-6	470906	1098	**Chlorfenvinphos**	2_Pest	Clofenvinfos	Phosphoric acid, 2-Chloro-1-(2,4-dichlorophenyl)ethenyl diethyl ester	C12H14Cl3O4P	C12H14Cl3O4P	359.57	CCOP(=O)(OCC)O\C(=C/Cl)\c1ccc(Cl)cc1Cl	InChI=1/C12H14Cl3O4P/c1-3-17-20(16,18-4-2)19-12(8-13)10-6-5-9(14)7-11(10)15/h5-8H,3-4H2,1-2H3/b12-8-	3.562	3.562	1	1	1
49866-87-7	49866877	4903	**Difenzoquat**	2_Pest		Difenzoquat		C17H17N2	249.34	C[n+]1c(cc(c2ccccc2)n1C)c3ccccc3	InChI=1/C17H17N2/c1-18-16(14-9-5-3-6-10-14)13-17(19(18)2)15-11-7-4-8-12-15/h3-13H,1-2H3/q+1	4.338	4.338	1	1	1
50471-44-8	50471448	661	**Vinclozolin**	2_Pest	Vinclozoline	Vinclozolin	C12H9Cl2NO3	C12H9Cl2NO3	286.12	CC1(OC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2)C=C	InChI=1/C12H9Cl2NO3/c1-3-12(2)10(16)15(11(17)18-12)9-5-7(13)4-8(14)6-9/h3-6H,1H2,2H3	3.662	3.662	1	1	1
50563-36-5	50563365	663	**Dimethachlor**	2_Pest		dimethachloor		C13H18ClNO2	255.75	COCCN(C(=O)CCl)c1c(C)cccc1C	InChI=1/C13H18ClNO2/c1-10-5-4-6-11(2)13(10)15(7-8-17-3)12(16)9-14/h4-6H,7-9H2,1-3H3	2.53	2.53	1	1	1
50594-66-6	50594666	4828	**Acifluorfen**	2_Pest	Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-	5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid	C14H7ClF3NO5	C14H6ClF3NO5	361.66	[O-]C(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	InChI=1/C14H7ClF3NO5/c15-10-5-7(14(16,17)18)1-4-12(10)24-8-2-3-11(19(22)23)9(6-8)13(20)21/h1-6H,(H,20,21)/p-1	3.047	3.047	1	1	1
51218-45-2	51218452	56	**Metolachlor**	2_Pest	Metolachlor	2-Chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)acetamide	C15H22ClNO2	C15H22ClNO2	283.8	CCc1cccc(C)c1N(C(C)COC)C(=O)CCl	InChI=1/C15H22ClNO2/c1-5-13-8-6-7-11(2)15(13)17(14(18)9-16)12(3)10-19-4/h6-8,12H,5,9-10H2,1-4H3	3.364	3.363	1	1	1
51276-47-2	51276472	4969	**Glufosinate**	2_Pest		2-Amino-4-(hydroxymethylphosphinyl)butanoic acid		C5H11NO4P	181.13	CP(=O)([O-])CCC([NH3+])C(=O)[O-]	InChI=1/C5H12NO4P/c1-11(9,10)3-2-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)(H,9,10)/p-1	-5.493	-5.492	1	1	1
51630-58-1	51630581	1111	**Fenvalerate**	2_Pest	Fenvalerate	Fenvalerate	C25H22ClNO3	C25H22ClNO3	419.91	CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c3ccc(Cl)cc3	InChI=1/C25H22ClNO3/c1-17(2)24(18-11-13-20(26)14-12-18)25(28)30-23(16-27)19-7-6-10-22(15-19)29-21-8-4-3-5-9-21/h3-15,17,23-24H,1-2H3	6.564	6.564	1	1	1
51707-55-2	51707552	5158	**Thidiazuron**	2_Pest		N-Phenyl-N'-1,2,3-thiadiazol-5-ylurea		C9H8N4OS	220.26	O=C(Nc1ccccc1)Nc2cnns2	InChI=1/C9H8N4OS/c14-9(12-8-6-10-13-15-8)11-7-4-2-1-3-5-7/h1-6H,(H2,11,12,14)	1.192	1.192	1	1	1
52315-07-8	52315078	1099	**Cypermethrin**	2_Pest		3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid cyano(3-phenoxyphenyl)methyl ester		C22H19Cl2NO3	416.31	CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	InChI=1/C22H19Cl2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-14)27-15-8-4-3-5-9-15/h3-12,17-18,20H,1-2H3	5.304	5.304	1	1	1
5234-68-4	5234684	673	**Carboxin**	2_Pest	Carboxin	5,6-Dihydro-2-methyl-N-phenyl-1,4-oxathiin-3-carboxamide	C12H13NO2S	C12H13NO2S	235.31	CC1=C(SCCO1)C(=O)Nc2ccccc2	InChI=1/C12H13NO2S/c1-9-11(16-8-7-15-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3,(H,13,14)	1.6	1.6	1	1	1
52-68-6	52686	677	**Trichlorfon**	2_Pest	Metrifonate	(2,2,2-Trichloro-1-hydroxyethyl)phosphonic acid, Dimethyl ester	C4H8Cl3O4P	C4H8Cl3O4P	257.44	COP(=O)(OC)C(O)C(Cl)(Cl)Cl	InChI=1/C4H8Cl3O4P/c1-10-12(9,11-2)3(8)4(5,6)7/h3,8H,1-2H3	0.753	0.753	1	1	1
52888-80-9	52888809	60	**Prosulfocarb**	2_Pest		Prosulfocarb			251.39	CCCN(CCC)C(=O)SCC1=CC=CC=C1	InChI=1S/C14H21NOS/c1-3-10-15(11-4-2)14(16)17-12-13-8-6-5-7-9-13/h5-9H,3-4,10-12H2,1-2H3			1	1	1
52918-63-5	52918635	679	**Deltamethrin**	2_Pest	Cyclopropanecarboxylic acid, 3-(2,2-dibromoethenyl)-2,2-dimethyl-cyano(3-phenoxyphenyl)methyl ester, [1R-[1.alpha.(S*),3.alpha.]]-	(1R,3R)-3-(2,2-Dibromoethenyl)-2,2-dimethylcyclopropanecarboxylic acid (S)cyano(3-phenoxyphenyl)methyl ester	C22H19Br2NO3	C22H19Br2NO3	505.22	CC1(C)[C@@H](C=C(Br)Br)[C@H]1C(=O)O[C@H](C#N)c2cccc(Oc3ccccc3)c2	InChI=1/C22H19Br2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-14)27-15-8-4-3-5-9-15/h3-12,17-18,20H,1-2H3/t17-,18+,20-/m0/s1	5.522	5.522	1	1	1
53112-28-0	53112280	681	**Pyrimethanil**	2_Pest		pyremethanil			199.26	CC1=CC(=NC(=N1)NC2=CC=CC=C2)C	InChI=1S/C12H13N3/c1-9-8-10(2)14-12(13-9)15-11-6-4-3-5-7-11/h3-8H,1-2H3,(H,13,14,15)			1	1	1
55179-31-2	55179312	693	**Bitertanol**	2_Pest		bitertanol		C20H23N3O2	337.43	CC(C)(C)C(O)C(Oc1ccc(cc1)c2ccccc2)n3cncn3	InChI=1/C20H23N3O2/c1-20(2,3)18(24)19(23-14-21-13-22-23)25-17-11-9-16(10-12-17)15-7-5-4-6-8-15/h4-14,18-19,24H,1-3H3	4.1	4.101	1	1	1
55219-65-3	55219653	694	**Triadimenol**	2_Pest	Ethanol, 2-(4-chlorophenoxy)-1-ter butyl-2-(1H-1,2,4-triazole-1-yl)-	Triadimenol	C14H18ClN3O2	C14H18ClN3O2	295.77	CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n2cncn2	InChI=1/C14H18ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h4-9,12-13,19H,1-3H3	3.247	3.247	1	1	1
55283-68-6	55283686	695	**Ethalfluralin**	2_Pest		Ethalfluralin		C13H15F3N3O4	333.27	CC[NH+](CC(=C)C)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	InChI=1/C13H14F3N3O4/c1-4-17(7-8(2)3)12-10(18(20)21)5-9(13(14,15)16)6-11(12)19(22)23/h5-6H,2,4,7H2,1,3H3/p+1	2.479	3.169	1	1	1
55285-14-8	55285148	696	**Carbosulfan**	2_Pest	Carbosulfan	carbosulfan	C20H32N2O3S	C20H32N2O3S	380.55	CCCCN(CCCC)SN(C)C(=O)Oc1cccc2CC(C)(C)Oc12	InChI=1/C20H32N2O3S/c1-6-8-13-22(14-9-7-2)26-21(5)19(23)24-17-12-10-11-16-15-20(3,4)25-18(16)17/h10-12H,6-9,13-15H2,1-5H3	5.402	5.402	1	1	1
55335-06-3	55335063	698	**Triclopyr**	2_Pest	Acetic acid, [(3,5,6-trichloro-2-pyridinyl)oxy]-	((3,5,6-Trichloro-2-pyridyl)oxy)acetic acid	C7H4Cl3NO3	C7H3Cl3NO3	256.47	[O-]C(=O)COc1nc(Cl)c(Cl)cc1Cl	InChI=1/C7H4Cl3NO3/c8-3-1-4(9)7(11-6(3)10)14-2-5(12)13/h1H,2H2,(H,12,13)/p-1	1.412	2.884	1	1	1
55-38-9	55389	699	**Fenthion**	2_Pest	Fenthion	O,O-Dimethyl O-[3-Methyl-4-	C10H15O3PS2	C10H15O3PS2	278.33	COP(=S)(OC)Oc1ccc(SC)c(C)c1	InChI=1/C10H15O3PS2/c1-8-7-9(5-6-10(8)16-4)13-14(15,11-2)12-3/h5-7H,1-4H3	3.338	3.338	1	1	1
55512-33-9	55512339	701	**Pyridate**	2_Pest		pyridaat		C19H23ClN2O2S	378.92	CCCCCCCCSC(=O)Oc1cc(Cl)nnc1c2ccccc2	InChI=1/C19H23ClN2O2S/c1-2-3-4-5-6-10-13-25-19(23)24-16-14-17(20)21-22-18(16)15-11-8-7-9-1	7.155	7.155	1	1	1
555-37-3	555373	5063	**Neburon**	2_Pest	Urea, N-butyl-N'-(3,4-dichlorophenyl)-N-methyl-	Neburon	C12H16Cl2N2O	C12H16Cl2N2O	275.18	CCCCN(C)C(=O)Nc1ccc(Cl)c(Cl)c1	InChI=1/C12H16Cl2N2O/c1-3-4-7-16(2)12(17)15-9-5-6-10(13)11(14)8-9/h5-6,8H,3-4,7H2,1-2H3,(H,15,17)	3.809	3.809	1	1	1
5598-13-0	5598130	709	**Chlorpyrifos-Methyl**	2_Pest	o,o-Dimethyl-o-(3,5,6-trichloro-2-	O,O-Dimethyl O-(3,5,6-trichloro-2-pyridinyl)	C7H9Cl3NO3PS	C7H7Cl3NO3PS	322.54	COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl	InChI=1/C7H7Cl3NO3PS/c1-12-15(16,13-2)14-7-5(9)3-4(8)6(10)11-7/h3H,1-2H3	3.901	3.901	1	1	1
563-12-2	563122	711	**Ethion**	2_Pest	Ethion	Phosphorodithioic acid, S,S'-Methylene O,O,O',O'-tetraethyl ester	C9H22O4P2S4	C9H22O4P2S4	384.48	CCOP(=S)(OCC)SCSP(=S)(OCC)OCC	InChI=1/C9H22O4P2S4/c1-5-10-14(16,11-6-2)18-9-19-15(17,12-7-3)13-8-4/h5-9H2,1-4H3	3.781	3.781	1	1	1
56-38-2	56382	713	**Parathion**	2_Pest	Ethyl parathion (o,o-diethyl-o-p-nitrophenylthiophosphate)	Parathion-ethyl	C10H14NO5PS	C10H14NO5PS	291.26	CCOP(=S)(OCC)Oc1ccc(cc1)[N+](=O)[O-]	InChI=1/C10H14NO5PS/c1-3-14-17(18,15-4-2)16-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3	2.902	2.902	1	1	1
57018-04-9	57018049	718	**Tolclofos-methyl**	2_Pest	Tolclofos methyl	tolclofos-methyl	C9H11Cl2O3PS	C9H11Cl2O3PS	301.13	COP(=S)(OC)Oc1c(Cl)cc(C)cc1Cl	InChI=1/C9H11Cl2O3PS/c1-6-4-7(10)9(8(11)5-6)14-15(16,12-2)13-3/h4-5H,1-3H3	4.125	4.125	1	1	1
57646-30-7	57646307	725	**Furalaxyl**	2_Pest		furalaxyl		C17H19NO4	301.34	COC(=O)[C@H](C)N(C(=O)c1occc1)c2c(C)cccc2C	InChI=1/C17H19NO4/c1-11-7-5-8-12(2)15(11)18(13(3)17(20)21-4)16(19)14-9-6-10-22-14/h5-10,13H,1-4H3/t13-/m0/s1	3.379	3.379	1	1	1
57837-19-1	57837191	726	**Metalaxyl**	2_Pest	DL-Alanine, N-(2,6-dimethylphenyl)-N-(methoxyacetyl)-, methyl ester	Metalaxyl	C15H21NO4	C15H21NO4	279.34	COCC(=O)N(C(C)C(=O)OC)c1c(C)cccc1C	InChI=1/C15H21NO4/c1-10-7-6-8-11(2)14(10)16(13(17)9-19-4)12(3)15(18)20-5/h6-8,12H,9H2,1-5H3	2.056	2.056	1	1	1
57966-95-7	57966957	727	**Cymoxanil**	2_Pest		cymoxanil		C7H10N4O3	198.19	CCNC(=O)NC(=O)\C(=N\OC)\C#N	InChI=1/C7H10N4O3/c1-3-9-7(13)10-6(12)5(4-8)11-14-2/h3H2,1-2H3,(H2,9,10,12,13)/b11-5+	-0.491	-0.491	1	1	1
58138-08-2	58138082	5176	**Tridiphane**	2_Pest	Tridiphane	Tridiphane	C10H7Cl5O		320.43	C1C(O1)(CC(Cl)(Cl)Cl)C2=CC(=CC(=C2)Cl)Cl	InChI=1S/C10H7Cl5O/c11-7-1-6(2-8(12)3-7)9(5-16-9)4-10(13,14)15/h1-3H,4-5H2			1	1	1
58-89-9	58899	68	**Lindane**	2_Pest	Lindane	(1a,2a,3b,4a,5a,6b)-1,2,3,4,5,6-Hexachlorocyclohexane	C6H6Cl6	C6H6Cl6	290.83	Cl[C@@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H](Cl)[C@H]1Cl	InChI=1/C6H6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6H/t1-,2-,3-,4+,5+,6+	4.163	4.163	1	1	1
5902-51-2	5902512	5149	**Terbacil**	2_Pest	Terbacil	5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)pyrimidinedione	C9H13ClN2O2	C9H13ClN2O2	216.67	CC1=C(Cl)C(=O)N(C(=O)N1)C(C)(C)C	InChI=1/C9H13ClN2O2/c1-5-6(10)7(13)12(8(14)11-5)9(2,3)4/h1-4H3,(H,11,14)	1.007	1.007	1	1	1
5915-41-3	5915413	70	**Terbuthylazine**	2_Pest	Terbuthylazine	6-Chloro-N-(1,1-dimethylethyl)-N'-ethyl-1,3,5-triazine-2,4-diamine	C9H16ClN5	C9H16ClN5	229.72	CCNc1nc(Cl)nc(NC(C)(C)C)n1	InChI=1/C9H16ClN5/c1-5-11-7-12-6(10)13-8(14-7)15-9(2,3)4/h5H2,1-4H3,(H2,11,12,13,14,15)	1.795	1.795	1	1	1
60168-88-9	60168889	747	**Fenarimol**	2_Pest	Fenarimol	Fenarimol	C17H12Cl2N2O	C17H12Cl2N2O	331.2	OC(c1ccc(Cl)cc1)(c2cncnc2)c3ccccc3Cl	InChI=1/C17H12Cl2N2O/c18-14-7-5-12(6-8-14)17(22,13-9-20-11-21-10-13)15-3-1-2-4-16(15)19/h1-11,22H	3.827	3.827	1	1	1
60207-90-1	60207901	748	**Propiconazole**	2_Pest		1-[[2-(2,4-Dichlorophenyl)-4-propyl 1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole		C15H17Cl2N3O2	342.23	CCCC1COC(Cn2cncn2)(O1)c3ccc(Cl)cc3Cl	InChI=1/C15H17Cl2N3O2/c1-2-3-12-7-21-15(22-12,8-20-10-18-9-19-20)13-5-4-11(16)6-14(13)17/h4-6,9-10,12H,2-3,7-8H2,1H3	3.8	3.8	1	1	1
60-51-5	60515	753	**Dimethoate**	2_Pest	Dimethoate	Phosphorodithioic acid, O,O-Dimethyl S-[2-methylamino)-2-oxoethyl]ester	C5H12NO3PS2	C5H12NO3PS2	229.26	CNC(=O)CSP(=S)(OC)OC	InChI=1/C5H12NO3PS2/c1-6-5(7)4-12-10(11,8-2)9-3/h4H2,1-3H3,(H,6,7)	0.352	0.352	1	1	1
61213-25-0	61213250	4960	**Flurochloridone**	2_Pest		fluorchloridon		C12H10Cl2F3NO	312.12	FC(F)(F)c1cccc(c1)N2CC(CCl)C(Cl)C2=O	InChI=1/C12H10Cl2F3NO/c13-5-7-6-18(11(19)10(7)14)9-3-1-2-8(4-9)12(15,16)17/h1-4,7,10H,5-6H2	3.306	3.306	1	1	1
62-73-7	62737	4897	**Dichlorvos**	2_Pest	Dimethyl-2,2-dichlorovinyl phosphate	Phosphoric acid 2,2-dichloroethenyl dimethyl ester	C4H7Cl2O4P	C4H7Cl2O4P	220.98	COP(=O)(OC)OC=C(Cl)Cl	InChI=1/C4H7Cl2O4P/c1-8-11(7,9-2)10-3-4(5)6/h3H,1-2H3	0.473	0.473	1	1	1
62850-32-2	62850322	4946	**Fenothiocarb**	2_Pest		Fenothiocarb			253.37	CN(C)C(=O)SCCCCOC1=CC=CC=C1	InChI=1S/C13H19NO2S/c1-14(2)13(15)17-11-7-6-10-16-12-8-4-3-5-9-12/h3-5,8-9H,6-7,10-11H2,1-2H3			1	1	1
63-25-2	63252	76	**Carbaryl**	2_Pest	Carbaril	Carbaryl	C12H11NO2	C12H11NO2	201.23	CNC(=O)Oc1cccc2ccccc12	InChI=1/C12H11NO2/c1-13-12(14)15-11-8-4-6-9-5-2-3-7-10(9)11/h2-8H,1H3,(H,13,14)	2.502	2.502	1	1	1
63284-71-9	63284719	773	**Nuarimol**	2_Pest		nuarimol		C17H12ClFN2O	314.75	Oc1ncncc1C(c2ccc(F)cc2)c3ccccc3Cl	InChI=1/C17H12ClFN2O/c18-15-4-2-1-3-13(15)16(11-5-7-12(19)8-6-11)14-9-20-10-21-17(14)22/h1-10,16H,(H,20,21,22)	4.476	4.476	1	1	1
640-15-3	640153	775	**Thiometon**	2_Pest	Thiometon	S-[2-(Ethylthio)ethyl]O,O-dimethyl ester phosphorodithioic acid	C6H15O2PS3	C6H15O2PS3	246.35	CCSCCSP(=S)(OC)OC	InChI=1/C6H15O2PS3/c1-4-11-5-6-12-9(10,7-2)8-3/h4-6H2,1-3H3	2.255	2.255	1	1	1
64902-72-3	64902723	783	**Chlorsulfuron**	2_Pest		chloorsulfuron		C12H11ClN5O4S	357.78	COc1nc(C)nc(NC(=O)[N-]S(=O)(=O)c2ccccc2Cl)n1	InChI=1/C12H12ClN5O4S/c1-7-14-10(17-12(15-7)22-2)16-11(19)18-23(20,21)9-6-4-3-5-8(9)13/h3-6H,1-2H3,(H2,14,15,16,17,18,19)/p-1	1.962	1.686	1	1	1
66215-27-8	66215278	4881	**Cyromazine**	2_Pest		N-Cyclopropyl-1,3,5-triazine-2,4,6-triamine		C6H10N6	166.19	Nc1nc(N)nc(NC2CC2)n1	InChI=1/C6H10N6/c7-4-10-5(8)12-6(11-4)9-3-1-2-3/h3H,1-2H2,(H5,7,8,9,10,11,12)	-0.159	-0.161	1	1	1
66230-04-4	66230044	786	**Esfenvalerate**	2_Pest	Benzeneacetic acid, 4-chloro-.alpha.-(1-methylethyl)-, cyano (3-phenoxyphenyl)methyl ester,(S-(R*,R*))-	4-Chloro-a-(1-methylethyl)benzeneacetic acid [S-(R*,R*)]-Cyano-(3-phenoxyphenyl)methyl ester	C25H22ClNO3		419.91	CC(C)C(C1=CC=C(C=C1)Cl)C(=O)OC(C#N)C2=CC(=CC=C2)OC3=CC=CC=C3	InChI=1S/C25H22ClNO3/c1-17(2)24(18-11-13-20(26)14-12-18)25(28)30-23(16-27)19-7-6-10-22(15-19)29-21-8-4-3-5-9-21			1	1	1
66246-88-6	66246886	787	**Penconazole**	2_Pest		penconazool		C13H15Cl2N3	284.19	CCCC(Cn1cncn1)c2ccc(Cl)cc2Cl	InChI=1/C13H15Cl2N3/c1-2-3-10(7-18-9-16-8-17-18)12-5-4-11(14)6-13(12)15/h4-6,8-10H,2-3,7H2,1H3	4.261	4.261	1	1	1
66332-96-5	66332965	4961	**Flutolanil**	2_Pest	Flutolanil	N-[3-(1-Methylethoxy)phenyl]-2-(trifluoromethyl)benzamide	C17H16F3NO2		323.32	CC(C)OC1=CC=CC(=C1)NC(=O)C2=CC=CC=C2C(F)(F)F	InChI=1S/C17H16F3NO2/c1-11(2)23-13-7-5-6-12(10-13)21-16(22)14-8-3-4-9-15(14)17(18,19)20/h3-11H,1-2H3,(H,21,22)			1	1	1
668-34-8	668348	790	**Fentin**	2_Pest		Trifenyltin			350.01	C1=CC=C(C=C1)[Sn+](C2=CC=CC=C2)C3=CC=CC=C3	InChI=1S/3C6H5.Sn/c3*1-2-4-6-5-3-1;/h3*1-5H;/q;;;+1			1	1	1
66841-25-6	66841256	5167	**Tralomethrin**	2_Pest		2,2-Dimethyl-3-(1,2,2,2-tetrabromoethyl)cyclopropane carboxylic acid, Cyano(3-phenoxyphenyl)methyl ester		C22H19Br4NO3	665.04	CC1(C)C(C(Br)C(Br)(Br)Br)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	InChI=1/C22H19Br4NO3/c1-21(2)17(19(23)22(24,25)26)18(21)20(28)30-16(12-27)13-7-6-10-15(11-13)29-14-8-4-3-5-9-14/h3-11,16-19H,1-2H3	6.926	6.926	1	1	1
67129-08-2	67129082	81	**Metazachlor**	2_Pest	Acetamide, 2-chloro-N-(2,6-dimethylphenyl)-N-(1H-pyrazol-1-ylmethyl)-	2-Chloro-N-(2,6-dimethylphenyl)-N-(1H-pyrazol-1-ylmethyl)acetamide	C14H16ClN3O	C14H16ClN3O	277.76	Cc1cccc(C)c1N(Cn2cccn2)C(=O)CCl	InChI=1/C14H16ClN3O/c1-11-5-3-6-12(2)14(11)18(13(19)9-15)10-17-8-4-7-16-17/h3-8H,9-10H2,1-2H3	2.942	2.941	1	1	1
67306-00-7	67306007	792	**Fenpropidin**	2_Pest		Fenpropidin			273.46	CC(CC1=CC=C(C=C1)C(C)(C)C)CN2CCCCC2	InChI=1S/C19H31N/c1-16(15-20-12-6-5-7-13-20)14-17-8-10-18(11-9-17)19(2,3)4/h8-11,16H,5-7,12-15H2,1-4H3			1	1	1
67375-30-8	67375308	1108	**alpha-Cypermethrin**	2_Pest		(1S,3S)-rel-3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (R)-cyano(3-phenoxyphenyl)methyl ester			416.31	CC1(C(C1C(=O)OC(C#N)C2=CC(=CC=C2)OC3=CC=CC=C3)C=C(Cl)Cl)C	InChI=1S/C22H19Cl2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-14)27-15-8-4-3-5-9-15/h3-1			1	1	1
67564-91-4	67564914	4949	**Fenpropimorph**	2_Pest		fenpropimorf		C20H33NO	303.49	CC(CN1C[C@@H](C)O[C@@H](C)C1)Cc2ccc(cc2)C(C)(C)C	InChI=1/C20H33NO/c1-15(12-21-13-16(2)22-17(3)14-21)11-18-7-9-19(10-8-18)20(4,5)6/h7-10,15-17H,11-14H2,1-6H3/t15?,16-,17+	4.843	4.581	1	1	1
67747-09-5	67747095	797	**Prochloraz**	2_Pest		prochloraz		C15H16Cl3N3O2	376.67	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)n2ccnc2	InChI=1/C15H16Cl3N3O2/c1-2-4-20(15(22)21-5-3-19-10-21)6-7-23-14-12(17)8-11(16)9-13(14)18/h3,5,8-10H,2,4,6-7H2,1H3	4.406	4.408	1	1	1
68694-11-1	68694111	802	**Triflumizole**	2_Pest		Triflumizole			345.76	CCCOCC(=NC1=C(C=C(C=C1)Cl)C(F)(F)F)N2C=CN=C2	InChI=1S/C15H15ClF3N3O/c1-2-7-23-9-14(22-6-5-20-10-22)21-13-4-3-11(16)8-12(13)15(17,18)19/h3-6,8,10H,2,7,9H2,1H3			1	1	1
6923-22-4	6923224	803	**Monocrotophos**	2_Pest	Monocrotophos	Dimethylphosphoric acid, (E)-(Methylamino)-3-oxo-1-propenyl ester	C7H14NO5P	C7H14NO5P	223.17	CNC(=O)\C=C(/C)\OP(=O)(OC)OC	InChI=1/C7H14NO5P/c1-6(5-7(9)8-2)13-14(10,11-3)12-4/h5H,1-4H3,(H,8,9)/b6-5+	-0.63	-0.63	1	1	1
69377-81-7	69377817	805	**Fluroxypyr**	2_Pest		fluroxypyr			255.03	C(C(=O)O)OC1=NC(=C(C(=C1Cl)N)Cl)F	InChI=1S/C7H5Cl2FN2O3/c8-3-5(11)4(9)7(12-6(3)10)15-1-2(13)14/h1H2,(H2,11,12)(H,13,14)			1	1	1
69806-34-4	69806344	810	**Haloxyfop**	2_Pest		2-[4-[[3-Chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoic acid			361.7	CC(C(=O)O)OC1=CC=C(C=C1)OC2=C(C=C(C=N2)C(F)(F)F)Cl	InChI=1S/C15H11ClF3NO4/c1-8(14(21)22)23-10-2-4-11(5-3-10)24-13-12(16)6-9(7-20-13)15(17,18)19/h2-8H,1H3,(H,21,22)			1	1	1
7003-89-6	7003896	4871	**Chlormequat**	2_Pest		chloormequat			122.62	C[N+](C)(C)CCCl	InChI=1S/C5H13ClN/c1-7(2,3)5-4-6/h4-5H2,1-3H3/q+1			1	1	1
70124-77-5	70124775	811	**Flucythrinate**	2_Pest		4-(Difluoromethoxy)-alpha-(1-methylethyl)benzeneacetic acid cyano(3-phenoxyphenyl)methyl ester		C26H41F2NO4	451.47	CC(C)C(C1CCC(CC1)OC(F)F)C(=O)OC(C#N)C2CCCC(C2)OC3CCCCC3	InChI=1/C26H41F2NO4/c1-17(2)24(18-11-13-21(14-12-18)32-26(27)28)25(30)33-23(16-29)19-7-6-10-22(15-19)31-20-8-4-3-5-9-20/h17-24,26H,3-15H2,1-2H3	6.641	6.641	1	1	1
70630-17-0	70630170	1113	**Metalaxyl-M**	2_Pest		N-(2,6-Dimethylphenyl)-N-(methoxyacetyl)-D-alanine methyl ester			279.34	CC1=C(C(=CC=C1)C)N(C(C)C(=O)OC)C(=O)COC	InChI=1S/C15H21NO4/c1-10-7-6-8-11(2)14(10)16(13(17)9-19-4)12(3)15(18)20-5/h6-8,12H,9H2,1-5H3/t12-/m1/s1			1	1	1
709-98-8	709988	816	**Propanil**	2_Pest	Propanamide, N-(3,4-dichlorophenyl)-	N-(3,4-Dichlorophenyl)propanamide	C9H9Cl2NO	C9H9Cl2NO	218.08	CCC(=O)Nc1ccc(Cl)c(Cl)c1	InChI=1/C9H9Cl2NO/c1-2-9(13)12-6-3-4-7(10)8(11)5-6/h3-5H,2H2,1H3,(H,12,13)	2.946	2.946	1	1	1
71626-11-4	71626114	823	**Benalaxyl**	2_Pest		N-(2,6-Dimethylphenyl)-N-(2-phenylacetyl)alanine methyl ester		C20H23NO3	325.41	COC(=O)[C@H](C)N(C(=O)Cc1ccccc1)c2c(C)cccc2C	InChI=1/C20H23NO3/c1-14-9-8-10-15(2)19(14)21(16(3)20(23)24-4)18(22)13-17-11-6-5-7-12-17/h5-12,16H,13H2,1-4H3/t16-/m0/s1	4.019	4.019	1	1	1
71751-41-2	71751412	1097	**Abamectin**	2_Pest		Avermectin B1			873.09	CCC(C)C1C(C=CC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)	InChI=1S/C49H74O14/c1-11-26(2)45-29(5)17-18-48(63-45)23-35-20-34(62-48)16-15-28(4)44(60-41-22-39(55-10)46(32(8			1	1	1
72178-02-0	72178020	824	**Fomesafen**	2_Pest		Fomesafen		C15H9ClF3N2O6S	438.77	CS(=O)(=O)[N-]C(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	InChI=1/C15H10ClF3N2O6S/c1-28(25,26)20-14(22)10-7-9(3-4-12(10)21(23)24)27-13-5-2-8(6-11(13)16)15(17,18)19/h2-7H,1H3,(H,20,22)/p-1	3.777	3.777	1	1	1
72490-01-8	72490018	825	**Fenoxycarb**	2_Pest		[2-(4-Phenoxyphenoxy)ethyl]carbamic acid ethyl ester		C17H19NO4	301.34	CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1	InChI=1/C17H19NO4/c1-2-20-17(19)18-12-13-21-14-8-10-16(11-9-14)22-15-6-4-3-5-7-15/h3-11H,2,12-13H2,1H3,(H,18,19)	3.558	3.558	1	1	1
7287-19-6	7287196	87	**Prometryn**	2_Pest	1,3,5-Triazine-2,4-diamine, N,N'-bis(1-methylethyl)-6-(methylthio)-	2,4-bis(Isopropylamino)-6-methylthio-S-triazine	C10H19N5S	C10H19N5S	241.37	CSc1nc(NC(C)C)nc(NC(C)C)n1	InChI=1/C10H19N5S/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,12,13,14,15)	2.175	2.175	1	1	1
731-27-1	731271	827	**Tolylfluanid**	2_Pest	Tolylfluanid	tolylfluanid	C10H13Cl2FN2O2S2	C10H13Cl2FN2O2S2	347.26	CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccc(C)cc1	InChI=1/C10H13Cl2FN2O2S2/c1-8-4-6-9(7-5-8)15(18-10(11,12)13)19(16,17)14(2)3/h4-7H,1-3H3	4.324	4.324	1	1	1
732-11-6	732116	828	**Phosmet**	2_Pest	Phosmet	S-[(1,3-Dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]O,O-dimethyl ester, Phosphorodithioic acid	C11H12NO4PS2	C11H12NO4PS2	317.32	COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O	InChI=1/C11H12NO4PS2/c1-15-17(18,16-2)19-7-12-10(13)8-5-3-4-6-9(8)11(12)14/h3-6H,7H2,1-2H3	1.955	1.955	1	1	1
74051-80-2	74051802	834	**Sethoxydim**	2_Pest	Sethoxydim	2-[1-(Ethoxyimino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one	C17H29NO3S	C17H28NO3S	327.49	CCCC(=NOCC)C1=C([O-])CC(CC(C)SCC)CC1=O	InChI=1/C17H29NO3S/c1-5-8-14(18-21-6-2)17-15(19)10-13(11-16(17)20)9-12(4)22-7-3/h12-13,19H,5-11H2,1-4H3/p-1	2.545	2.565	1	1	1
74070-46-5	74070465	835	**Aclonifen**	2_Pest		Aclonifen		C12H9ClN2O3	264.67	Nc1c(Cl)c(Oc2ccccc2)ccc1[N+](=O)[O-]	InChI=1/C12H9ClN2O3/c13-11-10(18-8-4-2-1-3-5-8)7-6-9(12(11)14)15(16)17/h1-7H,14H2	3.202	3.202	1	1	1
74223-64-6	74223646	836	**Metsulfuron-methyl**	2_Pest		2-[[[[(4-Methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]amino]sulfonyl]benzoic acid methyl ester			381.37	CC1=NC(=NC(=N1)OC)NC(=O)NS(=O)(=O)C2=CC=CC=C2C(=O)OC	InChI=1S/C14H15N5O6S/c1-8-15-12(18-14(16-8)25-3)17-13(21)19-26(22,23)10-7-5-4-6-9(10)11(20)24-2/h4-7H,1-3H3,(H			1	1	1
74738-17-3	74738173	4948	**Fenpiclonil**	2_Pest		fenpiclonil			237.09	C1=CC(=C(C(=C1)Cl)Cl)C2=CNC=C2C#N	InChI=1S/C11H6Cl2N2/c12-10-3-1-2-8(11(10)13)9-6-15-5-7(9)4-14/h1-3,5-6,15H			1	1	1
75-99-0	75990	4884	**Dalapon**	2_Pest	Propanoic acid, 2,2-dichloro-	2,2-Dichloropropanoic acid	C3H4Cl2O2	C3H3Cl2O2	142.97	CC(Cl)(Cl)C(=O)[O-]	InChI=1/C3H4Cl2O2/c1-3(4,5)2(6)7/h1H3,(H,6,7)/p-1	-0.55	-0.55	1	1	1
759-94-4	759944	869	**EPTC**	2_Pest	Carbamothioic acid, dipropyl-, S-ethyl ester	N,N-dipropylcarbamothioic acid S-ethyl ester	C9H19NOS	C9H19NOS	189.32	CCCN(CCC)C(=O)SCC	InChI=1/C9H19NOS/c1-4-7-10(8-5-2)9(11)12-6-3/h4-8H2,1-3H3	2.874	2.874	1	1	1
76578-12-6	76578126	5116	**Quizalofop**	2_Pest		2-[4-[(6-Chloro-2-quinoxalinyl)oxy]phenoxy]propanoic acid			344.76	CC(C(=O)O)OC1=CC=C(C=C1)OC2=CN=C3C=C(C=CC3=N2)Cl	InChI=1S/C17H13ClN2O4/c1-10(17(21)22)23-12-3-5-13(6-4-12)24-16-9-19-15-8-11(18)2-7-14(15)20-16/h2-10H,1H3,(H,2			1	1	1
76674-21-0	76674210	875	**Flutriafol**	2_Pest		Flutriafol			301.3	C1=CC=C(C(=C1)C(CN2C=NC=N2)(C3=CC=C(C=C3)F)O)F	InChI=1S/C16H13F2N3O/c17-13-7-5-12(6-8-13)16(22,9-21-11-19-10-20-21)14-3-1-2-4-15(14)18/h1-8,10-11,22H,9H2			1	1	1
76738-62-0	76738620	5082	**Paclobutrazol**	2_Pest		(R*,R*)-(+-)-beta[(4-Chlorophenyl)methyl]-alpha-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol			293.8	CC(C)(C)C(C(CC1=CC=C(C=C1)Cl)N2C=NC=N2)O	InChI=1S/C15H20ClN3O/c1-15(2,3)14(20)13(19-10-17-9-18-19)8-11-4-6-12(16)7-5-11/h4-7,9-10,13-14,20H,8H2,1-3H3/t1			1	1	1
76-87-9	76879	1110	**Fentin hydroxide**	2_Pest	Stannane, hydroxytriphenyl-	Hydroxytriphenylstannane	C18H16OSn	C18H16OSn	367.01	O[Sn](c1ccccc1)(c2ccccc2)c3ccccc3	InChI=1/3C6H5.H2O.Sn/c3*1-2-4-6-5-3-1;;/h3*1-5H;1H2;/q;;;;+1/p-1	4.576	4.576	1	1	1
77732-09-3	77732093	5080	**Oxadixyl**	2_Pest		Oxadixyl			278.31	CC1=C(C(=CC=C1)C)N(C(=O)COC)N2CCOC2=O	InChI=1S/C14H18N2O4/c1-10-5-4-6-11(2)13(10)16(12(17)9-19-3)15-7-8-20-14(15)18/h4-6H,7-9H2,1-3H3			1	1	1
7786-34-7	7786347	5035	**Mevinphos**	2_Pest	Mevinphos	3-[(Dimethoxyphosphinyl)oxy]-2-butenoic acid Methyl ester	C7H13O6P	C7H13O6P	224.15	COC(=O)\C=C(/C)\OP(=O)(OC)OC	InChI=1/C7H13O6P/c1-6(5-7(8)10-2)13-14(9,11-3)12-4/h5H,1-4H3/b6-5+	0.018	0.018	1	1	1
78587-05-0	78587050	4974	**Hexythiazox**	2_Pest		Hexythiazox (DPX-Y5893)			352.89	CC1C(SC(=O)N1C(=O)NC2CCCCC2)C3=CC=C(C=C3)Cl	InChI=1S/C17H21ClN2O2S/c1-11-15(12-7-9-13(18)10-8-12)23-17(22)20(11)16(21)19-14-5-3-2-4-6-14/h7-11,14-15H,2-6H			1	1	1
786-19-6	786196	898	**carbophenothion**	2_Pest	Carbofenotion	Carbofenthion	C11H16ClO2PS3	C11H16ClO2PS3	342.87	CCOP(=S)(OCC)SCSc1ccc(Cl)cc1	InChI=1/C11H16ClO2PS3/c1-3-13-15(16,14-4-2)18-9-17-11-7-5-10(12)6-8-11/h5-8H,3-4,9H2,1-2H3	4.827	4.827	1	1	1
79241-46-6	79241466	4954	**Fluazifop-P-butyl**	2_Pest		Fluazifop-p-butyl			383.37	CCCCOC(=O)C(C)OC1=CC=C(C=C1)OC2=NC=C(C=C2)C(F)(F)F	InChI=1S/C19H20F3NO4/c1-3-4-11-25-18(24)13(2)26-15-6-8-16(9-7-15)27-17-10-5-14(12-23-17)19(20,21)22/h5-10,12-1			1	1	1
79277-27-3	79277273	918	**Thifensulfuron-methyl**	2_Pest		Thiameturon-methyl			387.4	CC1=NC(=NC(=N1)OC)NC(=O)NS(=O)(=O)C2=C(SC=C2)C(=O)OC	InChI=1S/C12H13N5O6S2/c1-6-13-10(16-12(14-6)23-3)15-11(19)17-25(20,21)7-4-5-24-8(7)9(18)22-2/h4-5H,1-3H3,(H2,1			1	1	1
79538-32-2	79538322	922	**Tefluthrin**	2_Pest		Tefluthrin			418.74	CC1=C(C(=C(C(=C1F)F)COC(=O)C2C(C2(C)C)C=C(C(F)(F)F)Cl)F)F	InChI=1S/C17H14ClF7O2/c1-6-11(19)13(21)7(14(22)12(6)20)5-27-15(26)10-8(16(2,3)10)4-9(18)17(23,24)25/h4,8,10H,5H			1	1	1
79622-59-6	79622596	925	**Fluazinam**	2_Pest		fluazinam			465.1	C1=C(C=NC(=C1Cl)NC2=C(C=C(C(=C2[N+](=O)[O-])Cl)C(F)(F)F)[N+](=O)[O-])C(F)(F)F	InChI=1S/C13H4Cl2F6N4O4/c14-6-1-4(12(16,17)18)3-22-11(6)23-9-7(24(26)27)2-5(13(19,20)21)8(15)10(9)25(28)29/h1-3			1	1	1
79983-71-4	79983714	930	**Hexaconazole**	2_Pest		alpha-Butyl-alpha-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol			314.22	CCCCC(CN1C=NC=N1)(C2=C(C=C(C=C2)Cl)Cl)O	InChI=1S/C14H17Cl2N3O/c1-2-3-6-14(20,8-19-10-17-9-18-19)12-5-4-11(15)7-13(12)16/h4-5,7,9-10,20H,2-3,6,8H2,1H3			1	1	1
80-33-1	80331	935	**Chlorfenson**	2_Pest	4-Chlorophenyl 4-chlorobenzenesulfonate	chloorfenson	C12H8Cl2O3S	C12H8Cl2O3S	303.16	Clc1ccc(OS(=O)(=O)c2ccc(Cl)cc2)cc1	InChI=1/C12H8Cl2O3S/c13-9-1-5-11(6-2-9)17-18(15,16)12-7-3-10(14)4-8-12/h1-8H	4.293	4.293	1	1	1
81335-37-7	81335377	4977	**Imazaquin**	2_Pest		Imazaquin			311.34	CC(C)C1(C(=O)NC(=N1)C2=NC3=CC=CC=C3C=C2C(=O)O)C	InChI=1S/C17H17N3O3/c1-9(2)17(3)16(23)19-14(20-17)13-11(15(21)22)8-10-6-4-5-7-12(10)18-13/h4-9H,1-3H3,(H,21,22			1	1	1
81777-89-1	81777891	941	**Clomazone**	2_Pest	Dimethazone	Clomazone	C12H14ClNO2		239.7	CC1(CON(C1=O)CC2=CC=CC=C2Cl)C	InChI=1S/C12H14ClNO2/c1-12(2)8-16-14(11(12)15)7-9-5-3-4-6-10(9)13/h3-6H,7-8H2,1-2H3			1	1	1
82097-50-5	82097505	944	**Triasulfuron**	2_Pest		2-(2-Chloroethoxy)-N-[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide			401.83	CC1=NC(=NC(=N1)OC)NC(=O)NS(=O)(=O)C2=CC=CC=C2OCCCl	InChI=1S/C14H16ClN5O5S/c1-9-16-12(19-14(17-9)24-2)18-13(21)20-26(22,23)11-6-4-3-5-10(11)25-8-7-15/h3-6H,7-8H2,			1	1	1
82558-50-7	82558507	946	**Isoxaben**	2_Pest		isoxaben			332.4	CCC(C)(CC)C1=NOC(=C1)NC(=O)C2=C(C=CC=C2OC)OC	InChI=1S/C18H24N2O4/c1-6-18(3,7-2)14-11-15(24-20-14)19-17(21)16-12(22-4)9-8-10-13(16)23-5/h8-11H,6-7H2,1-5H3,(			1	1	1
82560-54-1	82560541	947	**Benfuracarb**	2_Pest		2-Methyl-4-(1-methylethyl)-7-oxo-8-oxa-3-thia-2,4-diazadecanoic acid, 2,3-Dihydro-2,2-dimethyl-7-benzofuranyl ester			410.54	CCOC(=O)CCN(C(C)C)SN(C)C(=O)OC1=CC=CC2=C1OC(C2)(C)C	InChI=1S/C20H30N2O5S/c1-7-25-17(23)11-12-22(14(2)3)28-21(6)19(24)26-16-10-8-9-15-13-20(4,5)27-18(15)16/h8-10,1			1	1	1
82657-04-3	82657043	948	**Bifenthrin**	2_Pest		3-(2-Chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-cyclopropanecarboxylic acid, cis-(2-Methyl[1,1'-biphenyl]3-yl)methy			422.87	CC1=C(C=CC=C1COC(=O)C2C(C2(C)C)C=C(C(F)(F)F)Cl)C3=CC=CC=C3	InChI=1S/C23H22ClF3O2/c1-14-16(10-7-11-17(14)15-8-5-4-6-9-15)13-29-21(28)20-18(22(20,2)3)12-19(24)23(25,26)27/h			1	1	1
82-68-8	82688	5115	**Quintozene**	2_Pest	Benzene, pentachloronitro-	Pentachloronitrobenzene	C6Cl5NO2	C6Cl5NO2	295.34	[O-][N+](=O)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	InChI=1/C6Cl5NO2/c7-1-2(8)4(10)6(12(13)14)5(11)3(1)9	5.046	5.046	1	1	1
83055-99-6	83055996	949	**Bensulfuron-methyl**	2_Pest		2-[[[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]methyl]benzoic acid methyl ester			410.41	COC1=CC(=NC(=N1)NC(=O)NS(=O)(=O)CC2=CC=CC=C2C(=O)OC)OC	InChI=1S/C16H18N4O7S/c1-25-12-8-13(26-2)18-15(17-12)19-16(22)20-28(23,24)9-10-6-4-5-7-11(10)14(21)27-3/h4-8H,9			1	1	1
83121-18-0	83121180	5144	**Teflubenzuron**	2_Pest		teflubenzuron			381.11	C1=CC(=C(C(=C1)F)C(=O)NC(=O)NC2=CC(=C(C(=C2F)Cl)F)Cl)F	InChI=1S/C14H6Cl2F4N2O2/c15-5-4-8(12(20)10(16)11(5)19)21-14(24)22-13(23)9-6(17)2-1-3-7(9)18/h1-4H,(H2,21,22,23,			1	1	1
83164-33-4	83164334	951	**Diflufenican**	2_Pest		diflufenican			394.3	C1=CC(=CC(=C1)OC2=C(C=CC=N2)C(=O)NC3=C(C=C(C=C3)F)F)C(F)(F)F	InChI=1S/C19H11F5N2O2/c20-12-6-7-16(15(21)10-12)26-17(27)14-5-2-8-25-18(14)28-13-4-1-3-11(9-13)19(22,23)24/h1-			1	1	1
834-12-8	834128	953	**ametryn**	2_Pest	1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(1-methylethyl)-6-(methylthio)-	N-Ethyl-N'-((1-methylethyl)-6-methylthio)-1,3,5-triazine-2,4-diamine	C9H17N5S	C9H17N5S	227.34	CCNc1nc(NC(C)C)nc(SC)n1	InChI=1/C9H17N5S/c1-5-10-7-12-8(11-6(2)3)14-9(13-7)15-4/h6H,5H2,1-4H3,(H2,10,11,12,13,14)	1.798	1.796	1	1	1
83657-24-3	83657243	955	**Diniconazole**	2_Pest		Diniconazol			326.23	CC(C)(C)C(C(=CC1=C(C=C(C=C1)Cl)Cl)N2C=NC=N2)O	InChI=1S/C15H17Cl2N3O/c1-15(2,3)14(21)13(20-9-18-8-19-20)6-10-4-5-11(16)7-12(10)17/h4-9,14,21H,1-3H3/b13-6-			1	1	1
84087-01-4	84087014	958	**Quinclorac**	2_Pest		3,7-Dichloro-8-quinolinecarboxylic acid			242.06	C1=CC(=C(C2=NC=C(C=C21)Cl)C(=O)O)Cl	InChI=1S/C10H5Cl2NO2/c11-6-3-5-1-2-7(12)8(10(14)15)9(5)13-4-6/h1-4H,(H,14,15)			1	1	1
841-06-5	841065	959	**Methoprotryne**	2_Pest	Methoprotryne	N-(3-Methoxypropyl)-N'(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine	C11H21N5OS	C11H21N5OS	271.39	COCCCNc1nc(NC(C)C)nc(SC)n1	InChI=1/C11H21N5OS/c1-8(2)13-10-14-9(12-6-5-7-17-3)15-11(16-10)18-4/h8H,5-7H2,1-4H3,(H2,12,13,14,15,16)	1.38	1.38	1	1	1
85509-19-9	85509199	967	**Flusilazole**	2_Pest		1-[[Bis(4-fluorophenyl)methylsilyl]methyl]-1H-1,2,4-triazole			315.4	C[Si](CN1C=NC=N1)(C2=CC=C(C=C2)F)C3=CC=C(C=C3)F	InChI=1S/C16H15F2N3Si/c1-22(12-21-11-19-10-20-21,15-6-2-13(17)3-7-15)16-8-4-14(18)5-9-16/h2-11H,12H2,1H3			1	1	1
86479-06-3	86479063	971	**Hexaflumuron**	2_Pest		Hexaflumuron			461.15	C1=CC(=C(C(=C1)F)C(=O)NC(=O)NC2=CC(=C(C(=C2)Cl)OC(C(F)(F)F)F)Cl)F	InChI=1S/C16H8Cl2F6N2O3/c17-7-4-6(5-8(18)12(7)29-16(23,24)14(21)22)25-15(28)26-13(27)11-9(19)2-1-3-10(11)20/h1-			1	1	1
86-50-0	86500	972	**Azinphos-methyl**	2_Pest	Azinphos-Methyl	Azinophosmethyl	C10H12N3O3PS2	C10H12N3O3PS2	317.33	COP(=S)(OC)SCN1N=Nc2ccccc2C1=O	InChI=1/C10H12N3O3PS2/c1-15-17(18,16-2)19-7-13-10(14)8-5-3-4-6-9(8)11-12-13/h3-6H,7H2,1-2H3	2.925	2.925	1	1	1
87392-12-9	87392129	1115	**S-Metolachlor**	2_Pest		2-Chloro-N-(2-ethyl-6-methylphenyl)-N-[(1S)-2-methoxy-1-methylethyl]acetamide			283.8	CCC1=CC=CC(=C1N(C(C)COC)C(=O)CCl)C	InChI=1S/C15H22ClNO2/c1-5-13-8-6-7-11(2)15(13)17(14(18)9-16)12(3)10-19-4/h6-8,12H,5,9-10H2,1-4H3/t12-/m0/s1			1	1	1
87674-68-8	87674688	1109	**Dimethenamid**	2_Pest		Dimethenamid			275.8	CC1=CSC(=C1N(C(C)COC)C(=O)CCl)C	InChI=1S/C12H18ClNO2S/c1-8-7-17-10(3)12(8)14(11(15)5-13)9(2)6-16-4/h7,9H,5-6H2,1-4H3			1	1	1
87820-88-0	87820880	981	**Tralkoxydim**	2_Pest		2-[1-(Ethoxyimino)propyl]-3-hydroxy-5-(2,4,6-trimethylphenyl)-2-cyclohexen-1-one			329.44	CCC(=C1C(=O)CC(CC1=O)C2=C(C=C(C=C2C)C)C)NOCC	InChI=1S/C20H27NO3/c1-6-16(21-24-7-2)20-17(22)10-15(11-18(20)23)19-13(4)8-12(3)9-14(19)5/h8-9,15,21H,6-7,10-11H			1	1	1
886-50-0	886500	104	**Terbutryn**	2_Pest	Terbutryn	Terbutryne	C10H19N5S	C10H19N5S	241.37	CCNc1nc(NC(C)(C)C)nc(SC)n1	InChI=1/C10H19N5S/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,12,13,14,15)	2.003	2.001	1	1	1
88671-89-0	88671890	984	**Myclobutanil**	2_Pest		Myclobutanil			288.79	CCCCC(CN1C=NC=N1)(C#N)C2=CC=C(C=C2)Cl	InChI=1S/C15H17ClN4/c1-2-3-8-15(9-17,10-20-12-18-11-19-20)13-4-6-14(16)7-5-13/h4-7,11-12H,2-3,8,10H2,1H3			1	1	1
90717-03-6	90717036	1003	**Quinmerac**	2_Pest		quinmerac			221.64	CC1=CN=C2C(=C1)C=CC(=C2C(=O)O)Cl	InChI=1S/C11H8ClNO2/c1-6-4-7-2-3-8(12)9(11(14)15)10(7)13-5-6/h2-5H,1H3,(H,14,15)			1	1	1
91465-08-6	91465086	5001	**Lambda-Cyhalothrin**	2_Pest		3-[(1Z)-2-Chloro-3,3,3-trifluoro-1-propen-1-yl]-2,2-dimethylcyclopropanecarboxylic acid (1S,3S)-rel-(R)-cyano(3-phenoxyphenyl)methyl ester			449.86	CC1(C(C1C(=O)OC(C#N)C2=CC(=CC=C2)OC3=CC=CC=C3)C=C(C(F)(F)F)Cl)C	InChI=1S/C23H19ClF3NO3/c1-22(2)17(12-19(24)23(25,26)27)20(22)21(29)31-18(13-28)14-7-6-10-16(11-14)30-15-8-4-3-			1	1	1
919-86-8	919868	1010	**Demeton-S-methyl**	2_Pest	Demeton-S-methyl	S-[2-(Ethylthio)ethyl]O,O-dimethyl ester phosphorothioic acid	C6H15O3PS2	C6H15O3PS2	230.29	CCSCCSP(=O)(OC)OC	InChI=1/C6H15O3PS2/c1-4-11-5-6-12-10(7,8-2)9-3/h4-6H2,1-3H3	1.356	1.356	1	1	1
93-65-2	93652	108	**Mecoprop**	2_Pest	Propanoic acid, 2-(4-chloro-2-methylphenoxy)-	2-(4-Chloro-2-methylphenoxy)propanoic acid	C10H11ClO3	C10H10ClO3	214.65	CC(Oc1ccc(Cl)cc1C)C(=O)[O-]	InChI=1/C10H11ClO3/c1-6-5-8(11)3-4-9(6)14-7(2)10(12)13/h3-5,7H,1-2H3,(H,12,13)/p-1	1.455	1.456	1	1	1
94125-34-5	94125345	1021	**Prosulfuron**	2_Pest		Prosulfuron			419.39	CC1=NC(=NC(=N1)OC)NC(=O)NS(=O)(=O)C2=CC=CC=C2CCC(F)(F)F	InChI=1S/C15H16F3N5O4S/c1-9-19-12(22-14(20-9)27-2)21-13(24)23-28(25,26)11-6-4-3-5-10(11)7-8-15(16,17)18/h3-6H			1	1	1
94361-06-5	94361065	1022	**Cyproconazole**	2_Pest		Cyproconazole			291.79	CC(C1CC1)C(CN2C=NC=N2)(C3=CC=C(C=C3)Cl)O	InChI=1S/C15H18ClN3O/c1-11(12-2-3-12)15(20,8-19-10-17-9-18-19)13-4-6-14(16)7-5-13/h4-7,9-12,20H,2-3,8H2,1H3			1	1	1
944-22-9	944229	1023	**Fonofos**	2_Pest	Fonofos	Ethylphosphonodithioic acid, O-Ethyl S-phenyl ester	C10H15OPS2	C10H15OPS2	246.33	CCOP(=S)(CC)Sc1ccccc1	InChI=1/C10H15OPS2/c1-3-11-12(13,4-2)14-10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3	3.413	3.413	1	1	1
94-74-6	94746	110	**MCPA**	2_Pest	Azacyclotridecan-2-one	(4-Chloro-2-methylphenoxy)acetic acid	C9H9ClO3	C9H8ClO3	200.62	Cc1cc(Cl)ccc1OCC(=O)[O-]	InChI=1/C9H9ClO3/c1-6-4-7(10)2-3-8(6)13-5-9(11)12/h2-4H,5H2,1H3,(H,11,12)/p-1	0.971	0.972	1	1	1
94-75-7	94757	111	**2,4-D**	2_Pest	(2,4-Dichlorophenoxy)acetic acid	(2,4-Dichlorophenoxy)acetic acid	C8H6Cl2O3	C8H5Cl2O3	221.04	[O-]C(=O)COc1ccc(Cl)cc1Cl	InChI=1/C8H6Cl2O3/c9-5-1-2-7(6(10)3-5)13-4-8(11)12/h1-3H,4H2,(H,11,12)/p-1	1.149	1.15	1	1	1
94-81-5	94815	5015	**MCPB**	2_Pest	4-(4-Chloro-2-methylphenoxy)butanoic acid	4-(4-Chloro-2-methylphenoxy)butanoic acid	C11H13ClO3	C11H12ClO3	228.68	Cc1cc(Cl)ccc1OCCCC(=O)[O-]	InChI=1/C11H13ClO3/c1-8-7-9(12)4-5-10(8)15-6-2-3-11(13)14/h4-5,7H,2-3,6H2,1H3,(H,13,14)/p-1	1.541	1.571	1	1	1
94-82-6	94826	4327	**2,4-DB**	2_Pest	Butanoic acid, 4-(2,4-dichlorophenoxy)-	4-(2,4-Dichlorophenoxy)butanoic acid	C10H10Cl2O3	C10H9Cl2O3	249.09	[O-]C(=O)CCCOc1ccc(Cl)cc1Cl	InChI=1/C10H10Cl2O3/c11-7-3-4-9(8(12)6-7)15-5-1-2-10(13)14/h3-4,6H,1-2,5H2,(H,13,14)/p-1	1.719	1.761	1	1	1
950-37-8	950378	1025	**Methidathion**	2_Pest	Methidathion	Phosphorodithioic acid, S-((5-methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl)O,O-dimethyl ester	C6H11N2O4PS3	C6H11N2O4PS3	302.33	COC1=NN(CSP(=S)(OC)OC)C(=O)S1	InChI=1/C6H11N2O4PS3/c1-10-5-7-8(6(9)16-5)4-15-13(14,11-2)12-3/h4H2,1-3H3	2.357	2.357	1	1	1
95266-40-3	95266403	1026	**Trinexapac-Ethyl**	2_Pest		Cimecticarb			252.27	CCOC(=O)C1CC(=O)C(=C(C2CC2)O)C(=O)C1	InChI=1S/C13H16O5/c1-2-18-13(17)8-5-9(14)11(10(15)6-8)12(16)7-3-4-7/h7-8,16H,2-6H2,1H3			1	1	1
95465-99-9	95465999	1027	**Cadusafos**	2_Pest		Cadusafos			270.39	CCC(C)SP(=O)(OCC)SC(C)CC	InChI=1S/C10H23O2PS2/c1-6-9(4)14-13(11,12-8-3)15-10(5)7-2/h9-10H,6-8H2,1-5H3			1	1	1
95617-09-7	95617097	4947	**Fenoxaprop**	2_Pest		(+-)-2-[4-[(6-Chloro-2-benzoxazolyl)oxy]phenoxy]propanoic acid			333.73	CC(C(=O)O)OC1=CC=C(C=C1)OC2=NC3=C(O2)C=C(C=C3)Cl	InChI=1S/C16H12ClNO5/c1-9(15(19)20)21-11-3-5-12(6-4-11)22-16-18-13-7-2-10(17)8-14(13)23-16/h2-9H,1H3,(H,19,20)			1	1	1
96489-71-3	96489713	1055	**Pyridaben**	2_Pest		Pyridaben			364.94	CC(C)(C)C1=CC=C(C=C1)CSC2=C(C(=O)N(N=C2)C(C)(C)C)Cl	InChI=1S/C19H25ClN2OS/c1-18(2,3)14-9-7-13(8-10-14)12-24-15-11-21-22(19(4,5)6)17(23)16(15)20/h7-11H,12H2,1-6H3			1	1	1
99105-77-8	99105778	1083	**Sulcotrione**	2_Pest		sulcotrion			328.77	CS(=O)(=O)C1=CC(=C(C=C1)C(=O)C2C(=O)CCCC2=O)Cl	InChI=1S/C14H13ClO5S/c1-21(19,20)8-5-6-9(10(15)7-8)14(18)13-11(16)3-2-4-12(13)17/h5-7,13H,2-4H2,1H3			1	1	1
99129-21-2	99129212	1084	**Clethodim**	2_Pest		Clethodim			359.92	CCC(=C1C(=O)CC(CC1=O)CC(C)SCC)NOCC=CCl	InChI=1S/C17H26ClNO3S/c1-4-14(19-22-8-6-7-18)17-15(20)10-13(11-16(17)21)9-12(3)23-5-2/h6-7,12-13,19H,4-5,8-11H			1	1	1
99-30-9	99309	1085	**Dicloran**	2_Pest	2,6-Dichloro-4-nitroaniline	2,6-Dichloro-4-nitrobenzenamine	C6H4Cl2N2O2	C6H4Cl2N2O2	207.02	Nc1c(Cl)cc(cc1Cl)[N+](=O)[O-]	InChI=1/C6H4Cl2N2O2/c7-4-1-3(10(11)12)2-5(8)6(4)9/h1-2H,9H2	2.306	2.306	1	1	1
2458-08-4	2458084	1246	**12-Ketochenodeoxycholic acid**	3_REACH		3a,7a-dihydroxy-12-oxo-5ß-cholan-24-oic acid		C24H37O5	406.56	C[C@H](CCC(=O)[O-])[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC(=O)[C@]	InChI=1/C24H38O5/c1-13(4-7-21(28)29)16-5-6-17-22-18(12-20(27)24(16,17)3)23(2)9-8-15(25)10-14(23)11-19(22)26/h13-19,22,25-26H,4-12H2,1-3H3,(H,28,29)/p-1/t13-,14+,15-,16-,17+,18+,19-,22+,23+,24-/m1/s1	1.539	1.735	1	1	1
2478-10-6	2478106	1247	**4-hydroxybutyl acrylate**	3_REACH		4-hydroxybutyl acrylate		C7H12O3	144.17	OCCCCOC(=O)C=C	InChI=1/C7H12O3/c1-2-7(9)10-6-4-3-5-8/h2,8H,1,3-6H2	0.821	0.821	1	1	1
2536-05-2	2536052	1249	**2,2'-methylenediphenyl diisocyanate**	3_REACH		2,2'-methylenediphenyl diisocyanate		C15H10N2O2	250.26	O=C=Nc1ccccc1Cc2ccccc2N=C=O	InChI=1/C15H10N2O2/c18-10-16-14-7-3-1-5-12(14)9-13-6-2-4-8-15(13)17-11-19/h1-8H,9H2	3.525	3.525	1	1	1
2550-02-9	2550029	1250	**triethoxypropylsilane**	3_REACH	Silane, triethoxypropyl-	triethoxypropylsilane	C9H22O3Si	C9H22O3Si	206.36	CCC[Si](OCC)(OCC)OCC	InChI=1/C9H22O3Si/c1-5-9-13(10-6-2,11-7-3)12-8-4/h5-9H2,1-4H3	4.079	4.079	1	1	1
2550-06-3	2550063	1251	**trichloro(3-chloropropyl)silane**	3_REACH	Silane, trichloro(3-chloropropyl)-	trichloro(3-chloropropyl)silane	C3H6Cl4Si	C3H6Cl4Si	211.98	ClCCC[Si](Cl)(Cl)Cl	InChI=1/C3H6Cl4Si/c4-2-1-3-8(5,6)7/h1-3H2	4.064	4.064	1	1	1
2554-06-5	2554065	1252	**2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane**	3_REACH	2,4,6,8-Tetravinyl-2,4,6,8-tetramethylcyclotetrasiloxane	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	C12H24O4Si4	C12H24O4Si4	344.66	C[Si]1(O[Si](C)(O[Si](C)(O[Si](C)(O1)C=C)C=C)C=C)C=C	InChI=1/C12H24O4Si4/c1-9-17(5)13-18(6,10-2)15-20(8,12-4)16-19(7,11-3)14-17/h9-12H,1-4H2,5-8H3	7.23	7.23	1	1	1
2643-07-4	2643074	1253	**p-[(2-chloroethyl)ethylamino]benzaldehyde**	3_REACH	p-([2-Chloroethyl]ethylamino)benzaldehyde	p-[(2-chloroethyl)ethylamino]benzaldehyde	C11H14ClNO	C11H14ClNO	211.69	CCN(CCCl)c1ccc(C=O)cc1	InChI=1/C11H14ClNO/c1-2-13(8-7-12)11-5-3-10(9-14)4-6-11/h3-6,9H,2,7-8H2,1H3	2.765	2.763	1	1	1
2680-03-7	2680037	1254	**N,N-dimethylacrylamide**	3_REACH	2-propenamide, N,N-dimethyl	N,N-dimethylacrylamide	C5H9NO	C5H9NO	99.134	CN(C)C(=O)C=C	InChI=1/C5H9NO/c1-4-5(7)6(2)3/h4H,1H2,2-3H3	0.277	0.277	1	1	1
3081-01-4	3081014	1257	**N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine**	3_REACH		N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine		C19H26N2	282.43	CC(C)CCC(C)Nc1ccc(Nc2ccccc2)cc1	InChI=1/C19H26N2/c1-15(2)9-10-16(3)20-18-11-13-19(14-12-18)21-17-7-5-4-6-8-17/h4-8,11-16,20-21H,9-10H2,1-3H3	5.602	5.152	1	1	1
3302-10-1	3302101	1259	**3,5,5-trimethylhexanoic acid**	3_REACH	3,5,5-Trimethylhexanoic acid	3,5,5-trimethylhexanoic acid	C9H18O2	C9H17O2	158.24	CC(CC(=O)[O-])CC(C)(C)C	InChI=1/C9H18O2/c1-7(5-8(10)11)6-9(2,3)4/h7H,5-6H2,1-4H3,(H,10,11)/p-1	1.066	1.145	1	1	1
3452-07-1	3452071	1261	**Icos-1-ene**	3_REACH	1-Eicosene	icos-1-ene	C20H40	C20H40	280.54	CCCCCCCCCCCCCCCCCCC=C	InChI=1/C20H40/c1-3-5-7-9-11-13-15-17-19-20-18-16-14-12-10-8-6-4-2/h3H,1,4-20H2,2H3	9.104	9.104	0	1	1
3913-02-8	3913028	1263	**2-butyloctan-1-ol**	3_REACH	1-Octanol, 2-butyl-	2-butyloctan-1-ol	C12H26O	C12H26O	186.34	CCCCCCC(CO)CCCC	InChI=1/C12H26O/c1-3-5-7-8-10-12(11-13)9-6-4-2/h12-13H,3-11H2,1-2H3	4.483	4.483	1	1	1
4130-08-9	4130089	1265	**triacetoxyvinylsilane**	3_REACH	Triacetoxy(vinyl)silane	triacetoxyvinylsilane	C8H12O6Si	C8H12O6Si	232.26	CC(=O)OC(=C(OC(=O)C)OC(=O)C)[SiH3]	InChI=1/C8H12O6Si/c1-4(9)12-7(15)8(13-5(2)10)14-6(3)11/h1-3,15H3	3.761	3.761	1	1	1
4223-03-4	4223034	1266	**N-(1,1,3,3-tetramethylbutyl)acrylamide**	3_REACH	2-Propenamide, n-1,1,3,3-tetramethylbutyl-	N-(1,1,3,3-tetramethylbutyl)acrylamide	C11H21NO	C11H21NO	183.3	CC(C)(C)CC(C)(C)NC(=O)C=C	InChI=1/C11H21NO/c1-7-9(13)12-11(5,6)8-10(2,3)4/h7H,1,8H2,2-6H3,(H,12,13)	2.44	2.44	1	1	1
4292-10-8	4292108	1267	**(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide**	3_REACH		(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide		C19H38N2O3	342.53	CCCCCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]	InChI=1/C19H38N2O3/c1-4-5-6-7-8-9-10-11-12-14-18(22)20-15-13-16-21(2,3)17-19(23)24/h4-17H2,1-3H3,(H-,20,22,23,24)	1	1	1	1	1
4719-04-4	4719044	117	**2,2',2''-(hexahydro-1,3,5-triazine-1,3,5-triyl)triethanol**	3_REACH		1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol		C9H23N3O3	219.29	OCCN1C[NH+](CCO)C[NH+](CCO)C1	InChI=1/C9H21N3O3/c13-4-1-10-7-11(2-5-14)9-12(8-10)3-6-15/h13-15H,1-9H2/p+2	-4.377	-3.048	1	1	1
5117-12-4	5117124	4397	**4-(1-oxo-2-propenyl)-morpholine**	3_REACH	N-Acryloylmorpholine	4-(1-oxo-2-propenyl)-morpholine	C7H11NO2		141.17	C=CC(=O)N1CCOCC1	InChI=1S/C7H11NO2/c1-2-7(9)8-3-5-10-6-4-8/h2H,1,3-6H2			1	1	1
6318-09-8	6318098	1282	**2,4,6-Tri(propan-2-yl)benzene-1,3-diamine**	3_REACH		1,3-Benzenediamine, 2,4,6-tris(1-methylethyl)-			234.39	CC(C)C1=CC(=C(C(=C1N)C(C)C)N)C(C)C	InChI=1S/C15H26N2/c1-8(2)11-7-12(9(3)4)15(17)13(10(5)6)14(11)16/h7-10H,16-17H2,1-6H3			1	1	1
6992-11-6	6992116	1287	**4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxynaphthalene-2-carboxamide**	3_REACH		4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxynaphthalene-2-carboxamide		C24H14Cl2N5O3	492.33	Oc1nc2cc(NC(=O)c3cc4ccccc4c(N=Nc5cc(Cl)ccc5Cl)c3[O-])ccc2[nH]1	InChI=1/C24H15Cl2N5O3/c25-13-5-7-17(26)19(10-13)30-31-21-15-4-2-1-3-12(15)9-16(22(21)32)23(33)27-14-6-8-18-20(11-14)29-24(34)28-18/h1-11,32H,(H,27,33)(H2,28,29,34)/p-1	6.091	6.793	1	1	1
7027-11-4	7027114	4392	**3-cyano-3,5,5-trimethylcyclohexanone**	3_REACH		3-cyano-3,5,5-trimethylcyclohexanone			165.24	CC1(CC(=O)CC(C1)(C)C#N)C	InChI=1S/C10H15NO/c1-9(2)4-8(12)5-10(3,6-9)7-11/h4-6H2,1-3H3			1	1	1

7651-02-7	7651027	1289	**N-[3-(dimethylamino)propyl]stearamide**	3_REACH	N-[3-(dimethylamino)propyl]octadecanamide	N-[3-(dimethylamino)propyl]stearamide	C23H48N2O	C23H49N2O	368.65	CCCCCCCCCCCCCCCCCC(=O)NCCC[NH+](C)C	InChI=1/C23H48N2O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23(26)24-21-19-22-25(2)3/h4-22H2,1-3H3,(H,24,26)/p+1	5.524	5.657	1	1	1
100-00-5	100005	119	**1-chloro-4-nitrobenzene**	3_REACH	Benzene, 1-chloro-4-nitro-	1-Chloro-4-nitrobenzene	C6H4ClNO2	C6H4ClNO2	157.56	[O-][N+](=O)c1ccc(Cl)cc1	InChI=1/C6H4ClNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H	2.388	2.388	1	1	1
100-01-6	100016	120	**4-nitroaniline**	3_REACH	p-Nitroaniline	4-Nitrobenzenamine	C6H6N2O2	C6H6N2O2	138.13	Nc1ccc(cc1)[N+](=O)[O-]	InChI=1/C6H6N2O2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H,7H2	0.977	0.977	1	1	1
100-02-7	100027	1	**4-nitrophenol**	3_REACH	Phenol, 4-nitro-	4-Nitrophenol	C6H5NO3	C6H4NO3	139.11	[O-]c1ccc(cc1)[N+](=O)[O-]	InChI=1/C6H5NO3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H/p-1	0.779	1.173	1	1	1
1001354-72-8	1001354728	4779	**3-Aminooctan-4-ol**	3_REACH		4-Octanol, 3-amino-			145.25	CCCCC(C(CC)N)O	InChI=1S/C8H19NO/c1-3-5-6-8(10)7(9)4-2/h7-8,10H,3-6,9H2,1-2H3			1	1	1
10016-20-3	10016203	1295	**cyclohexapentylose**	3_REACH	α-Cyclodextrin	cyclohexapentylose	C36H60O30	C36H60O30	972.85	OC[C@H]1O[C@@H]2O[C@H]3[C@H](O)[C@@H](O)[C@H](O[C@@H]3CO)O[C@H]4[C@H](O)[C@@H](O)[C@H](O	InChI=1/C36H60O30/c37-1-7-25-13(43)19(49)31(55-7)62-26-8(2-38)57-33(21(51)15(26)45)64-28-10(4-40)59-35(23(53)17(28)47)66-30-12(6-42)60-36(24(54)18(30)48)65-29-11(5-41)58-34(22(52)16(29)46)63-27-9(3-39)56-32(61-25)20(50)14(27)44/h7-54H,1-6H2/t7-,8-,9-,10-,11-,12-,13-,14-,15-,16-,17-,18-,19-,20-,21-,22-,23-,24-,25-,26-,27-,28-,29-,30-,31-,32-,33-,34-,35-,36-/m1/s1	-10.482	-10.482	1	1	1
100-18-5	100185	1296	**1,4-diisopropylbenzene**	3_REACH	Benzene, 1,4-bis(1-methylethyl)-	1,4-diisopropylbenzene	C12H18	C12H18	162.28	CC(C)c1ccc(cc1)C(C)C	InChI=1/C12H18/c1-9(2)11-5-7-12(8-6-11)10(3)4/h5-10H,1-4H3	4.218	4.218	1	1	1
100-20-9	100209	1297	**terephthaloyl dichloride**	3_REACH	1,4-Benzenedicarbonyl dichloride	terephthaloyl dichloride	C8H4Cl2O2	C8H4Cl2O2	203.02	ClC(=O)c1ccc(cc1)C(=O)Cl	InChI=1/C8H4Cl2O2/c9-7(11)5-1-2-6(4-3-5)8(10)12/h1-4H	2.242	2.242	1	1	1
100-21-0	100210	122	**terephthalic acid**	3_REACH	1,4-Benzenedicarboxylic acid	1,4-Benzenedicarboxylic acid	C8H6O4	C8H4O4	166.13	[O-]C(=O)c1ccc(cc1)C(=O)[O-]	InChI=1/C8H6O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H,(H,9,10)(H,11,12)/p-2	-1.859	-1.831	1	1	1
1003-52-7	1003527	1302	**4-methyloxazole-5-carbonitrile**	3_REACH		4-methyloxazole-5-carbonitrile		C5H4N2O	108.1	Cc1ncoc1C#N	InChI=1/C5H4N2O/c1-4-5(2-6)8-3-7-4/h3H,1H3	0.18	0.18	1	1	1
100-37-8	100378	123	**2-diethylaminoethanol**	3_REACH	Ethanol, 2-(diethylamino)-	2-(Diethylamino)ethanol	C6H15NO	C6H16NO	117.19	CC[NH+](CC)CCO	InChI=1/C6H15NO/c1-3-7(4-2)5-6-8/h8H,3-6H2,1-2H3/p+1	-1.083	-1.034	1	1	1
10042-59-8	10042598	1306	**2-propylheptan-1-ol**	3_REACH		2-propylheptan-1-ol		C10H22O	158.29	CCCCCC(CO)CCC	InChI=1/C10H22O/c1-3-5-6-8-10(9-11)7-4-2/h10-11H,3-9H2,1-2H3	3.57	3.57	1	1	1
100-46-9	100469	127	**benzylamine**	3_REACH	Benzylamine	Benzylamine	C7H9N	C7H10N	107.16	[NH3+]Cc1ccccc1	InChI=1/C7H9N/c8-6-7-4-2-1-3-5-7/h1-5H,6,8H2/p+1	-0.069	0.095	1	1	1
100-47-0	100470	128	**benzonitrile**	3_REACH	Benzonitrile	Benzonitrile	C7H5N	C7H5N	103.13	N#Cc1ccccc1	InChI=1/C7H5N/c8-6-7-4-2-1-3-5-7/h1-5H	1.708	1.708	1	1	1
100-51-6	100516	129	**benzyl alcohol**	3_REACH	Benzyl alcohol	Benzenemethanol	C7H8O	C7H8O	108.14	OCc1ccccc1	InChI=1/C7H8O/c8-6-7-4-2-1-3-5-7/h1-5,8H,6H2	1.225	1.225	1	1	1
100-52-7	100527	130	**benzaldehyde**	3_REACH	Benzaldehyde	Benzaldehyde	C7H6O	C7H6O	106.12	O=Cc1ccccc1	InChI=1/C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H	1.589	1.589	1	1	1
100-54-9	100549	131	**nicotinonitrile**	3_REACH	3-Pyridinecarbonitrile	3-Pyridinecarbonitrile	C6H4N2	C6H4N2	104.11	N#Cc1cccnc1	InChI=1/C6H4N2/c7-4-6-2-1-3-8-5-6/h1-3,5H	0.558	0.558	1	1	1
100-61-8	100618	133	**N-methylaniline**	3_REACH	Aniline, N-methyl-	N-Methylaniline	C7H9N	C7H9N	107.16	CNc1ccccc1	InChI=1/C7H9N/c1-8-7-5-3-2-4-6-7/h2-6,8H,1H3	1.638	1.638	1	1	1
100-63-0	100630	134	**phenylhydrazine**	3_REACH	Hydrazine, phenyl-	Phenylhydrazine	C6H8N2	C6H8N2	108.15	NNc1ccccc1	InChI=1/C6H8N2/c7-8-6-4-2-1-3-5-6/h1-5,8H,7H2	1.105	1.105	1	1	1
100-64-1	100641	135	**cyclohexanone oxime**	3_REACH	Cyclohexanone, oxime	Cyclohexanone, Oxime	C6H11NO	C6H11NO	113.16	ON=C1CCCCC1	InChI=1/C6H11NO/c8-7-6-4-2-1-3-5-6/h8H,1-5H2	1.381	1.381	1	1	1
100-69-6	100696	1309	**2-vinylpyridine**	3_REACH	Pyridine, 2-ethenyl-	2-vinylpyridine	C7H7N	C7H7N	105.14	C=Cc1ccccn1	InChI=1/C7H7N/c1-2-7-5-3-4-6-8-7/h2-6H,1H2	1.659	1.661	1	1	1
10081-67-1	10081671	1310	**4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline**	3_REACH		4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline		C30H31N	405.59	CC(C)(c1ccccc1)c2ccc(Nc3ccc(cc3)C(C)(C)c4ccccc4)cc2	InChI=1/C30H31N/c1-29(2,23-11-7-5-8-12-23)25-15-19-27(20-16-25)31-28-21-17-26(18-22-28)30(3,4)24-13-9-6-10-14-24/h5-22,31H,1-4H3	8.245	8.245	1	1	1
100-83-4	100834	138	**3-hydroxybenzaldehyde**	3_REACH	Benzaldehyde, 3-hydroxy-	3-Hydroxybenzaldehyde	C7H6O2	C7H6O2	122.12	Oc1cccc(C=O)c1	InChI=1/C7H6O2/c8-5-6-2-1-3-7(9)4-6/h1-5,9H	1.347	1.338	1	1	1
100-97-0	100970	2	**methenamine**	3_REACH	Hexamethylenetetramine	Hexamethylenetetramine	C6H12N4	C6H12N4	140.19	C1N2CN3CN(CN1C3)C2	InChI=1/C6H12N4/c1-7-2-9-4-8(1)5-10(3-7)6-9/h1-6H2	0.085	0.049	1	1	1
10097-02-6	10097026	4315	**2,2-bis(hydroxymethyl)butanoic acid**	3_REACH		2,2-bis(hydroxymethyl)butanoic acid			148.16	CCC(CO)(CO)C(=O)O	InChI=1S/C6H12O4/c1-2-6(3-7,4-8)5(9)10/h7-8H,2-4H2,1H3,(H,9,10)			1	1	1
101-02-0	101020	140	**triphenyl phosphite**	3_REACH	Phosphorous acid, triphenyl ester	Triphenyl ester, Phosphorous acid	C18H15O3P	C18H15O3P	310.29	O(P(Oc1ccccc1)Oc2ccccc2)c3ccccc3	InChI=1/C18H15O3P/c1-4-10-16(11-5-1)19-22(20-17-12-6-2-7-13-17)21-18-14-8-3-9-15-18/h1-15H	4.337	4.337	1	1	1
101-14-4	101144	1315	**4,4'-methylenebis[2-chloroaniline]**	3_REACH	Aniline), methylene bis-4,4'-(2-chloro-	4,4'-methylenebis[2-chloroaniline]	C13H12Cl2N2	C13H12Cl2N2	267.16	Nc1ccc(Cc2ccc(N)c(Cl)c2)cc1Cl	InChI=1/C13H12Cl2N2/c14-10-6-8(1-3-12(10)16)5-9-2-4-13(17)11(15)7-9/h1-4,6-7H,5,16-17H2	3.64	3.64	1	1	1
101-20-2	101202	143	**triclocarban**	3_REACH	3,4,4'-Trichloro carbanilide	Triclocarban	C13H9Cl3N2O	C13H9Cl3N2O	315.59	Clc1ccc(NC(=O)Nc2ccc(Cl)c(Cl)c2)cc1	InChI=1/C13H9Cl3N2O/c14-8-1-3-9(4-2-8)17-13(19)18-10-5-6-11(15)12(16)7-10/h1-7H,(H2,17,18,19)	4.516	4.516	1	1	1
101238-01-1	101238011	1317	**2,2,6,6-Tetramethylpiperidin-4-yl dodecanoate**	3_REACH		2,2,6,6-Tetramethylpiperidin-4-yl dodecanoate			339.57	CCCCCCCCCCCC(=O)OC1CC(NC(C1)(C)C)(C)C	InChI=1S/C21H41NO2/c1-6-7-8-9-10-11-12-13-14-15-19(23)24-18-16-20(2,3)22-21(4,5)17-18/h18,22H,6-17H2,1-5H3			1	1	1
101-37-1	101371	1318	**2,4,6-triallyloxy-1,3,5-triazine**	3_REACH	2,4,6-Triallyloxy-1,3,5-triazine	2,4,6-triallyloxy-1,3,5-triazine	C12H15N3O3	C12H15N3O3	249.27	C=CCOc1nc(OCC=C)nc(OCC=C)n1	InChI=1/C12H15N3O3/c1-4-7-16-10-13-11(17-8-5-2)15-12(14-10)18-9-6-3/h4-6H,1-3,7-9H2	3.309	3.309	1	1	1
1013-88-3	1013883	4621	**diphenylmethanimine**	3_REACH	Benzenemethanimine, α-phenyl-	Benzenemethanimine, a-phenyl-	C13H11N		181.24	C1=CC=C(C=C1)C(=N)C2=CC=CC=C2	InChI=1S/C13H11N/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,14H			1	1	1
101-39-3	101393	1320	**alpha-Methylcinnamaldehyde**	3_REACH	2-Propenal, 2-methyl-3-phenyl-	a-methylcinnamaldehyde	C10H10O	C10H10O	146.19	C\C(=C/c1ccccc1)\C=O	InChI=1/C10H10O/c1-9(8-11)7-10-5-3-2-4-6-10/h2-8H,1H3/b9-7+	2.395	2.395	1	1	1
101-41-7	101417	1321	**methyl phenylacetate**	3_REACH	Benzeneacetic acid, methyl ester	methyl phenylacetate	C9H10O2	C9H10O2	150.18	COC(=O)Cc1ccccc1	InChI=1/C9H10O2/c1-11-9(10)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3	1.72	1.72	1	1	1
101-43-9	101439	1322	**cyclohexyl methacrylate**	3_REACH	2-Propenoic acid, 2-methyl-, cyclohexyl ester	cyclohexyl methacrylate	C10H16O2	C10H16O2	168.24	CC(=C)C(=O)OC1CCCCC1	InChI=1/C10H16O2/c1-8(2)10(11)12-9-6-4-3-5-7-9/h9H,1,3-7H2,2H3	3.023	3.023	1	1	1
101-54-2	101542	1323	**N-(4-aminophenyl)aniline**	3_REACH	1,4-Benzenediamine, N-phenyl-	N-(4-aminophenyl)aniline	C12H12N2	C12H12N2	184.24	Nc1ccc(Nc2ccccc2)cc1	InChI=1/C12H12N2/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9,14H,13H2	2.633	2.633	1	1	1
101-68-8	101688	1325	**4,4'-methylenediphenyl diisocyanate**	3_REACH	Benzene, 1,1'-methylenebis[4-isocyanato-	4,4'-methylenediphenyl diisocyanate	C15H10N2O2	C15H10N2O2	250.26	O=C=Nc1ccc(Cc2ccc(cc2)N=C=O)cc1	InChI=1/C15H10N2O2/c18-10-16-14-5-1-12(2-6-14)9-13-3-7-15(8-4-13)17-11-19/h1-8H,9H2	3.525	3.525	1	1	1
1017183-70-8	1017183708	4503	**3-(4-fluorophenyl)-2-methylpropanoylchloride**	3_REACH		SOLE 3			200.64	CC(CC1=CC=C(C=C1)F)C(=O)Cl	InChI=1S/C10H10ClFO/c1-7(10(11)13)6-8-2-4-9(12)5-3-8/h2-5,7H,6H2,1H3			1	1	1
101-72-4	101724	1326	**N-isopropyl-N'-phenyl-p-phenylenediamine**	3_REACH	P-phenylenediamine, n-isopropyl-n-phenyl-	N-isopropyl-N'-phenyl-p-phenylenediamine	C15H18N2	C15H18N2	226.32	CC(C)Nc1ccc(Nc2ccccc2)cc1	InChI=1/C15H18N2/c1-12(2)16-14-8-10-15(11-9-14)17-13-6-4-3-5-7-13/h3-12,16-17H,1-2H3	3.915	3.485	1	1	1
101-77-9	101779	1328	**4,4'-methylenedianiline**	3_REACH	Benzenamine, 4,4'-methylenebis-	4,4'-methylenedianiline	C13H14N2	C13H14N2	198.27	Nc1ccc(Cc2ccc(N)cc2)cc1	InChI=1/C13H14N2/c14-12-5-1-10(2-6-12)9-11-3-7-13(15)8-4-11/h1-8H,9,14-15H2	2.311	2.308	1	1	1
101-80-4	101804	1329	**4,4'-oxydianiline**	3_REACH	Benzenamine, 4,4'-oxybis-	4,4'-oxydianiline	C12H12N2O	C12H12N2O	200.24	Nc1ccc(Oc2ccc(N)cc2)cc1	InChI=1/C12H12N2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H,13-14H2	1.897	1.889	1	1	1
101-84-8	101848	150	**diphenyl ether**	3_REACH	Diphenyl ether	1,1'-Oxybisbenzene	C12H10O	C12H10O	170.21	O(c1ccccc1)c2ccccc2	InChI=1/C12H10O/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10H	3.39	3.39	1	1	1
101-96-2	101962	1331	**N,N'-di-sec-butyl-p-phenylenediamine**	3_REACH	N,N'-Di-sec-butyl-p-phenylenediamine	N,N'-di-sec-butyl-p-phenylenediamine	C14H24N2	C14H24N2	220.36	CCC(C)Nc1ccc(NC(C)CC)cc1	InChI=1/C14H24N2/c1-5-11(3)15-13-7-9-14(10-8-13)16-12(4)6-2/h7-12,15-16H,5-6H2,1-4H3	3.947	3.917	1	1	1
102-01-2	102012	1334	**acetoacetanilide**	3_REACH	Butanamide, 3-oxo-N-phenyl-	acetoacetanilide	C10H11NO2	C10H11NO2	177.2	CC(=O)CC(=O)Nc1ccccc1	InChI=1/C10H11NO2/c1-8(12)7-10(13)11-9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,11,13)	0.861	0.861	1	1	1
102-06-7	102067	1335	**1,3-diphenylguanidine**	3_REACH	Guanidine, N,N'-diphenyl-	1,3-diphenylguanidine	C13H13N3	C13H14N3	211.27	N=C(Nc1ccccc1)[NH2+]c2ccccc2	InChI=1/C13H13N3/c14-13(15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H,(H3,14,15,16)/p+1	2.596	2.599	1	1	1
102-08-9	102089	151	**1,3-diphenyl-2-thiourea**	3_REACH		N,N'-Diphenylthiourea		C13H13N2S	228.32	S=C(Nc1ccccc1)[NH2+]c2ccccc2	InChI=1/C13H12N2S/c16-13(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10H,(H2,14,15,16)/p+1	3.913	3.908	1	1	1
102-09-0	102090	1336	**diphenyl carbonate**	3_REACH	Diphenyl carbonate	diphenyl carbonate	C13H10O3	C13H10O3	214.22	O=C(Oc1ccccc1)Oc2ccccc2	InChI=1/C13H10O3/c14-13(15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H	3.817	3.817	1	1	1
10233-13-3	10233133	1339	**isopropyl laurate**	3_REACH	Isopropyl laurate	isopropyl laurate	C15H30O2	C15H30O2	242.4	CCCCCCCCCCCC(=O)OC(C)C	InChI=1/C15H30O2/c1-4-5-6-7-8-9-10-11-12-13-15(16)17-14(2)3/h14H,4-13H2,1-3H3	5.52	5.52	1	1	1
102-36-3	102363	1341	**3,4-dichlorophenyl isocyanate**	3_REACH	Benzene, 1,2-dichloro-4-isocyanato-	3,4-dichlorophenyl isocyanate	C7H3Cl2NO	C7H3Cl2NO	188.01	Clc1ccc(cc1Cl)N=C=O	InChI=1/C7H3Cl2NO/c8-6-2-1-5(10-4-11)3-7(6)9/h1-3H	3.019	3.019	1	1	1
10254-57-6	10254576	1344	**4,4'-methylene bis(dibutyldithiocarbamate)**	3_REACH		4,4'-methylene bis(dibutyldithiocarbamate)		C19H38N2S4	422.79	CCCCN(CCCC)C(=S)SCSC(=S)N(CCCC)CCCC	InChI=1/C19H38N2S4/c1-5-9-13-20(14-10-6-2)18(22)24-17-25-19(23)21(15-11-7-3)16-12-8-4/h5-17H2,1-4H3	9.525	9.525	1	1	1
102-60-3	102603	1347	**1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol**	3_REACH		1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol		C14H33N2O4	292.42	CC(O)CN(CC[NH+](CC(C)O)CC(C)O)CC(C)O	InChI=1/C14H32N2O4/c1-11(17)7-15(8-12(2)18)5-6-16(9-13(3)19)10-14(4)20/h11-14,17-20H,5-10H2,1-4H3/p+1	-1.75	-1.538	1	1	1
102-69-2	102692	154	**tripropylamine**	3_REACH	1-Propanamine, N,N-dipropyl-	N,N-Dipropyl-1-propanamine	C9H21N	C9H22N	143.28	CCC[NH+](CCC)CCC	InChI=1/C9H21N/c1-4-7-10(8-5-2)9-6-3/h4-9H2,1-3H3/p+1	1.376	1.397	1	1	1
102-71-6	102716	155	**2,2',2''-nitrilotriethanol**	3_REACH	Triethanolamine	Triethanolamine	C6H15NO3	C6H16NO3	149.19	OCC[NH+](CCO)CCO	InChI=1/C6H15NO3/c8-4-1-7(2-5-9)3-6-10/h8-10H,1-6H2/p+1	-2.859	-1.855	1	1	1
102-76-1	102761	1352	**triacetin**	3_REACH	1,2,3-Propanetriol, triacetate	triacetin	C9H14O6	C9H14O6	218.21	CC(=O)OCC(COC(=O)C)OC(=O)C	InChI=1/C9H14O6/c1-6(10)13-4-9(15-8(3)12)5-14-7(2)11/h9H,4-5H2,1-3H3	-0.271	-0.271	1	1	1
102-77-2	102772	1353	**2-(morpholinothio)benzothiazole**	3_REACH	Morpholine, 4-(2-benzothiazolylthio)-	2-(morpholinothio)benzothiazole	C11H12N2OS2	C11H12N2OS2	252.36	C1CN(CCO1)Sc2nc3ccccc3s2	InChI=1/C11H12N2OS2/c1-2-4-10-9(3-1)12-11(15-10)16-13-5-7-14-8-6-13/h1-4H,5-8H2	2.399	2.399	1	1	1
102-81-8	102818	1354	**2-dibutylaminoethanol**	3_REACH	Ethanol, 2-(dibutylamino)-	2-dibutylaminoethanol	C10H23NO	C10H24NO	173.3	CCCC[NH+](CCO)CCCC	InChI=1/C10H23NO/c1-3-5-7-11(9-10-12)8-6-4-2/h12H,3-10H2,1-2H3/p+1	0.877	0.932	1	1	1
102-82-9	102829	156	**tributylamine**	3_REACH	Tributylamine	Tributylamine	C12H27N	C12H28N	185.36	CCCC[NH+](CCCC)CCCC	InChI=1/C12H27N/c1-4-7-10-13(11-8-5-2)12-9-6-3/h4-12H2,1-3H3/p+1	2.745	2.788	1	1	1
102985-93-3	102985933	4723	**2,2-dimethyl-3-oxopropyl dodecanoate**	3_REACH		2,2-dimethyl-3-oxopropyl dodecanoate			284.44	CCCCCCCCCCCC(=O)OCC(C)(C)C=O	InChI=1S/C17H32O3/c1-4-5-6-7-8-9-10-11-12-13-16(19)20-15-17(2,3)14-18/h14H,4-13,15H2,1-3H3			1	1	1
103-09-3	103093	1359	**2-ethylhexyl acetate**	3_REACH	Acetic acid, 2-ethylhexyl ester	2-ethylhexyl acetate	C10H20O2	C10H20O2	172.27	CCCCC(CC)COC(=O)C	InChI=1/C10H20O2/c1-4-6-7-10(5-2)8-12-9(3)11/h10H,4-8H2,1-3H3	3.037	3.037	1	1	1
103-11-7	103117	159	**2-ethylhexyl acrylate**	3_REACH	2-Propenoic acid, 2-ethylhexyl ester	2-Ethylhexyl acrylate	C11H20O2	C11H20O2	184.28	CCCCC(CC)COC(=O)C=C	InChI=1/C11H20O2/c1-4-7-8-10(5-2)9-13-11(12)6-3/h6,10H,3-5,7-9H2,1-2H3	3.735	3.735	1	1	1
103-23-1	103231	160	**bis(2-ethylhexyl) adipate**	3_REACH	Di(2-ethylhexyl)adipate	bis(2-Ethylhexyl)ester hexanedioic acid	C22H42O4	C22H42O4	370.57	CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC	InChI=1/C22H42O4/c1-5-9-13-19(7-3)17-25-21(23)15-11-12-16-22(24)26-18-20(8-4)14-10-6-2/h19-20H,5-18H2,1-4H3	7.037	7.037	1	1	1
103-26-4	103264	1362	**methyl cinnamate**	3_REACH	2-Propenoic acid, 3-phenyl-, methyl ester	methyl cinnamate	C10H10O2	C10H10O2	162.19	COC(=O)\C=C\c1ccccc1	InChI=1/C10H10O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7+	2.153	2.153	1	1	1
10326-41-7	10326417	161	**(R)-lactic acid**	3_REACH		(R)-lactic acid		C3H5O3	90.078	C[C@@H](O)C(=O)[O-]	InChI=1/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)/p-1/t2-/m1/s1	-1.867	-1.863	1	1	1
103-45-7	103457	1367	**phenethyl acetate**	3_REACH	Acetic acid, 2-phenylethyl ester	phenethyl acetate	C10H12O2	C10H12O2	164.2	CC(=O)OCCc1ccccc1	InChI=1/C10H12O2/c1-9(11)12-8-7-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3	1.925	1.925	1	1	1
103-49-1	103491	1368	**dibenzylamine**	3_REACH	Dibenzylamine	dibenzylamine	C14H15N	C14H16N	197.28	C([NH2+]Cc1ccccc1)c2ccccc2	InChI=1/C14H15N/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10,15H,11-12H2/p+1	1.72	2.048	1	1	1
103-50-4	103504	1369	**dibenzyl ether**	3_REACH	Benzene, 1,1'-[oxybis(methylene)]bis-	dibenzyl ether	C14H14O	C14H14O	198.26	C(OCc1ccccc1)c2ccccc2	InChI=1/C14H14O/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10H,11-12H2	3.217	3.217	1	1	1
103-60-6	103606	1374	**2-phenoxyethyl isobutyrate**	3_REACH	2-Phenoxyethyl isobutyrate	2-phenoxyethyl isobutyrate	C12H16O3	C12H16O3	208.26	CC(C)C(=O)OCCOc1ccccc1	InChI=1/C12H16O3/c1-10(2)12(13)15-9-8-14-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3	2.782	2.782	1	1	1
103694-68-4	103694684	4367	**Trimethylbenzenepropanol**	3_REACH		3-(2,2-dimethyl-3-hydroxypropyl)toluene			178.28	CC1=CC(=CC=C1)CC(C)(C)CO	InChI=1S/C12H18O/c1-10-5-4-6-11(7-10)8-12(2,3)9-13/h4-7,13H,8-9H2,1-3H3			1	1	1
103-69-5	103695	162	**N-ethylaniline**	3_REACH	Benzenamine, N-ethyl-	N-Ethylaniline	C8H11N	C8H11N	121.18	CCNc1ccccc1	InChI=1/C8H11N/c1-2-9-8-6-4-3-5-7-8/h3-7,9H,2H2,1H3	1.987	1.986	1	1	1
103-71-9	103719	1378	**phenyl isocyanate**	3_REACH	Benzene, isocyanato-	phenyl isocyanate	C7H5NO	C7H5NO	119.12	O=C=Nc1ccccc1	InChI=1/C7H5NO/c9-6-8-7-4-2-1-3-5-7/h1-5H	1.69	1.69	1	1	1
103-74-2	103742	163	**2-(2-pyridyl)ethanol**	3_REACH	2-Pyridineethanol	2-Pyridineethanol	C7H9NO	C7H9NO	123.16	OCCc1ccccn1	InChI=1/C7H9NO/c9-6-4-7-3-1-2-5-8-7/h1-3,5,9H,4,6H2	0.538	0.543	1	1	1
103-83-3	103833	164	**benzyldimethylamine**	3_REACH	Benzenemethanamine, N,N-	N,N-Dimethylbenzylamine	C9H13N	C9H14N	135.21	C[NH+](C)Cc1ccccc1	InChI=1/C9H13N/c1-10(2)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3/p+1	0.342	0.656	1	1	1
103-95-7	103957	1382	**3-p-cumenyl-2-methylpropionaldehyde**	3_REACH	3-(4-Isopropylphenyl)-2-methylpropionaldehyde	3-p-cumenyl-2-methylpropionaldehyde	C13H18O	C13H18O	190.29	CC(Cc1ccc(cc1)C(C)C)C=O	InChI=1/C13H18O/c1-10(2)13-6-4-12(5-7-13)8-11(3)9-14/h4-7,9-11H,8H2,1-3H3	3.629	3.629	1	1	1
10411-92-4	10411924	1383	**cis-4-tert-butylcyclohexyl acetate**	3_REACH	Cyclohexyl, 4-tert-butyl-, acetate (mostly cis-)	cis-4-tert-butylcyclohexyl acetate	C12H22O2	C12H22O2	198.31	CC(=O)O[C@@H]1CC[C@@H](CC1)C(C)(C)C	InChI=1/C12H22O2/c1-9(13)14-11-7-5-10(6-8-11)12(2,3)4/h10-11H,5-8H2,1-4H3/t10-,11+	3.045	3.045	1	1	1
10420-33-4	10420334	1387	**dimethyl acetylsuccinate**	3_REACH		dimethyl acetylsuccinate		C8H11O5	188.18	COC(=O)C[C-](C(=O)C)C(=O)OC	InChI=1/C8H11O5/c1-5(9)6(8(11)13-3)4-7(10)12-2/h4H2,1-3H3/q-1	-0.057	-0.06	1	1	1
104-23-4	104234	1388	**4'-aminoazobenzene-4-sulphonic acid**	3_REACH		4'-aminoazobenzene-4-sulphonic acid		C12H10N3O3S	277.31	Nc1ccc(cc1)N=Nc2ccc(cc2)S(=O)(=O)[O-]	InChI=1/C12H11N3O3S/c13-9-1-3-10(4-2-9)14-15-11-5-7-12(8-6-11)19(16,17)18/h1-8H,13H2,(H,16,17,18)/p-1/b15-14+	0.54	0.542	1	1	1
104-38-1	104381	1393	**2,2'-p-phenylenedioxydiethanol**	3_REACH		2,2'-p-phenylenedioxydiethanol		C10H14O4	198.22	OCCOc1ccc(OCCO)cc1	InChI=1/C10H14O4/c11-5-7-13-9-1-2-10(4-3-9)14-8-6-12/h1-4,11-12H,5-8H2	0.718	0.718	1	1	1
104468-21-5	104468215	4316	**2,2-dimethyl 3-methyl-3-butenyl propanoate**	3_REACH		2,2-dimethyl 3-methyl-3-butenyl propanoate			170.25	CC(=C)CCOC(=O)C(C)(C)C	InChI=1S/C10H18O2/c1-8(2)6-7-12-9(11)10(3,4)5/h1,6-7H2,2-5H3			1	1	1
104-55-2	104552	168	**cinnamaldehyde**	3_REACH	Cinnamylaldehyde	3-Phenyl-2-propenal	C9H8O	C9H8O	132.16	O=C\C=C\c1ccccc1	InChI=1/C9H8O/c10-8-4-7-9-5-2-1-3-6-9/h1-8H/b7-4+	1.949	1.949	1	1	1
104-61-0	104610	1395	**nonan-4-olide**	3_REACH	2(3H)-Furanone, dihydro-5-pentyl-	nonan-4-olide	C9H16O2	C9H16O2	156.22	CCCCCC1CCC(=O)O1	InChI=1/C9H16O2/c1-2-3-4-5-8-6-7-9(10)11-8/h8H,2-7H2,1H3	2.546	2.546	1	1	1
104-66-5	104665	1397	**1,2-diphenoxyethane**	3_REACH	Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-	1,2-diphenoxyethane	C14H14O2	C14H14O2	214.26	C(COc1ccccc1)Oc2ccccc2	InChI=1/C14H14O2/c1-3-7-13(8-4-1)15-11-12-16-14-9-5-2-6-10-14/h1-10H,11-12H2	3.445	3.445	1	1	1
104-67-6	104676	1398	**undecan-4-olide**	3_REACH	2(3H)-Furanone, 5-heptyldihydro-	undecan-4-olide	C11H20O2	C11H20O2	184.28	CCCCCCCC1CCC(=O)O1	InChI=1/C11H20O2/c1-2-3-4-5-6-7-10-8-9-11(12)13-10/h10H,2-9H2,1H3	3.458	3.458	1	1	1
104-68-7	104687	1399	**2-(2-phenoxyethoxy)ethanol**	3_REACH		2-(2-phenoxyethoxy)ethanol		C10H14O3	182.22	OCCOCCOc1ccccc1	InChI=1/C10H14O3/c11-6-7-12-8-9-13-10-4-2-1-3-5-10/h1-5,11H,6-9H2	1.143	1.143	1	1	1
1047-16-1	1047161	1400	**5,12-dihydroquino[2,3-b]acridine-7,14-dione**	3_REACH		5,12-dihydroquino[2,3-b]acridine-7,14-dione		C20H10N2O2	312.33	[O-]c1c2ccccc2nc3cc4c([O-])c5ccccc5nc4cc13	InChI=1/C20H12N2O2/c23-19-11-5-1-3-7-15(11)21-17-10-18-14(9-13(17)19)22-16-8-4-2-6-12(16)20(14)24/h1-10H,(H,21,23)(H,22,24)/p-2	2.985	3.945	1	1	1
104-75-6	104756	169	**2-ethylhexylamine**	3_REACH	1-Hexanamine, 2-ethyl-	2-Ethylhexyl amine	C8H19N	C8H20N	129.25	CCCCC(CC)C[NH3+]	InChI=1/C8H19N/c1-3-5-6-8(4-2)7-9/h8H,3-7,9H2,1-2H3/p+1	1.364	1.364	1	1	1
104-76-7	104767	170	**2-ethylhexan-1-ol**	3_REACH	1-Hexanol, 2-ethyl-	2-Ethylhexanol	C8H18O	C8H18O	144.26	CCCCC(CC)CO	InChI=1/C8H18O/c1-3-5-6-8(4-2)7-9/h8-9H,3-7H2,1-2H3	2.658	2.658	1	1	1
104-88-1	104881	171	**4-chlorobenzaldehyde**	3_REACH	Benzaldehyde, 4-chloro-	4-Chlorobenzaldehyde	C7H5ClO	C7H5ClO	140.57	Clc1ccc(C=O)cc1	InChI=1/C7H5ClO/c8-7-3-1-6(5-9)2-4-7/h1-5H	2.253	2.253	1	1	1
104-90-5	104905	172	**5-ethyl-2-methylpyridine**	3_REACH	Pyridine, 5-ethyl-2-methyl-	5-Ethyl-2-methylpyridine	C8H11N	C8H11N	121.18	CCc1ccc(C)nc1	InChI=1/C8H11N/c1-3-8-5-4-7(2)9-6-8/h4-6H,3H2,1-2H3	1.904	1.976	1	1	1
104-93-8	104938	1403	**4-methylanisole**	3_REACH	Benzene, 1-methoxy-4-methyl-	4-methylanisole	C8H10O	C8H10O	122.17	COc1ccc(C)cc1	InChI=1/C8H10O/c1-7-3-5-8(9-2)6-4-7/h3-6H,1-2H3	2.299	2.299	1	1	1
105-05-5	105055	1405	**1,4-diethylbenzene**	3_REACH	Benzene, 1,4-diethyl-	1,4-diethylbenzene	C10H14	C10H14	134.22	CCc1ccc(CC)cc1	InChI=1/C10H14/c1-3-9-5-7-10(4-2)8-6-9/h5-8H,3-4H2,1-2H3	3.714	3.714	1	1	1
10543-57-4	10543574	175	**N,N'-ethylenebis[N-acetylacetamide]**	3_REACH	N,N,N',N'-Tetraacetylethylenediamine	N,N'-1,2-Ethanediylbis N-acetylacetamide	C10H16N2O4	C10H16N2O4	228.25	CC(=O)N(CCN(C(=O)C)C(=O)C)C(=O)C	InChI=1/C10H16N2O4/c1-7(13)11(8(2)14)5-6-12(9(3)15)10(4)16/h5-6H2,1-4H3	-1.454	-1.454	1	1	1
105-53-3	105533	177	**diethyl malonate**	3_REACH	Propanedioic acid, diethyl ester	Propanedioic acid, Diethyl ester	C7H12O4	C7H11O4	160.17	CCOC(=O)[CH-]C(=O)OCC	InChI=1/C7H12O4/c1-3-10-6(8)5-7(9)11-4-2/h5H,3-4H2,1-2H3/q-1	1.243	1.238	1	1	1
105-55-5	105555	178	**1,3-diethyl-2-thiourea**	3_REACH	Diethyl-2-thiourea	1,3-Diethylthiourea	C5H12N2S	C5H12N2S	132.23	CCNC(=S)NCC	InChI=1/C5H12N2S/c1-3-6-5(8)7-4-2/h3-4H2,1-2H3,(H2,6,7,8)	1.355	1.355	1	1	1
105-56-6	105566	1415	**ethyl cyanoacetate**	3_REACH	Acetic acid, cyano-, ethyl ester	ethyl cyanoacetate	C5H7NO2	C5H7NO2	113.12	CCOC(=O)CC#N	InChI=1/C5H7NO2/c1-2-8-5(7)3-4-6/h2-3H2,1H3	0.429	0.429	1	1	1
105-59-9	105599	1416	**2,2'-methyliminodiethanol**	3_REACH	Methyldiethanolamine	2,2'-methyliminodiethanol	C5H13NO2	C5H14NO2	119.17	C[NH+](CCO)CCO	InChI=1/C5H13NO2/c1-6(2-4-7)3-5-8/h7-8H,2-5H2,1H3/p+1	-2.32	-1.777	1	1	1
105-60-2	105602	180	**Caprolactam**	3_REACH	Caprolactam	Hexahydro-2H-azepin-2-one	C6H11NO	C6H11NO	113.16	O=C1CCCCCN1	InChI=1/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)	0.541	0.541	1	1	1
10563-26-5	10563265	1417	**N,N'-bis(3-aminopropyl)ethylenediamine**	3_REACH		N,N'-bis(3-aminopropyl)ethylenediamine		C8H25N4	174.3	[NH3+]CCCNCC[NH2+]CCC[NH3+]	InChI=1/C8H22N4/c9-3-1-5-11-7-8-12-6-2-4-10/h11-12H,1-10H2/p+3	-5.387	-3.803	1	1	1
10563-29-8	10563298	1418	**N'-(3-aminopropyl)-N,N-dimethylpropane-1,3-diamine**	3_REACH		N'-(3-aminopropyl)-N,N-dimethylpropane-1,3-diamine		C8H23N3	159.28	CN(C)CCC[NH2+]CCC[NH3+]	InChI=1/C8H21N3/c1-11(2)8-4-7-10-6-3-5-9/h10H,3-9H2,1-2H3/p+2	-3.017	-3.059	1	1	1
105-67-9	105679	181	**2,4-xylenol**	3_REACH	Phenol, 2,4-dimethyl-	2,4-Dimethylphenol	C8H10O	C8H10O	122.17	Cc1ccc(O)c(C)c1	InChI=1/C8H10O/c1-6-3-4-8(9)7(2)5-6/h3-5,9H,1-2H3	2.56	2.56	1	1	1
105-75-9	105759	182	**dibutyl fumarate**	3_REACH	2-Butenedioic acid (e), dibutyl ester	(E)-2-Butenedioic acid, Dibutyl ester	C12H20O4	C12H20O4	228.29	CCCCOC(=O)\C=C\C(=O)OCCCC	InChI=1/C12H20O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h7-8H,3-6,9-10H2,1-2H3/b8-7+	3.147	3.147	1	1	1
105-76-0	105760	183	**dibutyl maleate**	3_REACH	2-Butenedioic acid (Z)-, dibutyl ester	Dibutyl maleate	C12H20O4	C12H20O4	228.29	CCCCOC(=O)\C=C/C(=O)OCCCC	InChI=1/C12H20O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h7-8H,3-6,9-10H2,1-2H3/b8-7-	3.147	3.147	1	1	1
105812-81-5	105812815	4223	**(-)-trans-4-(4'-fluorophenyl)-3-hydroxymethyl-N-methylpiperidine**	3_REACH		(-)-trans-4-(4'-fluorophenyl)-3-hydroxymethyl-N-methylpiperidine			223.29	CN1CCC(C(C1)CO)C2=CC=C(C=C2)F	InChI=1S/C13H18FNO/c1-15-7-6-13(11(8-15)9-16)10-2-4-12(14)5-3-10/h2-5,11,13,16H,6-9H2,1H3/t11-,13-/m0/s1			1	1	1
105827-91-6	105827916	4348	**2-chloro-5-chloromethylthiazole**	3_REACH		2-chloro-5-chloromethylthiazole			168.05	C1=C(SC(=N1)Cl)CCl	InChI=1S/C4H3Cl2NS/c5-1-3-2-7-4(6)8-3/h2H,1H2			1	1	1
105-83-9	105839	1420	**N,N-bis(3-aminopropyl)methylamine**	3_REACH	1,3-Propanediamine, N-(3-aminopropyl)-N-methyl-	N,N-bis(3-aminopropyl)methylamine	C7H19N3	C7H22N3	145.25	C[NH+](CCC[NH3+])CCC[NH3+]	InChI=1/C7H19N3/c1-10(6-2-4-8)7-3-5-9/h2-9H2,1H3/p+3	-4.784	-3.952	1	1	1
105-95-3	105953	1422	**1,4-dioxacycloheptadecane-5,17-dione**	3_REACH	Ethylene brassylate	1,4-dioxacycloheptadecane-5,17-dione	C15H26O4	C15H26O4	270.37	O=C1CCCCCCCCCCCC(=O)OCCO1	InChI=1/C15H26O4/c16-14-10-8-6-4-2-1-3-5-7-9-11-15(17)19-13-12-18-14/h1-13H2	4.016	4.016	1	1	1
105-99-7	105997	184	**dibutyl adipate**	3_REACH	Hexanedioic acid, dibutyl ester	Dibutyl adipate	C14H26O4	C14H26O4	258.36	CCCCOC(=O)CCCCC(=O)OCCCC	InChI=1/C14H26O4/c1-3-5-11-17-13(15)9-7-8-10-14(16)18-12-6-4-2/h3-12H2,1-2H3	3.661	3.661	1	1	1
106-02-5	106025	1425	**pentadecan-15-olide**	3_REACH	Oxacyclohexadecan-2-one	pentadecan-15-olide	C15H28O2	C15H28O2	240.39	O=C1CCCCCCCCCCCCCCO1	InChI=1/C15H28O2/c16-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-17-15/h1-14H2	5.294	5.294	1	1	1
106-20-7	106207	1430	**bis(2-ethylhexyl)amine**	3_REACH	1-Hexanamine, 2-ethyl-N-(2-ethylhexyl)-	bis(2-ethylhexyl)amine	C16H35N	C16H36N	241.46	CCCCC(CC)C[NH2+]CC(CC)CCCC	InChI=1/C16H35N/c1-5-9-11-15(7-3)13-17-14-16(8-4)12-10-6-2/h15-17H,5-14H2,1-4H3/p+1	4.586	4.588	1	1	1
106-21-8	106218	1431	**3,7-dimethyloctan-1-ol**	3_REACH	3,7-Dimethyl-1-octanol	3,7-dimethyloctan-1-ol	C10H22O	C10H22O	158.29	CC(C)CCCC(C)CCO	InChI=1/C10H22O/c1-9(2)5-4-6-10(3)7-8-11/h9-11H,4-8H2,1-3H3	3.299	3.299	1	1	1
106-22-9	106229	185	**citronellol**	3_REACH	6-Octen-1-ol, 3,7-dimethyl-	3,7-Dimethyl-6-octen-1-ol	C10H20O	C10H20O	156.27	CC(CCO)CCC=C(C)C	InChI=1/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h5,10-11H,4,6-8H2,1-3H3	3.049	3.049	1	1	1
106-23-0	106230	1432	**citronellal**	3_REACH	6-Octenal, 3,7-dimethyl-	citronellal	C10H18O	C10H18O	154.25	CC(CCC=C(C)C)CC=O	InChI=1/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,8,10H,4,6-7H2,1-3H3	3.018	3.018	1	1	1
106-24-1	106241	186	**geraniol**	3_REACH	2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-	(2E)-3,7-Dimethyl-2,6-octadien-1-ol	C10H18O	C10H18O	154.25	CC(=CCC\C(=C\CO)\C)C	InChI=1/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,7,11H,4,6,8H2,1-3H3/b10-7+	2.934	2.934	1	1	1
106-25-2	106252	187	**nerol**	3_REACH	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	nerol	C10H18O	C10H18O	154.25	CC(=CCC\C(=C/CO)\C)C	InChI=1/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,7,11H,4,6,8H2,1-3H3/b10-7-	2.934	2.934	1	1	1
106-26-3	106263	1433	**(Z)-3,7-dimethylocta-2,6-dienal**	3_REACH	β-Citral	(Z)-3,7-dimethylocta-2,6-dienal	C10H16O	C10H16O	152.24	CC(=CCC\C(=C/C=O)\C)C	InChI=1/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5,7-8H,4,6H2,1-3H3/b10-7-	3.19	3.19	1	1	1
106-43-4	106434	190	**4-chlorotoluene**	3_REACH	Benzene, 1-chloro-4-methyl-	1-Chloro-4-methylbenzene	C7H7Cl	C7H7Cl	126.59	Cc1ccc(Cl)cc1	InChI=1/C7H7Cl/c1-6-2-4-7(8)5-3-6/h2-5H,1H3	2.98	2.98	1	1	1
106-44-5	106445	191	**p-cresol**	3_REACH	Phenol, 4-methyl-	4-Methylphenol	C7H8O	C7H8O	108.14	Cc1ccc(O)cc1	InChI=1/C7H8O/c1-6-2-4-7(8)5-3-6/h2-5,8H,1H3	2.074	2.073	1	1	1
106461-41-0	106461410	4581	**2,4-dihydro-4-(4-(4-(4-hydroxyphenyl)-1-piperazinyl)phenyl)-2-(1-methylpropyl)-3H-1,2,4-triazol-3-one**	3_REACH		3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-[4-[4-(4-hydroxyphenyl)-1-piperazinyl]phenyl]-2-(1-methylpropyl)-			393.5	CCC(C)N1C(=O)N(C=N1)C2=CC=C(C=C2)N3CCN(CC3)C4=CC=C(C=C4)O	InChI=1S/C22H27N5O2/c1-3-17(2)27-22(29)26(16-23-27)20-6-4-18(5-7-20)24-12-14-25(15-13-24)19-8-10-21(28)11-9-19/			1	1	1
106-46-7	106467	192	**1,4-dichlorobenzene**	3_REACH	Benzene, 1,4-dichloro-	1,4-Dichlorobenzene	C6H4Cl2	C6H4Cl2	147	Clc1ccc(Cl)cc1	InChI=1/C6H4Cl2/c7-5-1-2-6(8)4-3-5/h1-4H	3.158	3.158	1	1	1
106-47-8	106478	193	**4-chloroaniline**	3_REACH	p-Chloroaniline	4-Chloroaniline	C6H6ClN	C6H6ClN	127.58	Nc1ccc(Cl)cc1	InChI=1/C6H6ClN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2	1.747	1.747	1	1	1
106-48-9	106489	194	**4-chlorophenol**	3_REACH	p-Chlorophenol	4-Chlorophenol	C6H5ClO	C6H5ClO	128.56	Oc1ccc(Cl)cc1	InChI=1/C6H5ClO/c7-5-1-3-6(8)4-2-5/h1-4,8H	2.252	2.248	1	1	1
106-49-0	106490	195	**p-toluidine**	3_REACH	p-Toluidine	p-Toluidine	C7H9N	C7H9N	107.16	Cc1ccc(N)cc1	InChI=1/C7H9N/c1-6-2-4-7(8)5-3-6/h2-5H,8H2,1H3	1.569	1.569	1	1	1
106-50-3	106503	196	**p-phenylenediamine**	3_REACH	1,4-Benzenediamine	p-Phenylenediamine	C6H8N2	C6H8N2	108.15	Nc1ccc(N)cc1	InChI=1/C6H8N2/c7-5-1-2-6(8)4-3-5/h1-4H,7-8H2	0.336	0.277	1	1	1
106-51-4	106514	197	**p-benzoquinone**	3_REACH	p-Benzoquinone	Quinone	C6H4O2	C6H4O2	108.1	O=C1C=CC(=O)C=C1	InChI=1/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H	0.687	0.687	1	1	1
1067-33-0	1067330	199	**dibutyltin di(acetate)**	3_REACH	Dibutyltin diacetate	Bis(acetyloxy)dibutylstannane	C12H24O4Sn	C8H18Sn	351.01	CCCC[Sn+2]CCCC	InChI=1/2C4H9.Sn/c2*1-3-4-2;/h2*1,3-4H2,2H3;/q;;+2	3.548	3.548	1	1	1
106-79-6	106796	1446	**dimethyl sebacate**	3_REACH	Decanedioic acid, dimethyl ester	dimethyl sebacate	C12H22O4	C12H22O4	230.3	COC(=O)CCCCCCCCC(=O)OC	InChI=1/C12H22O4/c1-15-11(13)9-7-5-3-4-6-8-10-12(14)16-2/h3-10H2,1-2H3	2.829	2.829	1	1	1
106797-53-9	106797539	4354	**2-hydroxy-4'-hydroxyethoxy-2-methylpropiophenone**	3_REACH		2-hydroxy-4'-hydroxyethoxy-2-methylpropiophenone			224.26	CC(C)(C(=O)C1=CC=C(C=C1)OCCO)O	InChI=1S/C12H16O4/c1-12(2,15)11(14)9-3-5-10(6-4-9)16-8-7-13/h3-6,13,15H,7-8H2,1-2H3			1	1	1
106-91-2	106912	1449	**2,3-epoxypropyl methacrylate**	3_REACH	2-Propenoic acid, 2-methyl-, oxiranylmethyl ester	2,3-epoxypropyl methacrylate	C7H10O3	C7H10O3	142.15	CC(=C)C(=O)OCC1CO1	InChI=1/C7H10O3/c1-5(2)7(8)10-4-6-3-9-6/h6H,1,3-4H2,2H3	0.881	0.881	1	1	1
1071-22-3	1071223	1455	**3-(trichlorosilyl)propiononitrile**	3_REACH	β-Trichlorosilylpropionitrile	3-(trichlorosilyl)propiononitrile	C3H4Cl3NSi	C3H4Cl3NSi	188.52	Cl[Si](Cl)(Cl)CCC#N	InChI=1/C3H4Cl3NSi/c4-8(5,6)3-1-2-7/h1,3H2	3.056	3.056	1	1	1
1072-63-5	1072635	1457	**1-vinylimidazole**	3_REACH	N-Vinylimidazole	1-vinylimidazole	C5H6N2	C5H6N2	94.119	C=Cn1ccnc1	InChI=1/C5H6N2/c1-2-7-4-3-6-5-7/h2-5H,1H2	0.007	0.643	1	1	1
1073-69-4	1073694	1461	**(4-chlorophenyl)hydrazine**	3_REACH		(4-chlorophenyl)hydrazine		C6H7ClN2	142.59	NNc1ccc(Cl)cc1	InChI=1/C6H7ClN2/c7-5-1-3-6(9-8)4-2-5/h1-4,9H,8H2	1.77	1.77	1	1	1
107-41-5	107415	219	**2-methylpentane-2,4-diol**	3_REACH	2,4-Pentanediol, 2-methyl-	2-Methyl-2,4-pentanediol	C6H14O2	C6H14O2	118.18	CC(O)CC(C)(C)O	InChI=1/C6H14O2/c1-5(7)4-6(2,3)8/h5,7-8H,4H2,1-3H3	0.124	0.124	1	1	1
107-56-2	107562	1465	**O,O-diisopropyl hydrogen dithiophosphate**	3_REACH		O,O-diisopropyl hydrogen dithiophosphate		C6H15O2PS2	214.29	CC(C)OP(=S)(S)OC(C)C	InChI=1/C6H15O2PS2/c1-5(2)7-9(10,11)8-6(3)4/h5-6H,1-4H3,(H,10,11)	2.563	2.563	1	1	1
107-58-4	107584	1466	**N-tert-butylacrylamide**	3_REACH	2-Propenamide, N-(1,1-dimethylethyl)-	N-tert-butylacrylamide	C7H13NO	C7H13NO	127.19	CC(C)(C)NC(=O)C=C	InChI=1/C7H13NO/c1-5-6(9)8-7(2,3)4/h5H,1H2,2-4H3,(H,8,9)	1.002	1.002	1	1	1
107-66-4	107664	1467	**dibutyl hydrogen phosphate**	3_REACH		dibutyl hydrogen phosphate		C8H18O4P	210.21	CCCCOP(=O)([O-])OCCCC	InChI=1/C8H19O4P/c1-3-5-7-11-13(9,10)12-8-6-4-2/h3-8H2,1-2H3,(H,9,10)/p-1	0.793	0.796	1	1	1
107737-97-3	107737973	4619	**2,2-Dimethyl-3-(3-methylphenyl)propanal**	3_REACH		Benzenepropanal, a,a,3-trimethyl-			176.26	CC1=CC(=CC=C1)CC(C)(C)C=O	InChI=1S/C12H16O/c1-10-5-4-6-11(7-10)8-12(2,3)9-13/h4-7,9H,8H2,1-3H3			1	1	1
107-75-5	107755	1468	**7-hydroxycitronellal**	3_REACH	Hydroxycitronellal	7-hydroxycitronellal	C10H20O2	C10H20O2	172.27	CC(CCCC(C)(C)O)CC=O	InChI=1/C10H20O2/c1-9(6-8-11)5-4-7-10(2,3)12/h8-9,12H,4-7H2,1-3H3	1.917	1.917	1	1	1
107-88-0	107880	1470	**butane-1,3-diol**	3_REACH	1,3-Butanediol	butane-1,3-diol	C4H10O2	C4H10O2	90.122	CC(O)CCO	InChI=1/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3	-0.458	-0.458	1	1	1
107898-54-4	107898544	4225	**Supersantol**	3_REACH		(+/-) trans-3,3-dimethyl-5-(2,2,3-trimethyl-cyclopent-3-en-1-yl)pent-4-en-2-ol			222.37	CC1=CCC(C1(C)C)C=CC(C)(C)C(C)O	InChI=1S/C15H26O/c1-11-7-8-13(15(11,5)6)9-10-14(3,4)12(2)16/h7,9-10,12-13,16H,8H2,1-6H3			1	1	1
107-92-6	107926	224	**butyric acid**	3_REACH	Butanoic acid	Butanoic acid	C4H8O2	C4H7O2	88.106	CCCC(=O)[O-]	InChI=1/C4H8O2/c1-2-3-4(5)6/h2-3H2,1H3,(H,5,6)/p-1	-0.556	-0.524	1	1	1
107-93-7	107937	225	**trans-crotonic acid**	3_REACH	Crotonic acid	(E)-2-Butenoic acid	C4H6O2	C4H5O2	86.09	C\C=C\C(=O)[O-]	InChI=1/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/p-1/b3-2+	-0.579	-0.561	1	1	1
107-96-0	107960	1473	**3-mercaptopropionic acid**	3_REACH	3-Thiolpropanoic acid	3-mercaptopropionic acid	C3H6O2S	C3H5O2S	106.14	[O-]C(=O)CCS	InChI=1/C3H6O2S/c4-3(5)1-2-6/h6H,1-2H2,(H,4,5)/p-1	-1.132	-1.121	1	1	1
108-39-4	108394	237	**m-cresol**	3_REACH	Phenol, 3-methyl-	3-Methylphenol	C7H8O	C7H8O	108.14	Cc1cccc(O)c1	InChI=1/C7H8O/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H3	2.074	2.073	1	1	1
108-42-9	108429	238	**3-chloroaniline**	3_REACH	m-Chloroaniline	3-Chloroaniline	C6H6ClN	C6H6ClN	127.58	Nc1cccc(Cl)c1	InChI=1/C6H6ClN/c7-5-2-1-3-6(8)4-5/h1-4H,8H2	1.747	1.747	1	1	1
108-44-1	108441	239	**m-toluidine**	3_REACH	Benzenamine, 3-methyl-	m-Toluidine	C7H9N	C7H9N	107.16	Cc1cccc(N)c1	InChI=1/C7H9N/c1-6-3-2-4-7(8)5-6/h2-5H,8H2,1H3	1.569	1.568	1	1	1
108-45-2	108452	1484	**m-phenylenediamine**	3_REACH	1,3-Benzenediamine	m-phenylenediamine	C6H8N2	C6H8N2	108.15	Nc1cccc(N)c1	InChI=1/C6H8N2/c7-5-2-1-3-6(8)4-5/h1-4H,7-8H2	0.336	0.333	1	1	1
108-46-3	108463	240	**resorcinol**	3_REACH	Resorcinol	1,3-Benzenediol	C6H6O2	C6H6O2	110.11	Oc1cccc(O)c1	InChI=1/C6H6O2/c7-5-2-1-3-6(8)4-5/h1-4,7-8H	1.346	1.333	1	1	1
108-67-8	108678	242	**mesitylene**	3_REACH	Benzene, 1,3,5-trimethyl-	Mesitylene	C9H12	C9H12	120.19	Cc1cc(C)cc(C)c1	InChI=1/C9H12/c1-7-4-8(2)6-9(3)5-7/h4-6H,1-3H3	3.288	3.288	1	1	1
108-68-9	108689	243	**3,5-xylenol**	3_REACH	Phenol, 3,5-dimethyl-	3,5-Dimethylphenol	C8H10O	C8H10O	122.17	Cc1cc(C)cc(O)c1	InChI=1/C8H10O/c1-6-3-7(2)5-8(9)4-6/h3-5,9H,1-2H3	2.56	2.559	1	1	1
108-69-0	108690	244	**3,5-xylidine**	3_REACH	Benzenamine, 3,5-dimethyl-	3,5-Xylidine	C8H11N	C8H11N	121.18	Cc1cc(C)cc(N)c1	InChI=1/C8H11N/c1-6-3-7(2)5-8(9)4-6/h3-5H,9H2,1-2H3	2.055	2.054	1	1	1
108-78-1	108781	4	**melamine**	3_REACH	1,3,5-Triazine-2,4,6-triamine	melamine	C3H6N6	C3H6N6	126.13	Nc1nc(N)nc(N)n1	InChI=1/C3H6N6/c4-1-7-2(5)9-3(6)8-1/h(H6,4,5,6,7,8,9)	-0.732	-0.733	1	1	1
108-80-5	108805	245	**cyanuric acid**	3_REACH	1,3,5-Triazine-2,4,6(1H,3H,5H)-	Isocyanuric acid	C3H3N3O3	C3HN3O3	129.08	O=C1NC(=O)[N-]C(=O)[N-]1	InChI=1/C3H3N3O3/c7-1-4-2(8)6-3(9)5-1/h(H3,4,5,6,7,8,9)/p-2	-0.453	-0.442	1	1	1
108-83-8	108838	1490	**2,6-dimethylheptan-4-one**	3_REACH	4-Heptanone, 2,6-dimethyl-	2,6-dimethylheptan-4-one	C9H18O	C9H18O	142.24	CC(C)CC(=O)CC(C)C	InChI=1/C9H18O/c1-7(2)5-9(10)6-8(3)4/h7-8H,5-6H2,1-4H3	2.645	2.645	1	1	1
108-93-0	108930	250	**cyclohexanol**	3_REACH	Cyclohexanol	Cyclohexanol	C6H12O	C6H12O	100.16	OC1CCCCC1	InChI=1/C6H12O/c7-6-4-2-1-3-5-6/h6-7H,1-5H2	1.5	1.5	1	1	1
108-95-2	108952	252	**phenol**	3_REACH	Phenol	Phenol	C6H6O	C6H6O	94.113	Oc1ccccc1	InChI=1/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H	1.588	1.587	1	1	1
108-98-5	108985	1491	**benzenethiol**	3_REACH	Benzenethiol	benzenethiol	C6H6S	C6H5S	110.18	[S-]c1ccccc1	InChI=1/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H/p-1	2.269	2.261	1	1	1
109-13-7	109137	1494	**tert-butyl peroxyisobutyrate**	3_REACH		tert-butyl peroxyisobutyrate		C8H16O3	160.21	CC(C)C(=O)OOC(C)(C)C	InChI=1/C8H16O3/c1-6(2)7(9)10-11-8(3,4)5/h6H,1-5H3	1.741	1.741	1	1	1
109-16-0	109160	1495	**2,2'-ethylenedioxydiethyl dimethacrylate**	3_REACH	2-Propenoic acid, 2-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl)	2,2'-ethylenedioxydiethyl dimethacrylate	C14H22O6	C14H22O6	286.32	CC(=C)C(=O)OCCOCCOCCOC(=O)C(=C)C	InChI=1/C14H22O6/c1-11(2)13(15)19-9-7-17-5-6-18-8-10-20-14(16)12(3)4/h1,3,5-10H2,2,4H3	1.887	1.887	1	1	1
109-52-4	109524	256	**valeric acid**	3_REACH	Pentanoic acid	Pentanoic acid	C5H10O2	C5H9O2	102.13	CCCCC(=O)[O-]	InChI=1/C5H10O2/c1-2-3-4-5(6)7/h2-4H2,1H3,(H,6,7)/p-1	-0.1	-0.065	1	1	1
109-77-3	109773	266	**malononitrile**	3_REACH	Malononitrile	Malononitrile	C3H2N2	C3H2N2	66.065	N#CCC#N	InChI=1/C3H2N2/c4-2-1-3-5/h1H2	0.104	0.104	1	1	1
110-15-6	110156	274	**succinic acid**	3_REACH	Butanedioic acid	Succinic acid	C4H6O4	C4H4O4	118.09	[O-]C(=O)CCC(=O)[O-]	InChI=1/C4H6O4/c5-3(6)1-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)/p-2	-3.308	-3.031	1	1	1
110-16-7	110167	275	**maleic acid**	3_REACH	2-Butenedioic acid (Z)-	Maleic acid	C4H4O4	C4H2O4	116.07	[O-]C(=O)\C=C/C(=O)[O-]	InChI=1/C4H4O4/c5-3(6)1-2-4(7)8/h1-2H,(H,5,6)(H,7,8)/p-2/b2-1-	-2.91	-2.71	1	1	1
110-25-8	110258	1515	**(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine**	3_REACH		(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine		C21H38NO3	353.55	CCCCCCCC\C=C/CCCCCCCC(=O)N(C)CC(=O)[O-]	InChI=1/C21H39NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20(23)22(2)19-21(24)25/h10-11H,3-9,12-19H2,1-2H3,(H,24,25)/p-1/b11-10-	4.652	4.661	1	1	1
110-41-8	110418	1519	**2-methylundecanal**	3_REACH	Undecanal, 2-methyl-	2-methylundecanal	C12H24O	C12H24O	184.32	CCCCCCCCCC(C)C=O	InChI=1/C12H24O/c1-3-4-5-6-7-8-9-10-12(2)11-13/h11-12H,3-10H2,1-2H3	4.596	4.596	1	1	1
110-42-9	110429	1520	**methyl decanoate**	3_REACH	Decanoic acid, methyl ester	methyl decanoate	C11H22O2	C11H22O2	186.29	CCCCCCCCCC(=O)OC	InChI=1/C11H22O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-10H2,1-2H3	3.881	3.881	1	1	1
110-44-1	110441	1521	**hexa-2,4-dienoic acid**	3_REACH	2,4-Hexadienoic acid, (E,E)-	hexa-2,4-dienoic acid	C6H8O2	C6H7O2	112.13	CC=CC=CC(=O)[O-]	InChI=1/C6H8O2/c1-2-3-4-5-6(7)8/h2-5H,1H3,(H,7,8)/p-1	-0.111	-0.09	1	1	1
110-63-4	110634	1526	**butane-1,4-diol**	3_REACH	1,4-Butanediol	butane-1,4-diol	C4H10O2	C4H10O2	90.122	OCCCCO	InChI=1/C4H10O2/c5-3-1-2-4-6/h5-6H,1-4H2	-0.256	-0.256	1	1	1
110-64-5	110645	1527	**but-2-ene-1,4-diol**	3_REACH	2-Butene-1,4-diol	but-2-ene-1,4-diol	C4H8O2	C4H8O2	88.106	OCC=CCO	InChI=1/C4H8O2/c5-3-1-2-4-6/h1-2,5-6H,3-4H2	-0.43	-0.43	1	1	1
110-65-6	110656	281	**but-2-yne-1,4-diol**	3_REACH	2-Butyne-1,4-diol	2-Butyne-1,4-diol	C4H6O2	C4H6O2	86.09	OCC#CCO	InChI=1/C4H6O2/c5-3-1-2-4-6/h5-6H,3-4H2	-0.307	-0.307	1	1	1
110-77-0	110770	283	**2-(ethylthio)ethanol**	3_REACH	Ethanol, 2-(ethylthio)-	2-(Ethylthio)ethanol	C4H10OS	C4H10OS	106.19	CCSCCO	InChI=1/C4H10OS/c1-2-6-4-3-5/h5H,2-4H2,1H3	0.604	0.604	1	1	1
110-93-0	110930	291	**6-methylhept-5-en-2-one**	3_REACH	5-Hepten-2-one, 6-methyl-	6-Methyl-5-hepten-2-one	C8H14O	C8H14O	126.2	CC(=CCCC(=O)C)C	InChI=1/C8H14O/c1-7(2)5-4-6-8(3)9/h5H,4,6H2,1-3H3	1.933	1.933	1	1	1
110964-79-9	110964799	1534	**4-(methylsulfonyl)-2-nitrobenzoic acid**	3_REACH		4-(methylsulfonyl)-2-nitrobenzoic acid			245.21	CS(=O)(=O)C1=CC(=C(C=C1)C(=O)O)[N+](=O)[O-]	InChI=1S/C8H7NO6S/c1-16(14,15)5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3,(H,10,11)			1	1	1
110-97-4	110974	292	**1,1'-iminodipropan-2-ol**	3_REACH	Diisopropanolamine	1,1'-Iminobis-2-propanol	C6H15NO2	C6H16NO2	133.19	CC(O)C[NH2+]CC(C)O	InChI=1/C6H15NO2/c1-5(8)3-7-4-6(2)9/h5-9H,3-4H2,1-2H3/p+1	-1.771	-1.652	1	1	1
111-11-5	111115	1538	**methyl octanoate**	3_REACH	Octanoic acid, methyl ester	methyl octanoate	C9H18O2	C9H18O2	158.24	CCCCCCCC(=O)OC	InChI=1/C9H18O2/c1-3-4-5-6-7-8-9(10)11-2/h3-8H2,1-2H3	2.969	2.969	1	1	1
111-14-8	111148	293	**heptanoic acid**	3_REACH	Heptanoic acid	Heptanoic acid	C7H14O2	C7H13O2	130.19	CCCCCCC(=O)[O-]	InChI=1/C7H14O2/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3,(H,8,9)/p-1	0.813	0.838	1	1	1
111-18-2	111182	1540	**N,N,N',N'-tetramethylhexamethylenediamine**	3_REACH	(CH3)2N(CH2)6N(CH3)2	N,N,N',N'-tetramethylhexamethylenediamine	C10H24N2	C10H26N2	172.32	C[NH+](C)CCCCCC[NH+](C)C	InChI=1/C10H24N2/c1-11(2)9-7-5-6-8-10-12(3)4/h5-10H2,1-4H3/p+2	-1.108	-1.005	1	1	1
111-21-7	111217	1542	**2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate**	3_REACH	Ethanol, 2,2'-[1,2-ethanediylbis(oxy)]bis-, diacetate	2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate	C10H18O6	C10H18O6	234.25	CC(=O)OCCOCCOCCOC(=O)C	InChI=1/C10H18O6/c1-9(11)15-7-5-13-3-4-14-6-8-16-10(2)12/h3-8H2,1-2H3	-0.402	-0.402	1	1	1
111-27-3	111273	294	**hexan-1-ol**	3_REACH	1-Hexanol	1-Hexanol	C6H14O	C6H14O	102.18	CCCCCCO	InChI=1/C6H14O/c1-2-3-4-5-6-7/h7H,2-6H2,1H3	1.883	1.883	1	1	1
111-30-8	111308	296	**glutaral**	3_REACH	Glutaral	Pentanedial	C5H8O2	C5H8O2	100.12	O=CCCCC=O	InChI=1/C5H8O2/c6-4-2-1-3-5-7/h4-5H,1-3H2	0.14	0.14	1	1	1
111-40-0	111400	299	**2,2'-iminodi(ethylamine)**	3_REACH	1,2-Ethanediamine, N-(2-aminoethyl)-	Diethylene triamine	C4H13N3	C4H14N3	103.17	NCC[NH2+]CCN	InChI=1/C4H13N3/c5-1-3-7-4-2-6/h7H,1-6H2/p+1	-3.105	-3.127	1	1	1
111-41-1	111411	1547	**2-(2-aminoethylamino)ethanol**	3_REACH	Ethanol, 2-[(2-aminoethyl)amino]-	2-(2-aminoethylamino)ethanol	C4H12N2O	C4H13N2O	104.16	NCC[NH2+]CCO	InChI=1/C4H12N2O/c5-1-2-6-3-4-7/h6-7H,1-5H2/p+1	-2.815	-2.8	1	1	1
111-42-2	111422	300	**2,2'-iminodiethanol**	3_REACH	Diethanolamine	Diethanolamine	C4H11NO2	C4H12NO2	105.14	OCC[NH2+]CCO	InChI=1/C4H11NO2/c6-3-1-5-2-4-7/h5-7H,1-4H2/p+1	-2.526	-2.346	1	1	1
111-44-4	111444	301	**bis(2-chloroethyl) ether**	3_REACH	Beta,beta'-dichlorodiethyl ether	2,2'-Dichlorodiethyl ether	C4H8Cl2O	C4H8Cl2O	143.01	ClCCOCCCl	InChI=1/C4H8Cl2O/c5-1-3-7-4-2-6/h1-4H2	1.38	1.38	1	1	1
111-46-6	111466	302	**2,2'-oxydiethanol**	3_REACH	Ethanol, 2,2'-oxybis-	Diethylene glycol	C4H10O3	C4H10O3	106.12	OCCOCCO	InChI=1/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2	-1.029	-1.029	1	1	1
111-64-8	111648	1551	**octanoyl chloride**	3_REACH	Octanoyl chloride	octanoyl chloride	C8H15ClO	C8H15ClO	162.66	CCCCCCCC(=O)Cl	InChI=1/C8H15ClO/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3	3.319	3.319	1	1	1
111-69-3	111693	307	**adiponitrile**	3_REACH	Hexanedinitrile	Hexanedinitrile	C6H8N2	C6H8N2	108.15	N#CCCCCC#N	InChI=1/C6H8N2/c7-5-3-1-2-4-6-8/h1-4H2	1.051	1.051	1	1	1
111-70-6	111706	308	**heptan-1-ol**	3_REACH	1-Heptanol	1-Heptanol	C7H16O	C7H16O	116.2	CCCCCCCO	InChI=1/C7H16O/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3	2.339	2.339	1	1	1
1117-31-3	1117313	1555	**1,3-butylene diacetate**	3_REACH	1,3-Butanediol, diacetate	1,3-butylene diacetate	C8H14O4	C8H14O4	174.2	CC(CCOC(=O)C)OC(=O)C	InChI=1/C8H14O4/c1-6(12-8(3)10)4-5-11-7(2)9/h6H,4-5H2,1-3H3	0.3	0.3	1	1	1
111-75-1	111751	1556	**2-butylaminoethanol**	3_REACH	Ethanol, 2-(butylamino)-	2-butylaminoethanol	C6H15NO	C6H16NO	117.19	CCCC[NH2+]CCO	InChI=1/C6H15NO/c1-2-3-4-7-5-6-8/h7-8H,2-6H2,1H3/p+1	-0.658	-0.649	1	1	1
111-76-2	111762	309	**2-butoxyethanol**	3_REACH	2-n-Butoxy-1-ethanol	2-Butoxyethanol	C6H14O2	C6H14O2	118.18	CCCCOCCO	InChI=1/C6H14O2/c1-2-3-5-8-6-4-7/h7H,2-6H2,1H3	0.839	0.839	1	1	1
111-77-3	111773	310	**2-(2-methoxyethoxy)ethanol**	3_REACH	Ethanol, 2-(2-methoxyethoxy)-	2-(2-Methoxyethoxy)ethanol	C5H12O3	C5H12O3	120.15	COCCOCCO	InChI=1/C5H12O3/c1-7-4-5-8-3-2-6/h6H,2-5H2,1H3	-0.62	-0.62	1	1	1
1117-86-8	1117868	1557	**octane-1,2-diol**	3_REACH	1,2-Octanediol	octane-1,2-diol	C8H18O2	C8H18O2	146.23	CCCCCCC(O)CO	InChI=1/C8H18O2/c1-2-3-4-5-6-8(10)7-9/h8-10H,2-7H2,1H3	1.828	1.828	1	1	1
111-81-9	111819	1558	**methyl undec-10-enoate**	3_REACH	10-Undecenoic acid, methyl ester	methyl undec-10-enoate	C12H22O2	C12H22O2	198.31	COC(=O)CCCCCCCCC=C	InChI=1/C12H22O2/c1-3-4-5-6-7-8-9-10-11-12(13)14-2/h3H,1,4-11H2,2H3	3.946	3.946	1	1	1
111-82-0	111820	1559	**methyl laurate**	3_REACH	Dodecanoic acid, methyl ester	methyl laurate	C13H26O2	C13H26O2	214.35	CCCCCCCCCCCC(=O)OC	InChI=1/C13H26O2/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h3-12H2,1-2H3	4.793	4.793	1	1	1
111-85-3	111853	1561	**1-chlorooctane**	3_REACH	Octane, 1-chloro-	1-chlorooctane	C8H17Cl	C8H17Cl	148.68	CCCCCCCCCl	InChI=1/C8H17Cl/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3	4	4	1	1	1
111-86-4	111864	313	**octylamine**	3_REACH	1-Octanamine	n-Octylamine	C8H19N	C8H20N	129.25	CCCCCCCC[NH3+]	InChI=1/C8H19N/c1-2-3-4-5-6-7-8-9/h2-9H2,1H3/p+1	1.501	1.504	1	1	1
111-87-5	111875	314	**octan-1-ol**	3_REACH	1-Octanol	1-Octanol	C8H18O	C8H18O	130.23	CCCCCCCCO	InChI=1/C8H18O/c1-2-3-4-5-6-7-8-9/h9H,2-8H2,1H3	2.795	2.795	1	1	1
111-88-6	111886	1563	**octane-1-thiol**	3_REACH	1-Octanethiol	octane-1-thiol	C8H18S	C8H18S	146.3	CCCCCCCCS	InChI=1/C8H18S/c1-2-3-4-5-6-7-8-9/h9H,2-8H2,1H3	3.766	3.766	1	1	1
111-90-0	111900	315	**2-(2-ethoxyethoxy)ethanol**	3_REACH	Ethanol, 2-(2-ethoxyethoxy)-	2'-(2-Ethoxyethoxy)ethanol	C6H14O3	C6H14O3	134.18	CCOCCOCCO	InChI=1/C6H14O3/c1-2-8-5-6-9-4-3-7/h7H,2-6H2,1H3	-0.272	-0.272	1	1	1
111-91-1	111911	316	**bis(2-chloroethoxy)methane**	3_REACH	Methane, bis(2-chloroethoxy)-	1,1'-[Methylenebis(oxy)]bis[2-chloroethane]	C5H10Cl2O2	C5H10Cl2O2	173.04	ClCCOCOCCCl	InChI=1/C5H10Cl2O2/c6-1-3-8-5-9-4-2-7/h1-5H2	1.232	1.232	1	1	1
111-92-2	111922	317	**dibutylamine**	3_REACH	1-Butanamine, N-butyl-	N-Butyl-1-butanamine	C8H19N	C8H20N	129.25	CCCC[NH2+]CCCC	InChI=1/C8H19N/c1-3-5-7-9-8-6-4-2/h9H,3-8H2,1-2H3/p+1	1.21	1.212	1	1	1
1120-21-4	1120214	1567	**undecane**	3_REACH	Undecane	undecane	C11H24	C11H24	156.31	CCCCCCCCCCC	InChI=1/C11H24/c1-3-5-7-9-11-10-8-6-4-2/h3-11H2,1-2H3	5.389	5.389	1	1	1
1120-24-7	1120247	1568	**decyldimethylamine**	3_REACH	1-Decanamine, N,N-dimethyl-	decyldimethylamine	C12H27N	C12H28N	185.36	CCCCCCCCCC[NH+](C)C	InChI=1/C12H27N/c1-4-5-6-7-8-9-10-11-12-13(2)3/h4-12H2,1-3H3/p+1	2.825	2.877	1	1	1
112-02-7	112027	7	**cetrimonium chloride**	3_REACH		N,N,N-Trimethyl-1-hexadecanaminium, Chloride		C19H42N	320.01	CCCCCCCCCCCCCCCC[N+](C)(C)C	InChI=1/C19H42N/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)4/h5-19H2,1-4H3/q+1	5.768	5.768	1	1	1
1120-36-1	1120361	1569	**tetradec-1-ene**	3_REACH	1-Tetradecene	tetradec-1-ene	C14H28	C14H28	196.38	CCCCCCCCCCCCC=C	InChI=1/C14H28/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3H,1,4-14H2,2H3	6.367	6.367	1	1	1
112-05-0	112050	320	**nonanoic acid**	3_REACH	Nonanoic acid	Nonanoic acid	C9H18O2	C9H17O2	158.24	CCCCCCCCC(=O)[O-]	InChI=1/C9H18O2/c1-2-3-4-5-6-7-8-9(10)11/h2-8H2,1H3,(H,10,11)/p-1	1.725	1.75	1	1	1

1120-71-4	1120714	1572	**1,3-propanesultone**	3_REACH	1,2-Oxathiolane, 2,2-dioxide	1,3-propanesultone	C3H6O3S	C3H6O3S	122.14	O=S1(=O)CCCO1	InChI=1/C3H6O3S/c4-7(5)3-1-2-6-7/h1-3H2	-0.494	-0.494	1	1	1
112-07-2	112072	1573	**2-butoxyethyl acetate**	3_REACH	2-Butoxyethyl acetate	2-butoxyethyl acetate	C8H16O3	C8H16O3	160.21	CCCCOCCOC(=O)C	InChI=1/C8H16O3/c1-3-4-5-10-6-7-11-8(2)9/h3-7H2,1-2H3	1.218	1.218	1	1	1
112-15-2	112152	1577	**2-(2-ethoxyethoxy)ethyl acetate**	3_REACH	Ethanol, 2-(2-ethoxyethoxy)-, acetate	2-(2-ethoxyethoxy)ethyl acetate	C8H16O4	C8H16O4	176.21	CCOCCOCCOC(=O)C	InChI=1/C8H16O4/c1-3-10-4-5-11-6-7-12-8(2)9/h3-7H2,1-2H3	0.108	0.108	1	1	1
112-16-3	112163	1578	**lauroyl chloride**	3_REACH	Dodecanoyl chloride	lauroyl chloride	C12H23ClO	C12H23ClO	218.77	CCCCCCCCCCCC(=O)Cl	InChI=1/C12H23ClO/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h2-11H2,1H3	5.144	5.144	1	1	1
112-18-5	112185	321	**dodecyldimethylamine**	3_REACH	1-Dodecanamine, N,N-dimethyl-	N,N-Dimethyl-1-dodecanamine	C14H31N	C14H32N	213.41	CCCCCCCCCCCC[NH+](C)C	InChI=1/C14H31N/c1-4-5-6-7-8-9-10-11-12-13-14-15(2)3/h4-14H2,1-3H3/p+1	3.737	3.789	1	1	1
112-25-4	112254	1580	**2-hexyloxyethanol**	3_REACH	Ethanol, 2-(hexyloxy)-	2-hexyloxyethanol	C8H18O2	C8H18O2	146.23	CCCCCCOCCO	InChI=1/C8H18O2/c1-2-3-4-5-7-10-8-6-9/h9H,2-8H2,1H3	1.752	1.752	1	1	1
112-27-6	112276	322	**2,2'-(ethylenedioxy)diethanol**	3_REACH	Triethylene glycol	Triethylene glycol	C6H14O4	C6H14O4	150.17	OCCOCCOCCO	InChI=1/C6H14O4/c7-1-3-9-5-6-10-4-2-8/h7-8H,1-6H2	-1.16	-1.16	1	1	1
112-29-8	112298	324	**1-bromodecane**	3_REACH	Decane, 1-bromo-	1-Bromodecane	C10H21Br	C10H21Br	221.19	CCCCCCCCCCBr	InChI=1/C10H21Br/c1-2-3-4-5-6-7-8-9-10-11/h2-10H2,1H3	5.056	5.056	1	1	1
112-30-1	112301	325	**decan-1-ol**	3_REACH	1-Decanol	1-Decanol	C10H22O	C10H22O	158.29	CCCCCCCCCCO	InChI=1/C10H22O/c1-2-3-4-5-6-7-8-9-10-11/h11H,2-10H2,1H3	3.707	3.707	1	1	1
112-31-2	112312	1581	**decanal**	3_REACH	Decanal	decanal	C10H20O	C10H20O	156.27	CCCCCCCCCC=O	InChI=1/C10H20O/c1-2-3-4-5-6-7-8-9-10-11/h10H,2-9H2,1H3	3.677	3.677	1	1	1
112-33-4	112334	1583	**2-[2-(3-aminopropoxy)ethoxy]ethanol**	3_REACH	Polyglycolamine	2-[2-(3-aminopropoxy)ethoxy]ethanol	C7H17NO3	C7H18NO3	163.22	[NH3+]CCCOCCOCCO	InChI=1/C7H17NO3/c8-2-1-4-10-6-7-11-5-3-9/h9H,1-8H2/p+1	-2.392	-2.37	1	1	1
112-34-5	112345	326	**2-(2-butoxyethoxy)ethanol**	3_REACH	2-(2-Butoxyethoxy)ethanol	Butyldiglycol	C8H18O3	C8H18O3	162.23	CCCCOCCOCCO	InChI=1/C8H18O3/c1-2-3-5-10-7-8-11-6-4-9/h9H,2-8H2,1H3	0.708	0.708	1	1	1
112-35-6	112356	1584	**2-(2-(2-methoxyethoxy)ethoxy)ethanol**	3_REACH	Ethanol, 2-[2-(2-methoxyethoxy)ethoxy]-	2-(2-(2-methoxyethoxy)ethoxy)ethanol	C7H16O4	C7H16O4	164.2	COCCOCCOCCO	InChI=1/C7H16O4/c1-9-4-5-11-7-6-10-3-2-8/h8H,2-7H2,1H3	-0.751	-0.751	1	1	1
112-36-7	112367	327	**bis(2-ethoxyethyl) ether**	3_REACH	Ethane, 1,1'-oxybis[2-ethoxy-	Diethylene glycol diethyl ether	C8H18O3	C8H18O3	162.23	CCOCCOCCOCC	InChI=1/C8H18O3/c1-3-9-5-7-11-8-6-10-4-2/h3-8H2,1-2H3	0.486	0.486	1	1	1
112-38-9	112389	1585	**undec-10-enoic acid**	3_REACH	Undecylenic Acid	undec-10-enoic acid	C11H20O2	C11H19O2	184.28	[O-]C(=O)CCCCCCCCC=C	InChI=1/C11H20O2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h2H,1,3-10H2,(H,12,13)/p-1	2.247	2.272	1	1	1
112-40-3	112403	1587	**dodecane**	3_REACH	n-Dodecane	dodecane	C12H26	C12H26	170.34	CCCCCCCCCCCC	InChI=1/C12H26/c1-3-5-7-9-11-12-10-8-6-4-2/h3-12H2,1-2H3	5.845	5.845	1	1	1
112-41-4	112414	1588	**dodec-1-ene**	3_REACH	1-Dodecene	dodec-1-ene	C12H24	C12H24	168.32	CCCCCCCCCCC=C	InChI=1/C12H24/c1-3-5-7-9-11-12-10-8-6-4-2/h3H,1,4-12H2,2H3	5.455	5.455	1	1	1
112-42-5	112425	329	**undecan-1-ol**	3_REACH	1-Undecanol	1-Undecanol	C11H24O	C11H24O	172.31	CCCCCCCCCCCO	InChI=1/C11H24O/c1-2-3-4-5-6-7-8-9-10-11-12/h12H,2-11H2,1H3	4.164	4.164	1	1	1
112-44-7	112447	1589	**undecanal**	3_REACH	Undecanal	undecanal	C11H22O	C11H22O	170.3	CCCCCCCCCCC=O	InChI=1/C11H22O/c1-2-3-4-5-6-7-8-9-10-11-12/h11H,2-10H2,1H3	4.133	4.133	1	1	1
112-45-8	112458	1590	**undec-10-enal**	3_REACH	10-Undecenal	undec-10-enal	C11H20O	C11H20O	168.28	C=CCCCCCCCCC=O	InChI=1/C11H20O/c1-2-3-4-5-6-7-8-9-10-11-12/h2,11H,1,3-10H2	3.743	3.743	1	1	1
112-49-2	112492	330	**1,2-bis(2-methoxyethoxy)ethane**	3_REACH	2,5,8,11-Tetraoxadodecane	2,5,8,11-Tetraoxadodecane	C8H18O4	C8H18O4	178.23	COCCOCCOCCOC	InChI=1/C8H18O4/c1-9-3-5-11-7-8-12-6-4-10-2/h3-8H2,1-2H3	-0.343	-0.343	1	1	1
112-50-5	112505	331	**2-(2-(2-ethoxyethoxy)ethoxy)ethanol**	3_REACH	Ethanol, 2-[2-(2-ethoxyethoxy)ethoxy]-	Triethyleneglycolmonoethyl ether	C8H18O4	C8H18O4	178.23	CCOCCOCCOCCO	InChI=1/C8H18O4/c1-2-10-5-6-12-8-7-11-4-3-9/h9H,2-8H2,1H3	-0.402	-0.402	1	1	1
112-53-8	112538	332	**dodecan-1-ol**	3_REACH	1-Dodecanol	1-Dodecanol	C12H26O	C12H26O	186.34	CCCCCCCCCCCCO	InChI=1/C12H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3	4.62	4.62	1	1	1
112-54-9	112549	333	**dodecanal**	3_REACH	Dodecanal	Dodecanal	C12H24O	C12H24O	184.32	CCCCCCCCCCCC=O	InChI=1/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h12H,2-11H2,1H3	4.59	4.59	1	1	1
112-55-0	112550	1592	**dodecane-1-thiol**	3_REACH	1-Dodecanethiol	dodecane-1-thiol	C12H26S	C12H26S	202.4	CCCCCCCCCCCCS	InChI=1/C12H26S/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3	5.591	5.591	1	1	1
112-59-4	112594	1593	**2-(2-hexyloxyethoxy)ethanol**	3_REACH	2-(2-Hexyloxyethoxy)ethanol	2-(2-hexyloxyethoxy)ethanol	C10H22O3	C10H22O3	190.28	CCCCCCOCCOCCO	InChI=1/C10H22O3/c1-2-3-4-5-7-12-9-10-13-8-6-11/h11H,2-10H2,1H3	1.621	1.621	1	1	1
112-67-4	112674	1597	**palmitoyl chloride**	3_REACH	Palmitoyl chloride	palmitoyl chloride	C16H31ClO	C16H31ClO	274.88	CCCCCCCCCCCCCCCC(=O)Cl	InChI=1/C16H31ClO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3	6.969	6.969	1	1	1
112-69-6	112696	1598	**hexadecyldimethylamine**	3_REACH	1-Hexadecanamine, N,N-dimethyl-	hexadecyldimethylamine	C18H39N	C18H40N	269.52	CCCCCCCCCCCCCCCC[NH+](C)C	InChI=1/C18H39N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2)3/h4-18H2,1-3H3/p+1	5.562	5.614	1	1	1
112-72-1	112721	1599	**tetradecanol**	3_REACH	1-Tetradecanol	tetradecanol	C14H30O	C14H30O	214.39	CCCCCCCCCCCCCCO	InChI=1/C14H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h15H,2-14H2,1H3	5.532	5.532	1	1	1
112-73-2	112732	1600	**bis(2-butoxyethyl) ether**	3_REACH	Butane, 1,1'-[oxybis(2,1-ethanediyloxy)]bis-	bis(2-butoxyethyl) ether	C12H26O3	C12H26O3	218.34	CCCCOCCOCCOCCCC	InChI=1/C12H26O3/c1-3-5-7-13-9-11-15-12-10-14-8-6-4-2/h3-12H2,1-2H3	2.446	2.446	1	1	1
112-75-4	112754	1601	**dimethyl(tetradecyl)amine**	3_REACH	1-Tetradecanamine, N,N-dimethyl-	dimethyl(tetradecyl)amine	C16H35N	C16H36N	241.46	CCCCCCCCCCCCCC[NH+](C)C	InChI=1/C16H35N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17(2)3/h4-16H2,1-3H3/p+1	4.65	4.701	1	1	1
112-76-5	112765	1602	**stearoyl chloride**	3_REACH	Stearic acid chloride	stearoyl chloride	C18H35ClO	C18H35ClO	302.93	CCCCCCCCCCCCCCCCCC(=O)Cl	InChI=1/C18H35ClO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-17H2,1H3	7.881	7.881	1	1	1
112-85-6	112856	1608	**docosanoic acid**	3_REACH	Docosanoic acid	docosanoic acid	C22H44O2	C22H43O2	340.59	CCCCCCCCCCCCCCCCCCCCCC(=O)[O-]	InChI=1/C22H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24/h2-21H2,1H3,(H,23,24)/p-1	7.656	7.681	0	0	1
112-88-9	112889	1609	**octadec-1-ene**	3_REACH	1-Octadecene	octadec-1-ene	C18H36	C18H36	252.49	CCCCCCCCCCCCCCCC=C	InChI=1/C18H36/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3H,1,4-18H2,2H3	8.192	8.192	0	1	1
112-92-5	112925	1611	**octadecan-1-ol**	3_REACH	1-Octadecanol	octadecan-1-ol	C18H38O	C18H38O	270.5	CCCCCCCCCCCCCCCCCCO	InChI=1/C18H38O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h19H,2-18H2,1H3	7.357	7.357	1	1	1
1134-94-7	1134947	4363	**2-Phenylsulfanylaniline**	3_REACH		2-phenylthioaniline			201.29	C1=CC=C(C(=C1)SC2=CC=CC=C2N	InChI=1S/C12H11NS/c13-11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/h1-9H,13H2			1	1	1
114772-54-2	114772542	1625	**4'-(Bromomethyl)-2-cyanobiphenyl**	3_REACH		[1,1'-Biphenyl]-2-carbonitrile, 4'-(bromomethyl)			272.15	C1=CC=C(C(=C1)C#N)C2=CC=C(C=C2)CBr	InChI=1S/C14H10BrN/c15-9-11-5-7-12(8-6-11)14-4-2-1-3-13(14)10-16/h1-8H,9H2			1	1	1
115-27-5	115275	1635	**1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride**	3_REACH	Chlorendic anhydride	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	C9H2Cl6O3	C9H2Cl6O3	370.83	ClC1=C(Cl)C2(Cl)C3C(C(=O)OC3=O)C1(Cl)C2(Cl)Cl	InChI=1/C9H2Cl6O3/c10-3-4(11)8(13)2-1(5(16)18-6(2)17)7(3,12)9(8,14)15/h1-2H	2.707	2.707	1	1	1
1154308-86-7	1154308867	1636	**N-(2-Hydroxyethyl)-3,5,5-trimethylhexanamide**	3_REACH		N-(2-hydroxyethyl)-3,5,5-trimethylhexanamide			201.31	CC(CC(=O)NCCO)CC(C)(C)C	InChI=1/C11H23NO2/c1-9(8-11(2,3)4)7-10(14)12-5-6-13/h9,13H,5-8H2,1-4H3,(H,12,14) AuxInfo=1/1/N:12,6,13,14,9,10,2,			1	1	1
115-70-8	115708	1638	**2-amino-2-ethylpropanediol**	3_REACH	2-Amino-2-ethyl-1,3-propanediol	2-amino-2-ethylpropanediol	C5H13NO2	C5H14NO2	119.17	CCC(C)([NH3+])C(O)O	InChI=1/C5H13NO2/c1-3-5(2,6)4(7)8/h4,7-8H,3,6H2,1-2H3/p+1	-1.426	-1.296	1	1	1
115-77-5	115775	341	**pentaerythritol**	3_REACH	1,3-Propanediol, 2,2-bis(hydroxymethyl)-	2,2-bis(Hydroxymethyl)-1,3-propanediol	C5H12O4	C5H12O4	136.15	OCC(CO)(CO)CO	InChI=1/C5H12O4/c6-1-5(2-7,3-8)4-9/h6-9H,1-4H2	-2.165	-2.165	1	1	1
115-86-6	115866	9	**triphenyl phosphate**	3_REACH	Triphenylphosphate	Phosphoric acid, Triphenyl ester	C18H15O4P	C18H15O4P	326.29	O=P(Oc1ccccc1)(Oc2ccccc2)Oc3ccccc3	InChI=1/C18H15O4P/c19-23(20-16-10-4-1-5-11-16,21-17-12-6-2-7-13-17)22-18-14-8-3-9-15-18/h1-15H	4.938	4.938	1	1	1
115-95-7	115957	1640	**linalyl acetate**	3_REACH	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate	linalyl acetate	C12H20O2	C12H20O2	196.29	CC(=CCCC(C)(OC(=O)C)C=C)C	InChI=1/C12H20O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h6,8H,1,7,9H2,2-5H3	3.114	3.114	1	1	1
115-96-8	115968	10	**tris(2-chloroethyl) phosphate**	3_REACH	Phosphoric acid, tri-2-chloroethyl ester	tris(beta-Chloroethylphosphate)	C6H12Cl3O4P	C6H12Cl3O4P	285.49	ClCCOP(=O)(OCCCl)OCCCl	InChI=1/C6H12Cl3O4P/c7-1-4-11-14(10,12-5-2-8)13-6-3-9/h1-6H2	1.644	1.644	1	1	1
116-37-0	116370	1648	**1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol**	3_REACH	Propane, 2,2-bis[4-(2-hydroxypropyloxy)phenyl]-	1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol	C21H28O4	C21H28O4	344.45	CC(O)COc1ccc(cc1)C(C)(C)c2ccc(OCC(C)O)cc2	InChI=1/C21H28O4/c1-15(22)13-24-19-9-5-17(6-10-19)21(3,4)18-7-11-20(12-8-18)25-14-16(2)23/h5-12,15-16,22-23H,13-14H2,1-4H3	3.906	3.906	1	1	1
116539-55-0	116539550	1651	**(1S)-3-(methylamino)-1-(2-thienyl)propan-1-ol**	3_REACH		(1S)-3-(methylamino)-1-(2-thienyl)propan-1-ol			171.26	CNCCC(C1=CC=CS1)O	InChI=1S/C8H13NOS/c1-9-5-4-7(10)8-3-2-6-11-8/h2-3,6-7,9-10H,4-5H2,1H3/t7-/m0/s1			1	1	1
116-75-6	116756	1653	**1,4-bis(mesitylamino)anthraquinone**	3_REACH		1,4-bis(mesitylamino)anthraquinone		C32H30N2O2	474.61	Cc1cc(C)c(Nc2ccc(Nc3c(C)cc(C)cc3C)c4C(=O)c5ccccc5C(=O)c24)c(C)c1	InChI=1/C32H30N2O2/c1-17-13-19(3)29(20(4)14-17)33-25-11-12-26(34-30-21(5)15-18(2)16-22(30)6)28-27(25)31(35)23-9-7-8-10-24(23)32(28)36/h7-16,33-34H,1-6H3	8.825	8.825	1	1	1
117-08-8	117088	1655	**tetrachlorophthalic anhydride**	3_REACH	1,3-Isobenzofurandione, 4,5,6,7-tetrachloro-	tetrachlorophthalic anhydride	C8Cl4O3	C8Cl4O3	285.9	Clc1c(Cl)c(Cl)c2C(=O)OC(=O)c2c1Cl	InChI=1/C8Cl4O3/c9-3-1-2(8(14)15-7(1)13)4(10)6(12)5(3)11	3.961	3.961	1	1	1
117-21-5	117215	1657	**3-chlorophthalic anhydride**	3_REACH		3-chlorophthalic anhydride		C8H3ClO3	182.56	Clc1cccc2C(=O)OC(=O)c12	InChI=1/C8H3ClO3/c9-5-3-1-2-4-6(5)8(11)12-7(4)10/h1-3H	1.968	1.968	1	1	1
117-61-3	117613	1661	**benzidine-2,2'-disulphonic acid**	3_REACH		benzidine-2,2'-disulphonic acid		C12H10N2O6S2	344.37	Nc1ccc(c2ccc(N)cc2S(=O)(=O)[O-])c(c1)S(=O)(=O)[O-]	InChI=1/C12H12N2O6S2/c13-7-1-3-9(11(5-7)21(15,16)17)10-4-2-8(14)6-12(10)22(18,19)20/h1-6H,13-14H2,(H,15,16,17)(H,18,19,20)/p-2	-3.969	-5.036	1	1	1
117-81-7	117817	346	**bis(2-ethylhexyl) phthalate**	3_REACH	Bis(2-ethylhexyl)phthalate	1,2-Benzenedicarboxylic acid, bis(2-Ethylhexyl)ester	C24H38O4	C24H38O4	390.56	CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	InChI=1/C24H38O4/c1-5-9-13-19(7-3)17-27-23(25)21-15-11-12-16-22(21)24(26)28-18-20(8-4)14-10-6-2/h11-12,15-16,19-20H,5-10,13-14,17-18H2,1-4H3	7.574	7.574	1	1	1
118135-28-7	118135287	1666	**8-tert-Butyl-2-(chloromethyl)-1,4-dioxaspiro[4.5]decane**	3_REACH		1,4-Dioxaspiro[4.5]decane, 2-(chloromethyl)-8-(1,1-dimethylethyl)-			246.78	CC(C)(C)C1CCC2(CC1)OCC(O2)CCl	InChI=1S/C13H23ClO2/c1-12(2,3)10-4-6-13(7-5-10)15-9-11(8-14)16-13/h10-11H,4-9H2,1-3H3			1	1	1
118-45-6	118456	1670	**4-chlorophthalic anhydride**	3_REACH		4-chlorophthalic anhydride		C8H3ClO3	182.56	Clc1ccc2C(=O)OC(=O)c2c1	InChI=1/C8H3ClO3/c9-4-1-2-5-6(3-4)8(11)12-7(5)10/h1-3H	1.968	1.968	1	1	1
118-48-9	118489	1671	**4H-3,1-benzoxazine-2,4(1H)-dione**	3_REACH	Isatoic anhydride	4H-3,1-benzoxazine-2,4(1H)-dione	C8H5NO3	C8H5NO3	163.13	O=C1Nc2ccccc2C(=O)O1	InChI=1/C8H5NO3/c10-7-5-3-1-2-4-6(5)9-8(11)12-7/h1-4H,(H,9,11)	1.212	1.212	1	1	1
118-58-1	118581	1674	**benzyl salicylate**	3_REACH	Benzoic acid, 2-hydroxy-, phenylmethyl ester	benzyl salicylate	C14H12O3	C14H12O3	228.25	Oc1ccccc1C(=O)OCc2ccccc2	InChI=1/C14H12O3/c15-13-9-5-4-8-12(13)14(16)17-10-11-6-2-1-3-7-11/h1-9,15H,10H2	3.026	3.018	1	1	1
118-60-5	118605	1675	**2-ethylhexyl salicylate**	3_REACH	Salicylic acid, 2-ethylhexyl ester	2-ethylhexyl salicylate	C15H22O3	C15H22O3	250.34	CCCCC(CC)COC(=O)c1ccccc1O	InChI=1/C15H22O3/c1-3-5-8-12(4-2)11-18-15(17)13-9-6-7-10-14(13)16/h6-7,9-10,12,16H,3-5,8,11H2,1-2H3	4.46	4.388	1	1	1
118-69-4	118694	1676	**2,6-dichlorotoluene**	3_REACH	Benzene, 1,3-dichloro-2-methyl-	2,6-dichlorotoluene	C7H6Cl2	C7H6Cl2	161.03	Cc1c(Cl)cccc1Cl	InChI=1/C7H6Cl2/c1-5-6(8)3-2-4-7(5)9/h2-4H,1H3	3.644	3.644	1	1	1
118-75-2	118752	1677	**tetrachloro-p-benzoquinone**	3_REACH	p-Benzoquinone, 2,3,5,6-tetrachloro-	tetrachloro-p-benzoquinone	C6Cl4O2	C6Cl4O2	245.88	ClC1=C(Cl)C(=O)C(=C(Cl)C1=O)Cl	InChI=1/C6Cl4O2/c7-1-2(8)6(12)4(10)3(9)5(1)11	2.162	2.162	1	1	1
118-79-6	118796	348	**2,4,6-tribromophenol**	3_REACH	Phenol, 2,4,6-tribromo-	2,4,6-Tribromophenol	C6H3Br3O	C6H2Br3O	330.82	[O-]c1c(Br)cc(Br)cc1Br	InChI=1/C6H3Br3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H/p-1	3.129	3.388	1	1	1
118-82-1	118821	1679	**2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol**	3_REACH	Phenol, 4,4'-methylenebis[2,6-bis(1,1-dimethylethyl)-	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	C29H44O2	C29H44O2	424.67	CC(C)(C)c1cc(Cc2cc(c(O)c(c2)C(C)(C)C)C(C)(C)C)cc(c1O)C(C)(C)C	InChI=1/C29H44O2/c1-26(2,3)20-14-18(15-21(24(20)30)27(4,5)6)13-19-16-22(28(7,8)9)25(31)23(17-19)29(10,11)12/h14-17,30-31H,13H2,1-12H3	8.922	8.922	0	1	1
1189-08-8	1189088	1682	**1-methyltrimethylene dimethacrylate**	3_REACH	1,3-Butanediol, bis(2-methylpropenoate)	1-methyltrimethylene dimethacrylate	C12H18O4	C12H18O4	226.27	CC(CCOC(=O)C(=C)C)OC(=O)C(=C)C	InChI=1/C12H18O4/c1-8(2)11(13)15-7-6-10(5)16-12(14)9(3)4/h10H,1,3,6-7H2,2,4-5H3	2.588	2.588	1	1	1
118-92-3	118923	1683	**anthranilic acid**	3_REACH	Anthranilic acid	anthranilic acid	C7H7NO2	C7H6NO2	137.14	Nc1ccccc1C(=O)[O-]	InChI=1/C7H7NO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,8H2,(H,9,10)/p-1	-0.761	-0.761	1	1	1
118-96-7	118967	349	**2,4,6-trinitrotoluene**	3_REACH	Trinitrotoluene	2-Methyl-1,3,5-trinitrobenzene	C7H5N3O6	C7H5N3O6	227.13	Cc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C7H5N3O6/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10(15)16/h2-3H,1H3	1.999	1.999	1	1	1
119-17-5	119175	1686	**m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphonic acid**	3_REACH		m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphonic acid		C10H9N2O4S	254.27	CC1=NN(C(=O)C1)c2cccc(c2)S(=O)(=O)[O-]	InChI=1/C10H10N2O4S/c1-7-5-10(13)12(11-7)8-3-2-4-9(6-8)17(14,15)16/h2-4,6H,5H2,1H3,(H,14,15,16)/p-1	-1.789	0.455	1	1	1
119313-12-1	119313121	4343	**2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone**	3_REACH		2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone			366.51	CCC(CC1=CC=CC=C1)(C(=O)C2=CC=C(C=C2)N3CCOCC3)N(C)C	InChI=1S/C23H30N2O2/c1-4-23(24(2)3,18-19-8-6-5-7-9-19)22(26)20-10-12-21(13-11-20)25-14-16-27-17-15-25/h5-13H,4,			1	1	1
119462-56-5	119462565	4277	**1,3-bis(3-methyl-2,5-dioxo-1H-pyrrolinylmethyl)benzene**	3_REACH		1,3-bis(3-methyl-2,5-dioxo-1H-pyrrolinylmethyl)benzene			324.34	CC1=CC(=O)N(C1=O)CC2=CC(=CC=C2)CN3C(=O)C=C(C3=O)C	InChI=1S/C18H16N2O4/c1-11-6-15(21)19(17(11)23)9-13-4-3-5-14(8-13)10-20-16(22)7-12(2)18(20)24/h3-8H,9-10H2,1-2H3			1	1	1
119-53-9	119539	1694	**benzoin**	3_REACH	Ethanone, 2-hydroxy-1,2-diphenyl-	benzoin	C14H12O2	C14H12O2	212.25	OC(C(=O)c1ccccc1)c2ccccc2	InChI=1/C14H12O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10,13,15H	2.616	2.616	1	1	1
119-61-9	119619	354	**benzophenone**	3_REACH	Benzophenone	Benzophenone	C13H10O	C13H10O	182.22	O=C(c1ccccc1)c2ccccc2	InChI=1/C13H10O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	3.234	3.234	1	1	1
119-64-2	119642	355	**1,2,3,4-tetrahydronaphthalene**	3_REACH	Tetralin	1,2,3,4-Tetrahydronaphthalene	C10H12	C10H12	132.21	C1CCc2ccccc2C1	InChI=1/C10H12/c1-2-6-10-8-4-3-7-9(10)5-1/h1-2,5-6H,3-4,7-8H2	3.343	3.343	1	1	1
119-65-3	119653	356	**isoquinoline**	3_REACH	Isoquinoline	Isoquinoline	C9H7N	C9H7N	129.16	c1ccc2cnccc2c1	InChI=1/C9H7N/c1-2-4-9-7-10-6-5-8(9)3-1/h1-7H	1.587	1.595	1	1	1
119-80-2	119802	357	**2,2'-dithiodi(benzoic acid)**	3_REACH		Bis(2-carboxyphenyl)disulfide		C14H8O4S2	306.36	[O-]C(=O)c1ccccc1SSc2ccccc2C(=O)[O-]	InChI=1/C14H10O4S2/c15-13(16)9-5-1-3-7-11(9)19-20-12-8-4-2-6-10(12)14(17)18/h1-8H,(H,15,16)(H,17,18)/p-2	0.85	0.861	1	1	1
119851-28-4	119851284	1700	**1-[2-Chloro-4-(4-chlorophenoxy)phenyl]ethanone**	3_REACH		Ethanone, 1-[2-chloro-4-(4-chlorophenoxy)phenyl]-			281.14	CC(=O)C1=C(C=C(C=C1)OC2=CC=C(C=C2)Cl)Cl	InChI=1S/C14H10Cl2O2/c1-9(17)13-7-6-12(8-14(13)16)18-11-4-2-10(15)3-5-11/h2-8H,1H3			1	1	1
120068-79-3	120068793	4457	**PYRAZOLE MB 45897**	3_REACH		1H-Pyrazole-3-carbonitrile, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-			321.09	C1=C(C=C(C(=C1Cl)N2C(=CC(=N2)C#N)N)Cl)C(F)(F)F	InChI=1S/C11H5Cl2F3N4/c12-7-1-5(11(14,15)16)2-8(13)10(7)20-9(18)3-6(4-17)19-20/h1-3H,18H2			1	1	1
120100-77-8	120100778	1704	**2-Chloro-4-(methylsulfonyl)-3-[(2,2,2-trifluoroethoxy)methyl]benzoic acid**	3_REACH		2-Chloro-4-(methylsulfonyl)-3-((2,2,2-trifluoroethoxy)methyl) benzoic acid			346.71	CS(=O)(=O)C1=C(C(=C(C=C1)C(=O)O)Cl)COCC(F)(F)F	InChI=1S/C11H10ClF3O5S/c1-21(18,19)8-3-2-6(10(16)17)9(12)7(8)4-20-5-11(13,14)15/h2-3H,4-5H2,1H3,(H,16,17)			1	1	1
120-12-7	120127	358	**anthracene**	3_REACH	Anthracene	Anthracene	C14H10	C14H10	178.23	c1ccc2cc3ccccc3cc2c1	InChI=1/C14H10/c1-2-6-12-10-14-8-4-3-7-13(14)9-11(12)5-1/h1-10H	3.646	3.646	1	1	1
120-18-3	120183	12	**naphthalene-2-sulphonic acid**	3_REACH		2-Naphthalenesulfonic acid		C10H7O3S	208.24	[O-]S(=O)(=O)c1ccc2ccccc2c1	InChI=1/C10H8O3S/c11-14(12,13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H,11,12,13)/p-1	-0.174	-0.174	1	1	1
120298-38-6	120298386	4257	**(S,S)-trans-4-(acetylamino)-5,6-dihydro-6-methyl-7,7-dioxo-4H-thieno[2,3-b]thiopyran-2-sulfonamide**	3_REACH		(S,S)-trans-4-(acetylamino)-5,6-dihydro-6-methyl-7,7-dioxo-4H-thieno[2,3-b]thiopyran-2-sulfonamide			338.43	CC1CC(C2=C(S1(=O)=O)SC(=C2)S(=O)(=O)N)NC(=O)C	InChI=1S/C10H14N2O5S3/c1-5-3-8(12-6(2)13)7-4-9(20(11,16)17)18-10(7)19(5,14)15/h4-5,8H,3H2,1-2H3,(H,12,13)(H2,1			1	1	1
120-40-1	120401	13	**N,N-bis(2-hydroxyethyl)dodecanamide**	3_REACH		N,N-bis(2-hydroxyethyl)dodecanamide		C16H33NO3	287.44	CCCCCCCCCCCC(=O)N(CCO)CCO	InChI=1/C16H33NO3/c1-2-3-4-5-6-7-8-9-10-11-16(20)17(12-14-18)13-15-19/h18-19H,2-15H2,1H3	3.273	3.273	1	1	1
120-46-7	120467	1712	**1,3-diphenylpropane-1,3-dione**	3_REACH	1,3-Propanedione, 1,3-diphenyl-	1,3-diphenylpropane-1,3-dione	C15H12O2	C15H11O2	224.26	O=C([CH-]C(=O)c1ccccc1)c2ccccc2	InChI=1/C15H11O2/c16-14(12-7-3-1-4-8-12)11-15(17)13-9-5-2-6-10-13/h1-11H/q-1	3.154	3.168	1	1	1
120-47-8	120478	14	**ethyl 4-hydroxybenzoate**	3_REACH	Ethylparaben	ethyl 4-hydroxybenzoate	C9H10O3	C9H10O3	166.18	CCOC(=O)c1ccc(O)cc1	InChI=1/C9H10O3/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6,10H,2H2,1H3	1.792	1.763	1	1	1
120-55-8	120558	1714	**oxydiethylene dibenzoate**	3_REACH	Ethanol, 2,2'-oxybis-, dibenzoate	oxydiethylene dibenzoate	C18H18O5	C18H18O5	314.34	O=C(OCCOCCOC(=O)c1ccccc1)c2ccccc2	InChI=1/C18H18O5/c19-17(15-7-3-1-4-8-15)22-13-11-21-12-14-23-18(20)16-9-5-2-6-10-16/h1-10H,11-14H2	3.058	3.058	1	1	1
120-57-0	120570	1715	**piperonal**	3_REACH	Piperonal	piperonal	C8H6O3	C8H6O3	150.13	O=Cc1ccc2OCOc2c1	InChI=1/C8H6O3/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-4H,5H2	1.357	1.357	1	1	1
120570-77-6	120570776	1716	**2-(2-Formyloxyethoxy)ethyl formate**	3_REACH		Ethanol, 2,2'-oxybis-, 1,1'-diformate			162.14	C(COC=O)OCCOC=O	InChI=1S/C6H10O5/c7-5-10-3-1-9-2-4-11-6-8/h5-6H,1-4H2			1	1	1
120578-03-2	120578032	4461	**3-(2-(7-Chloroquinolin-2-yl)vinyl)benzaldehyde**	3_REACH		MONOALDEHYDE			293.75	C1=CC(=CC(=C1)C=O)C=CC2=NC3=C(C=CC(=C3)Cl)C=C2	InChI=1S/C18H12ClNO/c19-16-7-5-15-6-9-17(20-18(15)11-16)8-4-13-2-1-3-14(10-13)12-21/h1-12H/b8-4+			1	1	1
120-61-6	120616	1717	**dimethyl terephthalate**	3_REACH	1,4-Benzenedicarboxylic acid dimethyl ester	dimethyl terephthalate	C10H10O4	C10H10O4	194.19	COC(=O)c1ccc(cc1)C(=O)OC	InChI=1/C10H10O4/c1-13-9(11)7-3-5-8(6-4-7)10(12)14-2/h3-6H,1-2H3	1.54	1.54	1	1	1
120-78-5	120785	360	**di(benzothiazol-2-yl) disulphide**	3_REACH	Benzothiazyl disulfide	2,2'-Dithiobisbenzothiazole	C14H8N2S4	C14H8N2S4	332.49	S(Sc1nc2ccccc2s1)c3nc4ccccc4s3	InChI=1/C14H8N2S4/c1-3-7-11-9(5-1)15-13(17-11)19-20-14-16-10-6-2-4-8-12(10)18-14/h1-8H	5.79	5.79	1	1	1
120-80-9	120809	361	**pyrocatechol**	3_REACH	1,2-Benzenediol	1,2-Benzenediol	C6H6O2	C6H6O2	110.11	Oc1ccccc1O	InChI=1/C6H6O2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H	1.346	1.333	1	1	1
120-82-1	120821	362	**1,2,4-trichlorobenzene**	3_REACH	Benzene, 1,2,4-trichloro-	1,2,4-Trichlorobenzene	C6H3Cl3	C6H3Cl3	181.45	Clc1ccc(Cl)c(Cl)c1	InChI=1/C6H3Cl3/c7-4-1-2-5(8)6(9)3-4/h1-3H	3.823	3.823	1	1	1
120-83-2	120832	363	**2,4-dichlorophenol**	3_REACH	Phenol, 2,4-dichloro-	2,4-Dichlorophenol	C6H4Cl2O	C6H4Cl2O	163	Oc1ccc(Cl)cc1Cl	InChI=1/C6H4Cl2O/c7-4-1-2-6(9)5(8)3-4/h1-3,9H	2.916	2.814	1	1	1
120-93-4	120934	367	**2-imidazolidone**	3_REACH	2-Imidazolidinone	2-Imidazolidinone	C3H6N2O	C3H6N2O	86.096	O=C1NCCN1	InChI=1/C3H6N2O/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)	-0.812	-0.812	1	1	1
121219-07-6	121219076	4298	**1-Ethoxy-2,3-Difluorobenzene**	3_REACH		1-ethoxy-2,3-difluorobenzene			158.15	CCOC1=C(C(=CC=C1)F)F	InChI=1S/C8H8F2O/c1-2-11-7-5-3-4-6(9)8(7)10/h3-5H,2H2,1H3			1	1	1
121-32-4	121324	368	**3-ethoxy-4-hydroxybenzaldehyde**	3_REACH	3-Ethoxy-4-hydroxybenzaldehyde	3-Ethoxy-4-hydroxybenzaldehyde	C9H10O3	C9H9O3	166.18	CCOc1cc(C=O)ccc1[O-]	InChI=1/C9H10O3/c1-2-12-9-5-7(6-10)3-4-8(9)11/h3-6,11H,2H2,1H3/p-1	0.976	1.404	1	1	1
121-33-5	121335	369	**vanillin**	3_REACH	Benzaldehyde, 4-hydroxy-3-methoxy-	4-Hydroxy-3-methoxybenzaldehyde	C8H8O3	C8H7O3	152.15	COc1cc(C=O)ccc1[O-]	InChI=1/C8H8O3/c1-11-8-4-6(5-9)2-3-7(8)10/h2-5,10H,1H3/p-1	0.627	1.055	1	1	1
121-57-3	121573	372	**sulphanilic acid**	3_REACH	Benzenesulfonic acid, 4-amino-	Sulfanilic acid	C6H7NO3S	C6H6NO3S	173.19	Nc1ccc(cc1)S(=O)(=O)[O-]	InChI=1/C6H7NO3S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,7H2,(H,8,9,10)/p-1	-1.829	-1.805	1	1	1
121-60-8	121608	1730	**N-acetylsulphanilyl chloride**	3_REACH	P-acetamidobenzene sulfonyl chloride	N-acetylsulphanilyl chloride	C8H8ClNO3S	C8H8ClNO3S	233.67	CC(=O)Nc1ccc(cc1)S(=O)(=O)Cl	InChI=1/C8H8ClNO3S/c1-6(11)10-7-2-4-8(5-3-7)14(9,12)13/h2-5H,1H3,(H,10,11)	0.859	0.859	1	1	1
121-69-7	121697	373	**N,N-dimethylaniline**	3_REACH	Benzenamine, N,N-dimethyl-	N,N-Dimethylaniline	C8H11N	C8H11N	121.18	CN(C)c1ccccc1	InChI=1/C8H11N/c1-9(2)8-6-4-3-5-7-8/h3-7H,1-2H3	1.992	1.984	1	1	1
121-82-4	121824	375	**perhydro-1,3,5-trinitro-1,3,5-triazine**	3_REACH	1,3,5-Triazine, hexahydro-1,3,5-trinitro-	Hexahydro-1,3,5-trinitro-1,2,3-triazine	C3H6N6O6	C3H6N6O6	222.12	[O-][N+](=O)N1CN(CN(C1)[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C3H6N6O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H2	5.163	5.163	1	1	1
121-86-8	121868	376	**2-chloro-4-nitrotoluene**	3_REACH	Benzene, 2-chloro-1-methyl-4-nitro	2-Chloro-4-nitrotoluene	C7H6ClNO2	C7H6ClNO2	171.58	Cc1ccc(cc1Cl)[N+](=O)[O-]	InChI=1/C7H6ClNO2/c1-5-2-3-6(9(10)11)4-7(5)8/h2-4H,1H3	2.875	2.875	1	1	1
121-91-5	121915	1739	**isophthalic acid**	3_REACH	1,3-Benzenedicarboxylic acid	isophthalic acid	C8H6O4	C8H4O4	166.13	[O-]C(=O)c1cccc(c1)C(=O)[O-]	InChI=1/C8H6O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)(H,11,12)/p-2	-1.859	-1.821	1	1	1
122-00-9	122009	1740	**4'-methylacetophenone**	3_REACH	Ethanone, 1-(4-methylphenyl)-	4'-methylacetophenone	C9H10O	C9H10O	134.18	CC(=O)c1ccc(C)cc1	InChI=1/C9H10O/c1-7-3-5-9(6-4-7)8(2)10/h3-6H,1-2H3	2.056	2.056	1	1	1
122-01-0	122010	1741	**4-chlorobenzoyl chloride**	3_REACH	4-Chlorobenzoic acid chloride	4-chlorobenzoyl chloride	C7H4Cl2O	C7H4Cl2O	175.01	ClC(=O)c1ccc(Cl)cc1	InChI=1/C7H4Cl2O/c8-6-3-1-5(2-4-6)7(9)10/h1-4H	2.7	2.7	1	1	1
122-03-2	122032	377	**4-isopropylbenzaldehyde**	3_REACH	Benzaldehyde, 4-(1-methylethyl)-	4-(1-Methylethyl)benzaldehyde	C10H12O	C10H12O	148.21	CC(C)c1ccc(C=O)cc1	InChI=1/C10H12O/c1-8(2)10-5-3-9(7-11)4-6-10/h3-8H,1-2H3	2.783	2.783	1	1	1
122-20-3	122203	1743	**1,1',1''-nitrilotripropan-2-ol**	3_REACH	2-Propanol, 1,1',1''-nitrilotris-	1,1',1''-nitrilotripropan-2-ol	C9H21NO3	C9H22NO3	191.27	CC(O)C[NH+](CC(C)O)CC(C)O	InChI=1/C9H21NO3/c1-7(11)4-10(5-8(2)12)6-9(3)13/h7-9,11-13H,4-6H2,1-3H3/p+1	-1.727	-0.722	1	1	1
12225-08-0	12225080	1744	**N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2,5-dimethoxy-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide**	3_REACH		N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2,5-dimethoxy-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide		C27H23N6O7S	576.59	CNS(=O)(=O)c1cc(OC)c(cc1OC)N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4ccc5[nH]c(O)nc5c4	InChI=1/C27H24N6O7S/c1-28-41(37,38)23-13-21(39-2)20(12-22(23)40-3)32-33-24-16-7-5-4-6-14(16)10-17(25(24)34)26(35)29-15-8-9-18-19(11-15)31-27(36)30-18/h4-13,28,34H,1-3H3,(H,29,35)(H2,30,31,36)/p-1	3.64	3.762	1	1	1
12225-18-2	12225182	1745	**N-(4-chloro-2,5-dimethoxyphenyl)-2-[[2,5-dimethoxy-4-[(phenylamino)sulphonyl]phenyl]azo]-3-oxobutyramide**	3_REACH		N-(4-chloro-2,5-dimethoxyphenyl)-2-[[2,5-dimethoxy-4-[(phenylamino)sulphonyl]phenyl]azo]-3-oxobutyramide		C26H27ClN4O8S	591.04	COc1cc(NC(=O)C(N=Nc2cc(OC)c(cc2OC)S(=O)(=O)Nc3ccccc3)C(=O)C)c(OC)cc1Cl	InChI=1/C26H27ClN4O8S/c1-15(32)25(26(33)28-18-12-20(36-2)17(27)11-21(18)37-3)30-29-19-13-23(39-5)24(14-22(19)38-4)40(34,35)31-16-9-7-6-8-10-16/h6-14,25,31H,1-5H3,(H,28,33)	4.276	4.283	1	1	1
12236-62-3	12236623	1747	**2-[(4-chloro-2-nitrophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide**	3_REACH		2-[(4-chloro-2-nitrophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide		C17H13ClN6O5	416.79	CC(=O)C(N=Nc1ccc(Cl)cc1[N+](=O)[O-])C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C17H13ClN6O5/c1-8(25)15(23-22-12-4-2-9(18)6-14(12)24(28)29)16(26)19-10-3-5-11-13(7-10)21-17(27)20-11/h2-7,15H,1H3,(H,19,26)(H2,20,21,27)	3.564	3.564	1	1	1
12236-64-5	12236645	1748	**N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxynaphthalene-2-carboxamide**	3_REACH		N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxynaphthalene-2-carboxamide		C26H19ClN5O4	501.94	CC(=O)Nc1ccc(NC(=O)c2cc3ccccc3c(N=Nc4cc(ccc4Cl)C(=O)N)c2[O-])cc1	InChI=1/C26H20ClN5O4/c1-14(33)29-17-7-9-18(10-8-17)30-26(36)20-12-15-4-2-3-5-19(15)23(24(20)34)32-31-22-13-16(25(28)35)6-11-21(22)27/h2-13,34H,1H3,(H2,28,35)(H,29,33)(H,30,36)/p-1	3.734	4.437	1	1	1
122-39-4	122394	379	**diphenylamine**	3_REACH	Diphenylamine	Difenylamine	C12H11N	C12H11N	169.23	N(c1ccccc1)c2ccccc2	InChI=1/C12H11N/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10,13H	3.38	3.38	1	1	1
122-52-1	122521	1751	**triethyl phosphite**	3_REACH	Phosphorous acid, triethyl ester	triethyl phosphite	C6H15O3P	C6H15O3P	166.16	CCOP(OCC)OCC	InChI=1/C6H15O3P/c1-4-7-10(8-5-2)9-6-3/h4-6H2,1-3H3	0.094	0.094	1	1	1
122-57-6	122576	1752	**4-phenylbutenone**	3_REACH	3-Buten-2-one, 4-phenyl-	4-phenylbutenone	C10H10O	C10H10O	146.19	CC(=O)C=Cc1ccccc1	InChI=1/C10H10O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-8H,1H3	2.028	2.028	1	1	1
122-62-3	122623	1755	**bis(2-ethylhexyl) sebacate**	3_REACH	Decanedioic acid, bis(2-ethylhexyl) ester	bis(2-ethylhexyl) sebacate	C26H50O4	C26H50O4	426.68	CCCCC(CC)COC(=O)CCCCCCCCC(=O)OCC(CC)CCCC	InChI=1/C26H50O4/c1-5-9-17-23(7-3)21-29-25(27)19-15-13-11-12-14-16-20-26(28)30-22-24(8-4)18-10-6-2/h23-24H,5-22H2,1-4H3	8.862	8.862	1	1	1
122-99-6	122996	384	**2-phenoxyethanol**	3_REACH	2-Phenoxyethanol	2-Phenoxyethanol	C8H10O2	C8H10O2	138.17	OCCOc1ccccc1	InChI=1/C8H10O2/c9-6-7-10-8-4-2-1-3-5-8/h1-5,9H,6-7H2	1.274	1.274	1	1	1
123-04-6	123046	1760	**3-(chloromethyl)heptane**	3_REACH	3-Chloromethyl heptane	3-(chloromethyl)heptane	C8H17Cl	C8H17Cl	148.68	CCCCC(CC)CCl	InChI=1/C8H17Cl/c1-3-5-6-8(4-2)7-9/h8H,3-7H2,1-2H3	3.863	3.863	1	1	1
123-05-7	123057	1761	**2-ethylhexanal**	3_REACH	Hexanal, 2-ethyl-	2-ethylhexanal	C8H16O	C8H16O	128.22	CCCCC(CC)C=O	InChI=1/C8H16O/c1-3-5-6-8(4-2)7-9/h7-8H,3-6H2,1-2H3	2.771	2.771	1	1	1
123-11-5	123115	1763	**anisaldehyde**	3_REACH	Benzaldehyde, 4-methoxy-	anisaldehyde	C8H8O2	C8H8O2	136.15	COc1ccc(C=O)cc1	InChI=1/C8H8O2/c1-10-8-4-2-7(6-9)3-5-8/h2-6H,1H3	1.572	1.572	1	1	1
123-17-1	123171	1764	**2,6,8-trimethylnonan-4-ol**	3_REACH	4-Nonanol, 2,6,8-trimethyl-	2,6,8-trimethylnonan-4-ol	C12H26O	C12H26O	186.34	CC(C)CC(C)CC(O)CC(C)C	InChI=1/C12H26O/c1-9(2)6-11(5)8-12(13)7-10(3)4/h9-13H,6-8H2,1-5H3	3.995	3.995	1	1	1
123-30-8	123308	386	**4-aminophenol**	3_REACH	Phenol, 4-amino-	4-Aminophenol	C6H7NO	C6H7NO	109.13	Nc1ccc(O)cc1	InChI=1/C6H7NO/c7-5-1-3-6(8)4-2-5/h1-4,8H,7H2	0.841	0.785	1	1	1
123-31-9	123319	388	**hydroquinone**	3_REACH	Hydroquinone	1,4-Benzenediol	C6H6O2	C6H6O2	110.11	Oc1ccc(O)cc1	InChI=1/C6H6O2/c7-5-1-2-6(8)4-3-5/h1-4,7-8H	1.346	1.343	1	1	1
123-39-7	123397	392	**N-methylformamide**	3_REACH	Formamide, N-methyl-	N-Methylformamide	C2H5NO	C2H5NO	59.069	CNC=O	InChI=1/C2H5NO/c1-3-2-4/h2H,1H3,(H,3,4)	-0.705	-0.705	1	1	1
123-42-2	123422	393	**4-hydroxy-4-methylpentan-2-one**	3_REACH	4-Hydroxy-4-methylpentan-2-one	4-Hydroxy-4-methyl-2-pentanone	C6H12O2	C6H12O2	116.16	CC(=O)CC(C)(C)O	InChI=1/C6H12O2/c1-5(7)4-6(2,3)8/h8H,4H2,1-3H3	0.054	0.054	1	1	1
123-68-2	123682	1773	**allyl hexanoate**	3_REACH	Hexanoic acid, 2-propenyl ester	allyl hexanoate	C9H16O2	C9H16O2	156.22	CCCCCC(=O)OCC=C	InChI=1/C9H16O2/c1-3-5-6-7-9(10)11-8-4-2/h4H,2-3,5-8H2,1H3	2.673	2.673	1	1	1
123-77-3	123773	1775	**C,C'-azodi(formamide)**	3_REACH	Diazenedicarboxamide	C,C'-azodi(formamide)	C2H4N4O2	C2H4N4O2	116.08	NC(=O)N=NC(=O)N	InChI=1/C2H4N4O2/c3-1(7)5-6-2(4)8/h(H2,3,7)(H2,4,8)/b6-5+	0.194	0.194	1	1	1
1238449-42-7	1238449427	1776	**bis(2-propylheptyl) carbonate**	3_REACH		bis(2-propylheptyl) carbonate			342.56	CCCCCC(CCC)COC(=O)OCC(CCC)CCCCC	InChI=1S/C21H42O3/c1-5-9-11-15-19(13-7-3)17-23-21(22)24-18-20(14-8-4)16-12-10-6-2/h19-20H,5-18H2,1-4			1	1	1
123-96-6	123966	399	**octan-2-ol**	3_REACH	2-Octanol	2-Octanol	C8H18O	C8H18O	130.23	CCCCCCC(C)O	InChI=1/C8H18O/c1-3-4-5-6-7-8(2)9/h8-9H,3-7H2,1-2H3	2.716	2.716	1	1	1
124-04-9	124049	400	**adipic acid**	3_REACH	Hexanedioic acid	Hexanedioic acid	C6H10O4	C6H8O4	146.14	[O-]C(=O)CCCCC(=O)[O-]	InChI=1/C6H10O4/c7-5(8)3-1-2-4-6(9)10/h1-4H2,(H,7,8)(H,9,10)/p-2	-2.395	-2.345	1	1	1
124-07-2	124072	401	**octanoic acid**	3_REACH	Octanoic acid	Octanoic acid	C8H16O2	C8H15O2	144.21	CCCCCCCC(=O)[O-]	InChI=1/C8H16O2/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3,(H,9,10)/p-1	1.269	1.294	1	1	1
124-09-4	124094	1783	**hexamethylenediamine**	3_REACH	1,6-Hexanediamine	hexamethylenediamine	C6H16N2	C6H18N2	116.21	[NH3+]CCCCCC[NH3+]	InChI=1/C6H16N2/c7-5-3-1-2-4-6-8/h1-8H2/p+2	-1.932	-1.926	1	1	1
124-13-0	124130	1786	**octanal**	3_REACH	Octanal	octanal	C8H16O	C8H16O	128.22	CCCCCCCC=O	InChI=1/C8H16O/c1-2-3-4-5-6-7-8-9/h8H,2-7H2,1H3	2.765	2.765	1	1	1
124-17-4	124174	1787	**2-(2-butoxyethoxy)ethyl acetate**	3_REACH	Ethanol, 2-(2-butoxyethoxy)-, acetate	2-(2-butoxyethoxy)ethyl acetate	C10H20O4	C10H20O4	204.27	CCCCOCCOCCOC(=O)C	InChI=1/C10H20O4/c1-3-4-5-12-6-7-13-8-9-14-10(2)11/h3-9H2,1-2H3	1.087	1.087	1	1	1
124-18-5	124185	402	**decane**	3_REACH	Decane	Decane	C10H22	C10H22	142.29	CCCCCCCCCC	InChI=1/C10H22/c1-3-5-7-9-10-8-6-4-2/h3-10H2,1-2H3	4.933	4.933	1	1	1
1241-94-7	1241947	403	**2-ethylhexyl diphenyl phosphate**	3_REACH	Phosphoric acid, 2-ethylhexyl diphenyl ester	Phosphoric acid, 2-Ethylhexyl diphenyl ester	C20H27O4P	C20H27O4P	362.41	CCCCC(CC)COP(=O)(Oc1ccccc1)Oc2ccccc2	InChI=1/C20H27O4P/c1-3-5-12-18(4-2)17-22-25(21,23-19-13-8-6-9-14-19)24-20-15-10-7-11-16-20/h6-11,13-16,18H,3-5,12,17H2,1-2H3	6.191	6.191	1	1	1
124-19-6	124196	1788	**nonanal**	3_REACH	Nonanal	nonanal	C9H18O	C9H18O	142.24	CCCCCCCCC=O	InChI=1/C9H18O/c1-2-3-4-5-6-7-8-9-10/h9H,2-8H2,1H3	3.221	3.221	1	1	1
124-26-5	124265	1789	**stearamide**	3_REACH	Octadecanamide	stearamide	C18H37NO	C18H37NO	283.5	CCCCCCCCCCCCCCCCCC(=O)N	InChI=1/C18H37NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-17H2,1H3,(H2,19,20)	6.677	6.677	1	1	1
124-28-7	124287	1790	**dimantine**	3_REACH	1-Octadecanamine, N,N-dimethyl-	dimantine	C20H43N	C20H44N	297.57	CCCCCCCCCCCCCCCCCC[NH+](C)C	InChI=1/C20H43N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(2)3/h4-20H2,1-3H3/p+1	6.474	6.526	1	1	1
124-30-1	124301	1791	**octadecylamine**	3_REACH	1-Octadecanamine	octadecylamine	C18H39N	C18H40N	269.52	CCCCCCCCCCCCCCCCCC[NH3+]	InChI=1/C18H39N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-19H2,1H3/p+1	6.063	6.066	1	1	1
124655-09-0	124655090	4568	**tert-butyl2-[(4R,6S)-6-(hydroxymethyl)-2,2-dimethyl-1,3-dioxan-4-yl]acetate**	3_REACH		BHA (LSM0922)			260.33	CC1(OC(CC(O1)CO)CC(=O)OC(C)(C)C	InChI=1S/C13H24O5/c1-12(2,3)18-11(15)7-9-6-10(8-14)17-13(4,5)16-9/h9-10,14H,6-8H2,1-5H3/t9-,10+/m1/s1			1	1	1
125-12-2	125122	1796	**exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate**	3_REACH	Isobornyl acetate	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	C12H20O2	C12H20O2	196.29	CC(=O)O[C@H]1C[C@@H]2CC[C@@]1(C)C2(C)C	InChI=1/C12H20O2/c1-8(13)14-10-7-9-5-6-12(10,4)11(9,2)3/h9-10H,5-7H2,1-4H3/t9-,10-,12+/m0/s1	2.354	2.354	1	1	1
12542-30-2	12542302	1797	**hexahydro-4,7-methano-1H-indenyl acrylate**	3_REACH		hexahydro-4,7-methano-1H-indenyl acrylate		C13H16O2	204.27	C=CC(=O)OC1C=CC2C3CCC(C3)C12	InChI=1/C13H16O2/c1-2-12(14)15-11-6-5-10-8-3-4-9(7-8)13(10)11/h2,5-6,8-11,13H,1,3-4,7H2	2.598	2.598	1	1	1
125971-57-5	125971575	1800	**(2Z)-2-Benzylidene-4-methyl-3-oxo-N-phenylpentanamide**	3_REACH		BIBEA			293.37	CC(C)C(=O)C(=CC1=CC=CC=C1)C(=O)NC2=CC=CC=C2	InChI=1S/C19H19NO2/c1-14(2)18(21)17(13-15-9-5-3-6-10-15)19(22)20-16-11-7-4-8-12-16/h3-14H,1-2H3,(H,20,22)/b17-1			1	1	1
125971-96-2	125971962	4497	**4-(4-F-PHENYL)-4-OXO-3-PHENYL-2-ISOBUTYRYL-N-PHENYL BUTANAMID**	3_REACH		Benzenebutanamide, 4-fluoro-a-(2-methyl-1-oxopropyl)-?-oxo-N,ß-diphenyl-			417.48	CC(C)C(=O)C(C(C1=CC=CC=C1)C(=O)C2=CC=C(C=C2)F)C(=O)NC3=CC=CC=C3	InChI=1S/C26H24FNO3/c1-17(2)24(29)23(26(31)28-21-11-7-4-8-12-21)22(18-9-5-3-6-10-18)25(30)19-13-15-20(27)16-14-			1	1	1
126-33-0	126330	406	**tetrahydrothiophene 1,1-dioxide**	3_REACH	Thiophene, tetrahydro-, 1,1-dioxide	2,3,4,5-Tetrahydrothiophene-1,1-dioxide	C4H8O2S	C4H8O2S	120.17	O=S1(=O)CCCC1	InChI=1/C4H8O2S/c5-7(6)3-1-2-4-7/h1-4H2	0.24	0.24	1	1	1
126586-91-2	126586912	4597	**N2-[1-(S)-ethoxycarbonyl-3-phenylpropyl]-N6-trifluoroacetyl-L-lysyl-N2-carboxy anhydride**	3_REACH		EPTL			414.43	CCOC(=O)[C@H](CCC1=CC=CC=C1)N1[C@@H](CCCCNC(=O)C(F)(F)F)C(=O)OC1=O				1	1	1
126-71-6	126716	18	**triisobutyl phosphate**	3_REACH	Triisobutyl phosphate	Triisobutyl phosphate	C12H27O4P	C12H27O4P	266.32	CC(C)COP(=O)(OCC(C)C)OCC(C)C	InChI=1/C12H27O4P/c1-10(2)7-14-17(13,15-8-11(3)4)16-9-12(5)6/h10-12H,7-9H2,1-6H3	3.224	3.224	1	1	1
126-73-8	126738	19	**tributyl phosphate**	3_REACH	Tri-n-butylphosphate	Phosphoric acid, Tributyl ester	C12H27O4P	C12H27O4P	266.32	CCCCOP(=O)(OCCCC)OCCCC	InChI=1/C12H27O4P/c1-4-7-10-14-17(13,15-11-8-5-2)16-12-9-6-3/h4-12H2,1-3H3	3.634	3.634	1	1	1
127-47-9	127479	1812	**retinyl acetate**	3_REACH	Retinol, acetate	retinyl acetate	C22H32O2	C22H30O3	328.5	CC(=O)OC(=O)\C=C(/C)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C	InChI=1/C22H30O3/c1-16(9-7-10-17(2)15-21(24)25-19(4)23)12-13-20-18(3)11-8-14-22(20,5)6/h7,9-10,12-13,15H,8,11,14H2,1-6H3/b10-7+,13-12+,16-9+,17-15+	5.56	5.56	1	1	1
128-37-0	128370	413	**2,6-di-tert-butyl-p-cresol**	3_REACH	Butylated hydroxytoluene	2,6-bis(1,1-Dimethylethyl)-4-methylphenol	C15H24O	C15H24O	220.36	Cc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C	InChI=1/C15H24O/c1-10-8-11(14(2,3)4)13(16)12(9-10)15(5,6)7/h8-9,16H,1-7H3	4.874	4.874	1	1	1
128-39-2	128392	1820	**2,6-di-tert-butylphenol**	3_REACH	Phenol, 2,6-bis(1,1-dimethylethyl)-	2,6-di-tert-butylphenol	C14H22O	C14H22O	206.33	CC(C)(C)c1cccc(c1O)C(C)(C)C	InChI=1/C14H22O/c1-13(2,3)10-8-7-9-11(12(10)15)14(4,5)6/h7-9,15H,1-6H3	4.388	4.388	1	1	1
128-69-8	128698	1822	**perylene-3,4:9,10-tetracarboxylic dianhydride**	3_REACH	3,4,9,10-Perylenetetracarboxylic dianhydride	perylene-3,4:9,10-tetracarboxylic dianhydride	C24H8O6	C24H8O6	392.32	O=C1OC(=O)c2ccc3c4ccc5C(=O)OC(=O)c6ccc(c7ccc1c2c37)c4c56	InChI=1/C24H8O6/c25-21-13-5-1-9-10-2-6-15-20-16(24(28)30-23(15)27)8-4-12(18(10)20)11-3-7-14(22(26)29-21)19(13)17(9)11/h1-8H	3.801	3.801	1	1	1
129-00-0	129000	21	**pyrene**	3_REACH	Pyrene	Pyrene	C16H10	C16H10	202.26	c1cc2ccc3cccc4ccc(c1)c2c34	InChI=1/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H	3.945	3.945	1	1	1
129909-90-6	129909906	415	**Amicarbazone**	3_REACH		4-Amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide			241.3	CC(C)C1=NN(C(=O)N1N)C(=O)NC(C)(C)C	InChI=1S/C10H19N5O2/c1-6(2)7-13-15(9(17)14(7)11)8(16)12-10(3,4)5/h6H,11H2,1-5H3,(H,12,16)			1	1	1
13048-33-4	13048334	1837	**hexamethylene diacrylate**	3_REACH		hexamethylene diacrylate		C12H18O4	226.27	C=CC(=O)OCCCCCCOC(=O)C=C	InChI=1/C12H18O4/c1-3-11(13)15-9-7-5-6-8-10-16-12(14)4-2/h3-4H,1-2,5-10H2	2.81	2.81	1	1	1
130755-46-3	130755463	1842	**4,4'-dithiobis[5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1H-pyrazole]**	3_REACH		1H-Pyrazole-3-carbonitrile, 4,4'-dithiobis[5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-			704.3	C1=C(C=C(C(=C1Cl)N2C(=C(C(=N2)C#N)SSC3=C(N(N=C3C#N)C4=C(C=C(C=C4Cl)C(F)(F)F)Cl)N)N)Cl)C(F)(F)F	InChI=1S/C22H8Cl4F6N8S2/c23-9-1-7(21(27,28)29)2-10(24)15(9)39-19(35)17(13(5-33)37-39)41-42-18-14(6-34)38-40(20			1	1	1
13076-17-0	13076170	1843	**Lactide, D-**	3_REACH		1,4-Dioxane-2,5-dione, 3,6-dimethyl-, (3R,6R)-			144.13	CC1C(=O)OC(C(=O)O1)C	InChI=1S/C6H8O4/c1-3-5(7)10-4(2)6(8)9-3/h3-4H,1-2H3/t3-,4-/m1/s1			1	1	1
130841-23-5	130841235	1844	**Benzene,1,4-dichloro-2-(1,1,2,3,3,3-hexafluoropropoxy)-5-nitro-**	3_REACH		1,4-dichloro-2-(1,1,2,3,3,3-hexafluoropropoxy)-5-nitrobenzene			358.02	C1=C(C(=CC(=C1Cl)OC(C(C(F)(F)F)F)(F)F)Cl)[N+](=O)[O-]	InChI=1S/C9H3Cl2F6NO3/c10-3-2-6(4(11)1-5(3)18(19)20)21-9(16,17)7(12)8(13,14)15/h1-2,7H			1	1	1
131-11-3	131113	417	**dimethyl phthalate**	3_REACH	Dimethyl phthalate	1,2-Benzenedicarboxylic acid, Dimethyl ester	C10H10O4	C10H10O4	194.19	COC(=O)c1ccccc1C(=O)OC	InChI=1/C10H10O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-6H,1-2H3	1.54	1.54	1	1	1
131-17-9	131179	418	**diallyl phthalate**	3_REACH	1,2-Benzenedicarboxylic acid, di-2-propenyl ester	Phthalic acid diallylester	C14H14O4	C14H14O4	246.26	C=CCOC(=O)c1ccccc1C(=O)OCC=C	InChI=1/C14H14O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h3-8H,1-2,9-10H2	2.774	2.774	1	1	1
13122-18-4	13122184	1847	**tert-butyl 3,5,5-trimethylperoxyhexanoate**	3_REACH		tert-butyl 3,5,5-trimethylperoxyhexanoate		C13H26O8	230.35	COOC(CC(=O)OC(C)(C)C)CC(C)(OOC)OOC	InChI=1S/C13H26O8/c1-12(2,3)18-11(14)8-10(19-15-5)9-13(4,20-16-6)21-17-7/h10H,8-9H2,1-7H3	0.636	0.636	1	1	1
13127-18-9	13127189	1848	**Erythromycin oxime**	3_REACH		Erythromycin, 9-oxime			748.95	CCC1C(C(C(C(=NO)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C	InChI=1S/C37H68N2O13/c1-14-25-37(10,45)30(41)20(4)27(38-46)18(2)16-35(8,44)32(52-34-28(40)24(39(11)12)15-19(3)			1	1	1
1315251-11-6	1315251116	1849	**7,7,8,9,9-pentamethyl-6,7,8,9-tetrahydro-5H-cyclopenta[h]quinazoline**	3_REACH		7,7,8,9,9-pentamethyl-6,7,8,9-tetrahydro-5H-cyclopenta[h]quinazoline			242.37	C[C@H]1C(C)(C)C2=C(C3=NC=NC=C3CC2)C1(C)C	InChI=1S/C16H22N2/c1-10-15(2,3)12-7-6-11-8-17-9-18-14(11)13(12)16(10,4)5/h8-10H,6-7H2,1-5H3/t10-/m0/s1 AuxInfo=			1	1	1
131538-00-6	131538006	4321	**2,3-bis((2-mercaptoethyl)thio)-1-propanethiol**	3_REACH		2,3-bis((2-mercaptoethyl)thio)-1-propanethiol			260.52	C(CSCC(CS)SCCS)S	InChI=1S/C7H16S5/c8-1-3-11-6-7(5-10)12-4-2-9/h7-10H,1-6H2			1	1	1
131-56-6	131566	1850	**2,4-dihydroxybenzophenone**	3_REACH	Methanone, (2,4-dihydroxyphenyl)phenyl-	2,4-dihydroxybenzophenone	C13H10O3	C13H9O3	214.22	Oc1cc([O-])ccc1C(=O)c2ccccc2	InChI=1/C13H10O3/c14-10-6-7-11(12(15)8-10)13(16)9-4-2-1-3-5-9/h1-8,14-15H/p-1	2.046	2.427	1	1	1
131-57-7	131577	22	**oxybenzone**	3_REACH	Oxybenzone	(2-Hydroxy-4-methoxyphenyl)phenylmethanone	C14H12O3	C14H12O3	228.25	COc1ccc(C(=O)c2ccccc2)c(O)c1	InChI=1/C14H12O3/c1-17-11-7-8-12(13(15)9-11)14(16)10-5-3-2-4-6-10/h2-9,15H,1H3	2.975	2.971	1	1	1
13170-23-5	13170235	1851	**diacetoxydi-tert-butoxysilane**	3_REACH		diacetoxydi-tert-butoxysilane		C12H24O6Si	292.4	CC(=O)O[Si](OC(=O)C)(OC(C)(C)C)OC(C)(C)C	InChI=1/C12H24O6Si/c1-9(13)15-19(16-10(2)14,17-11(3,4)5)18-12(6,7)8/h1-8H3	3.488	3.488	1	1	1
132694-65-6	132694656	4685	**4-[4-[(1-Oxo-2-propenyl)oxy]butoxy]benzoic acid 1,4-phenylene ester**	3_REACH		Unknown			602.64					1	1	1

1333-07-9	1333079	1866	**toluenesulphonamide**	3_REACH		toluenesulphonamide		C7H9NO2S	171.22	Cc1ccccc1S(=O)(=O)N	InChI=1/C7H9NO2S/c1-6-4-2-3-5-7(6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)	1.021	1.021	1	1	1
133467-41-1	133467411	4415	**4-[4-(2-ethylhexyloxy)phenyl](1,4-thiazinane-1,1-dioxide)**	3_REACH		4-[4-(2-ethylhexyloxy)phenyl](1,4-thiazinane-1,1-dioxide)			339.5	CCCCC(CC)COC1=CC=C(C=C1)N2CCS(CC2)([O-])[O-]	InChI=1S/C18H31NO3S/c1-3-5-6-16(4-2)15-22-18-9-7-17(8-10-18)19-11-13-23(20,21)14-12-19/h7-10,16,20-21H,3-6,11-1			1	1	1
13361-34-7	13361347	1870	**2-ethylhexyl cyanoacetate**	3_REACH	Acetic acid, cyano-, 2-ethylhexyl ester	2-ethylhexyl cyanoacetate	C11H19NO2	C11H19NO2	197.28	CCCCC(CC)COC(=O)CC#N	InChI=1/C11H19NO2/c1-3-5-6-10(4-2)9-14-11(13)7-8-12/h10H,3-7,9H2,1-2H3	3.097	3.097	1	1	1
133636-82-5	133636825	4540	**Spiro[bicyclo[3.1.1]heptane-3,1'-[2]cyclohexen]-4'-one, 2,6,6-trimethyl-, (1S,1'S,2S,5R)-**	3_REACH		(+)-(1S,2S,3S,5R)-2,6,6-Trimethylbicyclo(3.1.1)heptane-3-spiro-1'-(cyclohex-2'-en-4'-one)			218.34	CC1C2CC(C2(C)C)CC13CCC(=O)C=C3	InChI=1S/C15H22O/c1-10-13-8-11(14(13,2)3)9-15(10)6-4-12(16)5-7-15/h4,6,10-11,13H,5,7-9H2,1-3H3/t10-,11+,13-,15-/m			1	1	1
133-91-5	133915	1872	**3,5-diiodosalicylic acid**	3_REACH	3,5-Diiodo-2-hydroxybenzoic acid	3,5-diiodosalicylic acid	C7H4I2O3	C7H2I2O3	389.91	[O-]C(=O)c1cc(I)cc(I)c1[O-]	InChI=1/C7H4I2O3/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2,10H,(H,11,12)/p-2	0.196	0.9	1	1	1
13393-93-6	13393936	1873	**tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol**	3_REACH		tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol		C20H36O	292.51	CC(C)C1CCC2C(CCC3C(C)(CO)CCCC23C)C1	InChI=1/C20H36O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/h14-18,21H,5-13H2,1-4H3	5.359	5.359	1	1	1
13402-02-3	13402023	1875	**hexadecyl acrylate**	3_REACH	2-Propenoic acid, hexadecyl ester	hexadecyl acrylate	C19H36O2	C19H36O2	296.5	CCCCCCCCCCCCCCCCOC(=O)C=C	InChI=1/C19H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-19(20)4-2/h4H,2-3,5-18H2,1H3	7.521	7.521	1	1	1
134605-64-4	134605644	433	**1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl]benzoate**	3_REACH		2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]benzoic acid 1,1-dimethyl-2-oxo-2-(2-propenyloxy)ethyl ester			474.82	CC(C)(C(=O)OCC=C)OC(=O)C1=C(C=CC(=C1)N2C(=O)C=C(N(C2=O)C)C(F)(F)F)Cl	InChI=1S/C20H18ClF3N2O6/c1-5-8-31-17(29)19(2,3)32-16(28)12-9-11(6-7-13(12)21)26-15(27)10-14(20(22,23)24)25(4)1			1	1	1
134701-20-5	134701205	4329	**2,4-dimethyl-6-(1-methyl-pentadecyl)phenol**	3_REACH		2,4-dimethyl-6-(1-methyl-pentadecyl)phenol			346.6	CCCCCCCCCCCCCCC(C)C1=CC(=CC(=C1O)C)C	InChI=1S/C24H42O/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21(3)23-19-20(2)18-22(4)24(23)25/h18-19,21,25H,5-17H2,1-4			0	0	1
13472-08-7	13472087	1882	**2,2'-azobis[2-methylbutyronitrile]**	3_REACH		2,2'-azobis[2-methylbutyronitrile]		C10H16N4	192.27	CCC(C)(N=NC(C)(CC)C#N)C#N	InChI=1/C10H16N4/c1-5-9(3,7-11)13-14-10(4,6-2)8-12/h5-6H2,1-4H3	3.146	3.146	1	1	1
13501-76-3	13501763	1885	**(3-chloropropyl)diethoxymethylsilane**	3_REACH		(3-chloropropyl)diethoxymethylsilane		C8H19ClO2Si	209.77	CCOC([SiH3])(CCCCl)OCC	InChI=1/C8H19ClO2Si/c1-3-10-8(12,11-4-2)6-5-7-9/h3-7H2,1-2,12H3	5.653	5.653	1	1	1
13515-40-7	13515407	1887	**2-[(4-chloro-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide**	3_REACH		2-[(4-chloro-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide		C17H15ClN4O5	390.79	COc1ccccc1NC(=O)C(N=Nc2ccc(Cl)cc2[N+](=O)[O-])C(=O)C	InChI=1/C17H15ClN4O5/c1-10(23)16(17(24)19-13-5-3-4-6-15(13)27-2)21-20-12-8-7-11(18)9-14(12)22(25)26/h3-9,16H,1-2H3,(H,19,24)	3.732	3.732	1	1	1
135-19-3	135193	435	**2-naphthol**	3_REACH	2-Naphthalenol	2-Naphthol	C10H8O	C10H8O	144.17	Oc1ccc2ccccc2c1	InChI=1/C10H8O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7,11H	2.496	2.494	1	1	1
135590-91-9	135590919	436	**1-(2,4-Dichlorophenyl)-4,5-dihydro-5-methyl-1H-pyrazole-3,5-dicarboxylic acid 3,5-diethyl ester**	3_REACH		1-(2,4-Dichlorophenyl)-4,5-dihydro-5-methyl-1H-pyrazole-3,5-dicarboxylic acid 3,5-diethyl ester			373.24	CCOC(=O)C1=NN(C(C1)(C)C(=O)OCC)C2=C(C=C(C=C2)Cl)Cl	InChI=1S/C16H18Cl2N2O4/c1-4-23-14(21)12-9-16(3,15(22)24-5-2)20(19-12)13-7-6-10(17)8-11(13)18/h6-8H,4-5,9H2,1-3H3			1	1	1
136210-30-5	136210305	4527	**1,4-diethyl 2-{[4-({4-[(1,4-diethoxy-1,4-dioxobutan-2-yl)amino]cyclohexyl}methyl)cyclohexyl]amino}butanedioate**	3_REACH		Aspartic acid, N,N'-(methylenedi-4,1-cyclohexanediyl)bis-, 1,1',4,4'-tetraethyl ester			554.73	CCOC(=O)CC(C(=O)OCC)NC1CCC(CC1)CC2CCC(CC2)NC(CC(=O)OCC)C(=O)OCC	InChI=1S/C29H50N2O8/c1-5-36-26(32)18-24(28(34)38-7-3)30-22-13-9-20(10-14-22)17-21-11-15-23(16-12-21)31-25(29(3			1	1	1
136239-66-2	136239662	4294	**1-butoxy-2,3-difluorobenzene**	3_REACH		1-butoxy-2,3-difluorobenzene			186.2	CCCCOC1=C(C(=CC=C1)F)F	InChI=1S/C10H12F2O/c1-2-3-7-13-9-6-4-5-8(11)10(9)12/h4-6H,2-3,7H2,1H3			1	1	1
136465-81-1	136465811	4454	**PHIQ**	3_REACH		3-Isoquinolinecarboxamide, N-(1,1-dimethylethyl)decahydro-, (3S,4aS,8aS)-			238.38	CC(C)(C)NC(=O)C1CC2CCCCC2CN1	InChI=1S/C14H26N2O/c1-14(2,3)16-13(17)12-8-10-6-4-5-7-11(10)9-15-12/h10-12,15H,4-9H2,1-3H3,(H,16,17)/t10-,11+,12			1	1	1
1364731-90-7	1364731907	1900	**2,6-dimethylphenyl 4-hydroxybenzenesulfonate**	3_REACH		2,6-dimethylphenyl 4-hydroxybenzenesulfonate			278.33	Cc1cccc(c1OS(=O)(=O)c2ccc(cc2)O)C	InChI=1S/C14H14O4S/c1-10-4-3-5-11(2)14(10)18-19(16,17)13-8-6-12(15)7-9-13/h3-9,15H,1-2H3			1	1	1
13674-84-5	13674845	24	**tris(2-chloro-1-methylethyl) phosphate**	3_REACH		Tris(2-chloroethyl) phosphate		C9H18Cl3O4P	327.57	CC(CCl)OP(=O)(OC(C)CCl)OC(C)CCl	InChI=1/C9H18Cl3O4P/c1-7(4-10)14-17(13,15-8(2)5-11)16-9(3)6-12/h7-9H,4-6H2,1-3H3	2.776	2.776	1	1	1
13674-87-8	13674878	25	**tris[2-chloro-1-(chloromethyl)ethyl] phosphate**	3_REACH	Tris(1,3-dichloro-2-propyl) phosphate	1,3-Dichloro-2-propanol phosphate (3:1)	C9H15Cl6O4P	C9H15Cl6O4P	430.91	ClCC(CCl)OP(=O)(OC(CCl)CCl)OC(CCl)CCl	InChI=1/C9H15Cl6O4P/c10-1-7(2-11)17-20(16,18-8(3-12)4-13)19-9(5-14)6-15/h7-9H,1-6H2	3.726	3.726	1	1	1
13749-61-6	13749616	1909	**N-isopropylmethacrylamide**	3_REACH		N-isopropylmethacrylamide		C7H13NO	127.19	CC(C)NC(=O)C(=C)C	InChI=1/C7H13NO/c1-5(2)7(9)8-6(3)4/h6H,1H2,2-4H3,(H,8,9)	1.244	1.244	1	1	1
13752-51-7	13752517	1911	**4-[(morpholinothio)thioxomethyl]morpholine**	3_REACH		4-[(morpholinothio)thioxomethyl]morpholine		C9H16N2O2S2	248.37	S=C(SN1CCOCC1)N2CCOCC2	InChI=1/C9H16N2O2S2/c14-9(10-1-5-12-6-2-10)15-11-3-7-13-8-4-11/h1-8H2	1.294	1.294	1	1	1
137863-20-8	137863208	1913	**Valsartan benzyl ester**	3_REACH		L-Valine, N-(1-oxopentyl)-N-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, phenylmethyl ester			525.66	CCCCC(=O)N(CC1=CC=C(C=C1)C2=CC=CC=C2C3=NNN=N3)C(C(C)C)C(=O)OCC4=CC=CC=C4	InChI=1S/C31H35N5O3/c1-4-5-15-28(37)36(29(22(2)3)31(38)39-21-24-11-7-6-8-12-24)20-23-16-18-25(19-17-23)26-13-9-			1	1	1
138564-59-7	138564597	4458	**5-methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile**	3_REACH		3-Thiophenecarbonitrile, 5-methyl-2-[(2-nitrophenyl)amino]-			259.283	CC1=CC(=C(S1)NC2=CC=CC=C2[N+](=O)[O-])C#N	InChI=1S/C12H9N3O2S/c1-8-6-9(7-13)12(18-8)14-10-4-2-3-5-11(10)15(16)17/h2-6,14H,1H3			1	1	1
138-59-0	138590	445	**(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid**	3_REACH	Shikimic acid	Shikimic acid	C7H10O5	C7H9O5	174.15	O[C@@H]1CC(=C[C@@H](O)[C@H]1O)C(=O)[O-]	InChI=1/C7H10O5/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1,4-6,8-10H,2H2,(H,11,12)/p-1/t4-,5-,6-/m1/s1	-2.628	-2.624	1	1	1
139007-06-0	139007060	1915	**(E)-2-Ethoxy-N-(2-methyl-1-phenylpropylidene)ethylamine**	3_REACH		Ethanamine, 2-ethoxy-N-(2-methyl-1-phenylpropylidene)-			219.33	CCOCCN=C(C(C)C)c1ccccc1	InChI=1/C14H21NO/c1-4-16-11-10-15-14(12(2)3)13-8-6-5-7-9-13/h5-9,12H,4,10-11H2,1-3H3			1	1	1
139122-17-1	139122171	4737	**2-(3-chloro-2-oxo-2,3-dihydro-1H-indol-4-yl) ethyl benzoate**	3_REACH		2-(3-chloro-2-oxo-2,3-dihydro-1H-indol-4-yl) ethyl benzoate			315.76	C1=CC=C(C=C1)C(=O)OCCC2=C3C(C(=O)NC3=CC=C2)Cl	InChI=1S/C17H14ClNO3/c18-15-14-11(7-4-8-13(14)19-16(15)20)9-10-22-17(21)12-5-2-1-3-6-12/h1-8,15H,9-10H2,(H,19,20)			1	1	1
139-13-9	139139	27	**nitrilotriacetic acid**	3_REACH	Nitrilotriacetic acid	Nitrilotriacetic acid	C6H9NO6	C6H7NO6	191.14	[O-]C(=O)C[NH+](CC(=O)[O-])CC(=O)[O-]	InChI=1/C6H9NO6/c8-4(9)1-7(2-5(10)11)3-6(12)13/h1-3H2,(H,8,9)(H,10,11)(H,12,13)/p-2	-7.219	-7.191	1	1	1
139189-30-3	139189303	4566	**Phosphoric acid, P,P'-1,3-phenylene P,P,P',P'-tetrakis(2,6-dimethylphenyl) ester**	3_REACH		Phosphoric acid, P,P'-1,3-phenylene P,P,P',P' tetrakis(2,6-dimethylphenyl) ester			686.68	CC1=C(C(=CC=C1)C)OP(=O)(OC2=CC(=CC=C2)OP(=O)(OC3=C(C=CC=C3C)C)OC4=C(C=CC=C4C)C)OC5=C(C=CC	InChI=1S/C38H40O8P2/c1-25-14-9-15-26(2)35(25)43-47(39,44-36-27(3)16-10-17-28(36)4)41-33-22-13-23-34(24-33)42-4			0	0	1
139504-68-0	139504680	4286	**1-[(2-tert-butylcyclohexyl)oxy]butan-2-ol**	3_REACH		1-[(2-tert-butylcyclohexyl)oxy]butan-2-ol			228.38	CCC(COC1CCCCC1C(C)(C)C)O	InChI=1S/C14H28O2/c1-5-11(15)10-16-13-9-7-6-8-12(13)14(2,3)4/h11-13,15H,5-10H2,1-4H3			1	1	1
140-11-4	140114	448	**benzyl acetate**	3_REACH	Benzyl ethanoate	Benzyl acetate	C9H10O2	C9H10O2	150.18	CC(=O)OCc1ccccc1	InChI=1/C9H10O2/c1-8(10)11-7-9-5-3-2-4-6-9/h2-6H,7H2,1H3	1.604	1.604	1	1	1
140-29-4	140294	1926	**phenylacetonitrile**	3_REACH	Benzeneacetonitrile	phenylacetonitrile	C8H7N	C8H7N	117.15	N#CCc1ccccc1	InChI=1/C8H7N/c9-7-6-8-4-2-1-3-5-8/h1-5H,6H2	1.743	1.743	1	1	1
140-31-8	140318	449	**2-piperazin-1-ylethylamine**	3_REACH	N-(2-Aminoethyl)piperazine	1-(2-Aminoethyl)piperazine	C6H15N3	C6H17N3	129.21	[NH3+]CCN1CC[NH2+]CC1	InChI=1/C6H15N3/c7-1-4-9-5-2-8-3-6-9/h8H,1-7H2/p+2	-3.323	-2.951	1	1	1
14064-10-9	14064109	450	**diethyl chloromalonate**	3_REACH		Diethyl chloromalonate		C7H10ClO4	194.61	CCOC(=O)[C-](Cl)C(=O)OCC	InChI=1/C7H10ClO4/c1-3-11-6(9)5(8)7(10)12-4-2/h3-4H2,1-2H3/q-1	1.464	1.462	1	1	1
140-66-9	140669	451	**4-(1,1,3,3-tetramethylbutyl)phenol**	3_REACH	Phenol, 4-(1,1,3,3-tetramethylbutyl	4-(1,1,3,3-Tetramethylbutyl)phenol	C14H22O	C14H22O	206.33	CC(C)(C)CC(C)(C)c1ccc(O)cc1	InChI=1/C14H22O/c1-13(2,3)10-14(4,5)11-6-8-12(15)9-7-11/h6-9,15H,10H2,1-5H3	4.358	4.358	1	1	1
14073-97-3	14073973	1929	**L-menthan-3-one**	3_REACH		L-menthan-3-one		C10H18O	154.25	CC(C)C1CCC(C)CC1=O	InChI=1/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-9H,4-6H2,1-3H3	2.736	2.736	1	1	1
14078-41-2	14078412	1930	**3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diol**	3_REACH		3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diol			358.48	CC(C)(C)C1=C(C(=CC(=C1)OC)C2=CC(=CC(=C2O)C(C)(C)C)OC)O	InChI=1S/C22H30O4/c1-21(2,3)17-11-13(25-7)9-15(19(17)23)16-10-14(26-8)12-18(20(16)24)22(4,5)6/h9-12,23-24H,1-8H3			1	1	1
141-05-9	141059	454	**diethyl maleate**	3_REACH	2-Butenedioic acid (Z)-, diethyl ester	Diethyl maleate	C8H12O4	C8H12O4	172.18	CCOC(=O)\C=C/C(=O)OCC	InChI=1/C8H12O4/c1-3-11-7(9)5-6-8(10)12-4-2/h5-6H,3-4H2,1-2H3/b6-5-	1.187	1.187	1	1	1
141-10-6	141106	1932	**6,10-dimethylundeca-3,5,9-trien-2-one**	3_REACH	3,5,9-Undecatrien-2-one, 6,10-dimethyl-	6,10-dimethylundeca-3,5,9-trien-2-one	C13H20O	C13H20O	192.3	CC(=CCCC(=CC=CC(=O)C)C)C	InChI=1/C13H20O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h6-7,9-10H,5,8H2,1-4H3	3.736	3.736	1	1	1
141-17-3	141173	1933	**bis(2-(2-butoxyethoxy)ethyl) adipate**	3_REACH	Hexanedioic acid, bis[2-(2-butoxyethoxy)ethyl] ester	bis(2-(2-butoxyethoxy)ethyl) adipate	C22H42O8	C22H42O8	434.57	CCCCOCCOCCOC(=O)CCCCC(=O)OCCOCCOCCCC	InChI=1/C22H42O8/c1-3-5-11-25-13-15-27-17-19-29-21(23)9-7-8-10-22(24)30-20-18-28-16-14-26-12-6-4-2/h3-20H2,1-2H3	3.138	3.138	1	1	1
141-18-4	141184	1934	**bis(2-butoxyethyl) adipate**	3_REACH	di(Butoxyethyl)adipate	bis(2-butoxyethyl) adipate	C18H34O6	C18H34O6	346.46	CCCCOCCOC(=O)CCCCC(=O)OCCOCCCC	InChI=1/C18H34O6/c1-3-5-11-21-13-15-23-17(19)9-7-8-10-18(20)24-16-14-22-12-6-4-2/h3-16H2,1-2H3	3.4	3.4	1	1	1
141-27-5	141275	1935	**(E)-3,7-dimethylocta-2,6-dienal**	3_REACH	2,6-Octadienal, 3,7-dimethyl-, (E)-	(E)-3,7-dimethylocta-2,6-dienal	C10H16O	C10H16O	152.24	CC(=CCC\C(=C\C=O)\C)C	InChI=1/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5,7-8H,4,6H2,1-3H3/b10-7+	3.19	3.19	1	1	1
141-62-8	141628	1939	**decamethyltetrasiloxane**	3_REACH	Tetrasiloxane, decamethyl-	decamethyltetrasiloxane	C10H30O3Si4	C10H30O3Si4	310.69	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	InChI=1/C10H30O3Si4/c1-14(2,3)11-16(7,8)13-17(9,10)12-15(4,5)6/h1-10H3	7.098	7.098	1	1	1
141-63-9	141639	1940	**dodecamethylpentasiloxane**	3_REACH	Dodecamethylpentasiloxane	dodecamethylpentasiloxane	C12H36O4Si5	C12H36O4Si5	384.85	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	InChI=1/C12H36O4Si5/c1-17(2,3)13-19(7,8)15-21(11,12)16-20(9,10)14-18(4,5)6/h1-12H3	8.821	8.821	1	1	1
141-97-9	141979	459	**ethyl acetoacetate**	3_REACH	Butanoic acid, 3-oxo-, ethyl ester	3-Oxobutanoic acid, Ethyl ester	C6H10O3	C6H9O3	130.14	CCOC(=O)[CH-]C(=O)C	InChI=1/C6H9O3/c1-3-9-6(8)4-5(2)7/h4H,3H2,1-2H3/q-1	0.769	0.676	1	1	1
141-98-0	141980	460	**O-isopropyl ethylthiocarbamate**	3_REACH		Isopropyl ethylthionocarbamate		C6H13NOS	147.24	CCNC(=S)OC(C)C	InChI=1/C6H13NOS/c1-4-7-6(9)8-5(2)3/h5H,4H2,1-3H3,(H,7,9)	2.185	2.185	1	1	1
142-16-5	142165	1948	**bis(2-ethylhexyl) maleate**	3_REACH	2-Butenedioic acid (z), di-2-ethylhexyl ester	bis(2-ethylhexyl) maleate	C20H36O4	C20H36O4	340.5	CCCCC(CC)COC(=O)\C=C/C(=O)OCC(CC)CCCC	InChI=1/C20H36O4/c1-5-9-11-17(7-3)15-23-19(21)13-14-20(22)24-16-18(8-4)12-10-6-2/h13-14,17-18H,5-12,15-16H2,1-4H3/b14-13-	6.523	6.523	1	1	1
142-19-8	142198	1950	**allyl heptanoate**	3_REACH	Allyl heptanoate	allyl heptanoate	C10H18O2	C10H18O2	170.25	CCCCCCC(=O)OCC=C	InChI=1/C10H18O2/c1-3-5-6-7-8-10(11)12-9-4-2/h4H,2-3,5-9H2,1H3	3.129	3.129	1	1	1
14246-53-8	14246538	1956	**N-(1-oxooctyl)glycine**	3_REACH		N-(1-oxooctyl)glycine		C10H18NO3	201.27	CCCCCCCC(=O)NCC(=O)[O-]	InChI=1/C10H19NO3/c1-2-3-4-5-6-7-9(12)11-8-10(13)14/h2-8H2,1H3,(H,11,12)(H,13,14)/p-1	0.329	0.331	1	1	1
142-62-1	142621	462	**hexanoic acid**	3_REACH	Hexanoic acid	Hexanoic acid	C6H12O2	C6H11O2	116.16	CCCCCC(=O)[O-]	InChI=1/C6H12O2/c1-2-3-4-5-6(7)8/h2-5H2,1H3,(H,7,8)/p-1	0.356	0.382	1	1	1
142-90-5	142905	465	**dodecyl methacrylate**	3_REACH	2-Propenoic acid, 2-methyl-, dodecyl ester	2-Methyl-2-propenoic acid, Dodecyl ester	C16H30O2	C16H30O2	254.41	CCCCCCCCCCCCOC(=O)C(=C)C	InChI=1/C16H30O2/c1-4-5-6-7-8-9-10-11-12-13-14-18-16(17)15(2)3/h2,4-14H2,1,3H3	6.143	6.143	1	1	1
142-91-6	142916	1957	**isopropyl palmitate**	3_REACH	Isopropyl palmitate	isopropyl palmitate	C19H38O2	C19H38O2	298.51	CCCCCCCCCCCCCCCC(=O)OC(C)C	InChI=1/C19H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19(20)21-18(2)3/h18H,4-17H2,1-3H3	7.344	7.344	1	1	1
142-92-7	142927	466	**hexyl acetate**	3_REACH	Hexyl ethanoate	Hexyl acetate	C8H16O2	C8H16O2	144.21	CCCCCCOC(=O)C	InChI=1/C8H16O2/c1-3-4-5-6-7-10-8(2)9/h3-7H2,1-2H3	2.262	2.262	1	1	1
143-07-7	143077	468	**lauric acid**	3_REACH	Dodecanoic acid	Dodecanoic acid	C12H24O2	C12H23O2	200.32	CCCCCCCCCCCC(=O)[O-]	InChI=1/C12H24O2/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h2-11H2,1H3,(H,13,14)/p-1	3.094	3.119	1	1	1
143-08-8	143088	469	**nonan-1-ol**	3_REACH	1-Nonanol	1-Nonanol	C9H20O	C9H20O	144.26	CCCCCCCCCO	InChI=1/C9H20O/c1-2-3-4-5-6-7-8-9-10/h10H,2-9H2,1H3	3.251	3.251	1	1	1
143-22-6	143226	1959	**2-(2-(2-butoxyethoxy)ethoxy)ethanol**	3_REACH	Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	2-(2-(2-butoxyethoxy)ethoxy)ethanol	C10H22O4	C10H22O4	206.28	CCCCOCCOCCOCCO	InChI=1/C10H22O4/c1-2-3-5-12-7-9-14-10-8-13-6-4-11/h11H,2-10H2,1H3	0.578	0.578	1	1	1
143-24-8	143248	28	**bis(2-(2-methoxyethoxy)ethyl) ether**	3_REACH	CH3O[CH2CH2O]4CH3	bis(2-(2-methoxyethoxy)ethyl) ether	C10H22O5	C10H22O5	222.28	COCCOCCOCCOCCOC	InChI=1/C10H22O5/c1-11-3-5-13-7-9-15-10-8-14-6-4-12-2/h3-10H2,1-2H3	-0.474	-0.474	1	1	1
143-28-2	143282	1962	**(Z)-octadec-9-enol**	3_REACH	Oleyl Alcohol	(Z)-octadec-9-enol	C18H36O	C18H36O	268.49	CCCCCCCC\C=C/CCCCCCCCO	InChI=1/C18H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h9-10,19H,2-8,11-18H2,1H3/b10-9-	6.912	6.912	1	1	1
14338-82-0	14338820	1965	**dibutyl methylenedithiodi(acetate)**	3_REACH		dibutyl methylenedithiodi(acetate)		C13H24O4S2	308.46	CCCCOC(=O)CSCSCC(=O)OCCCC	InChI=1/C13H24O4S2/c1-3-5-7-16-12(14)9-18-11-19-10-13(15)17-8-6-4-2/h3-11H2,1-2H3	3.462	3.462	1	1	1
144-19-4	144194	1974	**2,2,4-trimethylpentane-1,3-diol**	3_REACH	1,3-Pentanediol, 2,2,4-trimethyl-	2,2,4-trimethylpentane-1,3-diol	C8H18O2	C8H18O2	146.23	CC(C)C(O)C(C)(C)CO	InChI=1/C8H18O2/c1-6(2)7(10)8(3,4)5-9/h6-7,9-10H,5H2,1-4H3	1.237	1.237	1	1	1
14433-76-2	14433762	471	**N,N-dimethyldecan-1-amide**	3_REACH	N,N-Dimethyldecanamide	N,N-Dimethyldecanamide	C12H25NO	C12H25NO	199.34	CCCCCCCCCC(=O)N(C)C	InChI=1/C12H25NO/c1-4-5-6-7-8-9-10-11-12(14)13(2)3/h4-11H2,1-3H3	3.439	3.439	1	1	1
144-62-7	144627	472	**oxalic acid**	3_REACH	Oxalic acid	Oxalic acid	C2H2O4	C2O4	90.034	[O-]C(=O)C(=O)[O-]	InChI=1/C2H2O4/c3-1(4)2(5)6/h(H,3,4)(H,5,6)/p-2	-3.377	-3.359	1	1	1
144-83-2	144832	29	**sulfapyridine**	3_REACH	Sulfapyridine	4-Amino-N-2-pyridinylbenzenesulfonamide	C11H11N3O2S	C11H11N3O2S	249.29	Nc1ccc(cc1)S(=O)(=O)Nc2ccccn2	InChI=1/C11H11N3O2S/c12-9-4-6-10(7-5-9)17(15,16)14-11-3-1-2-8-13-11/h1-8H,12H2,(H,13,14)	0.959	0.955	1	1	1
1453-58-3	1453583	1985	**3-methylpyrazole**	3_REACH	3(5)-methylpyrazole	3-methylpyrazole	C4H6N2	C4H6N2	82.108	Cc1cc[nH]n1	InChI=1/C4H6N2/c1-4-2-3-5-6-4/h2-3H,1H3,(H,5,6)	0.556	0.556	1	1	1
145783-14-8	145783148	1988	**4,6-dichloro-5-nitro-2-(propylthio)pyrimidine**	3_REACH		4,6-dichloro-5-nitro-2-(propylthio)pyrimidine			268.13	CCCSC1=NC(=C(C(=N1)Cl)[N+](=O)[O-])Cl	InChI=1S/C7H7Cl2N3O2S/c1-2-3-15-7-10-5(8)4(12(13)14)6(9)11-7/h2-3H2,1H3			1	1	1
1459-93-4	1459934	1990	**dimethyl isophthalate**	3_REACH	1,3-Benzenedicarboxylic acid dimethyl ester	dimethyl isophthalate	C10H10O4	C10H10O4	194.19	COC(=O)c1cccc(c1)C(=O)OC	InChI=1/C10H10O4/c1-13-9(11)7-4-3-5-8(6-7)10(12)14-2/h3-6H,1-2H3	1.54	1.54	1	1	1
146421-65-0	146421650	4455	**URACROSS P 3307**	3_REACH		URACROSS P 3307			400.52	C=COCCCCOC(=O)NCCCCCCNC(=O)OCCCCOC=C	InChI=1S/C20H36N2O6/c1-3-25-15-9-11-17-27-19(23)21-13-7-5-6-8-14-22-20(24)28-18-12-10-16-26-4-2/h3-4H,1-2,5-18H			1	1	1
14657-64-8	14657648	4379	**3-(hydroxyphenylphosphinyl)propanoic acid**	3_REACH		3-(hydroxyphenylphosphinyl)propanoic acid			214.16	C1=CC=C(C=C1)P(=O)(CCC(=O)O)O	InChI=1S/C9H11O4P/c10-9(11)6-7-14(12,13)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,11)(H,12,13)			1	1	1
147315-50-2	147315502	4308	**2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-((hexyl)oxy)phenol**	3_REACH		2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-((hexyl)oxy)phenol			425.54	CCCCCCOC1=CC(=O)C(=C2NC(=NC(=N2)C3=CC=CC=C3)C4=CC=CC=C4)C=C1	InChI=1S/C27H27N3O2/c1-2-3-4-11-18-32-22-16-17-23(24(31)19-22)27-29-25(20-12-7-5-8-13-20)28-26(30-27)21-14-9-6-			1	1	1
147504-92-5	147504925	4409	**4,6-bis[2-(4-hydroxyphenyl)isopropylidene]resorcinol**	3_REACH		4,6-bis[2-(4-hydroxyphenyl)isopropylidene]resorcinol			378.47	CC(C)(C1=CC=C(C=C1)O)C2=CC(=C(C=C2O)O)C(C)(C)C3=CC=C(C=C3)O	InChI=1S/C24H26O4/c1-23(2,15-5-9-17(25)10-6-15)19-13-20(22(28)14-21(19)27)24(3,4)16-7-11-18(26)12-8-16/h5-14,25-			1	1	1
1477-55-0	1477550	1997	**m-phenylenebis(methylamine)**	3_REACH	1,3-Benzenedimethanamine	m-phenylenebis(methylamine)	C8H12N2	C8H12N2	136.2	CNc1cccc(NC)c1	InChI=1/C8H12N2/c1-9-7-4-3-5-8(6-7)10-2/h3-6,9-10H,1-2H3	1.447	1.416	1	1	1
147-85-3	147853	1999	**L-proline**	3_REACH	Proline	L-proline	C5H9NO2	C5H9NO2	115.13	[O-]C(=O)[C@@H]1CCC[NH2+]1	InChI=1/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)/t4-/m0/s1	-2.843	-2.843	1	1	1
14814-09-6	14814096	2001	**3-(triethoxysilyl)propanethiol**	3_REACH		3-(triethoxysilyl)propanethiol		C9H22O3SSi	238.42	CCO[Si](CCCS)(OCC)OCC	InChI=1/C9H22O3SSi/c1-4-10-14(11-5-2,12-6-3)9-7-8-13/h13H,4-9H2,1-3H3	3.824	3.824	1	1	1
148528-05-6	148528056	2002	**2-Methyloctane-1,8-diamine**	3_REACH		2-Methyloctane-1,8-diamine			158.29	CC(CCCCCCN)CN	InChI=1S/C9H22N2/c1-9(8-11)6-4-2-3-5-7-10/h9H,2-8,10-11H2,1H3			1	1	1
14858-73-2	14858732	2004	**bis(2-ethylhexyl) carbonate**	3_REACH	Carbonic acid, bis(2-ethylhexyl) ester	bis(2-ethylhexyl) carbonate	C17H34O3	C17H34O3	286.46	CCCCC(CC)COC(=O)OCC(CC)CCCC	InChI=1/C17H34O3/c1-5-9-11-15(7-3)13-19-17(18)20-14-16(8-4)12-10-6-2/h15-16H,5-14H2,1-4H3	6.697	6.697	1	1	1
14901-07-6	14901076	477	**4-(2,6,6-trimethylcyclohex-1-ene-1-yl)but-3-ene-2-one**	3_REACH	4-(2,6,6-Trimethylcyclohex-1-en-1-yl)but-3-en-2-one	4-(2,6,6-trimethylcyclohex-1-ene-1-yl)but-3-ene-2-one	C13H20O	C13H20O	192.3	CC(=O)C=CC1=C(C)CCCC1(C)C	InChI=1/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8H,5-6,9H2,1-4H3	3.355	3.355	1	1	1
149-30-4	149304	478	**benzothiazole-2-thiol**	3_REACH	2-Mercaptobenzothiazole	2-Mercaptobenzothiazole	C7H5NS2	C7H4NS2	167.25	[S-]c1nc2ccccc2s1	InChI=1/C7H5NS2/c9-7-8-5-3-1-2-4-6(5)10-7/h1-4H,(H,8,9)/p-1	2.895	2.815	1	1	1
1493-13-6	1493136	2005	**trifluoromethanesulphonic acid**	3_REACH	CF3SO3H	trifluoromethanesulphonic acid	CHF3O3S	CF3O3S	150.07	[O-]S(=O)(=O)C(F)(F)F	InChI=1/CHF3O3S/c2-1(3,4)8(5,6)7/h(H,5,6,7)/p-1	-0.523	-0.523	1	1	1
149-57-5	149575	479	**2-ethylhexanoic acid**	3_REACH	Hexanoic acid, 2-ethyl-	2-Ethylhexanoic acid	C8H16O2	C8H15O2	144.21	CCCCC(CC)C(=O)[O-]	InChI=1/C8H16O2/c1-3-5-6-7(4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)/p-1	1.275	1.337	1	1	1
149-74-6	149746	2006	**dichloro(methyl)(phenyl)silane**	3_REACH	Silane, dichloromethylphenyl-	dichloro(methyl)(phenyl)silane	C7H8Cl2Si	C7H8Cl2Si	191.13	C[Si](Cl)(Cl)c1ccccc1	InChI=1/C7H8Cl2Si/c1-10(8,9)7-5-3-2-4-6-7/h2-6H,1H3	4.271	4.271	1	1	1
149850-30-6	149850306	5029	**methyl N-[3-acetylamino)-4-(2-cyano-4-nitrophenylazo)phenyl]-N-[(1-methoxy)acetyl]glycinate**	3_REACH		methyl N-[3-acetylamino)-4-(2-cyano-4-nitrophenylazo)phenyl]-N-[(1-methoxy)acetyl]glycinate			468.43	CC(=O)NC1=C(C=CC(=C1)N(CC(=O)OC)CC(=O)OC)N=NC2=C(C=C(C=C2)[N+](=O)[O-])C#N	InChI=1S/C21H20N6O7/c1-13(28)23-19-9-15(26(11-20(29)33-2)12-21(30)34-3)4-7-18(19)25-24-17-6-5-16(27(31)32)8-14(			1	1	1
150-76-5	150765	483	**mequinol**	3_REACH	Mequinol	4-Methoxyphenol	C7H8O2	C7H8O2	124.14	COc1ccc(O)cc1	InChI=1/C7H8O2/c1-9-7-4-2-6(8)3-5-7/h2-5,8H,1H3	1.571	1.571	1	1	1
150-78-7	150787	484	**1,4-dimethoxybenzene**	3_REACH	Benzene, 1,4-dimethoxy-	1,4-Dimethoxybenzene	C8H10O2	C8H10O2	138.17	COc1ccc(OC)cc1	InChI=1/C8H10O2/c1-9-7-3-5-8(10-2)6-4-7/h3-6H,1-2H3	1.797	1.797	1	1	1
150-84-5	150845	2012	**citronellyl acetate**	3_REACH	Citronellyl acetate	citronellyl acetate	C12H22O2	C12H22O2	198.31	CC(CCOC(=O)C)CCC=C(C)C	InChI=1/C12H22O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h6,11H,5,7-9H2,1-4H3	3.428	3.428	1	1	1
15214-89-8	15214898	2021	**2-acrylamido-2-methylpropanesulphonic acid**	3_REACH		2-acrylamido-2-methylpropanesulphonic acid		C7H12NO4S	207.25	CC(C)(CS(=O)(=O)[O-])NC(=O)C=C	InChI=1/C7H13NO4S/c1-4-6(9)8-7(2,3)5-13(10,11)12/h4H,1,5H2,2-3H3,(H,8,9)(H,10,11,12)/p-1	-2.187	-2.183	1	1	1
152402-98-7	152402987	2023	**2-[[(3-Methyl-4-nitro-pyridin-2-yl)methyl]sulfanyl]-1H-benzoimidazole**	3_REACH		1H-Benzimidazole, 2-[[(3-methyl-4-nitro-2-pyridinyl)methyl]thio]-			300.34	CC1=C(C=CN=C1CSC2=NC3=CC=CC=C3N2)[N+](=O)[O-]	InChI=1S/C14H12N4O2S/c1-9-12(15-7-6-13(9)18(19)20)8-21-14-16-10-4-2-3-5-11(10)17-14/h2-7H,8H2,1H3,(H,16,17)			1	1	1
15267-95-5	15267955	2025	**(chloromethyl)triethoxysilane**	3_REACH		(chloromethyl)triethoxysilane		C7H17ClO3Si	212.75	CCO[Si](CCl)(OCC)OCC	InChI=1/C7H17ClO3Si/c1-4-9-12(7-8,10-5-2)11-6-3/h4-7H2,1-3H3	3.508	3.508	1	1	1
1530-32-1	1530321	2028	**ethyltriphenylfosfonium bromide**	3_REACH		ethyltriphenylfosfonium bromide		C20H20P	371.26	CC[P+](c1ccccc1)(c2ccccc2)c3ccccc3	InChI=1/C20H20P/c1-2-21(18-12-6-3-7-13-18,19-14-8-4-9-15-19)20-16-10-5-11-17-20/h3-17H,2H2,1H3/q+1	5.487	5.487	1	1	1
15307-79-6	15307796	30	**sodium [2-[(2,6-dichlorophenyl)amino]phenyl]acetate**	3_REACH		2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid, Sodium salt (1:1)		C14H10Cl2NO2	318.14	[O-]C(=O)Cc1ccccc1Nc2c(Cl)cccc2Cl	InChI=1/C14H11Cl2NO2/c15-10-5-3-6-11(16)14(10)17-12-7-2-1-4-9(12)8-13(18)19/h1-7,17H,8H2,(H,18,19)/p-1	2.899	3.368	1	1	1
15356-60-2	15356602	486	**(+)-menthol**	3_REACH		(+)-menthol		C10H20O	156.27	CC(C)C1CCC(C)CC1O	InChI=1/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H,4-6H2,1-3H3	2.779	2.779	1	1	1
153719-38-1	153719381	4548	**N-nitro-N-(3-methyl-3,6-dihydro-2H-1,3,5-oxadiazin-4-yl)amine**	3_REACH		2H-1,3,5-Oxadiazin-4-amine, 3,6-dihydro-3-methyl-N-nitro-			160.14	CN1COCN=C1N[N+](=O)[O-]	InChI=1S/C4H8N4O3/c1-7-3-11-2-5-4(7)6-8(9)10/h2-3H2,1H3,(H,5,6)			1	1	1
15396-00-6	15396006	2033	**3-(trimethoxysilyl)propyl isocyanate**	3_REACH		3-(trimethoxysilyl)propyl isocyanate		C7H16NO4Si	205.29	CO[Si](CCC[NH+]=C=O)(OC)OC	InChI=1/C7H15NO4Si/c1-10-13(11-2,12-3)6-4-5-8-7-9/h4-6H2,1-3H3/p+1	2.175	2.175	1	1	1
154279-60-4	154279604	2034	**4,4'-methylenebis(N-sec-butylcyclohexanamine)**	3_REACH		4,4'-methylenebis(N-sec-butylcyclohexanamine)			322.58	CCC(C)NC1CCC(CC1)CC2CCC(CC2)NC(C)CC	InChI=1S/C21H42N2/c1-5-16(3)22-20-11-7-18(8-12-20)15-19-9-13-21(14-10-19)23-17(4)6-2/h16-23H,5-15H2,1-4H3			1	1	1
15471-17-7	15471177	2039	**1-(3-sulphonatopropyl)pyridinium**	3_REACH		1-(3-sulphonatopropyl)pyridinium		C8H11NO3S	201.25	[O-]S(=O)(=O)CCC[n+]1ccccc1	InChI=1/C8H11NO3S/c10-13(11,12)8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2	-1.343	-1.343	1	1	1
15520-10-2	15520102	2040	**2-methylpentane-1,5-diamine**	3_REACH		2-methylpentane-1,5-diamine		C6H18N2	116.21	CC(C[NH3+])CCC[NH3+]	InChI=1/C6H16N2/c1-6(5-8)3-2-4-7/h6H,2-5,7-8H2,1H3/p+2	-2.069	-1.982	1	1	1
15625-89-5	15625895	2046	**2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate**	3_REACH		2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate		C15H20O6	296.32	CCC(COC(=O)C=C)(COC(=O)C=C)COC(=O)C=C	InChI=1/C15H20O6/c1-5-12(16)19-9-15(8-4,10-20-13(17)6-2)11-21-14(18)7-3/h5-7H,1-3,8-11H2,4H3	2.612	2.612	1	1	1
156-43-4	156434	2048	**p-phenetidine**	3_REACH	4-Ethoxyaniline	p-phenetidine	C8H11NO	C8H11NO	137.18	CCOc1ccc(N)cc1	InChI=1/C8H11NO/c1-2-10-8-5-3-7(9)4-6-8/h3-6H,2,9H2,1H3	1.415	1.413	1	1	1
1570-64-5	1570645	495	**4-chloro-o-cresol**	3_REACH	Phenol, 4-chloro-2-methyl-	4-Chloro-2-methylphenol	C7H7ClO	C7H7ClO	142.59	Cc1cc(Cl)ccc1O	InChI=1/C7H7ClO/c1-5-4-6(8)2-3-7(5)9/h2-4,9H,1H3	2.738	2.736	1	1	1
15721-78-5	15721785	2055	**bis(4-(1,1,3,3-tetramethylbutyl)phenyl)amine**	3_REACH		bis(4-(1,1,3,3-tetramethylbutyl)phenyl)amine		C28H43N	393.66	CC(C)(C)CC(C)(C)c1ccc(Nc2ccc(cc2)C(C)(C)CC(C)(C)C)cc1	InChI=1/C28H43N/c1-25(2,3)19-27(7,8)21-11-15-23(16-12-21)29-24-17-13-22(14-18-24)28(9,10)20-26(4,5)6/h11-18,29H,19-20H2,1-10H3	8.921	8.921	0	0	1
15827-60-8	15827608	2059	**[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid**	3_REACH		[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid		C9H19N3O15P5	573.2	[O-]P(=O)([O-])CN(CC[NH+](CCN(CP(=O)([O-])[O-])CP(=O)([O-])[O-])CP(=O)([O-])[O-])CP(=O)([O-])[O-]	InChI=1/C9H28N3O15P5/c13-28(14,15)5-10(1-3-11(6-29(16,17)18)7-30(19,20)21)2-4-12(8-31(22,23)24)9-32(25,26)27/h1-9H2,(H2,13,14,15)(H2,16,17,18)(H2,19,20,21)(H2,22,23,24)(H2,25,26,27)/p-9	-15.76	-13.495	1	1	1
15834-04-5	15834045	2060	**2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate**	3_REACH		2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate		C25H44O8	472.62	CCCCC(=O)OCC(COC(=O)CCCC)(COC(=O)CCCC)COC(=O)CCCC	InChI=1/C25H44O8/c1-5-9-13-21(26)30-17-25(18-31-22(27)14-10-6-2,19-32-23(28)15-11-7-3)20-33-24(29)16-12-8-4/h5-20H2,1-4H3	5.668	5.668	1	1	1
15848-49-4	15848494	2062	**Ethyl 2-(cyclopent-2-EN-1-YL)acetate**	3_REACH		ethyl cyclopent-2-en-1-ylacetate			154.21	CCOC(=O)CC1CCC=C1	InChI=1S/C9H14O2/c1-2-11-9(10)7-8-5-3-4-6-8/h3,5,8H,2,4,6-7H2,1H3			1	1	1
15894-70-9	15894709	2065	**N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]**	3_REACH		N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]		C10H20N8	250.32	[NH2+]=C(NCCCCCCNC(=[NH2+])NC#N)NC#N	InChI=1/C10H18N8/c11-7-17-9(13)15-5-3-1-2-4-6-16-10(14)18-8-12/h1-6H2,(H3,13,15,17)(H3,14,16,18)/p+2	-0.121	-0.121	1	1	1
15993-42-7	15993427	2069	**N-(5-chloro-2-methoxyphenyl)-2-[(2-methoxy-4-nitrophenyl)azo]-3-oxobutyramide**	3_REACH		N-(5-chloro-2-methoxyphenyl)-2-[(2-methoxy-4-nitrophenyl)azo]-3-oxobutyramide		C18H17ClN4O6	420.81	COc1ccc(Cl)cc1NC(=O)C(N=Nc2ccc(cc2OC)[N+](=O)[O-])C(=O)C	InChI=1/C18H17ClN4O6/c1-10(24)17(18(25)20-14-8-11(19)4-7-15(14)28-2)22-21-13-6-5-12(23(26)27)9-16(13)29-3/h4-9,17H,1-3H3,(H,20,25)	3.715	3.716	1	1	1
16111-62-9	16111629	2079	**bis(2-ethylhexyl) peroxydicarbonate**	3_REACH		bis(2-ethylhexyl) peroxydicarbonate		C18H34O6	346.46	CCCCC(CC)COC(=O)OOC(=O)OCC(CC)CCCC	InChI=1/C18H34O6/c1-5-9-11-15(7-3)13-21-17(19)23-24-18(20)22-14-16(8-4)12-10-6-2/h15-16H,5-14H2,1-4H3	6.784	6.784	1	1	1
161462-35-7	161462357	4456	**1-cyclopropyl-3-(2-methylthio-4-trifluoromethylphenyl)-1,3-propanedione**	3_REACH		DCS			302.31	CSC1=C(C=CC(=C1)C(F)(F)F)C(=O)CC(=O)C2CC2	InChI=1S/C14H13F3O2S/c1-20-13-6-9(14(15,16)17)4-5-10(13)12(19)7-11(18)8-2-3-8/h4-6,8H,2-3,7H2,1H3			1	1	1
16219-75-3	16219753	2083	**5-ethylidene-8,9,10-trinorborn-2-ene**	3_REACH	Bicyclo[2.2.1]hept-2-ene, 5-ethylidene-	5-ethylidene-8,9,10-trinorborn-2-ene	C9H12	C9H12	120.19	CC=C1CC2CC1C=C2	InChI=1/C9H12/c1-2-8-5-7-3-4-9(8)6-7/h2-4,7,9H,5-6H2,1H3	2.426	2.426	1	1	1
162208-27-7	162208277	4901	**Diethyl thiophosphoril-(z)-(2-aminothiazol-4-yl)-(methoxyimino)acetate**	3_REACH		diethyl thiophosphoryl (Z)-(2-aminothiazol-4-yl)methoxyimino acetate			353.36	CCOP(=S)(OCC)OC(=O)C(=NOC)C1=CSC(=N1)N	InChI=1S/C10H16N3O5PS2/c1-4-16-19(20,17-5-2)18-9(14)8(13-15-3)7-6-21-10(11)12-7/h6H,4-5H2,1-3H3,(H2,11,12)/b13			1	1	1
16298-38-7	16298387	4407	**4,4'-methylenebis(2-isopropyl-6-methylaniline)**	3_REACH		4,4'-methylenebis(2-isopropyl-6-methylaniline)			310.49	CC1=C(C(=CC(=C1)CC2=CC(=C(C(=C2)C(C)C)N)C)C(C)C)N	InChI=1S/C21H30N2/c1-12(2)18-10-16(7-14(5)20(18)22)9-17-8-15(6)21(23)19(11-17)13(3)4/h7-8,10-13H,9,22-23H2,1-6H3			1	1	1
16415-12-6	16415126	2092	**hexadecyltrimethoxysilane**	3_REACH		hexadecyltrimethoxysilane		C19H42O3Si	346.63	CCCCCCCCCCCCCCCC[Si](OC)(OC)OC	InChI=1/C19H42O3Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(20-2,21-3)22-4/h5-19H2,1-4H3	8.963	8.963	1	1	1
164578-11-4	164578114	4335	**2,9-bis[N-[3-(diethylamino)propyl]sulfamoyl]-5H,12H-quino[2,3-b]acridin-7,14-dione**	3_REACH		2,9-bis[N-[3-(diethylamino)propyl]sulfamoyl]-5H,12H-quino[2,3-b]acridin-7,14-dione			696.9	[illegible]	[illegible]			1	1	1
165184-98-5	165184985	2096	**alpha-Hexylcinnamaldehyde**	3_REACH		alpha-Hexyl Cinnamic Aldehyde			216.32	CCCCCCC(=CC1=CC=CC=C1)C=O	InChI=1S/C15H20O/c1-2-3-4-6-11-15(13-16)12-14-9-7-5-8-10-14/h5,7-10,12-13H,2-4,6,11H2,1H3/b15-12+			1	1	1
16634-82-5	16634825	4584	**2-Chloro-N-(4-methylphenyl)acetamide**	3_REACH	2-Chloro-para-acetotoluidide	2-chloro-N-(4-methylphenyl)acetamide	C9H10ClNO		183.64	CC1=CC=C(C=C1)NC(=O)CCl	InChI=1S/C9H10ClNO/c1-7-2-4-8(5-3-7)11-9(12)6-10/h2-5H,6H2,1H3,(H,11,12)			1	1	1
166524-65-8	166524658	2105	**2-ethoxy-4,6-difluoropyrimidine**	3_REACH		2-ethoxy-4,6-difluoropyrimidine			160.13	CCOC1=NC(=CC(=N1)F)F	InChI=1S/C6H6F2N2O/c1-2-11-6-9-4(7)3-5(8)10-6/h3H,2H2,1H3			1	1	1
167004-78-6	167004786	2110	**3-[butoxy(methyl)phosphoryl]-1-**	3_REACH		Phosphinic acid, P-[3-(acetyloxy)-3-			261.26	CCCCOP(=O)(C)CCC(C#N)OC(=O)C	InChI=1S/C11H20NO4P/c1-4-5-7-15-17(3,14)8-6-11(9-12)16-10(2)13/h11H,4-8H2,1-3H3			1	1	1
16712-64-4	16712644	2111	**6-hydroxy-2-naphthoic acid**	3_REACH		6-hydroxy-2-naphthoic acid		C11H7O3	188.18	Oc1ccc2cc(ccc2c1)C(=O)[O-]	InChI=1/C11H8O3/c12-10-4-3-7-5-9(11(13)14)2-1-8(7)6-10/h1-6,12H,(H,13,14)/p-1	0.652	0.653	1	1	1
1696-20-4	1696204	2118	**4-acetylmorpholine**	3_REACH	Morpholine, 4-acetyl-	4-acetylmorpholine	C6H11NO2	C6H11NO2	129.16	CC(=O)N1CCOCC1	InChI=1/C6H11NO2/c1-6(8)7-2-4-9-5-3-7/h2-5H2,1H3	-0.733	-0.733	1	1	1
1704-62-7	1704627	2119	**2-[2-(dimethylamino)ethoxy]ethanol**	3_REACH	ethanol, 2-[2-(dimethylamino)ethoxy]-	2-[2-(dimethylamino)ethoxy]ethanol	C6H15NO2	C6H16NO2	133.19	C[NH+](C)CCOCCO	InChI=1/C6H15NO2/c1-7(2)3-5-9-6-4-8/h8H,3-6H2,1-2H3/p+1	-1.911	-1.314	1	1	1
1709-70-2	1709702	2121	**Tris-bht mesitylene**	3_REACH		3,3',3'',5,5',5''-hexa-tert-butyl-a,a',a''-(mesitylene-2,4,6-triyl)tri-p-cresol		C54H78O3	775.22	Cc1c(Cc2c(cc(O)cc2C(C)(C)C)C(C)(C)C)c(C)c(Cc3c(cc(O)cc3C(C)(C)C)C(C)(C)C)c(C)c1Cc4c(cc(O)cc4C(C)(C)C)C(C)(C)C(	InChI=1/C54H78O3/c1-31-37(28-40-43(49(4,5)6)22-34(55)23-44(40)50(7,8)9)32(2)39(30-42-47(53(16,17)18)26-36(57)27-48(42)54(19,20)21)33(3)38(31)29-41-45(51(10,11)12)24-35(56)25-46(41)52(13,14)15/h22-27,55-57H,28-30H2,1-21H3	16.888	16.854	0	0	1
1724-39-6	1724396	2126	**cyclododecanol**	3_REACH	Cyclododecanol	cyclododecanol	C12H24O	C12H24O	184.32	OC1CCCCCCCCCCC1	InChI=1/C12H24O/c13-12-10-8-6-4-2-1-3-5-7-9-11-12/h12-13H,1-11H2	4.237	4.237	1	1	1
172529-93-0	172529930	2128	**1,3-dimethyl 2-[2-(2-amino-6-chloro-9H-purin-9-yl)ethyl]propanedioate**	3_REACH		Propanedioic acid, 2-[2-(2-amino-6-chloro-9H-purin-9-yl)ethyl]-, 1,3-dimethyl ester			327.73	COC(=O)C(CCN1C=NC2=C1N=C(N=C2Cl)N)C(=O)OC	InChI=1S/C12H14ClN5O4/c1-21-10(19)6(11(20)22-2)3-4-18-5-15-7-8(13)16-12(14)17-9(7)18/h5-6H,3-4H2,1-2H3,(H2,14,1			1	1	1
1738-25-6	1738256	2132	**3-dimethylaminopropiononitrile**	3_REACH	Propanenitrile, 3-(dimethylamino)-	3-dimethylaminopropiononitrile	C5H10N2	C5H10N2	98.151	CN(C)CCC#N	InChI=1/C5H10N2/c1-7(2)5-3-4-6/h3,5H2,1-2H3	0.298	0.158	1	1	1
173904-11-5	173904115	2133	**N,N'-[cyclohexane-1,3-diylbis(methylene)]bis(2-methylpropan-1-imine)**	3_REACH		N,N'-[cyclohexane-1,3-diylbis(methylene)]bis(2-methylpropan-1-imine)			250.43	CC(C)C=NCC1CCCC(C1)CN=CC(C)C	InChI=1S/C16H30N2/c1-13(2)9-17-11-15-6-5-7-16(8-15)12-18-10-14(3)4/h9-10,13-16H,5-8,11-12H2,1-4H3			1	1	1
1739-84-0	1739840	2135	**1,2-dimethylimidazole**	3_REACH	1H-Imidazole, 1,2-dimethyl-	1,2-dimethylimidazole	C5H8N2	C5H9N2	96.135	Cc1[nH+]ccn1C	InChI=1/C5H8N2/c1-5-6-3-4-7(5)2/h3-4H,1-2H3/p+1	0.551	0.467	1	1	1
174489-43-1	174489431	2137	**1-(allyloxy)-2-methyl-1-oxopropan-2-yl 5-amino-2-chlorobenzoate**	3_REACH		1-(allyloxy)-2-methyl-1-oxopropan-2-yl 5-amino-2-chlorobenzoate			297.74	CC(C)(C(=O)OCC=C)OC(=O)C1=C(C=CC(=C1)N)Cl	InChI=1S/C14H16ClNO4/c1-4-7-19-13(18)14(2,3)20-12(17)10-8-9(16)5-6-11(10)15/h4-6,8H,1,7,16H2,2-3H3			1	1	1
174489-76-0	174489760	2138	**1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-nitrobenzoate**	3_REACH		1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-nitrobenzoate			327.72	Clc1ccc(cc1C(=O)OC(C(=O)OC\C=C)(C)C)[N+]([O-])=O	InChI=1S/C14H14ClNO6/c1-4-7-21-13(18)14(2,3)22-12(17)10-8-9(16(19)20)5-6-11(10)15/h4-6,8H,1,7H2,2-3H3			1	1	1
1746-23-2	1746232	2139	**p-tert-butylstyrene**	3_REACH	Styrene, p-tert-butyl-	p-tert-butylstyrene	C12H16	C12H16	160.26	CC(C)(C)c1ccc(C=C)cc1	InChI=1/C12H16/c1-5-10-6-8-11(9-7-10)12(2,3)4/h5-9H,1H2,2-4H3	3.782	3.782	1	1	1
1760-24-3	1760243	2145	**N-(3-(trimethoxysilyl)propyl)ethylenediamine**	3_REACH	N-(2-Aminoethyl-3-aminopropyl)trimethoxysilane	N-(3-(trimethoxysilyl)propyl)ethylenediamine	C8H22N2O3Si	C8H23N2O3Si	222.36	CO[Si](CCC[NH2+]CCN)(OC)OC	InChI=1/C8H22N2O3Si/c1-11-14(12-2,13-3)8-4-6-10-7-5-9/h10H,4-9H2,1-3H3/p+1	-0.111	-0.121	1	1	1
17689-77-9	17689779	2148	**triacetoxyethylsilane**	3_REACH		triacetoxyethylsilane		C8H14O6Si	234.28	CC[Si](OC(=O)C)(OC(=O)C)OC(=O)C	InChI=1/C8H14O6Si/c1-5-15(12-6(2)9,13-7(3)10)14-8(4)11/h5H2,1-4H3	1.928	1.928	1	1	1
176969-34-9	176969349	2150	**3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid**	3_REACH		3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid			176.12	CN1C=C(C(=N1)C(F)F)C(=O)O	InChI=1S/C6H6F2N2O2/c1-10-2-3(6(11)12)4(9-10)5(7)8/h2,5H,1H3,(H,11,12)			1	1	1
17796-82-6	17796826	2153	**N-(cyclohexylthio)phthalimide**	3_REACH		N-(cyclohexylthio)phthalimide		C14H15NO2S	261.34	O=C1N(SC2CCCCC2)C(=O)c3ccccc13	InChI=1/C14H15NO2S/c16-13-11-8-4-5-9-12(11)14(17)15(13)18-10-6-2-1-3-7-10/h4-5,8-10H,1-3,6-7H2	3.311	3.311	1	1	1
17832-28-9	17832289	2154	**4-(vinyloxy)butan-1-ol**	3_REACH		4-(vinyloxy)butan-1-ol		C6H12O2	116.16	OCCCCOC=C	InChI=1/C6H12O2/c1-2-8-6-4-3-5-7/h2,7H,1,3-6H2	0.424	0.424	1	1	1
17865-07-5	17865075	2155	**propyltriacetoxysilane**	3_REACH		propyltriacetoxysilane		C9H16O6Si	248.31	CCC[Si](OC(=O)C)(OC(=O)C)OC(=O)C	InChI=1/C9H16O6Si/c1-5-6-16(13-7(2)10,14-8(3)11)15-9(4)12/h5-6H2,1-4H3	2.385	2.385	1	1	1
17928-28-8	17928288	2158	**1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]trisiloxane**	3_REACH	Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-(trimethylsiloxy)-	1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]trisiloxane	C10H30O3Si4	C10H30O3Si4	310.69	C[Si](C)(C)O[Si](C)(O[Si](C)(C)C)O[Si](C)(C)C	InChI=1/C10H30O3Si4/c1-14(2,3)11-17(10,12-15(4,5)6)13-16(7,8)9/h1-10H3	7.098	7.098	1	1	1
18063-03-1	18063031	2163	**2,6-difluorobenzamide**	3_REACH	Benzamide, 2,6-difluoro-	2,6-difluorobenzamide	C7H5F2NO	C7H5F2NO	157.12	NC(=O)c1c(F)cccc1F	InChI=1/C7H5F2NO/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H2,10,11)	1.243	1.243	1	1	1
1809-19-4	1809194	2164	**dibutyl phosphonate**	3_REACH	Dibutyl hydrogen phosphite	dibutyl phosphonate	C8H19O3P	C8H19O3P	194.21	CCCCOP(=O)OCCCC	InChI=1/C8H19O3P/c1-3-5-7-10-12(9)11-8-6-4-2/h12H,3-8H2,1-2H3	1.63	1.63	1	1	1
18127-01-0	18127010	2166	**3-(4-tert-butylphenyl)propionaldehyde**	3_REACH		3-(4-tert-butylphenyl)propionaldehyde		C13H18O	190.29	CC(C)(C)c1ccc(CCC=O)cc1	InChI=1/C13H18O/c1-13(2,3)12-8-6-11(7-9-12)5-4-10-14/h6-10H,4-5H2,1-3H3	3.373	3.373	1	1	1
181587-01-9	181587019	4655	**Ethiprole**	3_REACH		1H-Pyrazole-3-carbonitrile, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-			397.21	CCS(=O)C1=C(N(N=C1C#N)C2=C(C=C(C=C2Cl)C(F)(F)F)Cl)N	InChI=1S/C13H9Cl2F3N4OS/c1-2-24(23)11-9(5-19)21-22(12(11)20)10-7(14)3-6(4-8(10)15)13(16,17)18/h3-4H,2,20H2,1H3			1	1	1
18171-19-2	18171192	2172	**(3-chloropropyl)dimethoxymethylsilane**	3_REACH		(3-chloropropyl)dimethoxymethylsilane		C6H15ClO2Si	182.72	COC([SiH3])(CCCCl)OC	InChI=1/C6H15ClO2Si/c1-8-6(10,9-2)4-3-5-7/h3-5H2,1-2,10H3	4.955	4.955	1	1	1
18379-25-4	18379254	2187	**trichloro(2,4,4-trimethylpentyl)silane**	3_REACH		trichloro(2,4,4-trimethylpentyl)silane		C8H17Cl3Si	247.67	CC(CC(C)(C)C)C[Si](Cl)(Cl)Cl	InChI=1/C8H17Cl3Si/c1-7(5-8(2,3)4)6-12(9,10)11/h7H,5-6H2,1-4H3	5.707	5.707	1	1	1
1843-03-4	1843034	2190	**4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol]**	3_REACH		4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol]		C37H52O3	544.82	CC(CC(c1cc(c(O)cc1C)C(C)(C)C)c2cc(c(O)cc2C)C(C)(C)C)c3cc(c(O)cc3C)C(C)(C)C	InChI=1/C37H52O3/c1-21(25-18-29(35(5,6)7)32(38)15-22(25)2)14-28(26-19-30(36(8,9)10)33(39)16-23(26)3)27-20-31(37(11,12)13)34(40)17-24(27)4/h15-21,28,38-40H,14H2,1-13H3	11.186	10.483	0	0	1
18479-58-8	18479588	2192	**2,6-dimethyloct-7-en-2-ol**	3_REACH	7-Octen-2-ol, 2,6-dimethyl-	2,6-dimethyloct-7-en-2-ol	C10H20O	C10H20O	156.27	CC(CCCC(C)(C)O)C=C	InChI=1/C10H20O/c1-5-9(2)7-6-8-10(3,4)11/h5,9,11H,1,6-8H2,2-4H3	2.782	2.782	1	1	1
1852-17-1	1852171	2196	**perhydropyrimidin-2-one**	3_REACH		perhydropyrimidin-2-one		C4H8N2O	100.12	O=C1NCCCN1	InChI=1/C4H8N2O/c7-4-5-2-1-3-6-4/h1-3H2,(H2,5,6,7)	-0.75	-0.75	1	1	1

18600-59-4	18600594	4312	**2,2-(1,4-phenylene)bis((4H-3,1-benzoxazine-4-one)**	3_REACH		2,2-(1,4-phenylene)bis((4H-3,1-benzoxazine-4-one)			368.35	C1=CC=C2C(=C1)C(=O)OC(=N2)C3=CC=C(C=C3)C4=NC5=CC=CC=C5C(=O)O4	InChI=1S/C22H12N2O4/c25-21-15-5-1-3-7-17(15)23-19(27-21)13-9-11-14(12-10-13)20-24-18-8-4-2-6-16(18)22(26)28-20/			1	1	1
1860-26-0	1860260	2200	**2-ethyl-N,N-bis(2-ethylhexyl)hexylamine**	3_REACH		2-ethyl-N,N-bis(2-ethylhexyl)hexylamine		C24H52N	353.68	CCCCC(CC)C[NH+](CC(CC)CCCC)CC(CC)CCCC	InChI=1/C24H51N/c1-7-13-16-22(10-4)19-25(20-23(11-5)17-14-8-2)21-24(12-6)18-15-9-3/h22-24H, 21H2,1-6H3/p+1	7.809	7.818	1	1	1
186817-80-1	186817801	2203	**Propanoic acid, 2-hydroxy-, 2-ethylhexyl ester, (2S)-**	3_REACH		Propanoic acid, 2-hydroxy-, 2-ethylhexyl ester (2S)-			202.29	CCCCC(CC)COC(=O)[C@H](C)O	InChI=1S/C11H22O3/c1-4-6-7-10(5-2)8-14-11(13)9(3)12/h9-10,12H,4-8H2,1-3H3/t9-,10?/m0/s1			1	1	1
1879-09-0	1879090	2209	**6-tert-butyl-2,4-xylenol**	3_REACH	6-Tert-butyl-2,4-xylenol	6-tert-butyl-2,4-xylenol	C12H18O	C12H18O	178.28	Cc1cc(C)c(O)c(c1)C(C)(C)C	InChI=1/C12H18O/c1-8-6-9(2)11(13)10(7-8)12(3,4)5/h6-7,13H,1-5H3	3.96	3.96	1	1	1
18835-33-1	18835331	2210	**hexacos-1-ene**	3_REACH	1-Hexacosene	hexacos-1-ene	C26H52	C26H52	364.7	CCCCCCCCCCCCCCCCCCCCCCCC=C	InChI=1/C26H52/c1-3-5-7-9-11-13-15-17-19-21-23-25-26-24-22-20-18-16-14-12-10-8-6-4-2/h3H,1,4-26H2,2H3	11.842	11.842	0	0	1
18835-34-2	18835342	2211	**octacos-1-ene**	3_REACH	1-Octacosene	octacos-1-ene	C28H56	C28H56	392.76	CCCCCCCCCCCCCCCCCCCCCCCCCC=C	InChI=1/C28H56/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h3H,1,4-28H2,2H3	12.754	12.754	0	1	1
1889-67-4	1889674	2214	**1,1'-(1,1,2,2-tetramethylethylene)dibenzene**	3_REACH	Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-	1,1'-(1,1,2,2-tetramethylethylene)dibenzene	C18H22	C18H22	238.37	CC(C)(c1ccccc1)C(C)(C)c2ccccc2	InChI=1/C18H22/c1-17(2,15-11-7-5-8-12-15)18(3,4)16-13-9-6-10-14-16/h5-14H,1-4H3	5.176	5.176	1	1	1
19234-20-9	19234209	2228	**2-(1-methylethoxy)ethyl acetate**	3_REACH		2-(1-methylethoxy)ethyl acetate		C7H14O3	146.19	CC(C)OCCOC(=O)C	InChI=1/C7H14O3/c1-6(2)9-4-5-10-7(3)8/h6H,4-5H2,1-3H3	0.616	0.616	1	1	1
19444-21-4	19444214	2233	**allyl 2-hydroxy-2-methylpropanoate**	3_REACH		allyl 2-hydroxy-2-methylpropanoate			144.17	CC(C)(C(=O)OCC=C)O	InChI=1S/C7H12O3/c1-4-5-10-6(8)7(2,3)9/h4,9H,1,5H2,2-3H3			1	1	1
1948-33-0	1948330	523	**2-tert-butylhydroquinone**	3_REACH	1,4-Benzenediol, 2-(1,1-dimethylethyl)-	2-(1,1-Dimethylethyl)-1,4-benzenediol	C10H14O2	C10H14O2	166.22	CC(C)(C)c1cc(O)ccc1O	InChI=1/C10H14O2/c1-10(2,3)8-6-7(11)4-5-9(8)12/h4-6,11-12H,1-3H3	2.746	2.746	1	1	1
1955-46-0	1955460	2235	**methyl 5-nitrohydrogen isophthalate**	3_REACH		methyl 5-nitrohydrogen.isophthalate		C9H6NO6	225.16	COC(=O)c1cc(cc(c1)N(=O)=O)C(=O)[O-]	InChI=1/C9H7NO6/c1-16-9(13)6-2-5(8(11)12)3-7(4-6)10(14)15/h2-4H,1H3,(H,11,12)/p-1	-0.265	-0.265	1	1	1
1962-75-0	1962750	525	**dibutyl terephthalate**	3_REACH	1,4-Benzenedicarboxylic acid, dibutyl...	1,4-Benzenedicarboxylic acid, Dibutyl ester	C16H22O4	C16H22O4	278.35	CCCCOC(=O)c1ccc(cc1)C(=O)OCCCC	InChI=1/C16H22O4/c1-3-5-11-19-15(17)13-7-9-14(10-8-13)16(18)20-12-6-4-2/h7-10H,3-6,11-12H2,	4.198	4.198	1	1	1
1975-78-6	1975786	2239	**decanenitrile**	3_REACH	Decanenitrile	decanenitrile	C10H19N	C10H19N	153.27	CCCCCCCCCC#N	InChI=1/C10H19N/c1-2-3-4-5-6-7-8-9-10-11/h2-9H2,1H3	3.904	3.904	1	1	1
1999-85-5	1999855	2247	**alpha,alpha'-Dihydroxy-1,3-diisopropylbenzene**	3_REACH	Noname	a,a,a',a'-tetramethyl-m-xylene-a,a'-diol	C12H18O2	C12H18O2	194.27	CC(C)(O)c1cccc(c1)C(C)(C)O	InChI=1/C12H18O2/c1-11(2,13)9-6-5-7-10(8-9)12(3,4)14/h5-8,13-14H,1-4H3	1.785	1.785	1	1	1
20030-30-2	20030302	2248	**2,5,6-trimethylcyclohex-2-en-1-one**	3_REACH	2,5,6-Trimethyl-2-cyclohexen-1-one	2,5,6-trimethylcyclohex-2-en-1-one	C9H14O	C9H14O	138.21	CC1CC=C(C)C(=O)C1C	InChI=1/C9H14O/c1-6-4-5-7(2)9(10)8(6)3/h5-6,8H,4H2,1-3H3	2.451	2.451	1	1	1
20120-33-6	20120336	2250	**dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate**	3_REACH		dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate		C6H14NO5P	211.16	COP(=O)(CCC(=O)NCO)OC	InChI=1/C6H14NO5P/c1-11-13(10,12-2)4-3-6(9)7-5-8/h8H,3-5H2,1-2H3,(H,7,9)	-1.754	-1.754	1	1	1
20292-08-4	20292084	2257	**2-ethylhexyl laurate**	3_REACH		2-ethylhexyl laurate		C20H40O2	312.54	CCCCCCCCCCCC(=O)OCC(CC)CCCC	InChI=1/C20H40O2/c1-4-7-9-10-11-12-13-14-15-17-20(21)22-18-19(6-3)16-8-5-2/h19H,4-18H2,1-3H3	7.81	7.81	1	1	1
20298-69-5	20298695	2258	**cis-2-tert-butylcyclohexyl acetate**	3_REACH		cis-2-tert-butylcyclohexyl acetate		C12H22O2	198.31	CC(=O)O[C@H]1CCCC[C@H]1C(C)(C)C	InChI=1/C12H22O2/c1-9(13)14-11-8-6-5-7-10(11)12(2,3)4/h10-11H,5-8H2,1-4H3/t10-,11+/m1/s1	3.112	3.112	1	1	1
2031-67-6	2031676	2259	**triethoxy(methyl)silane**	3_REACH	Silane, triethoxymethyl-	triethoxy(methyl)silane	C7H18O3Si	C7H18O3Si	178.3	CCO[Si](C)(OCC)OCC	InChI=1/C7H18O3Si/c1-5-8-11(4,9-6-2)10-7-3/h5-7H2,1-4H3	3.071	3.071	1	1	1
2040-90-6	2040906	4576	**2-chloro-6-fluoro-phenol**	3_REACH		2-chloro-6-fluoro-phenol			146.55					1	1	1
2044-64-6	2044646	2265	**N,N-dimethyl-3-oxobutyramide**	3_REACH	N,N-Dimethylacetoacetamide	N,N-dimethyl-3-oxobutyramide	C6H11NO2	C6H10NO2	129.16	CN(C)C(=O)[CH-]C(=O)C	InChI=1/C6H10NO2/c1-5(8)4-6(9)7(2)3/h4H,1-3H3/q-1	-0.51	-0.51	1	1	1
204918-22-9	204918229	2267	**1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-isocyanatobenzoate**	3_REACH		1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-isocyanatobenzoate			323.73	Clc1ccc(\N=C=O)cc1C(=O)OC(C(=O)OC\C=C)(C)C	InChI=1S/C15H14ClNO5/c1-4-7-21-14(20)15(2,3)22-13(19)11-8-10(17-9-18)5-6-12(11)16/h4-6,8H,1,7H2,2-3H3			1	1	1
20592-85-2	20592852	2271	**[nitrilotris(methylene)]trisphosphonic acid, sodium salt**	3_REACH		[nitrilotris(methylene)]trisphosphonic acid, sodium salt		C3H10NO9P3	299.05	OP(=O)([O-])C[NH+](CP(=O)(O)[O-])CP(=O)(O)[O-]	InChI=1/C3H12NO9P3/c5-14(6,7)1-4(2-15(8,9)10)3-16(11,12)13/h1-3H2,(H2,5,6,7)(H2,8,9,10)(H2,11,12,13)/p-2	-8.009	-8.859	1	1	1
20749-68-2	20749682	2272	**8,9,10,11-tetrachloro-12H-phthaloperin-12-one**	3_REACH		8,9,10,11-tetrachloro-12H-phthaloperin-12-one		C18H6Cl4N2O	408.07	Clc1c(Cl)c(Cl)c2C3=Nc4cccc5cccc(N3C(=O)c2c1Cl)c45	InChI=1/C18H6Cl4N2O/c19-13-11-12(14(20)16(22)15(13)21)18(25)24-9-6-2-4-7-3-1-5-8(10(7)9)23-17(11)24/h1-6H	6.012	5.909	1	1	1
2082-81-7	2082817	2277	**tetramethylene dimethacrylate**	3_REACH	1,4-Butylene glycol dimethacrylate	tetramethylene dimethacrylate	C12H18O4	C12H18O4	226.27	CC(=C)C(=O)OCCCCOC(=O)C(=C)C	InChI=1/C12H18O4/c1-9(2)11(13)15-7-5-6-8-16-12(14)10(3)4/h1,3,5-8H2,2,4H3	2.791	2.791	1	1	1
21282-97-3	21282973	2288	**2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate**	3_REACH		2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate		C10H13O5	214.22	CC(=O)[CH-]C(=O)OCCOC(=O)C(=C)C	InChI=1/C10H13O5/c1-7(2)10(13)15-5-4-14-9(12)6-8(3)11/h6H,1,4-5H2,2-3H3/q-1	1.404	1.311	1	1	1
2135-17-3	2135173	532	**flumetasone**	3_REACH		Flumethasone		C22H28F2O5	410.46	C[C@@H]1C[C@H]2[C@@H]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=	InChI=1/C22H28F2O5/c1-11-6-13-14-8-16(23)15-7-12(26)4-5-19(15,2)21(14,24)17(27)9-20(13,3)22(11,29)18(28)10-25/h4-5,7,11,13-14,16-17,25,27,29H,6,8-10H2,1-3H3/t11-,13+,14+,16+,17+,19+,20+,21+,22+/m1/s1	1.546	1.546	1	1	1
2146-71-6	2146716	2295	**vinyl laurate**	3_REACH		vinyl laurate		C14H26O2	226.36	CCCCCCCCCCCC(=O)OC=C	InChI=1/C14H26O2/c1-3-5-6-7-8-9-10-11-12-13-14(15)16-4-2/h4H,2-3,5-13H2,1H3	4.878	4.878	1	1	1
21542-96-1	21542961	2298	**N,N-dimethyldocosylamine**	3_REACH	dimethyldocosylamine	N,N-dimethyldocosylamine	C24H51N	C24H52N	353.68	CCCCCCCCCCCCCCCCCCCCCC[NH+](C)C	InChI=1/C24H51N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25(2)3/h4-24H2, 3H3/p+1	8.299	8.351	1	1	1
2156-97-0	2156970	533	**dodecyl acrylate**	3_REACH	Dodecyl acrylate	2-Propenoic acid, Dodecyl ester	C15H28O2	C15H28O2	240.39	CCCCCCCCCCCCOC(=O)C=C	InChI=1/C15H28O2/c1-3-5-6-7-8-9-10-11-12-13-14-17-15(16)4-2/h4H,2-3,5-14H2,1H3	5.696	5.696	1	1	1
2162-73-4	2162734	2299	**2,4,6-triisopropyl-m-phenylene diisocyanate**	3_REACH		2,4,6-triisopropyl-m-phenylene diisocyanate		C17H22N2O2	286.38	CC(C)c1cc(C(C)C)c(N=C=O)c(C(C)C)c1N=C=O	InChI=1/C17H22N2O2/c1-10(2)13-7-14(11(3)4)17(19-9-21)15(12(5)6)16(13)18-8-20/h7,10-12H,1-6H3	5.133	5.133	1	1	1
2162-74-5	2162745	2300	**bis(2,6-diisopropylphenyl)carbodiimide**	3_REACH		bis(2,6-diisopropylphenyl)carbodiimide		C25H34N2	362.56	CC(C)c1cccc(C(C)C)c1N=C=Nc2c(cccc2C(C)C)C(C)C	InChI=1/C25H34N2/c1-16(2)20-11-9-12-21(17(3)4)24(20)26-15-27-25-22(18(5)6)13-10-14-23(25)19(7)8/h9-14,16-19H,1-8H3	8.304	8.304	1	1	1
2163-00-0	2163000	2301	**1,6-dichlorohexane**	3_REACH	1,6-Dichlorohexane	1,6-dichlorohexane	C6H12Cl2	C6H12Cl2	155.07	ClCCCCCCCl	InChI=1/C6H12Cl2/c7-5-3-1-2-4-6-8/h1-6H2	3.066	3.066	1	1	1
2163-42-0	2163420	4357	**2-methyl-1,3-propanediol**	3_REACH	Propane-1,3-diol, 2-methyl-	2-methyl-1,3-propanediol	C4H10O2		90.122					1	1	1
21643-42-5	21643425	2302	**tetradecyl acrylate**	3_REACH	2-Propenoic acid, tetradecyl ester	tetradecyl acrylate	C17H32O2	C17H32O2	268.44	CCCCCCCCCCCCCCOC(=O)C=C	InChI=1/C17H32O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-17(18)4-2/h4H,2-3,5-16H2,1H3	6.609	6.609	1	1	1
21743-27-1	21743271	4770	**4-((Triethoxysilyl)methyl)morpholine**	3_REACH		4-((Triethoxysilyl)methyl)morpholine			263.41					1	1	1
2186-92-7	2186927	2308	**p-(dimethoxymethyl)anisole**	3_REACH		p-(dimethoxymethyl)anisole		C10H14O3	182.22	COC(OC)c1ccc(OC)cc1	InChI=1/C10H14O3/c1-11-9-6-4-8(5-7-9)10(12-2)13-3/h4-7,10H,1-3H3	1.686	1.686	1	1	1
22047-49-0	22047490	2316	**2-ethylhexyl stearate**	3_REACH		2-ethylhexyl stearate		C26H52O2	396.7	CCCCCCCCCCCCCCCCCC(=O)OCC(CC)CCCC	InChI=1/C26H52O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-26(27)28-24-25(6-3)22-8-5-2/h25H,4-24H2,1-3H3	10.547	10.547	1	1	1
220727-26-4	220727264	4596	**S-(3-(triethoxysilyl)propyl)octanethioate**	3_REACH		Y-15099			364.616	CCCCCCCC(=O)SCCC[Si](OCC)(OCC)OCC	InChI=1S/C17H36O4SSi/c1-5-9-10-11-12-14-17(18)22-15-13-16-23(19-6-2,20-7-3)21-8-4/h5-16H2,1-4H3			1	1	1
22094-93-5	22094935	2317	**2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]**	3_REACH		2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]		C36H32Cl4N6O4	754.51	CC(=O)C(N=Nc1cc(Cl)c(cc1Cl)c2cc(Cl)c(cc2Cl)N=NC(C(=O)C)C(=O)Nc3ccc(C)cc3C)C(=O)Nc4ccc(C)cc4C	InChI=1/C36H32Cl4N6O4/c1-17-7-9-29(19(3)11-17)41-35(49)33(21(5)47)45-43-31-15-25(37)23(13-27(31)39)24-14-28(40)32(16-26(24)38)44-46-34(22(6)48)36(50)42-30-10-8-18(2)12-20(30)4/h7-16,3 34H,1-6H3,(H,41,49)(H,42,50)	10.67	10.67	0	1	1
2210-79-9	2210799	2319	**2,3-epoxypropyl o-tolyl ether**	3_REACH	Oxirane, [(2-methylphenoxy)methy	2,3-epoxypropyl o-tolyl ether	C10H12O2	C10H12O2	164.2	Cc1ccccc1OCC2CO2	InChI=1/C10H12O2/c1-8-4-2-3-5-10(8)12-7-9-6-11-9/h2-5,9H,6-7H2,1H3	2.016	2.016	1	1	1
2216-51-5	2216515	538	**L-menthol**	3_REACH	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, [1R-(1α,2β,5α)]-	(1R,2S,5R)-(-)-Menthol	C10H20O	C10H20O	156.27	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O	InChI=1/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H,4-6H2,1-3H3/t8-,9+,10-/m1/s1	2.779	2.779	1	1	1
2224-33-1	2224331	2325	**butan-2-one O,O',O''-(vinylsilylidyne)trioxime**	3_REACH		butan-2-one O,O',O''-(vinylsilylidyne)trioxime		C14H27N3O3Si	313.48	CC\C(=N/O[Si](O\N=C(/C)\CC)(O\N=C(/C)\CC)C=C)\C	InChI=1/C14H27N3O3Si/c1-8-12(5)15-18-21(11-4,19-16-13(6)9-2)20-17-14(7)10-3/h11H,4,8-10H2, 2,5-7H3/b15-12-,16-13+,17-14+	3.868	3.626	1	1	1
2226-96-2	2226962	2327	**4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl**	3_REACH	1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	C9H18NO2	C9H20NO2	173.26	CC1(C)CC(O)CC(C)(C)[NH+]1O	InChI=1/C9H19NO2/c1-8(2)5-7(11)6-9(3,4)10(8)12/h7,11-12H,5-6H2,1-4H3/p+1	0.607	0.607	1	1	1
2235-00-9	2235009	2331	**1-vinylhexahydro-2H-azepin-2-one**	3_REACH		1-vinylhexahydro-2H-azepin-2-one		C8H13NO	139.2	C=CN1CCCCCC1=O	InChI=1/C8H13NO/c1-2-9-7-5-3-4-6-8(9)10/h2H,1,3-7H2	0.831	0.831	1	1	1
224049-04-1	224049041	2333	**isotianil**	3_REACH		3,4-dichloro-N-(2-cyanophenyl)isothiazole-5-carboxamide			298.15	C1=CC=C(C(=C1)C#N)NC(=O)C2=C(C(=NS2)Cl)Cl	InChI=1S/C11H5Cl2N3OS/c12-8-9(18-16-10(8)13)11(17)15-7-4-2-1-3-6(7)5-14/h1-4H,(H,15,17)			1	1	1
2243-62-1	2243621	542	**1,5-naphthylenediamine**	3_REACH	1,5-Naphthalenediamine	1,5-Naphthalenediamine	C10H10N2	C10H10N2	158.21	Nc1cccc2c(N)cccc12	InChI=1/C10H10N2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1-6H,11-12H2	1.245	1.244	1	1	1
2280-49-1	2280491	2338	**N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide**	3_REACH		N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide		C13H10Cl3NO2S2	382.72	ClC(Cl)(Cl)SN(c1ccccc1)S(=O)(=O)c2ccccc2	InChI=1/C13H10Cl3NO2S2/c14-13(15,16)20-17(11-7-3-1-4-8-11)21(18,19)12-9-5-2-6-10-12/h1-10H	6.11	6.11	1	1	1
22871-58-5	22871585	2340	**3-Amino-5-((2-hydroxyethyl)carbamoyl)-2,4,6-triiodobenzoic acid**	3_REACH		Benzoic acid, 3-amino-5-[[(2-hydroxyethyl)amino]carbonyl]-2,4,6-triiodo-			601.89	C(CO)NC(=O)C1=C(C(=C(C(=C1I)N)I)C(=O)O)I	InChI=1S/C10H9I3N2O4/c11-5-3(9(17)15-1-2-16)6(12)8(14)7(13)4(5)10(18)19/h16H,1-2,14H2,(H,15,17)(H,18,19)			1	1	1
22984-54-9	22984549	2341	**butan-2-one O,O',O''-(methylsilylidyne)trioxime**	3_REACH		butan-2-one O,O',O''-(methylsilylidyne)trioxime		C13H27N3O3Si	301.47	CC\C(=N/O[Si](C)(O\N=C(/C)\CC)O\N=C(/C)\CC)\C	InChI=1/C13H27N3O3Si/c1-8-11(4)14-17-20(7,18-15-12(5)9-2)19-16-13(6)10-3/h8-10H2,1-7H3/b14 11-,15-12+,16-13+	3.784	3.542	1	1	1
2312-35-8	2312358	548	**propargite**	3_REACH		2-[4-(1,1-Dimethylethyl)phenoxy]cyclohexyl-2-propynyl ester sulfurous acid		C19H26O4S	350.48	CC(C)(C)c1ccc(OC2CCCCC2OS(=O)OCC#C)cc1	InChI=1/C19H26O4S/c1-5-14-21-24(20)23-18-9-7-6-8-17(18)22-16-12-10-15(11-13-16)19(2,3)4/h1,10-13,17-18H,6-9,14H2,2-4H3	5.528	5.528	1	1	1
232938-43-1	232938431	4564	**3-(3-Tosylureido)phenyl p-toluenesulfonate**	3_REACH		DP 201			460.53	CC1=CC=C(C=C1)S(=O)(=O)NC(=O)NC2=CC(=CC=C2)OS(=O)(=O)C3=CC=C(C=C3)C	InChI=1S/C21H20N2O6S2/c1-15-6-10-19(11-7-15)30(25,26)23-21(24)22-17-4-3-5-18(14-17)29-31(27,28)20-12-8-16(2)9-			1	1	1
23410-40-4	23410404	2351	**N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine**	3_REACH	N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine	N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine	C9H24N2O2Si	C9H25N2O2Si	220.39	CO[Si](C)(CC(C)C[NH2+]CCN)OC	InChI=1/C9H24N2O2Si/c1-9(7-11-6-5-10)8-14(4,12-2)13-3/h9,11H,5-8,10H2,1-4H3/p+1	0.176	0.168	1	1	1
2362-14-3	2362143	2353	**4,4'-cyclohexylidenedi-o-cresol**	3_REACH		4,4'-cyclohexylidenedi-o-cresol		C20H24O2	296.41	Cc1cc(ccc1O)C2(CCCCC2)c3ccc(O)c(C)c3	InChI=1/C20H24O2/c1-14-12-16(6-8-18(14)21)20(10-4-3-5-11-20)17-7-9-19(22)15(2)13-17/h6-9,12-13,21-22H,3-5,10-11H2,1-2H3	5.748	5.747	1	1	1
2370-88-9	2370889	2355	**2,4,6,8-tetramethylcyclotetrasiloxane**	3_REACH	2,4,6,8-...	2,4,6,8-tetramethylcyclotetrasiloxane	C4H16O4Si4	C4H16O4Si4	236.48	C[SiH]1O[SiH](C)O[SiH](C)O[SiH](C)O1	InChI=1/C4H16O4Si4/c1-9-5-10(2)7-12(4)8-11(3)6-9/h9-12H,1-4H3	8.556	8.556	1	1	1
2372-82-9	2372829	554	**N-(3-aminopropyl)-N-dodecylpropane-1,3-diamine**	3_REACH		N1-(3-Aminopropyl)-N1-dodecyl-1,3-propanediamine		C18H43N3	299.55	CCCCCCCCCCCCN(CCC[NH3+])CCC[NH3+]	InChI=1/C18H41N3/c1-2-3-4-5-6-7-8-9-10-11-16-21(17-12-14-19)18-13-15-20/h2-20H2,1H3/p+2	1.755	1.767	1	1	1
23779-32-0	23779320	2358	**[3-(triethoxysilyl)propyl]urea**	3_REACH		[3-(triethoxysilyl)propyl]urea		C10H24N2O4Si	264.4	CCO[Si](CCCNC(=O)N)(OCC)OCC	InChI=1/C10H24N2O4Si/c1-4-14-17(15-5-2,16-6-3)9-7-8-12-10(11)13/h4-9H2,1-3H3,(H3,11,12,13)	2.375	2.375	1	1	1
23783-42-8	23783428	2359	**3,6,9,12-tetraoxotridecanol**	3_REACH	Tetraethyleneglycol monomethylether	3,6,9,12-tetraoxotridecanol	C9H20O5	C13H20O5	208.25	CC(=O)CCC(=O)CCC(=O)CCC(=O)CCO	InChI=1/C13H20O5/c1-10(15)2-3-11(16)4-5-12(17)6-7-13(18)8-9-14/h14H,2-9H2,1H3	-0.691	-0.691	1	1	1
2380-86-1	2380861	4816	**6-hydroxyindole**	3_REACH		6-hydroxyindole			133.15					1	1	1
23847-08-7	23847087	2360	**1,1'-dithiobis[hexahydro-2H-azepin-2-one]**	3_REACH		1,1'-dithiobis[hexahydro-2H-azepin-2-one]		C12H20N2O2S2	288.43	O=C1CCCCCN1SSN2CCCCCC2=O	InChI=1/C12H20N2O2S2/c15-11-7-3-1-5-9-13(11)17-18-14-10-6-2-4-8-12(14)16/h1-10H2	2.471	2.471	1	1	1
2385-77-5	2385775	2361	**(R)-3,7-dimethyloct-6-enal**	3_REACH	6-Octenal, 3,7-dimethyl-, (R)-	(R)-3,7-dimethyloct-6-enal	C10H18O	C10H18O	154.25	C[C@H](CCC=C(C)C)CC=O	InChI=1/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,8,10H,4,6-7H2,1-3H3/t10-/m1/s1	3.018	3.018	1	1	1
2386-87-0	2386870	2362	**7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate**	3_REACH		7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate		C14H20O4	252.31	O=C(OCC1CCC2OC2C1)C3CCC4OC4C3	InChI=1/C14H20O4/c15-14(9-2-4-11-13(6-9)18-11)16-7-8-1-3-10-12(5-8)17-10/h8-13H,1-7H2	1.461	1.461	1	1	1
2402-79-1	2402791	2367	**2,3,5,6-tetrachloropyridine**	3_REACH		2,3,5,6-tetrachloropyridine		C5HCl4N	216.88	Clc1cc(Cl)c(Cl)nc1Cl	InChI=1/C5HCl4N/c6-2-1-3(7)5(9)10-4(2)8/h1H	3.755	3.755	1	1	1
2403-88-5	2403885	2368	**2,2,6,6-tetramethylpiperidin-4-ol**	3_REACH	4-Piperidinol, 2,2,6,6-tetramethyl-	2,2,6,6-tetramethylpiperidin-4-ol	C9H19NO	C9H20NO	157.26	CC1(C)CC(O)CC(C)(C)[NH2+]1	InChI=1/C9H19NO/c1-8(2)5-7(11)6-9(3,4)10-8/h7,10-11H,5-6H2,1-4H3/p+1	-0.849	-0.834	1	1	1
2403-89-6	2403896	2369	**1,2,2,6,6-pentamethylpiperidin-4-ol**	3_REACH		1,2,2,6,6-pentamethylpiperidin-4-ol		C10H22NO	171.29	C[NH+]1C(C)(C)CC(O)CC1(C)C	InChI=1/C10H21NO/c1-9(2)6-8(12)7-10(3,4)11(9)5/h8,12H,6-7H2,1-5H3/p+1	-0.643	-0.642	1	1	1
24085-06-1	24085061	2372	**(5-Acetyl-2-acetyloxyphenyl)methyl acetate**	3_REACH		Ethanone, 1-[4-(acetyloxy)-3-[(acetyloxy)methyl]phenyl]-			250.25	CC(=O)C1=CC(=C(C=C1)OC(=O)C)COC(=O)C	InChI=1S/C13H14O5/c1-8(14)11-4-5-13(18-10(3)16)12(6-11)7-17-9(2)15/h4-6H,7H2,1-3H3			1	1	1
2409-55-4	2409554	2373	**2-tert-butyl-p-cresol**	3_REACH	Phenol, 2-(1,1-dimethylethyl)-4-methyl-	2-tert-butyl-p-cresol	C11H16O	C11H16O	164.25	Cc1ccc(O)c(c1)C(C)(C)C	InChI=1/C11H16O/c1-8-5-6-10(12)9(7-8)11(2,3)4/h5-7,12H,1-4H3	3.474	3.474	1	1	1
2416-94-6	2416946	558	**2,3,6-trimethylphenol**	3_REACH	Phenol, 2,3,6-trimethyl-	2,3,6-Trimethylphenol	C9H12O	C9H12O	136.19	Cc1ccc(C)c(O)c1C	InChI=1/C9H12O/c1-6-4-5-7(2)9(10)8(6)3/h4-5,10H,1-3H3	3.046	3.046	1	1	1
24199-46-0	24199460	2376	**6-methyloct-5-en-2-one**	3_REACH	6-Methyl-5-octen-2-one	6-methyloct-5-en-2-one	C9H16O	C9H16O	140.23	CCC(=CCCC(=O)C)C	InChI=1/C9H16O/c1-4-8(2)6-5-7-9(3)10/h6H,4-5,7H2,1-3H3	2.389	2.389	1	1	1
2421-28-5	2421285	2378	**benzophenone-3,3',4,4'-tetracarboxylic dianhydride**	3_REACH	Bis-(3-phthalyl anhydride) ketone	benzophenone-3,3',4,4'-tetracarboxylic dianhydride	C17H6O7	C17H6O7	322.23	O=C(c1ccc2C(=O)OC(=O)c2c1)c3ccc4C(=O)OC(=O)c4c3	InChI=1/C17H6O7/c18-13(7-1-3-9-11(5-7)16(21)23-14(9)19)8-2-4-10-12(6-8)17(22)24-15(10)20/h1-6H	2.181	2.181	1	1	1
2425-77-6	2425776	2381	**2-hexyldecan-1-ol**	3_REACH	1-Decanol, 2-hexyl-	2-hexyldecan-1-ol	C16H34O	C16H34O	242.45	CCCCCCCCC(CO)CCCCCC	InChI=1/C16H34O/c1-3-5-7-9-10-12-14-16(15-17)13-11-8-6-4-2/h16-17H,3-15H2,1-2H3	6.308	6.308	1	1	1
24279-39-8	24279398	4333	**2,6-dichloro-4-trifluoromethylaniline**	3_REACH	4-Amino-3,5-dichlorobenzotrifluoride	2,6-dichloro-4-trifluoromethylaniline	C7H4Cl2F3N		230.02	C1=C(C=C(C(=C1Cl)N)Cl)C(F)(F)F	InChI=1S/C7H4Cl2F3N/c8-4-1-3(7(10,11)12)2-5(9)6(4)13/h1-2H,13H2			1	1	1
24293-43-4	24293434	2384	**bis(2-ethylhexyl) 2,2'-thiobisacetate**	3_REACH		bis(2-ethylhexyl) 2,2'-thiobisacetate		C20H38O4S	374.58	CCCCC(CC)COC(=O)CSCC(=O)OCC(CC)CCCC	InChI=1/C20H38O4S/c1-5-9-11-17(7-3)13-23-19(21)15-25-16-20(22)24-14-18(8-4)12-10-6-2/h17-18H,5-16H2,1-4H3	6.242	6.242	1	1	1
2439-35-2	2439352	2391	**2-(dimethylamino)ethyl acrylate**	3_REACH	2-Propenoic acid, 2-(dimethylamino)ethyl ester	2-(dimethylamino)ethyl acrylate	C7H13NO2	C7H14NO2	143.19	C[NH+](C)CCOC(=O)C=C	InChI=1/C7H13NO2/c1-4-7(9)10-6-5-8(2)3/h4H,1,5-6H2,2-3H3/p+1	-0.704	-0.023	1	1	1
24424-99-5	24424995	2393	**di(tert-butyl) carbonate**	3_REACH		di(tert-butyl) carbonate		C9H18O3	218.25	CC(C)(C)OC(=O)OC(C)(C)C	InChI=1/C9H18O3/c1-8(2,3)11-7(10)12-9(4,5)6/h1-6H3	2.526	2.526	1	1	1
24468-13-1	24468131	2395	**2-ethylhexyl chloroformate**	3_REACH		2-ethylhexyl chloroformate		C9H17ClO2	192.69	CCCCC(CC)COC(=O)Cl	InChI=1/C9H17ClO2/c1-3-5-6-8(4-2)7-12-9(10)11/h8H,3-7H2,1-2H3	4.031	4.031	1	1	1
24549-06-2	24549062	2397	**6-ethyl-2-toluidine**	3_REACH	Benzenamine, 2-ethyl-6-methyl-	6-ethyl-2-toluidine	C9H13N	C9H13N	135.21	CCc1cccc(C)c1N	InChI=1/C9H13N/c1-3-8-6-4-5-7(2)9(8)10/h4-6H,3,10H2,1-2H3	2.512	2.511	1	1	1
2461-15-6	2461156	561	**[[(2-ethylhexyl)oxy]methyl]oxirane**	3_REACH	Oxirane, [[(2-ethylhexyl)oxy]methyl	[[(2-Ethylhexyl)oxy]methyl]oxirane	C11H22O2	C11H22O2	186.29	CCCCC(CC)COCC1CO1	InChI=1/C11H22O2/c1-3-5-6-10(4-2)7-12-8-11-9-13-11/h10-11H,3-9H2,1-2H3	2.783	2.783	1	1	1
24650-42-8	24650428	2400	**2,2-dimethoxy-1,2-diphenylethan-1-one**	3_REACH	Ethanone, 2,2-dimethoxy-1,2-diphenyl-	2,2-dimethoxy-1,2-diphenylethan-1-one	C16H16O3	C16H16O3	256.3	COC(OC)(C(=O)c1ccccc1)c2ccccc2	InChI=1/C16H16O3/c1-18-16(19-2,14-11-7-4-8-12-14)15(17)13-9-5-3-6-10-13/h3-12H,1-2H3	3.15	3.15	1	1	1
24800-44-0	24800440	2404	**[(methylethylene)bis(oxy)]dipropanol**	3_REACH		[(methylethylene)bis(oxy)]dipropanol		C9H20O4	192.26	CCC(O)OCC(C)OC(O)CC	InChI=1/C9H20O4/c1-4-8(10)12-6-7(3)13-9(11)5-2/h7-11H,4-6H2,1-3H3	0.845	0.845	1	1	1
24863-70-5	24863705	2405	**1-Cyclopentene-1-acetic acid, 3-oxo-2-pentyl-, methyl ester**	3_REACH		1-Cyclopentene-1-acetic acid, 3-oxo-2-pentyl-, methyl ester			224.3	CCCCCC1=C(CCC1=O)CC(=O)OC	InChI=1S/C13H20O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h3-9H2,1-2H3			1	1	1
2495-37-6	2495376	565	**benzyl methacrylate**	3_REACH	Benzyl methacrylate	Benzyl methacrylate	C11H12O2	C11H12O2	176.22	CC(=C)C(=O)OCc1ccccc1	InChI=1/C11H12O2/c1-9(2)11(12)13-8-10-6-4-3-5-7-10/h3-7H,1,8H2,2H3	2.748	2.748	1	1	1
2500-88-1	2500881	2411	**dioctadecyl disulphide**	3_REACH		dioctadecyl disulphide		C36H74S2	571.12	CCCCCCCCCCCCCCCCCCSSCCCCCCCCCCCCCCCCCC	InChI=1/C36H74S2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-38-36-34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h3-36H2,1-2H3	16.816	16.816	1	1	1
25013-15-4	25013154	2412	**vinyltoluene**	3_REACH		vinyltoluene		C9H10	118.18	Cc1ccccc1C=C	InChI=1/C9H10/c1-3-9-7-5-4-6-8(9)2/h3-7H,1H2,2H3	2.867	2.867	1	1	1
2512-29-0	2512290	2416	**2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-phenylbutyramide**	3_REACH		2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-phenylbutyramide		C17H16N4O4	340.34	CC(=O)C(N=Nc1ccc(C)cc1[N+](=O)[O-])C(=O)Nc2ccccc2	InChI=1/C17H16N4O4/c1-11-8-9-14(15(10-11)21(24)25)19-20-16(12(2)22)17(23)18-13-6-4-3-5-7-13/h3-10,16H,1-2H3,(H,18,23)	3.57	3.57	1	1	1
25265-71-8	25265718	566	**oxydipropanol**	3_REACH	Dipropylene glycol	Dipropylene glycol	C6H14O3		134.18	CC(CO)OCC(C)O	InChI=1S/C6H14O3/c1-5(8)4-9-6(2)3-7/h5-8H,3-4H2,1-2H3			1	1	1
25265-77-4	25265774	2426	**isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol**	3_REACH		isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol		C8H18O2	216.32	CC(C)C(O)C(C)(C)CO	InChI=1/C8H18O2/c1-6(2)7(10)8(3,4)5-9/h6-7,9-10H,5H2,1-4H3	1.237	1.237	1	1	1
2526-62-7	2526627	2427	**3-(trimethoxysilyl)propiononitrile**	3_REACH		3-(trimethoxysilyl)propiononitrile		C6H13NO3Si	175.26	CO[Si](CCC#N)(OC)OC	InChI=1/C6H13NO3Si/c1-8-11(9-2,10-3)6-4-5-7/h4,6H2,1-3H3	2.003	2.003	1	1	1
2528-61-2	2528612	2428	**heptanoyl chloride**	3_REACH	Heptanoyl chloride	heptanoyl chloride	C7H13ClO	C7H13ClO	148.63	CCCCCCC(=O)Cl	InChI=1/C7H13ClO/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3	2.863	2.863	1	1	1
25307-17-9	25307179	2429	**2,2'-(octadec-9-enylimino)bisethanol**	3_REACH		2,2'-(octadec-9-enylimino)bisethanol		C22H46NO2	355.61	CCCCCCCCC=CCCCCCCCC[NH+](CCO)CCO	InChI=1/C22H45NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23(19-21-24)20-22-25/h9-10,24-25H,2-8,11-22H2,1H3/p+1	4.951	5.258	1	1	1
2530-87-2	2530872	2430	**3-chloropropyltrimethoxysilane**	3_REACH	Silane, (3-chloropropyl)trimethoxy-	3-chloropropyltrimethoxysilane	C6H15ClO3Si	C6H15ClO3Si	198.72	CO[Si](CCCCl)(OC)OC	InChI=1/C6H15ClO3Si/c1-8-11(9-2,10-3)6-4-5-7/h4-6H2,1-3H3	3.011	3.011	1	1	1
25322-69-4	25322694	568	**Propane-1,2-diol, propoxylated**	3_REACH		Polypropylene glycol			134.175	CC(CO)OCC(C)O	InChI=1S/C6H14O3/c1-5(8)4-9-6(2)3-7/h5-8H,3-4H2,1-2H3			1	1	1
25498-49-1	25498491	2436	**[2-(2-methoxymethylethoxy)methylethoxy]propanol**	3_REACH		[2-(2-methoxymethylethoxy)methylethoxy]propanol		C10H22O4	206.28	CCC(O)OCCCOCCCOC	InChI=1/C10H22O4/c1-3-10(11)14-9-5-8-13-7-4-6-12-2/h10-11H,3-9H2,1-2H3	0.187	0.187	1	1	1
2550-26-7	2550267	2437	**4-phenylbutan-2-one**	3_REACH	4-Phenyl-2-butanone	4-phenylbutan-2-one	C10H12O	C10H12O	148.21	CC(=O)CCc1ccccc1	InChI=1/C10H12O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3	2.051	2.051	1	1	1
25601-41-6	25601416	2440	**Methyl 9-decenoate**	3_REACH		Methyl dec-9-enoate			184.28	COC(=O)CCCCCCCC=C	InChI=1S/C11H20O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3H,1,4-10H2,2H3			1	1	1
256473-04-8	256473048	2441	**2-Chloro-3-(2,2,2-trifluoroethoxy)pyridine**	3_REACH		2-Chloro-3-(2,2,2-trifluoroethoxy)pyridine.			211.57	c1cc(c(nc1)Cl)OCC(F)(F)F	InChI=1S/C7H5ClF3NO/c8-6-5(2-1-3-12-6)13-4-7(9,10)11/h1-3H,4H2			1	1	1
256473-05-9	256473059	2442	**2-(isopropylthio)-3-(2,2,2-trifluoroethoxy)pyridine**	3_REACH		2-(isopropylthio)-3-(2,2,2-trifluoroethoxy)pyridine			251.27	CC(C)SC1=C(OCC(F)(F)F)C=CC=N1				1	1	1
2568-90-3	2568903	2443	**1,1'-[methylenebis(oxy)]dibutane**	3_REACH	Butane, 1,1'-[methylenebis(oxy)]bis	1,1'-[methylenebis(oxy)]dibutane	C9H20O2	C9H20O2	160.26	CCCCOCOCCCC	InChI=1/C9H20O2/c1-3-5-7-10-9-11-8-6-4-2/h3-9H2,1-2H3	2.559	2.559	1	1	1
2602-34-8	2602348	2449	**[3-(2,3-epoxypropoxy)propyl]triethoxysilane**	3_REACH		[3-(2,3-epoxypropoxy)propyl]triethoxysilane		C12H26O5Si	278.42	CCO[Si](CCCOCC1CO1)(OCC)OCC	InChI=1/C12H26O5Si/c1-4-15-18(16-5-2,17-6-3)9-7-8-13-10-12-11-14-12/h12H,4-11H2,1-3H3	2.978	2.978	1	1	1
2605-79-0	2605790	2452	**N,N-dimethyldecylamine N-oxide**	3_REACH		N,N-dimethyldecylamine N-oxide		C12H27NO	201.35	CCCCCCCCCC[N+](C)(C)[O-]	InChI=1/C12H27NO/c1-4-5-6-7-8-9-10-11-12-13(2,3)14/h4-12H2,1-3H3	3.578	3.578	1	1	1
2612-57-9	2612579	2455	**2,4-dichlorophenyl isocyanate**	3_REACH		2,4-dichlorophenyl isocyanate		C7H3Cl2NO	188.01	Clc1ccc(N=C=O)c(Cl)c1	InChI=1/C7H3Cl2NO/c8-5-1-2-7(10-4-11)6(9)3-5/h1-3H	3.019	3.019	1	1	1
26159-31-9	26159319	572	**(±)-2-(6-methoxy-2-naphthyl)propionic acid**	3_REACH	2-(6-methoxy-2-naphthyl)propionic acid	(±)-2-(6-methoxy-2-naphthyl)propionic acid	C14H14O3	C14H13O3	230.26	COc1ccc2cc(ccc2c1)C(C)C(=O)[O-]	InChI=1/C14H14O3/c1-9(14(15)16)10-3-4-12-8-13(17-2)6-5-11(12)7-10/h3-9H,1-2H3,(H,15,16)/p-1	1.375	1.394	1	1	1
26218-04-2	26218042	4353	**2-ethylhexyl 4-aminobenzoate**	3_REACH		2-ethylhexyl 4-aminobenzoate			249.35	CCCCC(CC)COC(=O)C1=CC=C(C=C1)N	InChI=1S/C15H23NO2/c1-3-5-6-12(4-2)11-18-15(17)13-7-9-14(16)10-8-13/h7-10,12H,3-6,11,16H2,1-2H3			1	1	1
26272-90-2	26272902	2460	**hexadecyl chloroformate**	3_REACH		hexadecyl chloroformate		C17H33ClO2	304.9	CCCCCCCCCCCCCCCCOC(=O)Cl	InChI=1/C17H33ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-17(18)19/h2-16H2,1H3	7.818	7.818	1	1	1
2627-86-3	2627863	2461	**L-1-Phenylethylamine**	3_REACH	Benzenemethanamine, α-methyl-, (S)-	L-a-methylbenzylamine	C8H11N	C8H12N	121.18	C[C@H]([NH3+])c1ccccc1	InChI=1/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3/p+1/t7-/m0/s1	0.308	0.382	1	1	1
26364-65-8	26364658	4511	**2-thiazolidinylidenecyanamide**	3_REACH		Cyanamide, N-(4,5-dihydro-2-thiazolyl)-			127.17	C1CSC(=N1)NC#N	InChI=1S/C4H5N3S/c5-3-7-4-6-1-2-8-4/h1-2H2,(H,6,7)			1	1	1
26399-02-0	26399020	2468	**2-ethylhexyl oleate**	3_REACH		2-ethylhexyl oleate		C26H50O2	394.68	CCCCCCCC\C=C/CCCCCCCC(=O)OCC(CC)CCCC	InChI=1/C26H50O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-26(27)28-24-25(6-3)22-8-5-2/h14-15,25H,4-13,16-24H2,1-3H3/b15-14-	10.102	10.102	1	1	1
26523-78-4	26523784	2474	**tris(nonylphenyl) phosphite**	3_REACH		tris(nonylphenyl) phosphite		C45H69O3P	689.02	CCCCCCCCCc1ccccc1OP(Oc2ccccc2CCCCCCCCC)Oc3ccccc3CCCCCCCCC	InChI=1/C45H69O3P/c1-4-7-10-13-16-19-22-31-40-34-25-28-37-43(40)46-49(47-44-38-29-26-35-41(44)32-23-20-17-14-11-8-5-2)48-45-39-30-27-36-42(45)33-24-21-18-15-12-9-6-3/h25-30,34-39H, 4-24,31-33H2,1-3H3	16.744	16.744	1	0	1
26586-02-7	26586027	2480	**(E)-3-formylbut-2-enyl acetate**	3_REACH		(E)-3-formylbut-2-enyl acetate		C7H10O3	142.15	CC(=O)OC\C=C(/C)\C=O	InChI=1/C7H10O3/c1-6(5-8)3-4-10-7(2)9/h3,5H,4H2,1-2H3/b6-3+	0.652	0.652	1	1	1
26741-53-7	26741537	2485	**3,9-bis(2,4-di-tert-butylphenoxy)-**	3_REACH		3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-		C33H50O6P2	604.71	CC(C)(C)c1ccc(OP2OCC3(COP(Oc4ccc(cc4C(C)(C)C)C(C)(C)C)OC3)CO2)c(c1)C(C)(C)C	InChI=1/C33H50O6P2/c1-29(2,3)23-13-15-27(25(17-23)31(7,8)9)38-40-34-19-33(20-35-40)21-36-	6.491	6.491	0	0	1
26761-45-5	26761455	2487	**2,3-epoxypropyl neodecanoate**	3_REACH		2,3-epoxypropyl neodecanoate		C13H24O3	228.33	CCCCCCC(C)(C)C(=O)OCC1CO1	InChI=1/C13H24O3/c1-4-5-6-7-8-13(2,3)12(14)16-10-11-9-15-11/h11H,4-10H2,1-3H3	3.564	3.564	1	1	1
2687-91-4	2687914	2489	**1-ethylpyrrolidin-2-one**	3_REACH	1-Ethyl-2-pyrrolidinone	1-ethylpyrrolidin-2-one	C6H11NO	C6H11NO	113.16	CCN1CCCC1=O	InChI=1/C6H11NO/c1-2-7-5-3-4-6(7)8/h2-5H2,1H3	0.183	0.183	1	1	1
26896-20-8	26896208	2491	**neodecanoic acid**	3_REACH	Neodecanoic acid	neodecanoic acid	C10H20O2	C10H19O2	172.27	CCC(C)(CCC(C)(C)C)C(=O)[O-]	InChI=1/C10H20O2/c1-5-10(4,9(11)12)7-6-8(2,3)4/h5-7H2,1-4H3,(H,11,12)/p-1	1.944	2.103	1	1	1
2691-41-0	2691410	575	**octahydro-1,3,5,7-tetranitro-1,3,5,7-**	3_REACH	1,3,5,7-Tetrazocine, octahydro-	Octahydro-1,3,5,7-tetranitro-1,3,5,7-	C4H8N8O8	C4H8N8O8	296.16	[O-][N+](=O)N1CN(CN(CN(C1)[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C4H8N8O8/c13-9(14)5-1-6(10(15)16)3-8(12(19)20)4-7(2-5)11(17)18/h1-4H2	6.884	6.884	1	1	1
2705-87-5	2705875	2493	**allyl 3-cyclohexylpropionate**	3_REACH	Cyclohexanepropanoic acid, 2-propenyl ester	allyl 3-cyclohexylpropionate	C12H20O2	C12H20O2	196.29	C=CCOC(=O)CCC1CCCCC1	InChI=1/C12H20O2/c1-2-10-14-12(13)9-8-11-6-4-3-5-7-11/h2,11H,1,3-10H2	3.466	3.466	1	1	1
27458-94-2	27458942	2507	**isononyl alcohol**	3_REACH	Isononanol	isononyl alcohol	C9H20O	C9H20O	144.26	CC(CCO)CC(C)(C)C	InChI=1/C9H20O/c1-8(5-6-10)7-9(2,3)4/h8,10H,5-7H2,1-4H3	2.592	2.592	1	1	1
2752-17-2	2752172	2511	**2,2'-oxydi(ethylamine)**	3_REACH		2,2'-oxydi(ethylamine)		C4H14N2O	104.16	[NH3+]CCOCC[NH3+]	InChI=1/C4H12N2O/c5-1-3-7-4-2-6/h1-6H2/p+2	-3.618	-3.342	1	1	1
2778-42-9	2778429	2517	**1,3-bis(1-isocyanato-1-methylethyl)benzene**	3_REACH	1,3-Bis-(1-isocyanato-1-methylethyl)benzene	1,3-bis(1-isocyanato-1-methylethyl)benzene	C14H16N2O2	C14H16N2O2	244.3	CC(C)(N=C=O)c1cccc(c1)C(C)(C)N=C=O	InChI=1/C14H16N2O2/c1-13(2,15-9-17)11-6-5-7-12(8-11)14(3,4)16-10-18/h5-8H,1-4H3	2.729	2.728	1	1	1
2786-76-7	2786767	2520	**4-[[4-(aminocarbonyl)phenyl]azo]-N-(2-ethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide**	3_REACH		4-[[4-(aminocarbonyl)phenyl]azo]-N-(2-ethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide		C26H21N4O4	454.49	CCOc1ccccc1NC(=O)c2cc3ccccc3c(N=Nc4ccc(cc4)C(=O)N)c2[O-]	InChI=1/C26H22N4O4/c1-2-34-22-10-6-5-9-21(22)28-26(33)20-15-17-7-3-4-8-19(17)23(24(20)31)3 29-18-13-11-16(12-14-18)25(27)32/h3-15,31H,2H2,1H3,(H2,27,32)(H,28,33)/p-1	4.281	4.985	1	1	1
27955-94-8	27955948	4403	**4,4',4''-(ethan-1,1,1-triyl)triphenol**	3_REACH	Phenol, 4,4',4''-ethylidynetris-	4,4',4''-(ethan-1,1,1-triyl)triphenol	C20H18O3		306.36	CC(C1=CC=C(C=C1)O)(C2=CC=C(C=C2)O)C3=CC=C(C=C3)O	InChI=1S/C20H18O3/c1-20(14-2-8-17(21)9-3-14,15-4-10-18(22)11-5-15)16-6-12-19(23)13-7-16/h2-13,21-23H,1H3			1	1	1
2809-21-4	2809214	578	**etidronic acid**	3_REACH		1-hydroxy-ethylideen-1,1-difosfonzuur		C2H4O7P2	206.03	CC(O)(P(=O)([O-])[O-])P(=O)([O-])[O-]	InChI=1/C2H8O7P2/c1-2(3,10(4,5)6)11(7,8)9/h3H,1H3,(H2,4,5,6)(H2,7,8,9)/p-4	-5.055	-4.375	1	1	1
281-23-2	281232	579	**tricyclo[3.3.1.13,7]decane**	3_REACH	Adamantane	Adamantane	C10H16	C10H16	136.24	C1C2CC3CC(CC1C3)C2	InChI=1/C10H16/c1-7-2-9-4-8(1)5-10(3-7)6-9/h7-10H,1-6H2	3.001	3.001	1	1	1
28219-61-6	28219616	2525	**2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol**	3_REACH		2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol		C14H24O	208.35	CCC(=CCC1CC=C(C)C1(C)C)CO	InChI=1/C14H24O/c1-5-12(10-15)7-9-13-8-6-11(2)14(13,3)4/h6-7,13,15H,5,8-10H2,1-4H3	3.728	3.728	1	1	1
28479-22-3	28479223	2533	**3-chloro-p-tolyl isocyanate**	3_REACH		3-chloro-p-tolyl isocyanate		C8H6ClNO	167.6	Cc1ccc(cc1Cl)N=C=O	InChI=1/C8H6ClNO/c1-6-2-3-7(10-5-11)4-8(6)9/h2-4H,1H3	2.84	2.84	1	1	1
28535-81-1	28535811	2535	**Methyl 3alpha,7alpha-diacetoxy-12-oxo-5beta-cholanate**	3_REACH		methyl 3-a,7-a-diacetoxy-12-oxo-5-ß-cholan-24-oate		C29H44O7	504.66	COC(=O)CCC(C)C1CCC2C3C(CC4CC(CCC4(C)C3CC(=O)C12C)OC(=O)C)OC(=O)C	InChI=1/C29H44O7/c1-16(7-10-26(33)34-6)21-8-9-22-27-23(15-25(32)29(21,22)5)28(4)12-11-20(35 17(2)30)13-19(28)14-24(27)36-18(3)31/h16,19-24,27H,7-15H2,1-6H3	3.997	3.997	1	1	1
2855-13-2	2855132	2536	**3-aminomethyl-3,5,5-trimethylcyclohexylamine**	3_REACH		3-aminomethyl-3,5,5-trimethylcyclohexylamine		C10H24N2	170.3	CC1(C)CC([NH3+])CC(C)(C[NH3+])C1	InChI=1/C10H22N2/c1-9(2)4-8(12)5-10(3,6-9)7-11/h8H,4-7,11-12H2,1-3H3/p+2	-1.264	-1.25	1	1	1
28553-12-0	28553120	582	**di-"isononyl" phthalate**	3_REACH		Diisononylphthalate		C26H42O4	418.62	CC(C)CCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCC(C)C	InChI=1/C26H42O4/c1-21(2)15-9-5-7-13-19-29-25(27)23-17-11-12-18-24(23)26(28)30-20-14-8-6-1	8.351	8.351	1	1	1
2867-47-2	2867472	583	**2-dimethylaminoethyl methacrylate**	3_REACH	Dimethylaminoethyl methacrylate	(Dimethylamino)ethylmethacrylate	C8H15NO2	C8H16NO2	157.21	C[NH+](C)CCOC(=O)C(=C)C	InChI=1/C8H15NO2/c1-7(2)8(10)11-6-5-9(3)4/h1,5-6H2,2-4H3/p+1	-0.257	0.423	1	1	1
28768-32-3	28768323	2543	**4,4'-methylenebis[N,N-bis(2,3-epoxypropyl)aniline]**	3_REACH		4,4'-methylenebis[N,N-bis(2,3-epoxypropyl)aniline]		C25H30N2O4	422.53	C(C1CO1)N(CC2CO2)c3ccc(Cc4ccc(cc4)N(CC5CO5)CC6CO6)cc3	InChI=1/C25H30N2O4/c1-5-20(26(10-22-14-28-22)11-23-15-29-23)6-2-18(1)9-19-3-7-21(8-4-19)27(12-24-16-30-24)13-25-17-31-25/h1-8,22-25H,9-17H2	2.994	2.911	1	1	1
288-13-1	288131	43	**pyrazole**	3_REACH	1H-Pyrazole	1H-Pyrazole	C3H4N2	C3H4N2	68.081	c1cn[nH]c1	InChI=1/C3H4N2/c1-2-4-5-3-1/h1-3H,(H,4,5)	0.273	0.273	1	1	1
288-88-0	288880	584	**1,2,4-triazole**	3_REACH	1H-1,2,4-Triazole	1H-1,2,4-Triazole	C2H3N3	C2H3N3	69.07	c1nc[nH]n1	InChI=1/C2H3N3/c1-3-2-5-4-1/h1-2H,(H,3,4,5)	-0.41	-0.41	1	1	1
2896-70-0	2896700	2550	**2,2,6,6-tetramethyl-4-oxopiperidinooxy**	3_REACH	1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-oxo-	2,2,6,6-tetramethyl-4-oxopiperidinooxy	C9H16NO2	C9H17NO2	171.24	CC1(C)CC(=O)CC(C)(C)[NH+]1[O]	InChI=1/C9H17NO2/c1-8(2)5-7(11)6-9(3,4)10(8)12/h10H,5-6H2,1-4H3/q+1	1.03	1.03	1	1	1
2915-57-3	2915573	2559	**bis(2-ethylhexyl) succinate**	3_REACH	Dioctyl succinate	bis(2-ethylhexyl) succinate	C20H38O4	C20H38O4	342.52	CCCCC(CC)COC(=O)CCC(=O)OCC(CC)CCCC	InChI=1/C20H38O4/c1-5-9-11-17(7-3)15-23-19(21)13-14-20(22)24-16-18(8-4)12-10-6-2/h17-18H,5-16H2,1-4H3	6.125	6.125	1	1	1
29171-20-8	29171208	2560	**3,7-dimethyloct-6-en-1-yn-3-ol**	3_REACH	3,7-Dimethyl-6-octen-1-yn-3-ol	3,7-dimethyloct-6-en-1-yn-3-ol	C10H16O	C10H16O	152.24	CC(=CCCC(C)(O)C#C)C	InChI=1/C10H16O/c1-5-10(4,11)8-6-7-9(2)3/h1,7,11H,6,8H2,2-4H3	3.31	3.31	1	1	1
2920-38-9	2920389	2561	**p-phenylbenzonitrile**	3_REACH	4-Biphenylcarbonitrile	p-phenylbenzonitrile	C13H9N	C13H9N	179.22	N#Cc1ccc(cc1)c2ccccc2	InChI=1/C13H9N/c14-10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-9H	3.227	3.227	1	1	1
2935-90-2	2935902	2563	**methyl 3-mercaptopropionate**	3_REACH	Propanoic acid, 3-mercapto-, methyl ester	methyl 3-mercaptopropionate	C4H8O2S	C4H8O2S	120.17	COC(=O)CCS	InChI=1/C4H8O2S/c1-6-4(5)2-3-7/h7H,2-3H2,1H3	0.568	0.569	1	1	1
2942-59-8	2942598	2566	**2-chloronicotinic acid**	3_REACH		2-chloronicotinic acid		C6H3ClNO2	157.56	[O-]C(=O)c1cccnc1Cl	InChI=1/C6H4ClNO2/c7-5-4(6(9)10)2-1-3-8-5/h1-3H,(H,9,10)/p-1	-0.292	1.017	1	1	1
2943-75-1	2943751	2567	**triethoxyoctylsilane**	3_REACH	N-Octyltriethoxysilane	triethoxyoctylsilane	C14H32O3Si	C14H32O3Si	276.49	CCCCCCCC[Si](OCC)(OCC)OCC	InChI=1/C14H32O3Si/c1-5-9-10-11-12-13-14-18(15-6-2,16-7-3)17-8-4/h5-14H2,1-4H3	6.36	6.36	1	1	1
294-62-2	294622	587	**cyclododecane**	3_REACH	Cyclododecane	Cyclododecane	C12H24	C12H24	168.32	C1CCCCCCCCCCC1	InChI=1/C12H24/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-12H2	5.474	5.474	1	1	1
294-90-6	294906	4493	**1,4,7,10-tetraazacyclododecane**	3_REACH		1,4,7,10-Tetraazacyclododecane			172.28	C1CNCCNCCNCCN1	InChI=1S/C8H20N4/c1-2-10-5-6-12-8-7-11-4-3-9-1/h9-12H,1-8H2			1	1	1
29761-21-5	29761215	588	**isodecyl diphenyl phosphate**	3_REACH		Phosphoric acid, Isodecyl diphenyl ester		C22H31O4P	390.46	CC(C)CCCCCCCOP(=O)(Oc1ccccc1)Oc2ccccc2	InChI=1/C22H31O4P/c1-20(2)14-8-4-3-5-13-19-24-27(23,25-21-15-9-6-10-16-21)26-22-17-11-7-12-18-22/h6-7,9-12,15-18,20H,3-5,8,13-14,19H2,1-2H3	7.036	7.036	1	1	1
298-06-6	298066	591	**O,O-diethyl hydrogen phosphorodithioate**	3_REACH	Phosphorodithioic acid, o,o'-diethyl ester	O,O-Diethyl ester phosphorodithioic acid	C4H11O2PS2	C4H11O2PS2	186.23	CCOP(=S)(S)OCC	InChI=1/C4H11O2PS2/c1-3-5-7(8,9)6-4-2/h3-4H2,1-2H3,(H,8,9)	1.808	1.808	1	1	1
29806-73-3	29806733	2572	**2-ethylhexyl palmitate**	3_REACH		2-ethylhexyl palmitate		C24H48O2	368.65	CCCCCCCCCCCCCCCC(=O)OCC(CC)CCCC	InChI=1/C24H48O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-21-24(25)26-22-23(6-3)20-8-5-2/h23H,4-22H2,1-3H3	9.635	9.635	1	1	1
298-07-7	298077	592	**bis(2-ethylhexyl) hydrogen phosphate**	3_REACH	Bis(2-ethylhexyl)hydrogen phosphate	Di-2-(ethylhexyl)phosphoric acid	C16H35O4P	C16H34O4P	322.43	CCCCC(CC)COP(=O)([O-])OCC(CC)CCCC	InChI=1/C16H35O4P/c1-5-9-11-15(7-3)13-19-21(17,18)20-14-16(8-4)12-10-6-2/h15-16H,5-14H2,1-4H3,(H,17,18)/p-1	4.168	4.172	1	1	1
298-12-4	298124	2573	**glyoxylic acid**	3_REACH	Acetic acid, oxo-	glyoxylic acid	C2H2O3	C2HO3	74.035	[O-]C(=O)C=O	InChI=1/C2H2O3/c3-1-2(4)5/h1H,(H,4,5)/p-1	-1.881	-1.881	1	1	1
29911-28-2	29911282	2578	**1-(2-butoxy-1-methylethoxy)propan-2-ol**	3_REACH		1-(2-butoxy-1-methylethoxy)propan-2-ol		C10H22O3	190.28	CCCCOCC(C)OCC(C)O	InChI=1/C10H22O3/c1-4-5-6-12-8-10(3)13-7-9(2)11/h9-11H,4-8H2,1-3H3	1.463	1.463	1	1	1
29920-31-8	29920318	2579	**dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azoterephthalate**	3_REACH		dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azoterephthalate		C21H19N5O7	453.42	COC(=O)c1cc(cc(c1)C(=O)OC)N=NC(C(=O)C)C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C21H19N5O7/c1-10(27)17(18(28)22-13-4-5-15-16(9-13)24-21(31)23-15)26-25-14-7-11(19(29)32-2)6-12(8-14)20(30)33-3/h4-9,17H,1-3H3,(H,22,28)(H2,23,24,31)/b26-25+	2.716	2.716	1	1	1
29964-84-9	29964849	2581	**isodecyl methacrylate**	3_REACH		isodecyl methacrylate		C14H26O2	226.36	CC(C)CCCCCCCOC(=O)C(=C)C	InChI=1/C14H26O2/c1-12(2)10-8-6-5-7-9-11-16-14(15)13(3)4/h12H,3,5-11H2,1-2,4H3	5.026	5.026	1	1	1
2996-92-1	2996921	2582	**trimethoxyphenylsilane**	3_REACH	Silane, trimethoxyphenyl-	trimethoxyphenylsilane	C9H14O3Si	C9H14O3Si	198.29	CO[Si](OC)(OC)c1ccccc1	InChI=1/C9H14O3Si/c1-10-13(11-2,12-3)9-7-5-4-6-8-9/h4-8H,1-3H3	3.601	3.601	1	1	1
3030-47-5	3030475	2590	**bis(2-dimethylaminoethyl)(methyl)amine**	3_REACH		bis(2-dimethylaminoethyl)(methyl)amine		C9H24N3	173.31	CN(C)CC[NH+](C)CCN(C)C	InChI=1/C9H23N3/c1-10(2)6-8-12(5)9-7-11(3)4/h6-9H2,1-5H3/p+1	-0.964	-0.964	1	1	1
3031-66-1	3031661	2591	**hex-3-yne-2,5-diol**	3_REACH	3-Hexyne-2,5-diol	hex-3-yne-2,5-diol	C6H10O2	C6H10O2	114.14	CC(O)C#CC(C)O	InChI=1/C6H10O2/c1-5(7)3-4-6(2)8/h5-8H,1-2H3	0.447	0.447	1	1	1

3033-62-3	3033623	2592	**N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)**	3_REACH	Ethanamine, 2,2'-oxybis[N,N-dimethyl-	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	C8H20N2O	C8H22N2O	160.26	C[NH+](C)CCOCC[NH+](C)C	InChI=1/C8H20N2O/c1-9(2)5-7-11-8-6-10(3)4/h5-8H2,1-4H3/p+2	-2.794	-1.6	1	1	1
3047-32-3	3047323	2598	**3-ethyloxetane-3-methanol**	3_REACH	3-Ethyl-3-hydroxymethyl oxetane	3-ethyloxetane-3-methanol	C6H12O2	C6H12O2	116.16	CCC1(CO)COC1	InChI=1/C6H12O2/c1-2-6(3-7)4-8-5-6/h7H,2-5H2,1H3	0.148	0.148	1	1	1
3049-71-6	3049716	2600	**2,9-bis[4-(phenylazo)phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone**	3_REACH		2,9-bis[4-(phenylazo)phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone		C48H26N6O4	750.78	O=C1N(C(=O)c2ccc3c4ccc5C(=O)N(C(=O)c6ccc(c7ccc1c2c37)c4c56)c8ccc(cc8)N=Nc9ccccc9)c%10ccc(cc%10)N=Nc%	InChI=1/C48H26N6O4/c55-45-37-23-19-33-35-21-25-39-44-40(48(58)54(47(39)57)32-17-13-30(14-32)52-50-28-9-5-2-6-10-28)26-22-36(42(35)44)34-20-24-38(43(37)41(33)34)46(56)53(45)31-15-11-29(12-16-31)51-49-27-7-3-1-4-8-27/h1-26H	10.81	10.81	0	1	1
3061-75-4	3061754	2604	**docosanamide**	3_REACH		docosanamide		C22H45NO	339.61	CCCCCCCCCCCCCCCCCCCCCC(=O)N	InChI=1/C22H45NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24/h2-21H2,1H3,(H2,23,24)	8.502	8.502	1	1	1
30674-80-7	30674807	2606	**2-isocyanatoethyl methacrylate**	3_REACH		2-isocyanatoethyl methacrylate		C7H10NO3	155.15	CC(=C)C(=O)OCC[NH+]=C=O	InChI=1/C7H9NO3/c1-6(2)7(10)11-4-3-8-5-9/h1,3-4H2,2H3/p+1	0.993	0.993	1	1	1
3069-29-2	3069292	2608	**N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine**	3_REACH		N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine		C8H23N2O2Si	206.36	COC(OC)[SiH2]CCC[NH2+]CCN	InChI=1/C8H22N2O2Si/c1-11-8(12-2)13-7-3-5-10-6-4-9/h8,10H,3-7,9,13H2,1-2H3/p+1	1.174	1.164	1	1	1
3069-40-7	3069407	2609	**trimethoxyoctylsilane**	3_REACH	N-Octyltrimethoxysilane	trimethoxyoctylsilane	C11H26O3Si	C11H26O3Si	234.41	CCCCCCCC[Si](OC)(OC)OC	InChI=1/C11H26O3Si/c1-5-6-7-8-9-10-11-15(12-2,13-3)14-4/h5-11H2,1-4H3	5.313	5.313	1	1	1
3081-14-9	3081149	2612	**N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine**	3_REACH		N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine		C20H36N2	304.52	CC(C)CCC(C)Nc1ccc(NC(C)CCC(C)C)cc1	InChI=1/C20H36N2/c1-15(2)7-9-17(5)21-19-11-13-20(14-12-19)22-18(6)10-8-16(3)4/h11-18,21-22H,7-10H2,1-6H3	6.275	6.261	1	1	1
3089-16-5	3089165	2614	**4,11-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione**	3_REACH		4,11-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione		C20H8Cl2N2O2	381.22	[O-]c1c2cc3nc4c(Cl)cccc4c([O-])c3cc2nc5c(Cl)cccc15	InChI=1/C20H10Cl2N2O2/c21-13-5-1-3-9-17(13)23-15-8-12-16(7-11(15)19(9)25)24-18-10(20(12)26)2-6-14(18)22/h1-8H,(H,23,25)(H,24,26)/p-2	4.314	5.274	1	1	1
3089-17-6	3089176	2615	**2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione**	3_REACH		2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione		C20H8Cl2N2O2	381.22	[O-]c1c2cc(Cl)ccc2nc3cc4c([O-])c5cc(Cl)ccc5nc4cc13	InChI=1/C20H10Cl2N2O2/c21-9-1-3-15-11(5-9)19(25)13-8-18-14(7-17(13)23-15)20(26)12-6-10(22) 4-16(12)24-18/h1-8H,(H,23,25)(H,24,26)/p-2	4.314	5.274	1	1	1
31024-56-3	31024563	2617	**N-[3-(trimethoxysilyl)propyl]butylamine**	3_REACH		N-[3-(trimethoxysilyl)propyl]butylamine		C10H26NO3Si	235.4	CCCC[NH2+]CCC[Si](OC)(OC)OC	InChI=1/C10H25NO3Si/c1-5-6-8-11-9-7-10-15(12-2,13-3)14-4/h11H,5-10H2,1-4H3/p+1	2.047	2.048	1	1	1
31027-31-3	31027313	2618	**p-isopropylphenyl isocyanate**	3_REACH		p-isopropylphenyl isocyanate		C10H11NO	161.21	CC(C)c1ccc(cc1)N=C=O	InChI=1/C10H11NO/c1-8(2)9-3-5-10(6-4-9)11-7-12/h3-6,8H,1-2H3	2.884	2.884	1	1	1
3115-49-9	3115499	2619	**(4-nonylphenoxy)acetic acid**	3_REACH		(4-nonylphenoxy)acetic acid		C17H25O3	278.39	CCCCCCCCCc1ccc(OCC(=O)[O-])cc1	InChI=1/C17H26O3/c1-2-3-4-5-6-7-8-9-15-10-12-16(13-11-15)20-14-17(18)19/h10-13H,2-9,14H2,1H3,(H,18,19)/p-1	3.956	3.957	1	1	1
31335-74-7	31335747	2625	**2,2-dimethyl-1,3-propanediyl dioctanoate**	3_REACH		2,2-dimethyl-1,3-propanediyl dioctanoate		C21H40O4	356.55	CCCCCCCC(=O)OCC(C)(C)COC(=O)CCCCCCC	InChI=1/C21H40O4/c1-5-7-9-11-13-15-19(22)24-17-21(3,4)18-25-20(23)16-14-12-10-8-6-2/h5-18H2,1-4H3	6.67	6.67	1	1	1
3148-73-0	3148730	2627	**N,N'-diacetylhydrazine**	3_REACH	1,2-Diacetylhydrazine	N,N'-diacetylhydrazine	C4H8N2O2	C4H8N2O2	116.12	CC(=O)NNC(=O)C	InChI=1/C4H8N2O2/c1-3(7)5-6-4(2)8/h1-2H3,(H,5,7)(H,6,8)	-1.458	-1.458	1	1	1
3173-72-6	3173726	2631	**1,5-naphthylene diisocyanate**	3_REACH	Naphthalene, 1,5-diisocyanato-	1,5-naphthylene diisocyanate	C12H6N2O2	C12H6N2O2	210.19	O=C=Nc1cccc2c(cccc12)N=C=O	InChI=1/C12H6N2O2/c15-7-13-11-5-1-3-9-10(11)4-2-6-12(9)14-8-16/h1-6H	2.459	2.458	1	1	1
31775-20-9	31775209	2632	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-ethoxyphenyl)-3-oxobutyramide]**	3_REACH		2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-ethoxyphenyl)-3-oxobutyramide]		C36H33Cl2N6O6	717.62	CCOc1ccc(NC(=O)C(N=Nc2ccc(cc2Cl)c3ccc(N=N[C-](C(=O)C)C(=O)Nc4ccc(OCC)cc4)c(Cl)c3)C(=O)C)cc1	InChI=1/C36H33Cl2N6O6/c1-5-49-27-13-9-25(10-14-27)39-35(47)33(21(3)45)43-41-31-17-7-23(19-29(31)37)24-8-18-32(30(38)20-24)42-44-34(22(4)46)36(48)40-26-11-15-28(16-12-26)50-6-2/h7-20,33H,5-6H2,1-4H3,(H,39,47)(H,40,48)/q-1	8.061	8.219	1	1	1
31775-89-0	31775890	2633	**3-[(3-sulfanylbutanoyl)oxy]-2,2-bis{[(3-sulfanylbutanoyl)oxy]methyl}propyl 3-sulfanylbutanoate**	3_REACH		3-[(3-sulfanylbutanoyl)oxy]-2,2-bis{[(3-sulfanylbutanoyl)oxy]methyl}propyl 3-sulfanylbutanoate			544.77					1	1	1
31778-10-6	31778106	2634	**butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthyl]azo]benzoate**	3_REACH		butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthyl]azo]benzoate		C29H24N5O5	523.55	CCCCOC(=O)c1ccccc1N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4ccc5[nH]c(O)nc5c4	InChI=1/C29H25N5O5/c1-2-3-14-39-28(37)20-10-6-7-11-22(20)33-34-25-19-9-5-4-8-17(19)15-21(26(25)35)27(36)30-18-12-13-23-24(16-18)32-29(38)31-23/h4-13,15-16,35H,2-3,14H2,1H3,(H,30,36)(H2,31,32,38)/p-1	5.946	6.648	1	1	1
3179-47-3	3179473	2635	**decyl methacrylate**	3_REACH	Decyl methacrylate	decyl methacrylate	C14H26O2	C14H26O2	226.36	CCCCCCCCCCOC(=O)C(=C)C	InChI=1/C14H26O2/c1-4-5-6-7-8-9-10-11-12-16-14(15)13(2)3/h2,4-12H2,1,3H3	5.231	5.231	1	1	1
3179-63-3	3179633	2636	**3-dimethylaminopropan-1-ol**	3_REACH	1-Propanol, 3-(dimethylamino)-	3-dimethylaminopropan-1-ol	C5H13NO	C5H14NO	103.17	C[NH+](C)CCCO	InChI=1/C5H13NO/c1-6(2)4-3-5-7/h7H,3-5H2,1-2H3/p+1	-1.718	-1.56	1	1	1
3179-76-8	3179768	2637	**3-(diethoxymethylsilyl)propylamine**	3_REACH	1-Propanamine, 3-(diethoxymethylsilyl)-	3-(diethoxymethylsilyl)propylamine	C8H21NO2Si	C8H22NO2Si	191.35	CCO[Si](C)(CCC[NH3+])OCC	InChI=1/C8H21NO2Si/c1-4-10-12(3,11-5-2)8-6-7-9/h4-9H2,1-3H3/p+1	1.177	1.179	1	1	1
31837-42-0	31837420	2639	**2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzoic acid**	3_REACH		2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzoic acid		C18H14N5O5	381.35	CC(=O)C(N=Nc1ccccc1C(=O)[O-])C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C18H15N5O5/c1-9(24)15(23-22-12-5-3-2-4-11(12)17(26)27)16(25)19-10-6-7-13-14(8-10)2 18(28)20-13/h2-8,15H,1H3,(H,19,25)(H,26,27)(H2,20,21,28)/p-1	1.16	2.088	1	1	1
319002-92-1	319002921	4599	**Propyl (2S)-2-(2-methylbutan-2-yloxy)propanoate**	3_REACH		SCLAREOLATE			202.29	CCCOC(=O)C(C)OC(C)(C)CC	InChI=1S/C11H22O3/c1-6-8-13-10(12)9(3)14-11(4,5)7-2/h9H,6-8H2,1-5H3/t9-/m0/s1			1	1	1
3209-22-1	3209221	600	**1,2-dichloro-3-nitrobenzene**	3_REACH	Benzene, 1,2-dichloro-3-nitro-	1,2-Dichloro-3-nitrobenzene	C6H3Cl2NO2	C6H3Cl2NO2	192	[O-][N+](=O)c1cccc(Cl)c1Cl	InChI=1/C6H3Cl2NO2/c7-4-2-1-3-5(6(4)8)9(10)11/h1-3H	3.053	3.053	1	1	1
3234-85-3	3234853	2648	**tetradecyl myristate**	3_REACH	Tetradecanoic acid, tetradecyl ester	tetradecyl myristate	C28H56O2	C28H56O2	424.75	CCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCC	InChI=1/C28H56O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-30-28(29)26-24-22-20-18-16-14-12-10-8-6-4-2/h3-27H2,1-2H3	11.596	11.596	0	0	1
32388-55-9	32388559	2651	**Acetyl cedrene**	3_REACH		[3R-(3a,3aß,7ß,8aa)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one		C17H26O	246.39	CC1CCC2C(C)(C)C3CC12CC(=C3C)C(=O)C	InChI=1/C17H26O/c1-10-6-7-15-16(4,5)14-9-17(10,15)8-13(11(14)2)12(3)18/h10,14-15H,6-9H2,1-5H3	3.813	3.813	1	1	1
329-01-1	329011	2668	**3-(Trifluoromethyl)phenyl isocyanate**	3_REACH	Benzene, 1-isocyanato-3-(trifluoromethyl)-	a,a,a-trifluoro-3-tolyl isocyanate	C8H4F3NO	C8H4F3NO	187.12	FC(F)(F)c1cccc(c1)N=C=O	InChI=1/C8H4F3NO/c9-8(10,11)6-2-1-3-7(4-6)12-5-13/h1-4H	2.632	2.632	1	1	1
3290-92-4	3290924	2669	**propylidynetrimethyl trimethacrylate**	3_REACH		propylidynetrimethyl trimethacrylate		C18H26O6	338.4	CCC(COC(=O)C(=C)C)(COC(=O)C(=C)C)COC(=O)C(=C)C	InChI=1/C18H26O6/c1-8-18(9-22-15(19)12(2)3,10-23-16(20)13(4)5)11-24-17(21)14(6)7/h2,4,6,8-11H2,1,3,5,7H3	3.951	3.951	1	1	1
3296-90-0	3296900	2671	**2,2-bis(bromomethyl)propane-1,3-diol**	3_REACH	1,3-Propanediol, 2,2-bis(bromomethyl)-	2,2-bis(bromomethyl)propane-1,3-diol	C5H10Br2O2	C5H10Br2O2	261.95	OCC(CO)(CBr)CBr	InChI=1/C5H10Br2O2/c6-1-5(2-7,3-8)4-9/h8-9H,1-4H2	0.533	0.533	1	1	1
3320-83-0	3320830	2677	**2-chlorophenyl isocyanate**	3_REACH	Benzene, 1-chloro-2-isocyanato-	2-chlorophenyl isocyanate	C7H4ClNO	C7H4ClNO	153.57	Clc1ccccc1N=C=O	InChI=1/C7H4ClNO/c8-6-3-1-2-4-7(6)9-5-10/h1-4H	2.354	2.354	1	1	1
3332-27-2	3332272	2679	**N,N-dimethyltetradecylamine N-oxide**	3_REACH		N,N-dimethyltetradecylamine N-oxide		C16H35NO	257.46	CCCCCCCCCCCCCC[N+](C)(C)[O-]	InChI=1/C16H35NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17(2,3)18/h4-16H2,1-3H3	5.403	5.403	1	1	1
33329-35-0	33329350	2680	**N,N-bis[3-(dimethylamino)propyl]-N',N'-dimethylpropane-1,3-diamine**	3_REACH		N,N-bis[3-(dimethylamino)propyl]-N',N'-dimethylpropane-1,3-diamine		C15H39N4	272.49	C[NH+](C)CCCN(CCC[NH+](C)C)CCC[NH+](C)C	InChI=1/C15H36N4/c1-16(2)10-7-13-19(14-8-11-17(3)4)15-9-12-18(5)6/h7-15H2,1-6H3/p+3	-3.759	-2.2	1	1	1
33704-61-9	33704619	2684	**1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one**	3_REACH		1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one		C14H22O	206.33	CC1C(C)(C)C2=C(C(=O)CCC2)C1(C)C	InChI=1/C14H22O/c1-9-13(2,3)10-7-6-8-11(15)12(10)14(9,4)5/h9H,6-8H2,1-5H3	3.436	3.436	1	1	1
337906-36-2	337906362	2686	**2-(methoxymethyl)benzene-1,4-diamine**	3_REACH		2-(methoxymethyl)benzene-1,4-diamine			152.2	COCC1=C(C=CC(=C1)N)N	InChI=1S/C8H12N2O/c1-11-5-6-4-7(9)2-3-8(6)10/h2-4H,5,9-10H2,1H3			1	1	1
3407-42-9	3407429	2689	**3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol**	3_REACH		3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol		C16H28O	236.4	CC1C2CC(CC2C3CCCC(O)C3)C1(C)C	InChI=1/C16H28O/c1-10-14-8-12(16(10,2)3)9-15(14)11-5-4-6-13(17)7-11/h10-15,17H,4-9H2,1-3H3	3.842	3.842	1	1	1
34090-76-1	34090761	2690	**tetrahydro-4-methylphthalic anhydride**	3_REACH		tetrahydro-4-methylphthalic anhydride		C9H10O3	166.18	CC1CCC2=C(C1)C(=O)OC2=O	InChI=1/C9H10O3/c1-5-2-3-6-7(4-5)9(11)12-8(6)10/h5H,2-4H2,1H3	1.938	1.938	1	1	1
34206-40-1	34206401	2694	**butan-2-one O,O',O'',O'''-silanetetrayltetraoxime**	3_REACH		butan-2-one O,O',O'',O'''-silanetetrayltetraoxime		C16H32N4O4Si	372.55	CC\C(=N/O[Si](O\N=C(\C)/CC)(O\N=C(/C)\CC)O\N=C(/C)\CC)\C	InChI=1/C16H32N4O4Si/c1-9-13(5)17-21-25(22-18-14(6)10-2,23-19-15(7)11-3)24-20-16(8)12-4/h9-12H2,1-8H3/b17-13-, 18-14-, 19-15+, 20-16+	4.403	4.161	1	1	1
342-25-6	342256	2695	**2,4'-difluorobenzophenone**	3_REACH		2,4'-difluorobenzophenone		C13H8F2O	218.2	Fc1ccc(cc1)C(=O)c2ccccc2F	InChI=1/C13H8F2O/c14-10-7-5-9(6-8-10)13(16)11-3-1-2-4-12(11)15/h1-8H	3.645	3.645	1	1	1
34316-64-8	34316648	2700	**hexyl laurate**	3_REACH	hexyl dodecanoate	hexyl laurate	C18H36O2	C18H36O2	284.48	CCCCCCCCCCCC(=O)OCCCCCC	InChI=1/C18H36O2/c1-3-5-7-9-10-11-12-13-14-16-18(19)20-17-15-8-6-4-2/h3-17H2,1-2H3	7.034	7.034	1	1	1
3437-84-1	3437841	2701	**bisisobutyryl peroxide**	3_REACH		bisisobutyryl peroxide		C8H14O4	174.2	CC(C)C(=O)OOC(=O)C(C)C	InChI=1/C8H14O4/c1-5(2)7(9)11-12-8(10)6(3)4/h5-6H,1-4H3	1.723	1.723	1	1	1
34396-03-7	34396037	2702	**trimethoxy(2,4,4-trimethylpentyl)silane**	3_REACH		trimethoxy(2,4,4-trimethylpentyl)silane		C11H26O3Si	234.41	CO[Si](CC(C)CC(C)(C)C)(OC)OC	InChI=1/C11H26O3Si/c1-10(8-11(2,3)4)9-15(12-5,13-6)14-7/h10H,8-9H2,1-7H3	4.654	4.654	1	1	1
3452-97-9	3452979	609	**3,5,5-trimethylhexan-1-ol**	3_REACH	1-Hexanol, 3,5,5-trimethyl-	3,5,5-Trimethyl-1-hexanol	C9H20O	C9H20O	144.26	CC(CCO)CC(C)(C)C	InChI=1/C9H20O/c1-8(5-6-10)7-9(2,3)4/h8,10H,5-7H2,1-4H3	2.592	2.592	1	1	1
345-92-6	345926	2710	**bis(4-fluorophenyl) ketone**	3_REACH	4,4'-Difluorobenzophenone	bis(4-fluorophenyl) ketone	C13H8F2O	C13H8F2O	218.2	Fc1ccc(cc1)C(=O)c2ccc(F)cc2	InChI=1/C13H8F2O/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8H	3.645	3.645	1	1	1
34690-00-1	34690001	2714	**[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid**	3_REACH		[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid		C17H42N3O15P5	685.42	OP(=O)([O-])C[NH+](CCCCCC[NH+](CP(=O)(O)[O-])CP(=O)(O)[O-])CCCCCC[NH+](CP(=O)(O)[O-])CP(=O)(O)[O-]	InChI=1/C17H44N3O15P5/c21-36(22,23)13-18(9-5-1-3-7-11-19(14-37(24,25)26)15-38(27,28)29)10-2-4-8-12-20(16-39(30,31)32)17-40(33,34)35/h1-17H2,(H2,21,22,23)(H2,24,25,26)(H2,27,28,29)(H2,30,31,32)(H2,33,34,35)/p-2	-12.256	-11.727	1	1	1
34893-92-0	34893920	2717	**1,3-dichloro-5-isocyanatobenzene**	3_REACH	3,5-Dichlorophenyl isocyanate	1,3-dichloro-5-isocyanatobenzene	C7H3Cl2NO	C7H3Cl2NO	188.01	Clc1cc(Cl)cc(c1)N=C=O	InChI=1/C7H3Cl2NO/c8-5-1-6(9)3-7(2-5)10-4-11/h1-3H	3.019	3.019	1	1	1
350-46-9	350469	611	**1-fluoro-4-nitrobenzene**	3_REACH	Benzene, 1-fluoro-4-nitro-	1-Fluoro-4-nitrobenzene	C6H4FNO2	C6H4FNO2	141.1	[O-][N+](=O)c1ccc(F)cc1	InChI=1/C6H4FNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H	1.929	1.929	1	1	1
3508-98-3	3508983	4362	**2-phenylhexanenitrile**	3_REACH		2-phenylhexanenitrile			173.26					1	1	1
35265-04-4	35265044	2726	**2-[(1-methylpropyl)amino]ethanol**	3_REACH		2-[(1-methylpropyl)amino]ethanol		C6H16NO	117.19	CCC(C)[NH2+]CCO	InChI=1/C6H15NO/c1-3-6(2)7-4-5-8/h6-8H,3-5H2,1-2H3/p+1	-0.736	-0.644	1	1	1
35435-21-3	35435213	2734	**triethoxy(2,4,4-trimethylpentyl)silane**	3_REACH		triethoxy(2,4,4-trimethylpentyl)silane		C14H32O3Si	276.49	CCO[Si](CC(C)CC(C)(C)C)(OCC)OCC	InChI=1/C14H32O3Si/c1-8-15-18(16-9-2,17-10-3)12-13(4)11-14(5,6)7/h13H,8-12H2,1-7H3	5.701	5.701	1	1	1
3547-33-9	3547339	613	**2-(octylthio)ethanol**	3_REACH	Ethanol, 2-(octylthio)-	2-(Octylthio)ethanol	C10H22OS	C10H22OS	190.35	CCCCCCCCSCCO	InChI=1/C10H22OS/c1-2-3-4-5-6-7-9-12-10-8-11/h11H,2-10H2,1H3	3.409	3.409	1	1	1
35636-63-6	35636636	2742	**dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]terephthalate**	3_REACH		dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]terephthalate		C21H19N5O7	453.42	COC(=O)c1ccc(C(=O)OC)c(c1)N=NC(C(=O)C)C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C21H19N5O7/c1-10(27)17(18(28)22-12-5-7-14-16(9-12)24-21(31)23-14)26-25-15-8-11(19(29)32-2)4-6-13(15)20(30)33-3/h4-9,17H,1-3H3,(H,22,28)(H2,23,24,31)	2.716	2.716	1	1	1
3576-88-3	3576883	2746	**2,2'-iminobis[4,6-diamino-1,3,5-triazine]**	3_REACH		2,2'-iminobis[4,6-diamino-1,3,5-triazine]		C6H9N11	235.23	Nc1nc(N)nc(Nc2nc(N)nc(N)n2)n1	InChI=1/C6H9N11/c7-1-11-2(8)14-5(13-1)17-6-15-3(9)12-4(10)16-6/h(H9,7,8,9,10,11,12,13,14,15,16,17)	-0.887	-0.896	1	1	1
35836-72-7	35836727	2750	**2-Pinene-10-methyl acetate**	3_REACH		(1R,5S)-2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl) ethyl acetate			208.3	CC(=O)OCCC1=CCC2CC1C2(C)C	InChI=1S/C13H20O2/c1-9(14)15-7-6-10-4-5-11-8-12(10)13(11,2)3/h4,11-12H,5-8H2,1-3H3/t11-,12-/m0/s1			1	1	1
35948-25-5	35948255	2754	**6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide**	3_REACH		6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide		C12H9O2P	216.18	O=P1Oc2ccccc2c3ccccc13	InChI=1/C12H9O2P/c13-15-12-8-4-2-6-10(12)9-5-1-3-7-11(9)14-15/h1-8,15H	2.951	2.951	1	1	1
36177-92-1	36177921	2761	**N-butyl-2,2,6,6-tetramethylpiperidin-4-amine**	3_REACH		N-butyl-2,2,6,6-tetramethylpiperidin-4-amine		C13H30N2	212.38	CCCC[NH2+]C1CC(C)(C)[NH2+]C(C)(C)C1	InChI=1/C13H28N2/c1-6-7-8-14-11-9-12(2,3)15-13(4,5)10-11/h11,14-15H,6-10H2,1-5H3/p+2	-0.609	-0.529	1	1	1
3622-84-2	3622842	2763	**N-butylbenzenesulphonamide**	3_REACH	Benzenesulfonamide, N-butyl-	N-butylbenzenesulphonamide	C10H15NO2S	C10H15NO2S	213.3	CCCCNS(=O)(=O)c1ccccc1	InChI=1/C10H15NO2S/c1-2-3-9-11-14(12,13)10-7-5-4-6-8-10/h4-8,11H,2-3,9H2,1H3	2.069	2.072	1	1	1
3634-83-1	3634831	2766	**1,3-bis(isocyanatomethyl)benzene**	3_REACH		1,3-bis(isocyanatomethyl)benzene		C10H8N2O2	188.19	O=C=NCc1cccc(CN=C=O)c1	InChI=1/C10H8N2O2/c13-7-11-5-9-2-1-3-10(4-9)6-12-8-14/h1-4H,5-6H2	1.564	1.564	1	1	1
36443-68-2	36443682	2767	**ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)propionate]**	3_REACH		ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)propionate]		C34H50O8	586.77	Cc1cc(CCC(=O)OCCOCCOCCOC(=O)CCc2cc(C)c(O)c(c2)C(C)(C)C)cc(c1O)C(C)(C)C	InChI=1/C34H50O8/c1-23-19-25(21-27(31(23)37)33(3,4)5)9-11-29(35)41-17-15-39-13-14-40-16-18-42-30(36)12-10-26-20-24(2)32(38)28(22-26)34(6,7)8/h19-22,37-38H,9-18H2,1-8H3	7.198	7.198	1	1	1
36483-57-5	36483575	2768	**2,2-dimethylpropan-1-ol, tribromo derivative**	3_REACH		2,2-dimethylpropan-1-ol, tribromo derivative		C5H9Br3O	324.86	CC(C)(CO)C(Br)(Br)Br	InChI=1/C5H9Br3O/c1-4(2,3-9)5(6,7)8/h9H,3H2,1-2H3	2.765	2.765	1	1	1
36635-56-0	36635560	2772	**N-[[(4-methylphenyl)sulfonyl]methyl]formamide**	3_REACH		N-[[(4-methylphenyl)sulfonyl]methyl]formamide			213.26	CC1=CC=C(C=C1)S(=O)(=O)CNC=O	InChI=1S/C9H11NO3S/c1-8-2-4-9(5-3-8)14(12,13)7-10-6-11/h2-6H,7H2,1H3,(H,10,11)			1	1	1
36727-29-4	36727294	2775	**3,5,5-trimethylhexanoyl chloride**	3_REACH		3,5,5-trimethylhexanoyl chloride		C9H17ClO	176.69	CC(CC(=O)Cl)CC(C)(C)C	InChI=1/C9H17ClO/c1-7(5-8(10)11)6-9(2,3)4/h7H,5-6H2,1-4H3	3.117	3.117	1	1	1
36768-62-4	36768624	2776	**2,2,6,6-tetramethyl-4-piperidylamine**	3_REACH	4-Piperidinamine, 2,2,6,6-tetramethyl-	2,2,6,6-tetramethyl-4-piperidylamine	C9H20N2	C9H22N2	156.28	CC1(C)CC([NH3+])CC(C)(C)[NH2+]1	InChI=1/C9H20N2/c1-8(2)5-7(10)6-9(3,4)11-8/h7,11H,5-6,10H2,1-4H3/p+2	-2.144	-2.071	1	1	1
3681-71-8	3681718	2779	**(Z)-hex-3-enyl acetate**	3_REACH	3-Hexen-1-ol, acetate, (Z)-	(Z)-hex-3-enyl acetate	C8H14O2	C8H14O2	142.2	CC\C=C/CCOC(=O)C	InChI=1/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h4-5H,3,6-7H2,1-2H3/b5-4-	1.817	1.817	1	1	1
3687-22-7	3687227	4777	**2,4-Dinitro-6-(1-methylheptyl)phenol**	3_REACH		Phenol, 2-(1-methylheptyl)-4,6-dinitro-			296.32	CCCCCCC(C)C1=CC(=CC(=C1O)[N+](=O)[O-])[N+](=O)[O-]	InChI=1S/C14H20N2O5/c1-3-4-5-6-7-10(2)12-8-11(15(18)19)9-13(14(12)17)16(20)21/h8-10,17H,3-7H2,1-2H3			1	1	1
369634-22-0	369634220	4583	**Octalynol**	3_REACH		Unknown			140.18	[H][C@@]12CCC(C)(C)[C@H](O)[C@]1([H])[C@H](C)C=C(C)C2				1	1	1
3699-54-5	3699545	2788	**1-(2-hydroxyethyl)imidazolidin-2-one**	3_REACH	1-(2-Hydroxyethyl)-2-imidazolidinone	1-(2-hydroxyethyl)imidazolidin-2-one	C5H10N2O2	C5H10N2O2	130.15	OCCN1CCNC1=O	InChI=1/C5H10N2O2/c8-4-3-7-2-1-6-5(7)9/h8H,1-4H2,(H,6,9)	-1.146	-1.146	1	1	1
37052-78-1	37052781	2789	**1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione**	3_REACH		1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione		C8H8N2OS	180.23	COc1ccc2[nH]c(S)nc2c1	InChI=1/C8H8N2OS/c1-11-5-2-3-6-7(4-5)10-8(12)9-6/h2-4H,1H3,(H2,9,10,12)	2.23	2.23	1	1	1
3710-84-7	3710847	2791	**N,N-diethylhydroxylamine**	3_REACH	Ethanamine, N-ethyl-N-hydroxy-	N,N-diethylhydroxylamine	C4H11NO	C4H12NO	89.139	CC[NH+](O)CC	InChI=1/C4H11NO/c1-3-5(6)4-2/h6H,3-4H2,1-2H3/p+1	0.707	0.694	1	1	1
3717-40-6	3717406	2792	**N,N-Dimethyladamantan-1-amine**	3_REACH	N,N-Dimethyladamantylamine	Tricyclo[3.3.1.13,7]decan-1-amine, N,N-dimethyl-	C12H21N		179.31	CN(C)C12CC3CC(C1)CC(C3)C2	InChI=1S/C12H21N/c1-13(2)12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11H,3-8H2,1-2H3			1	1	1
372-09-8	372098	2794	**cyanoacetic acid**	3_REACH	Acetic acid, cyano-	cyanoacetic acid	C3H3NO2	C3H2NO2	85.063	[O-]C(=O)CC#N	InChI=1/C3H3NO2/c4-2-1-3(5)6/h1H2,(H,5,6)/p-1	-1.619	-1.619	1	1	1
373-44-4	373444	2796	**octamethylenediamine**	3_REACH	1,8-Diaminooctane	octamethylenediamine	C8H20N2	C8H22N2	144.26	[NH3+]CCCCCCCC[NH3+]	InChI=1/C8H20N2/c9-7-5-3-1-2-4-6-8-10/h1-10H2/p+2	-1.02	-1.013	1	1	1
3741-80-8	3741808	5041	**N-(1,1-dimethylethyl)bis(2-benzothiazolesulfen)amide**	3_REACH		N-(1,1-dimethylethyl)bis(2-benzothiazolesulfen)amide			403.61	CC(C)(C)N(SC1=NC2=CC=CC=C2S1)SC3=NC4=CC=CC=C4S3	InChI=1S/C18H17N3S4/c1-18(2,3)21(24-16-19-12-8-4-6-10-14(12)22-16)25-17-20-13-9-5-7-11-15(13)23-17/h4-11H,1-3H3			1	1	1
3748-13-8	3748138	2798	**m-bis(1-methylvinyl)benzene**	3_REACH	Benzene, 1,3-bis(1-methylethenyl)-	m-bis(1-methylvinyl)benzene	C12H14	C12H14	158.24	CC(=C)c1cccc(c1)C(=C)C	InChI=1/C12H14/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-8H,1,3H2,2,4H3	3.826	3.826	1	1	1
3749-87-9	3749879	2800	**Methyl 3,7-di-O-acetylcholate**	3_REACH		methyl 3-a,7-a-diacetoxy-12-a-hydroxy-5-ß-cholan-24-oate		C29H46O7	506.68	COC(=O)CCC(C)C1CCC2C3C(CC4CC(CCC4(C)C3CC(O)C12C)OC(=O)C)OC(=O)C	InChI=1/C29H46O7/c1-16(7-10-26(33)34-6)21-8-9-22-27-23(15-25(32)29(21,22)5)28(4)12-11-20(35 17(2)30)13-19(28)14-24(27)36-18(3)31/h16,19-25,27,32H,7-15H2,1-6H3	3.896	3.896	1	1	1
3779-63-3	3779633	2809	**(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene) isocyanate**	3_REACH		(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene) isocyanate		C24H39N6O6	504.59	O=C=[NH+]CCCCCCN1C(=O)N(CCCCCC[NH+]=C=O)C(=O)N(CCCCCC[NH+]=C=O)C1=O	InChI=1/C24H36N6O6/c31-19-25-13-7-1-4-10-16-28-22(34)29(17-11-5-2-8-14-26-20-32)24(36)30(23(28)35)18-12-6-3-9-15-27-21-33/h1-18H2/p+3	4.108	4.108	1	1	1
37971-36-1	37971361	2811	**2-phosphonobutane-1,2,4-tricarboxylic acid**	3_REACH		2-phosphonobutane-1,2,4-tricarboxylic acid		C7H7O9P	270.13	OC(=O)CC(CCC(=O)[O-])(CC(=O)[O-])P(=O)([O-])[O-]	InChI=1/C7H11O9P/c8-4(9)1-2-7(6(12)13,3-5(10)11)17(14,15)16/h1-3H2,(H,8,9)(H,10,11)(H,12,13)(H2,14,15,16)/p-4	-6.348	-4.76	1	1	1
38051-10-4	38051104	2812	**2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)**	3_REACH	Phosgard 2xc20	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	C13H24Cl6O8P2	C13H24Cl6O8P2	582.99	ClCCOP(=O)(OCCCl)OCC(CCl)(CCl)COP(=O)(OCCCl)OCCCl	InChI=1/C13H24Cl6O8P2/c14-1-5-22-28(20,23-6-2-15)26-11-13(9-18,10-19)12-27-29(21,24-7-3-16)25-8-4-17/h1-12H2	2.918	2.918	1	1	1
38083-17-9	38083179	620	**climbazole**	3_REACH		Climbazol		C15H17ClN2O2	292.77	CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n2ccnc2	InChI=1/C15H17ClN2O2/c1-15(2,3)13(19)14(18-9-8-17-10-18)20-12-6-4-11(16)5-7-12/h4-10,14H,1-3H3	3.766	4.401	1	1	1
3845-76-9	3845769	2822	**N-[3-(dimethylamino)propyl]acrylamide**	3_REACH		N-[3-(dimethylamino)propyl]acrylamide		C8H17N2O	156.23	C[NH+](C)CCCNC(=O)C=C	InChI=1/C8H16N2O/c1-4-8(11)9-6-5-7-10(2)3/h4H,1,5-7H2,2-3H3,(H,9,11)/p+1	-1.289	-1.156	1	1	1
3851-87-4	3851874	2823	**bis(3,5,5-trimethylhexanoyl) peroxide**	3_REACH		bis(3,5,5-trimethylhexanoyl) peroxide		C18H34O4	314.47	CC(CC(=O)OOC(=O)CC(C)CC(C)(C)C)CC(C)(C)C	InChI=1/C18H34O4/c1-13(11-17(3,4)5)9-15(19)21-22-16(20)10-14(2)12-18(6,7)8/h13-14H,9-12H2,1-8H3	4.955	4.955	1	1	1
3855-32-1	3855321	2824	**N-[3-(dimethylamino)propyl]-N,N',N'-trimethylpropane-1,3-diamine**	3_REACH		N-[3-(dimethylamino)propyl]-N,N',N'-trimethylpropane-1,3-diamine		C11H28N3	201.36	CN(C)CCC[NH+](C)CCCN(C)C	InChI=1/C11H27N3/c1-12(2)8-6-10-14(5)11-7-9-13(3)4/h6-11H2,1-5H3/p+1	-0.839	-1.149	1	1	1
38668-48-3	38668483	2825	**1,1'-(p-tolylimino)dipropan-2-ol**	3_REACH		1,1'-(p-tolylimino)dipropan-2-ol		C13H21NO2	223.32	CC(O)CN(CC(C)O)c1ccc(C)cc1	InChI=1/C13H21NO2/c1-10-4-6-13(7-5-10)14(8-11(2)15)9-12(3)16/h4-7,11-12,15-16H,8-9H2,1-3H3	2.154	1.987	1	1	1
3886-69-9	3886699	2827	**D-alpha-Methylbenzylamine**	3_REACH	Benzenemethanamine, α-methyl-, (R)-	D-a-methylbenzylamine	C8H11N	C8H12N	121.18	C[C@@H]([NH3+])c1ccccc1	InChI=1/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3/p+1/t7-/m1/s1	0.308	0.382	1	1	1
38888-98-1	38888981	2828	**(phenylethyl)benzene**	3_REACH		(phenylethyl)benzene		C14H14	182.27	CC(c1ccccc1)c2ccccc2	InChI=1/C14H14/c1-12(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-12H,1H3	4.056	4.056	1	1	1
393509-79-0	393509790	4634	**methyl 2-chlorosulfonyl-4-(methanesulfonylaminomethyl)benzoate**	3_REACH		AE F 156657			341.79	COC(=O)C1=C(C=C(CNS(C)(=O)=O)C=C1)S(Cl)(=O)=O	InChI=1S/C10H12ClNO6S2/c1-18-10(13)8-4-3-7(6-12-19(2,14)15)5-9(8)20(11,16)17/h3-5,12H,6H2,1-2H3 AuxInfo=1/0/N:			1	1	1
39515-51-0	39515510	625	**m-phenoxybenzaldehyde**	3_REACH		3-Phenoxybenzaldehyde		C13H10O2	198.22	O=Cc1cccc(Oc2ccccc2)c1	InChI=1/C13H10O2/c14-10-11-5-4-8-13(9-11)15-12-6-2-1-3-7-12/h1-10H	3.149	3.149	1	1	1
39670-09-2	39670092	2846	**2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate**	3_REACH		2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate		C12H22O5	246.3	CCOCCOCCOCCOC(=O)C(=C)C	InChI=1/C12H22O5/c1-4-14-5-6-15-7-8-16-9-10-17-12(13)11(2)3/h2,4-10H2,1,3H3	1.121	1.121	1	1	1
40306-75-0	40306750	2857	**3-acetamido-5-amino-4-hydroxybenzenesulphonic acid**	3_REACH		3-acetamido-5-amino-4-hydroxybenzenesulphonic acid		C8H9N2O5S	246.24	CC(=O)Nc1cc(cc(N)c1O)S(=O)(=O)[O-]	InChI=1/C8H10N2O5S/c1-4(11)10-7-3-5(16(13,14)15)2-6(9)8(7)12/h2-3,12H,9H2,1H3,(H,10,11)(H,13,14,15)/p-1	-2.951	-2.949	1	1	1
40601-76-1	40601761	2859	**1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6-xylyl]methyl]-1,3,5-triazine-2,4,6(1H,3H,5H)-trione**	3_REACH		1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6-xylyl]methyl]-1,3,5-triazine-2,4,6(1H,3H,5H)-trione		C42H57N3O6	699.94	Cc1cc(c(O)c(C)c1CN2C(=O)N(Cc3c(C)cc(c(O)c3C)C(C)(C)C)C(=O)N(Cc4c(C)cc(c(O)c4C)C(C)(C)C)C2=O)C(C)(C)C	InChI=1/C42H57N3O6/c1-22-16-31(40(7,8)9)34(46)25(4)28(22)19-43-37(49)44(20-29-23(2)17-32(41(10,11)12)35(47)26(29)5)39(51)45(38(43)50)21-30-24(3)18-33(42(13,14)15)36(48)27(30)6/h1 18,46-48H,19-21H2,1-15H3	11.1	11.1	1	1	1
4065-45-6	4065456	52	**sulisobenzone**	3_REACH		sulisobenzone		C14H11O6S	308.31	COc1cc(O)c(cc1S(=O)(=O)[O-])C(=O)c2ccccc2	InChI=1/C14H12O6S/c1-20-12-8-11(15)10(7-13(12)21(17,18)19)14(16)9-5-3-2-4-6-9/h2-8,15H,1H3,(H,17,18,19)/p-1	0.063	0.065	1	1	1
4073-98-7	4073987	2864	**4,4'-methylenebis(2,6-xylidine)**	3_REACH		4,4'-methylenebis(2,6-xylidine)		C17H22N2	254.38	Cc1cc(Cc2cc(C)c(N)c(C)c2)cc(C)c1N	InChI=1/C17H22N2/c1-10-5-14(6-11(2)16(10)18)9-15-7-12(3)17(19)13(4)8-15/h5-8H,9,18-19H2,1-4H3	4.256	4.254	1	1	1
40758-65-4	40758654	2865	**4,6-Dichloro-2-ethoxypyrimidine**	3_REACH		4,6-Dichloro-2-ethoxypyrimidine			193.04	CCOC1=NC(=CC(=N1)Cl)Cl	InChI=1S/C6H6Cl2N2O/c1-2-11-6-9-4(7)3-5(8)10-6/h3H,2H2,1H3			1	1	1
4083-64-1	4083641	629	**p-toluenesulphonyl isocyanate**	3_REACH	4-Methylbenzenesulfonyl isocyanate	4-Tosyl isocyanate	C8H7NO3S	C8H7NO3S	197.21	Cc1ccc(cc1)S(=O)(=O)N=C=O	InChI=1/C8H7NO3S/c1-7-2-4-8(5-3-7)13(11,12)9-6-10/h2-5H,1H3	1.105	1.105	1	1	1
4098-71-9	4098719	2867	**3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate**	3_REACH		3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate		C12H19N2O2	222.29	CC1(C)CC(CC(C)(CN=C=O)C1)[NH+]=C=O	InChI=1/C12H18N2O2/c1-11(2)4-10(14-9-16)5-12(3,6-11)7-13-8-15/h10H,4-7H2,1-3H3/p+1	2.165	2.151	1	1	1
41198-08-7	41198087	631	**Profenofos**	3_REACH		Phosphorothioic acid O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl ester		C11H15BrClO3PS	373.64	CCCSP(=O)(OCC)Oc1ccc(Br)cc1Cl	InChI=1/C11H15BrClO3PS/c1-3-7-18-17(14,15-4-2)16-11-6-5-9(12)8-10(11)13/h5-6,8H,3-4,7H2,1-2H3	4.79	4.79	1	1	1
41340-36-7	41340367	4309	**2-(7-ethyl-1H-indol-3-yl)ethanol**	3_REACH		2-(7-ethyl-1H-indol-3-yl)ethanol			189.26	CCC1=CC=CC2=C1NC=C2CCO	InChI=1S/C12H15NO/c1-2-9-4-3-5-11-10(6-7-14)8-13-12(9)11/h3-5,8,13-14H,2,6-7H2,1H3			1	1	1
41620-33-1	41620331	4337	**2-[[2-(acetyloxy)-3-(1,1-dimethylethyl)-5-methylphenyl]methyl]-6-(1,1-dimethylethyl)-4-methylphenol**	3_REACH		2-[[2-(acetyloxy)-3-(1,1-dimethylethyl)-5-methylphenyl]methyl]-6-(1,1-dimethylethyl)-4-methylphenol			382.54	CC1=CC(=C(C(=C1)C(C)(C)C)O)CC2=C(C(=CC(=C2)C)C(C)(C)C)OC(=O)C	InChI=1S/C25H34O3/c1-15-10-18(22(27)20(12-15)24(4,5)6)14-19-11-16(2)13-21(25(7,8)9)23(19)28-17(3)26/h10-13,27H,			1	1	1
4180-23-8	4180238	635	**(E)-anethole**	3_REACH	Anethole	1-Methoxy-4-(1E)-1-propenylbenzene	C10H12O	C10H12O	148.21	COc1ccc(\C=C\C)cc1	InChI=1/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3-8H,1-2H3/b4-3+	2.767	2.767	1	1	1
42019-78-3	42019783	2886	**4-chloro-4'-hydroxybenzophenone**	3_REACH	Methanone, (4-chlorophenyl)(4-hydroxyphenyl)-	4-chloro-4'-hydroxybenzophenone	C13H9ClO2	C13H9ClO2	232.67	Oc1ccc(cc1)C(=O)c2ccc(Cl)cc2	InChI=1/C13H9ClO2/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8,15H	3.656	3.595	1	1	1
42125-46-2	42125462	2889	**4-tert-butylcyclohexyl chloroformate**	3_REACH		4-tert-butylcyclohexyl chloroformate		C11H19ClO2	218.72	CC(C)(C)C1CCC(CC1)OC(=O)Cl	InChI=1/C11H19ClO2/c1-11(2,3)8-4-6-9(7-5-8)14-10(12)13/h8-9H,4-7H2,1-3H3	4.039	4.039	1	1	1
4245-76-5	4245765	2892	**610-029-6**	3_REACH	N-Methyl-N'-nitroguanidine	Guanidine, N-methyl-N'-nitro-	C2H6N4O2		118.1					1	1	1
4246-51-9	4246519	2893	**3,3'-oxybis(ethyleneoxy)bis(propylamine)**	3_REACH	Trioxa-1,13-tridecanediamine,4,7,10-,	3,3'-oxybis(ethyleneoxy)bis(propylamine)	C10H24N2O3	C10H26N2O3	220.32	[NH3+]CCCOCCOCCOCCC[NH3+]	InChI=1/C10H24N2O3/c11-3-1-5-13-7-9-15-10-8-14-6-2-4-12/h1-12H2/p+2	-3.755	-3.712	1	1	1
4253-34-3	4253343	2896	**methylsilanetriyl triacetate**	3_REACH	Methyltriacetoxysilane	methylsilanetriyl triacetate	C7H12O6Si	C7H12O6Si	220.25	CC(=O)O[Si](C)(OC(=O)C)OC(=O)C	InChI=1/C7H12O6Si/c1-5(8)11-14(4,12-6(2)9)13-7(3)10/h1-4H3	1.377	1.377	1	1	1
43057-68-7	43057687	4478	**2-Ethyl-2-methyl-1,3-dihydroperimidine**	3_REACH		C-24			212.3	CCC1(NC2=CC=CC3=C2C(=CC=C3)N1)C	InChI=1S/C14H16N2/c1-3-14(2)15-11-8-4-6-10-7-5-9-12(16-14)13(10)11/h4-9,15-16H,3H2,1-2H3			1	1	1
4378-61-4	4378614	2916	**4,10-dibromodibenzo[def,mno]chrysene-6,12-dione**	3_REACH		4,10-dibromodibenzo[def,mno]chrysene-6,12-dione		C22H8Br2O2	464.12	Brc1cc2C(=O)c3cccc4c(Br)cc5C(=O)c6cccc1c6c2c5c34	InChI=1/C22H8Br2O2/c23-15-7-14-19-17-9(15)3-1-5-11(17)21(25)13-8-16(24)10-4-2-6-12(22(14)26)18(10)20(13)19/h1-8H	5.81	5.81	1	1	1
4394-85-8	4394858	2918	**4-morpholinecarbaldehyde**	3_REACH	N-Formylmorpholine	4-morpholinecarbaldehyde	C5H9NO2	C5H9NO2	115.13	O=CN1CCOCC1	InChI=1/C5H9NO2/c7-5-6-1-3-8-4-2-6/h5H,1-4H2	-0.812	-0.812	1	1	1
4402-30-6	4402306	2919	**1,1'-(methylimino)dipropan-2-ol**	3_REACH		1,1'-(methylimino)dipropan-2-ol		C7H18NO2	147.22	CC(O)C[NH+](C)CC(C)O	InChI=1/C7H17NO2/c1-6(9)4-8(3)5-7(2)10/h6-7,9-10H,4-5H2,1-3H3/p+1	-1.565	-0.961	1	1	1
4404-43-7	4404437	641	**4,4'-bis[4-[bis(2-hydroxyethyl)amino]-6-anilino-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonic acid**	3_REACH		2,2'-(1,2-Ethenediyl)bis[5-[[4-bis(2-hydroxyethyl)amino]-6-(phenylamino)-1,3,5-triazin-2-yl]amino]benzenesulfonic acid		C40H44N12O10S2	917.01	OCCN(CCO)c1nc(Nc2ccccc2)nc(Nc3ccc(\C=C\c4ccc(Nc5nc(Nc6ccccc6)nc([nH+]5)N(CCO)CCO)cc4S(=O)(=O)[O-])c(c3	InChI=1/C40H44N12O10S2/c53-21-17-51(18-22-54)39-47-35(41-29-7-3-1-4-8-29)45-37(49-39)43-31-15-13-27(33(25-31)63(57,58)59)11-12-28-14-16-32(26-34(28)64(60,61)62)44-38-46-36(42-30-9-5-2-10-30)48-40(50-38)52(19-23-55)20-24-56/h1-16,25-26,53-56H,17-24H2,(H,57,58,59)(H,60,61,62)(H2,41,43,45,47,49)(H2,42,44,46,48,50)/b12-11+	-3.205	-2.555	1	1	1
4431-83-8	4431838	2921	**2,5,7,10-tetraoxaundecane**	3_REACH		2,5,7,10-tetraoxaundecane		C7H16O4	164.2	COCCOCOCCOC	InChI=1/C7H16O4/c1-8-3-5-10-7-11-6-4-9-2/h3-7H2,1-2H3	-0.36	-0.36	1	1	1
4443-26-9	4443269	2925	**1,3-dihydro-1,3-dioxo-2H-isoindole-2-hexanoic acid**	3_REACH		1,3-dihydro-1,3-dioxo-2H-isoindole-2-hexanoic acid		C14H14NO4	261.28	[O-]C(=O)CCCCCN1C(=O)c2ccccc2C1=O	InChI=1/C14H15NO4/c16-12(17)8-2-1-5-9-15-13(18)10-6-3-4-7-11(10)14(15)19/h3-4,6-7H,1-2,5,8-9H2,(H,16,17)/p-1	0.351	0.377	1	1	1
4457-71-0	4457710	2927	**3-methylpentane-1,5-diol**	3_REACH	1,5-Pentanediol, 3-methyl-	3-methylpentane-1,5-diol	C6H14O2	C6H14O2	118.18	CC(CCO)CCO	InChI=1/C6H14O2/c1-6(2-4-7)3-5-8/h6-8H,2-5H2,1H3	0.453	0.453	1	1	1
4488-57-7	4488577	2933	**3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene**	3_REACH	3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	C10H14	C10H14	134.22	C1CC2CC1C3CC=CC23	InChI=1/C10H14/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,7-10H,3-6H2	2.556	2.556	1	1	1
4500-29-2	4500292	2936	**2,2'-(cyclohexylimino)bisethanol**	3_REACH		2,2'-(cyclohexylimino)bisethanol		C10H22NO2	187.28	OCC[NH+](CCO)C1CCCCC1	InChI=1/C10H21NO2/c12-8-6-11(7-9-13)10-4-2-1-3-5-10/h10,12-13H,1-9H2/p+1	-0.462	-0.46	1	1	1
4511-42-6	4511426	2938	**(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione**	3_REACH		(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione		C6H8O4	144.13	C[C@@H]1OC(=O)[C@H](C)OC1=O	InChI=1/C6H8O4/c1-3-5(7)10-4(2)6(8)9-3/h3-4H,1-2H3/t3-,4-/m0/s1	0.382	0.382	1	1	1
4531-49-1	4531491	2939	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methoxyphenyl)-3-oxobutyramide]**	3_REACH		2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methoxyphenyl)-3-oxobutyramide]		C34H30Cl2N6O6	689.56	COc1ccccc1NC(=O)C(N=Nc2ccc(cc2Cl)c3ccc(N=NC(C(=O)C)C(=O)Nc4ccccc4OC)c(Cl)c3)C(=O)C	InChI=1/C34H30Cl2N6O6/c1-19(43)31(33(45)37-27-9-5-7-11-29(27)47-3)41-39-25-15-13-21(17-23(25)35)22-14-16-26(24(36)18-22)40-42-32(20(2)44)34(46)38-28-10-6-8-12-30(28)48-4/h5-18,31-32H,1-4H3,(H,37,45)(H,38,46)	7.364	7.364	1	1	1
4559-86-8	4559868	2943	**tetrabutylurea**	3_REACH	Urea, tetrabutyl-	tetrabutylurea	C17H36N2O	C17H36N2O	284.49	CCCCN(CCCC)C(=O)N(CCCC)CCCC	InChI=1/C17H36N2O/c1-5-9-13-18(14-10-6-2)17(20)19(15-11-7-3)16-12-8-4/h5-16H2,1-4H3	5.096	5.096	1	1	1
461-58-5	461585	2948	**cyanoguanidine**	3_REACH	Dicyandiamide	cyanoguanidine	C2H4N4	C2H5N4	84.086	NC(=[NH2+])NC#N	InChI=1/C2H4N4/c3-1-6-2(4)5/h(H4,4,5,6)/p+1	-0.953	-0.953	1	1	1
462-94-2	462942	2950	**pentamethylenediamine**	3_REACH	1,5-Diaminopentane	pentamethylenediamine	C5H14N2	C5H16N2	102.18	[NH3+]CCCCC[NH3+]	InChI=1/C5H14N2/c6-4-2-1-3-5-7/h1-7H2/p+2	-2.388	-2.382	1	1	1
4635-59-0	4635590	2951	**4-chlorobutyryl chloride**	3_REACH	Butanoyl chloride, 4-chloro-	4-chlorobutyryl chloride	C4H6Cl2O	C4H6Cl2O	141	ClCCCC(=O)Cl	InChI=1/C4H6Cl2O/c5-3-1-2-4(6)7/h1-3H2	1.474	1.474	1	1	1
4651-67-6	4651676	2954	**Nutriacholic acid**	3_REACH		3-a-hydroxy-7-oxo-5-ß-cholan-24-oic acid		C24H37O4	390.56	CC(CCC(=O)[O-])C1CCC2C3C(CCC12C)C4(C)CCC(O)CC4CC3=O	InChI=1/C24H38O4/c1-14(4-7-21(27)28)17-5-6-18-22-19(9-11-24(17,18)3)23(2)10-8-16(25)12-15(23)13-20(22)26/h14-19,22,25H,4-13H2,1-3H3,(H,27,28)/p-1	2.498	2.693	1	1	1
4672-38-2	4672382	2957	**propylphosphonic acid**	3_REACH		propylphosphonic acid		C3H8O3P	124.08	CCCP(=O)(O)[O-]	InChI=1/C3H9O3P/c1-2-3-7(4,5)6/h2-3H2,1H3,(H2,4,5,6)/p-1	-1.185	-1.212	1	1	1
470-82-6	470826	645	**cineole**	3_REACH	Eucalyptol	1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane	C10H18O	C10H18O	154.25	CC12CCC(CC1)C(C)(C)O2	InChI=1/C10H18O/c1-9(2)8-4-6-10(3,11-9)7-5-8/h8H,4-7H2,1-3H3	2.147	2.147	1	1	1
4724-48-5	4724485	2964	**octylphosphonic acid**	3_REACH		octylphosphonic acid		C8H18O3P	194.21	CCCCCCCCP(=O)(O)[O-]	InChI=1/C8H19O3P/c1-2-3-4-5-6-7-8-12(9,10)11/h2-8H2,1H3,(H2,9,10,11)/p-1	1.096	1.038	1	1	1
474-25-9	474259	2966	**chenodeoxycholic acid**	3_REACH		chenodeoxycholic acid		C24H39O4	392.58	C[C@H](CCC(=O)[O-])[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C	InChI=1/C24H40O4/c1-14(4-7-21(27)28)17-5-6-18-22-19(9-11-24(17,18)3)23(2)10-8-16(25)12-15(23)13-20(22)26/h14-20,22,25-26H,4-13H2,1-3H3,(H,27,28)/p-1/t14-,15+,16-,17-,18+,19+,20-,22+,23+,24-/m1/s1	2.54	2.736	1	1	1
479-27-6	479276	646	**1,8-naphthylenediamine**	3_REACH	1,8-Naphthalenediamine	1,8-Naphthalenediamine	C10H10N2	C10H10N2	158.21	Nc1cccc2cccc(N)c12	InChI=1/C10H10N2/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h1-6H,11-12H2	1.245	1.243	1	1	1
4813-57-4	4813574	2971	**octadecyl acrylate**	3_REACH	Octadecyl acrylate	octadecyl acrylate	C21H40O2	C21H40O2	324.55	CCCCCCCCCCCCCCCCCCOC(=O)C=C	InChI=1/C21H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-21(22)4-2/h4H,2-3,5-20H2,1H3	8.434	8.434	1	1	1
48145-04-6	48145046	2972	**2-phenoxyethyl acrylate**	3_REACH	beta.-Phenoxyethyl acrylate	2-phenoxyethyl acrylate	C11H12O3	C11H12O3	192.21	C=CC(=O)OCCOc1ccccc1	InChI=1/C11H12O3/c1-2-11(12)14-9-8-13-10-6-4-3-5-7-10/h2-7H,1,8-9H2	2.35	2.35	1	1	1
482-89-3	482893	647	**2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one**	3_REACH	c.i. Vat blue 1	2-(1,3-Dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	C16H10N2O2	C16H10N2O2	262.27	Oc1c([nH]c2ccccc12)C3=Nc4ccccc4C3=O	InChI=1/C16H10N2O2/c19-15-9-5-1-3-7-11(9)17-13(15)14-16(20)10-6-2-4-8-12(10)18-14/h1-8,17,19H	3.47	3.469	1	1	1
4904-61-4	4904614	648	**cyclododeca-1,5,9-triene**	3_REACH	1,5,9-Cyclododecatriene	1,5,9-Cyclododecatriene	C12H18	C12H18	162.28	C1CC=CCCC=CCCC=C1	InChI=1/C12H18/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,7-10H,3-6,11-12H2	4.14	4.14	1	1	1
4948-15-6	4948156	2983	**2,9-bis(3,5-dimethylphenyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone**	3_REACH		2,9-bis(3,5-dimethylphenyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone		C40H26N2O4	598.66	Cc1cc(C)cc(c1)N2C(=O)c3ccc4c5ccc6C(=O)N(C(=O)c7ccc(c8ccc(C2=O)c3c48)c5c67)c9cc(C)cc(C)c9	InChI=1/C40H26N2O4/c1-19-13-20(2)16-23(15-19)41-37(43)29-9-5-25-27-7-11-31-36-32(40(46)42(39(31)45)24-17-21(3)14-22(4)18-24)12-8-28(34(27)36)26-6-10-30(38(41)44)35(29)33(25)26/h5-18H,1-4H3	8.016	8.016	1	1	1
497-18-7	497187	2989	**carbonohydrazide**	3_REACH	Carbonic dihydrazide	carbonohydrazide	CH6N4O	CH4N4O	90.09	N[N-]C(=O)[N-]N	InChI=1/CH5N4O/c2-4-1(6)5-3/h2-3H2,(H-,4,5,6)/q-1/p-1	-1.819	-1.835	1	1	1

4979-32-2	4979322	2990	**N,N-dicyclohexylbenzothiazole-2-sulphenamide**	3_REACH		N,N-dicyclohexylbenzothiazole-2-sulphenamide		C19H26N2S2	346.56	C1CCC(CC1)N(Sc2nc3ccccc3s2)C4CCCCC4	InChI=1/C19H26N2S2/c1-3-9-15(10-4-1)21(16-11-5-2-6-12-16)23-19-20-17-13-7-8-14-18(17)22-19/h7-8,13-16H,1-6,9-12H2	6.427	6.427	1	1	1
50-21-5	50215	654	**lactic acid**	3_REACH	Propanoic acid, 2-hydroxy-	L-Lactic acid	C3H6O3	C3H5O3	90.078	CC(O)C(=O)[O-]	InChI=1/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)/p-1	-1.867	-1.863	1	1	1
502-44-3	502443	2999	**hexan-6-olide**	3_REACH	2-Oxepanone	hexan-6-olide	C6H10O2	C6H10O2	114.14	O=C1CCCCCO1	InChI=1/C6H10O2/c7-6-4-2-1-3-5-8-6/h1-5H2	1.188	1.188	1	1	1
5026-74-4	5026744	3000	**p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline**	3_REACH	N,N,N-Glycidyl p-aminophenol	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	C15H19NO4	C15H19NO4	277.32	C(Oc1ccc(cc1)N(CC2CO2)CC3CO3)C4CO4	InChI=1/C15H19NO4/c1-3-12(17-9-15-10-20-15)4-2-11(1)16(5-13-7-18-13)6-14-8-19-14/h1-4,13-15H,5-10H2	1.125	0.97	1	1	1
5036-48-6	5036486	3003	**1H-imidazole-1-propylamine**	3_REACH	1-(3-Aminopropyl)imidazole	1H-imidazole-1-propylamine	C6H11N3	C6H12N3	125.18	[NH3+]CCCn1ccnc1	InChI=1/C6H11N3/c7-2-1-4-9-5-3-8-6-9/h3,5-6H,1-2,4,7H2/p+1	-1.849	-1.211	1	1	1
503-74-2	503742	657	**isovaleric acid**	3_REACH	Butanoic acid, 3-methyl-	3-Methylbutanoic acid	C5H10O2	C5H9O2	102.13	CC(C)CC(=O)[O-]	InChI=1/C5H10O2/c1-4(2)3-5(6)7/h4H,3H2,1-2H3,(H,6,7)/p-1	-0.304	-0.275	1	1	1
504-29-0	504290	658	**2-pyridylamine**	3_REACH	2-Pyridinamine	2-Aminopyridine	C5H6N2	C5H6N2	94.119	Nc1ccccn1	InChI=1/C5H6N2/c6-5-3-1-2-4-7-5/h1-4H,(H2,6,7)	0.471	0.497	1	1	1
504-63-2	504632	660	**propane-1,3-diol**	3_REACH	1,3-Propanediol	1,3-Propanediol	C3H8O2	C3H8O2	76.095	OCCCO	InChI=1/C3H8O2/c4-2-1-3-5/h4-5H,1-3H2	-0.835	-0.835	1	1	1
506-30-9	506309	3012	**icosanoic acid**	3_REACH	Eicosanoic acid	icosanoic acid	C20H40O2	C20H39O2	312.54	CCCCCCCCCCCCCCCCCCCC(=O)[O-]	InChI=1/C20H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22/h2-19H2,1H3,(H,21,22)/p-1	6.743	6.769	1	1	1
507448-65-9	507448659	3018	**ethyl (2Z)-4,4,4-trifluoro-3-(methylamino)but-2-enoate**	3_REACH		ethyl (2Z)-4,4,4-trifluoro-3-(methylamino)but-2-enoate			197.16	CCOC(=O)C=C(C(F)(F)F)NC	InChI=1S/C7H10F3NO2/c1-3-13-6(12)4-5(11-2)7(8,9)10/h4,11H,3H2,1-2H3/b5-4-			1	1	1
5089-70-3	5089703	3022	**(3-chloropropyl)triethoxysilane**	3_REACH		(3-chloropropyl)triethoxysilane		C9H21ClO3Si	240.8	CCO[Si](CCCCl)(OCC)OCC	InChI=1/C9H21ClO3Si/c1-4-11-14(12-5-2,13-6-3)9-7-8-10/h4-9H2,1-3H3	4.057	4.057	1	1	1
5102-83-0	5102830	3025	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]**	3_REACH		2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]		C36H34Cl2N6O4	685.62	CC(=O)C(N=Nc1ccc(cc1Cl)c2ccc(N=NC(C(=O)C)C(=O)Nc3ccc(C)cc3C)c(Cl)c2)C(=O)Nc4ccc(C)cc4C	InChI=1/C36H34Cl2N6O4/c1-19-7-11-29(21(3)15-19)39-35(47)33(23(5)45)43-41-31-13-9-25(17-27(31)37)26-10-14-32(28(38)18-26)42-44-34(24(6)46)36(48)40-30-12-8-20(2)16-22(30)4/h7-18,33-34H,1-6H3,(H,39,47)(H,40,48)	9.342	9.342	1	1	1
51-03-6	51036	667	**2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether**	3_REACH	Piperonyl butoxide	Piperonyl butoxide	C19H30O5	C19H30O5	338.44	CCCCOCCOCCOCc1cc2OCOc2cc1CCC	InChI=1/C19H30O5/c1-3-5-7-20-8-9-21-10-11-22-14-17-13-19-18(23-15-24-19)12-16(17)6-4-2/h12-13H,3-11,14-15H2,1-2H3	3.867	3.867	1	1	1
51167-18-1	51167181	3028	**2'-[2,4-dichloro-5-(1-methylethoxy)phenyl]-2,2-dimethylpropionohydrazide**	3_REACH		2'-[2,4-dichloro-5-(1-methylethoxy)phenyl]-2,2-dimethylpropionohydrazide		C14H19Cl2N2O2	319.23	CC(C)Oc1cc(N[N-]C(=O)C(C)(C)C)c(Cl)cc1Cl	InChI=1/C14H20Cl2N2O2/c1-8(2)20-12-7-11(9(15)6-10(12)16)17-18-13(19)14(3,4)5/h6-8,17H,1-5H3,(H,18,19)/p-1	4.661	4.661	1	1	1
5124-30-1	5124301	3030	**4,4'-methylenedicyclohexyl diisocyanate**	3_REACH	Cyclohexane, 1,1'-methylenebis[4-isocyanato-	4,4'-methylenedicyclohexyl diisocyanate	C15H22N2O2	C15H24N2O2	262.36	O=C=[NH+]C1CCC(CC2CCC(CC2)[NH+]=C=O)CC1	InChI=1/C15H22N2O2/c18-10-16-14-5-1-12(2-6-14)9-13-3-7-15(8-4-13)17-11-19/h12-15H,1-9H2/p+2	3.412	3.494	1	1	1
51-28-5	51285	57	**2,4-dinitrophenol**	3_REACH	Phenol, 2,4-dinitro-	2,4-Dinitrophenol	C6H4N2O5	C6H3N2O5	184.11	[O-]c1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C6H4N2O5/c9-6-2-1-4(7(10)11)3-5(6)8(12)13/h1-3,9H/p-1	0.673	0.674	1	1	1
5131-66-8	5131668	3032	**1-butoxypropan-2-ol**	3_REACH	2-Propanol, 1-butoxy-	1-butoxypropan-2-ol	C7H16O2	C7H16O2	132.2	CCCCOCC(C)O	InChI=1/C7H16O2/c1-3-4-5-9-6-7(2)8/h7-8H,3-6H2,1-2H3	1.217	1.217	1	1	1
51920-12-8	51920128	3049	**N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-methyl-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide**	3_REACH		N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-methyl-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide		C27H23N6O6S	560.6	CNS(=O)(=O)c1cc(OC)c(cc1C)N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4ccc5[nH]c(O)nc5c4	InChI=1/C27H24N6O6S/c1-14-10-21(22(39-3)13-23(14)40(37,38)28-2)32-33-24-17-7-5-4-6-15(17)1 18(25(24)34)26(35)29-16-8-9-19-20(12-16)31-27(36)30-19/h4-13,28,34H,1-3H3,(H,29,35)(H2,30,31,36)/p-1	4.143	4.3	1	1	1
5208-93-5	5208935	3052	**3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol**	3_REACH		3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol		C15H24O	220.36	CC1=C(C=CC(C)(O)C=C)C(C)(C)CCC1	InChI=1/C15H24O/c1-6-15(5,16)11-9-13-12(2)8-7-10-14(13,3)4/h6,9,11,16H,1,7-8,10H2,2-5H3	3.87	3.87	1	1	1
521-18-6	521186	672	**androstanolone**	3_REACH	Stanolone	(5alpha,17beta)-17-Hydroxyandrostan-3-one	C19H30O2	C19H30O2	290.45	C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O	InChI=1/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)18/h12,14-17,21H,3-11H2,1-2H3/t12-,14-,15-,16-,17-,18-,19-/m0/s1	3.301	3.301	1	1	1
52449-76-0	52449760	3059	**Methyl 4-cyano-2-nitrobenzoate**	3_REACH		Benzoic acid, 4-cyano-2-nitro-, methyl ester			206.16	COC(=O)C1=C(C=C(C=C1)C#N)[N+](=O)[O-]	InChI=1S/C9H6N2O4/c1-15-9(12)7-3-2-6(5-10)4-8(7)11(13)14/h2-4H,1H3			1	1	1
52-51-7	52517	674	**bronopol**	3_REACH	Bronopol	2-Bromo-2-nitro-1,3-propanediol	C3H6BrNO4	C3H6BrNO4	200	OCC(Br)(CO)[N+](=O)[O-]	InChI=1/C3H6BrNO4/c4-3(1-6,2-7)5(8)9/h6-7H,1-2H2	0.056	0.056	1	1	1
52722-86-8	52722868	3072	**4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol**	3_REACH		4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol		C11H24NO2	201.31	CC1(C)CC(O)CC(C)(C)[NH+]1CCO	InChI=1/C11H23NO2/c1-10(2)7-9(14)8-11(3,4)12(10)5-6-13/h9,13-14H,5-8H2,1-4H3/p+1	-1.183	-1.182	1	1	1
5280-68-2	5280682	3074	**N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide**	3_REACH		N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide		C33H26ClN4O6	611.06	COc1cc(NC(=O)c2cc3ccccc3c(N=Nc4cc(ccc4OC)C(=O)Nc5ccccc5)c2[O-])c(OC)cc1Cl	InChI=1/C33H27ClN4O6/c1-42-27-14-13-20(32(40)35-21-10-5-4-6-11-21)16-26(27)37-38-30-22-12-7-9-19(22)15-23(31(30)39)33(41)36-25-18-28(43-2)24(34)17-29(25)44-3/h4-18,39H,1-3H3,(H,35,40)(H,36,41)/p-1	6.347	7.05	1	1	1
5280-80-8	5280808	3076	**3,3'-[(2,5-dimethyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]**	3_REACH		3,3'-[(2,5-dimethyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]		C44H36Cl4N8O6	916.66	CC(=O)[C-](Nc1cc(C)c(N[C-](C(=O)C)C(=O)N=Nc2cc(ccc2Cl)C(=O)Nc3cc(Cl)ccc3C)cc1C)C(=O)N=Nc4cc(ccc4Cl)C(=O)	InChI=1/C44H36Cl4N8O6/c1-21-7-11-29(45)19-35(21)51-41(59)27-9-13-31(47)37(17-27)53-55-43(61)39(25(5)57)49-33-15-24(4)34(16-23(33)3)50-40(26(6)58)44(62)56-54-38-18-28(10-14-32(38)48)42(60)52-36-20-30(46)12-8-22(36)2/h7-20,49-50H,1-6H3,(H,51,59)(H,52,60)/q-2	11.98	11.926	0	1	1
52829-07-9	52829079	3077	**bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate**	3_REACH		bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate		C28H54N2O4	480.74	CC1(C)CC(CC(C)(C)[NH2+]1)OC(=O)CCCCCCCCC(=O)OC2CC(C)(C)[NH2+]C(C)(C)C2	InChI=1/C28H52N2O4/c1-25(2)17-21(18-26(3,4)29-25)33-23(31)15-13-11-9-10-12-14-16-24(32)34-22-19-27(5,6)30-28(7,8)20-22/h21-22,29-30H,9-20H2,1-8H3/p+2	1.847	1.886	1	1	1
5283-66-9	5283669	678	**octyltrichlorosilane**	3_REACH	Octyltrichlorosilane	Trichlorooctylsilane	C8H17Cl3Si	C8H17Cl3Si	247.67	CCCCCCCC[Si](Cl)(Cl)Cl	InChI=1/C8H17Cl3Si/c1-2-3-4-5-6-7-8-12(9,10)11/h2-8H2,1H3	6.366	6.366	1	1	1
52846-56-7	52846567	3078	**N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(4-nitrophenyl)azo]-3-oxobutyramide**	3_REACH		N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(4-nitrophenyl)azo]-3-oxobutyramide		C17H14N6O5	382.34	CC(=O)C(N=Nc1ccc(cc1)[N+](=O)[O-])C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C17H14N6O5/c1-9(24)15(22-21-10-2-5-12(6-3-10)23(27)28)16(25)18-11-4-7-13-14(8-11)2 17(26)19-13/h2-8,15H,1H3,(H,18,25)(H2,19,20,26)	2.899	2.899	1	1	1
5292-45-5	5292455	680	**dimethyl 2-nitroterephthalate**	3_REACH		Dimethyl nitroterephthalate		C10H9NO6	239.18	COC(=O)c1ccc(C(=O)OC)c(c1)[N+](=O)[O-]	InChI=1/C10H9NO6/c1-16-9(12)6-3-4-7(10(13)17-2)8(5-6)11(14)15/h3-5H,1-2H3	1.435	1.435	1	1	1
5308-25-8	5308258	3087	**1-ethylpiperazine**	3_REACH	N-ethylpiperazine	1-ethylpiperazine	C6H14N2	C6H15N2	114.19	CCN1CC[NH2+]CC1	InChI=1/C6H14N2/c1-2-8-5-3-7-4-6-8/h7H,2-6H2,1H3/p+1	-1.141	-0.933	1	1	1
53-16-7	53167	61	**estrone**	3_REACH	3-Hydroxyestra-1,3,5(10)-trien-17-one	3-Hydroxyestra-1,3,5(10)trien-17-one	C18H22O2	C18H22O2	270.37	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CCC2=O	InChI=1/C18H22O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h3,5,10,14-16,19H,2,4,6-9H2,1H3/t14-,15-,16+,18+/m1/s1	3.938	3.938	1	1	1
53306-54-0	53306540	3094	**bis(2-propylheptyl) phthalate**	3_REACH		bis(2-propylheptyl) phthalate		C28H46O4	446.67	CCCCCC(CCC)COC(=O)c1ccccc1C(=O)OCC(CCC)CCCCC	InChI=1/C28H46O4/c1-5-9-11-17-23(15-7-3)21-31-27(29)25-19-13-14-20-26(25)28(30)32-22-24(16-4)18-12-10-6-2/h13-14,19-20,23-24H,5-12,15-18,21-22H2,1-4H3	9.398	9.398	0	0	1
5333-42-6	5333426	3096	**2-octyldodecan-1-ol**	3_REACH		2-octyldodecan-1-ol		C20H42O	298.56	CCCCCCCCCCC(CO)CCCCCCCC	InChI=1/C20H42O/c1-3-5-7-9-11-12-14-16-18-20(19-21)17-15-13-10-8-6-4-2/h20-21H,3-19H2,1-2H3	8.133	8.133	1	1	1
5333-84-6	5333846	3097	**1,2,3,6-tetrahydro-3-methylphthalic anhydride**	3_REACH	3-Methyltetrahydrophthalic anhydride	1,2,3,6-tetrahydro-3-methylphthalic anhydride	C9H10O3	C9H10O3	166.18	CC1C=CCC2C1C(=O)OC2=O	InChI=1/C9H10O3/c1-5-3-2-4-6-7(5)9(11)12-8(6)10/h2-3,5-7H,4H2,1H3	1.127	1.127	1	1	1
534-03-2	534032	3100	**2-aminopropane-1,3-diol**	3_REACH	2-Amino-1,3-propanediol	2-aminopropane-1,3-diol	C3H9NO2	C3H10NO2	91.111	[NH3+]C(CO)CO	InChI=1/C3H9NO2/c4-3(1-5)2-6/h3,5-6H,1-2,4H2/p+1	-2.703	-2.264	1	1	1
5343-92-0	5343920	3102	**pentane-1,2-diol**	3_REACH	1,2-Pentanediol	pentane-1,2-diol	C5H12O2	C5H12O2	104.15	CCCC(O)CO	InChI=1/C5H12O2/c1-2-3-5(7)4-6/h5-7H,2-4H2,1H3	0.459	0.459	1	1	1
53445-37-7	53445377	3103	**2,2,4(or 2,4,4)-trimethyladipic acid**	3_REACH		2,2,4(or 2,4,4)-trimethyladipic acid		C9H14O4	188.22	CC(CC(=O)[O-])CC(C)(C)C(=O)[O-]	InChI=1/C9H16O4/c1-6(4-7(10)11)5-9(2,3)8(12)13/h6H,4-5H2,1-3H3,(H,10,11)(H,12,13)/p-2	-1.264	-1.036	1	1	1
534-52-1	534521	682	**2-methyl-4,6-dinitro-phenol | DNOC**	3_REACH	Phenol, 2-methyl-4,6-dinitro-	2-Methyl-4,6-dinitrophenol	C7H6N2O5	C7H5N2O5	198.14	Cc1cc(cc(c1[O-])[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C7H6N2O5/c1-4-2-5(8(11)12)3-6(7(4)10)9(13)14/h2-3,10H,1H3/p-1	1.159	1.161	1	1	1
53651-69-7	53651697	3107	**Propanoic acid**	3_REACH		Propanoic acid, 2-hydroxy-, propyl ester, (2S)-			132.16	CCCOC(=O)C(C)O	InChI=1S/C6H12O3/c1-3-4-9-6(8)5(2)7/h5,7H,3-4H2,1-2H3/t5-/m0/s1			1	1	1
5372-81-6	5372816	683	**dimethyl 2-aminoterephthalate**	3_REACH	Aminoterephthalic acid, dimethyl ester	2-Amino-1,4-benzenedicarboxylic acid, Dimethyl ester	C10H11NO4	C10H11NO4	209.2	COC(=O)c1ccc(C(=O)OC)c(N)c1	InChI=1/C10H11NO4/c1-14-9(12)6-3-4-7(8(11)5-6)10(13)15-2/h3-5H,11H2,1-2H3	0.794	0.794	1	1	1
540-97-6	540976	3124	**dodecamethylcyclohexasiloxane**	3_REACH	Dodecamethylcyclohexasiloxane	dodecamethylcyclohexasiloxane	C12H36O6Si6	C12H36O6Si6	444.93	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	InChI=1/C12H36O6Si6/c1-19(2)13-20(3,4)15-22(7,8)17-24(11,12)18-23(9,10)16-21(5,6)14-19/h1-12H3	10.34	10.34	1	1	1
541-02-6	541026	3125	**decamethylcyclopentasiloxane**	3_REACH	Decamethylcyclopentasiloxane	decamethylcyclopentasiloxane	C10H30O5Si5	C10H30O5Si5	370.77	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	InChI=1/C10H30O5Si5/c1-16(2)11-17(3,4)13-19(7,8)15-20(9,10)14-18(5,6)12-16/h1-10H3	8.617	8.617	1	1	1
5413-60-5	5413605	3128	**3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate**	3_REACH	Dihydro-nordicyclopentadienyl acetate	3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate	C12H16O2	C12H16O2	192.26	CC(=O)OC1CC2CC1C3CC=CC23	InChI=1/C12H16O2/c1-7(13)14-12-6-8-5-11(12)10-4-2-3-9(8)10/h2-3,8-12H,4-6H2,1H3	1.766	1.766	1	1	1
541-73-1	541731	685	**1,3-dichlorobenzene**	3_REACH	Benzene, 1,3-dichloro-	1,3-Dichlorobenzene	C6H4Cl2	C6H4Cl2	147	Clc1cccc(Cl)c1	InChI=1/C6H4Cl2/c7-5-2-1-3-6(8)4-5/h1-4H	3.158	3.158	1	1	1
542-05-2	542052	3134	**3-oxoglutaric acid**	3_REACH		3-oxoglutaric acid		C5H4O5	146.1	[O-]C(=O)CC(=O)CC(=O)[O-]	InChI=1/C5H6O5/c6-3(1-4(7)8)2-5(9)10/h1-2H2,(H,7,8)(H,9,10)/p-2	-3.432	-3.422	1	1	1
5435-64-3	5435643	3140	**3,5,5-trimethylhexanal**	3_REACH	Hexanal, 3,5,5-trimethyl-	3,5,5-trimethylhexanal	C9H18O	C9H18O	142.24	CC(CC=O)CC(C)(C)C	InChI=1/C9H18O/c1-8(5-6-10)7-9(2,3)4/h6,8H,5,7H2,1-4H3	2.562	2.562	1	1	1
544-01-4	544014	3141	**diisopentyl ether**	3_REACH	Butane, 1,1'-oxybis[3-methyl-	diisopentyl ether	C10H22O	C10H22O	158.29	CC(C)CCOCCC(C)C	InChI=1/C10H22O/c1-9(2)5-7-11-8-6-10(3)4/h9-10H,5-8H2,1-4H3	3.211	3.211	1	1	1
54423-67-5	54423675	3143	**vinyl neononanoate**	3_REACH		vinyl neononanoate		C11H20O2	184.28	CC(C)(C)CCCCC(=O)OC=C	InChI=1/C11H20O2/c1-5-13-10(12)8-6-7-9-11(2,3)4/h5H,1,6-9H2,2-4H3	3.055	3.055	1	1	1
5466-77-3	5466773	3151	**2-ethylhexyl 4-methoxycinnamate**	3_REACH		2-ethylhexyl 4-methoxycinnamate		C18H26O3	290.4	CCCCC(CC)COC(=O)\C=C\c1ccc(OC)cc1	InChI=1/C18H26O3/c1-4-6-7-15(5-2)14-21-18(19)13-10-16-8-11-17(20-3)12-9-16/h8-13,15H,4-7,14H2,1-3H3/b13-10+	5.153	5.153	1	1	1
5468-75-7	5468757	3152	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide]**	3_REACH		2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide]		C34H30Cl2N6O4	657.56	CC(=O)C(N=Nc1ccc(cc1Cl)c2ccc(N=NC(C(=O)C)C(=O)Nc3ccccc3C)c(Cl)c2)C(=O)Nc4ccccc4C	InChI=1/C34H30Cl2N6O4/c1-19-9-5-7-11-27(19)37-33(45)31(21(3)43)41-39-29-15-13-23(17-25(29)35)24-14-16-30(26(36)18-24)40-42-32(22(4)44)34(46)38-28-12-8-6-10-20(28)2/h5-18,31-32H,1-4H3,(H,37,45)(H,38,46)	8.369	8.369	1	1	1
54839-24-6	54839246	3154	**2-ethoxy-1-methylethyl acetate**	3_REACH		2-ethoxy-1-methylethyl acetate		C7H14O3	146.19	CCOCC(C)OC(=O)C	InChI=1/C7H14O3/c1-4-9-5-6(2)10-7(3)8/h6H,4-5H2,1-3H3	0.616	0.616	1	1	1
54914-37-3	54914373	3156	**1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]cyclohexanemethylamine**	3_REACH		1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]cyclohexanemethylamine		C18H35N2	278.49	CC(C)\C=N\CC1(C)CC(CC(C)(C)C1)[NH+]=CC(C)C	InChI=1/C18H34N2/c1-14(2)10-19-13-18(7)9-16(20-11-15(3)4)8-17(5,6)12-18/h10-11,14-16H,8-9,1 13H2,1-7H3/p+1/b19-10+,20-11+	4.352	4.352	1	1	1
5521-31-3	5521313	3163	**2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone**	3_REACH		2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone		C26H14N2O4	418.41	CN1C(=O)c2ccc3c4ccc5C(=O)N(C)C(=O)c6ccc(c7ccc(C1=O)c2c37)c4c56	InChI=1/C26H14N2O4/c1-27-23(29)15-7-3-11-13-5-9-17-22-18(26(32)28(2)25(17)31)10-6-14(20(13)22)12-4-8-16(24(27)30)21(15)19(11)12/h3-10H,1-2H3	2.918	2.918	1	1	1
55314-16-4	55314164	3166	**611-255-8**	3_REACH		PYRENAMINE			176.22	CN(C)C=CC(=O)C1=CN=CC=C1	InChI=1S/C10H12N2O/c1-12(2)7-5-10(13)9-4-3-6-11-8-9/h3-8H,1-2H3/b7-5+			1	1	1
553-86-6	553866	3169	**(3H)-benzofuran-2-one**	3_REACH	2-Coumaranone	(3H)-benzofuran-2-one	C8H6O2	C8H6O2	134.13	O=C1Cc2ccccc2O1	InChI=1/C8H6O2/c9-8-5-6-3-1-2-4-7(6)10-8/h1-4H,5H2	1.466	1.466	1	1	1
554-00-7	554007	700	**2,4-dichloroaniline**	3_REACH	Benzenamine, 2,4-dichloro-	2,4-Dichloroaniline	C6H5Cl2N	C6H5Cl2N	162.02	Nc1ccc(Cl)cc1Cl	InChI=1/C6H5Cl2N/c7-4-1-2-6(9)5(8)3-4/h1-3H,9H2	2.412	2.412	1	1	1
556-67-2	556672	705	**octamethylcyclotetrasiloxane**	3_REACH	Cyclotetrasiloxane, octamethyl-	Octamethylcyclotetrasiloxane	C8H24O4Si4	C8H24O4Si4	296.62	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	InChI=1/C8H24O4Si4/c1-13(2)9-14(3,4)11-16(7,8)12-15(5,6)10-13/h1-8H3	6.893	6.893	1	1	1
5567-15-7	5567157	706	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]**	3_REACH		CI Pigment Yellow 83		C36H32Cl4N6O8	818.5	COc1cc(NC(=O)C(N=Nc2ccc(cc2Cl)c3ccc(N=NC(C(=O)C)C(=O)Nc4cc(OC)c(Cl)cc4OC)c(Cl)c3)C(=O)C)c(OC)cc1Cl	InChI=1/C36H32Cl4N6O8/c1-17(47)33(35(49)41-27-15-29(51-3)23(39)13-31(27)53-5)45-43-25-9-7-19(11-21(25)37)20-8-10-26(22(38)12-20)44-46-34(18(2)48)36(50)42-28-16-30(52-4)24(40)14-32(28)54-6/h7-16,33-34H,1-6H3,(H,41,49)(H,42,50)	8.66	8.66	1	1	1
556-88-7	556887	707	**1-nitroguanidine**	3_REACH	Guanidine, nitro-	Nitroguanidine	CH4N4O2	CH3N4O2	104.07	NC(=N)[N-][N+](=O)[O-]	InChI=1/CH3N4O2/c2-1(3)4-5(6)7/h(H3-,2,3,4)/p-1	1.323	1.323	1	1	1
5578-42-7	5578427	3177	**dichlorocyclohexylmethylsilane**	3_REACH	Cyclohexylmethyldichlorosilane	dichlorocyclohexylmethylsilane	C7H14Cl2Si	C7H14Cl2Si	197.18	[SiH3]C(Cl)(Cl)C1CCCCC1	InChI=1/C7H14Cl2Si/c8-7(9,10)6-4-2-1-3-5-6/h6H,1-5H2,10H3	6.669	6.669	1	1	1
5580-57-4	5580574	3178	**3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(3-chloro-o-tolyl)benzamide]**	3_REACH		3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(3-chloro-o-tolyl)benzamide]		C43H33Cl5N8O6	937.08	CC(=O)[C-](Nc1cc(Cl)c(N[C-](C(=O)C)C(=O)N=Nc2cc(ccc2Cl)C(=O)Nc3cccc(Cl)c3C)cc1C)C(=O)N=Nc4cc(ccc4Cl)C(=O	InChI=1/C43H33Cl5N8O6/c1-20-16-35(50-39(24(5)58)43(62)56-54-37-18-26(13-15-30(37)47)41(60)52-33-11-7-9-28(45)22(33)3)31(48)19-34(49)38(23(4)57)42(61)55-53-36-17-25(12-14-29(36)46)40(59)51-32-10-6-8-27(44)21(32)2/h6-19,49-50H,1-5H3,(H,51,59)(H,52,60)/q-2	12.158	12.104	1	0	1
5580-58-5	5580585	3179	**3,3'-[(2,5-dichloro-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]**	3_REACH		3,3'-[(2,5-dichloro-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]		C42H30Cl6N8O6	957.49	CC(=O)[C-](Nc1cc(Cl)c(N[C-](C(=O)C)C(=O)N=Nc2cc(ccc2Cl)C(=O)Nc3cc(Cl)ccc3C)cc1Cl)C(=O)N=Nc4cc(ccc4Cl)C(=	InChI=1/C42H30Cl6N8O6/c1-19-5-9-25(43)15-31(19)51-39(59)23-7-11-27(45)35(13-23)53-55-41(61)37(21(3)57)49-33-17-30(48)34(18-29(33)47)50-38(22(4)58)42(62)56-54-36-14-24(8-12-28(36)46)40(60)52-32-16-26(44)10-6-20(32)2/h5-18,49-50H,1-4H3,(H,51,59)(H,52,60)/q-2	12.337	12.282	1	0	0
55934-93-5	55934935	3182	**[(butoxymethylethoxy)methylethoxy]propan-1-ol**	3_REACH		[(butoxymethylethoxy)methylethoxy]propan-1-ol		C13H28O4	248.36	CCCCOCC(C)OCC(C)OC(O)CC	InChI=1/C13H28O4/c1-5-7-8-15-9-11(3)16-10-12(4)17-13(14)6-2/h11-14H,5-10H2,1-4H3	2.146	2.146	1	1	1
561-41-1	561411	3187	**4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol**	3_REACH		4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol		C24H30N3O	375.52	CNc1ccc(cc1)C(O)(c2ccc(cc2)N(C)C)c3ccc(cc3)[NH+](C)C	InChI=1/C24H29N3O/c1-25-21-12-6-18(7-13-21)24(28,19-8-14-22(15-9-19)26(2)3)20-10-16-23(17-11-20)27(4)5/h6-17,25,28H,1-5H3/p+1	2.754	3.555	1	1	1
56-18-8	56188	3188	**3,3'-iminodi(propylamine)**	3_REACH	3,3'-Iminobispropylamine	3,3'-iminodi(propylamine)	C6H17N3	C6H20N3	131.23	[NH3+]CCC[NH2+]CCC[NH3+]	InChI=1/C6H17N3/c7-3-1-5-9-6-2-4-8/h9H,1-8H2/p+3	-4.99	-4.432	1	1	1
56309-94-5	56309945	4472	**4-(1,4-dioxa-spiro[4.5]dec-8-yl)-cyclohexanone**	3_REACH		Cyclohexanone, 4-(1,4-dioxaspiro[4.5]dec-8-yl)-			238.33	C1CC(=O)CCC1C2CCC3(CC2)OCCO3	InChI=1S/C14H22O3/c15-13-3-1-11(2-4-13)12-5-7-14(8-6-12)16-9-10-17-14/h11-12H,1-10H2			1	1	1
56358-17-9	56358179	3192	**N-(2-ethylhexyl)naphthalen-2-amine**	3_REACH		N-(2-ethylhexyl)naphthalen-2-amine		C18H25N	255.41	CCCCC(CC)CNc1ccc2ccccc2c1	InChI=1/C18H25N/c1-3-5-8-15(4-2)14-19-18-12-11-16-9-6-7-10-17(16)13-18/h6-7,9-13,15,19H,3-5,8,14H2,1-2H3	5.563	5.562	1	1	1
56-41-7	56417	3198	**L-alanine**	3_REACH	Alanine	L-alanine	C3H7NO2	C3H7NO2	89.095	C[C@H]([NH3+])C(=O)[O-]	InChI=1/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)/t2-/m0/s1	-3.161	-3.161	1	1	1
56519-71-2	56519712	3200	**Propane-1,3-diyl dioctanoate**	3_REACH		Propane-1,3-diyl dioctanoate			328.49	CCCCCCCC(=O)OCCCOC(=O)CCCCCCC	InChI=1S/C19H36O4/c1-3-5-7-9-11-14-18(20)22-16-13-17-23-19(21)15-12-10-8-6-4-2/h3-17H2,1-2H3			1	1	1
56539-66-3	56539663	3201	**3-methoxy-3-methylbutan-1-ol**	3_REACH		3-methoxy-3-methylbutan-1-ol		C6H14O2	118.18	COC(C)(C)CCO	InChI=1/C6H14O2/c1-6(2,8-3)4-5-7/h7H,4-5H2,1-3H3	0.155	0.155	1	1	1
56677-60-2	56677602	3208	**tetradecyl chloroformate**	3_REACH		tetradecyl chloroformate		C15H29ClO2	276.85	CCCCCCCCCCCCCCOC(=O)Cl	InChI=1/C15H29ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-15(16)17/h2-14H2,1H3	6.905	6.905	1	1	1
56706-10-6	56706106	3209	**4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecane**	3_REACH		4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecane		C18H42O6S2Si2	474.83	CCO[Si](CCCSSCCC[Si](OCC)(OCC)OCC)(OCC)OCC	InChI=1/C18H42O6S2Si2/c1-7-19-27(20-8-2,21-9-3)17-13-15-25-26-16-14-18-28(22-10-4,23-11-5)2 12-6/h7-18H2,1-6H3	7.808	7.808	1	1	1
56718-71-9	56718719	3211	**p-(2-methoxyethyl)phenol**	3_REACH		p-(2-methoxyethyl)phenol		C9H12O2	152.19	COCCc1ccc(O)cc1	InChI=1/C9H12O2/c1-11-7-6-8-2-4-9(10)5-3-8/h2-5,10H,6-7H2,1H3	1.713	1.712	1	1	1
56-84-8	56848	3212	**aspartic acid**	3_REACH	Aspartic acid	aspartic acid	C4H7NO4	C4H6NO4	133.1	[NH3+]C(CC(=O)[O-])C(=O)[O-]	InChI=1/C4H7NO4/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H,6,7)(H,8,9)/p-1	-5.254	-5.248	1	1	1
56962-04-0	56962040	3217	**3-Bromo-5-chlorophenol**	3_REACH		3-Bromo-5-chlorophenol			207.46	C1=C(C=C(C=C1Cl)Br)O	InChI=1S/C6H4BrClO/c7-4-1-5(8)3-6(9)2-4/h1-3,9H			1	1	1
56973-87-6	56973876	4267	**1-(3,3-dimethylcyclohexyl)pent-4-en-1-one**	3_REACH		1-(3,3-dimethylcyclohexyl)pent-4-en-1-one			194.32	CC1(CCCC(C1)C(=O)CCC=C)C	InChI=1S/C13H22O/c1-4-5-8-12(14)11-7-6-9-13(2,3)10-11/h4,11H,1,5-10H2,2-3H3			1	1	1
57090-45-6	57090456	4249	**(R)-3-chloropropane-1,2-diol**	3_REACH		(R)-3-chloropropane-1,2-diol			110.54	C(C(CCl)O)O	InChI=1S/C3H7ClO2/c4-1-3(6)2-5/h3,5-6H,1-2H2/t3-/m0/s1			1	1	1
5726-19-2	5726192	3228	**2-methylcyclohexyl acetate**	3_REACH		2-methylcyclohexyl acetate		C9H16O2	156.22	CC1CCCCC1OC(=O)C	InChI=1/C9H16O2/c1-7-5-3-4-6-9(7)11-8(2)10/h7,9H,3-6H2,1-2H3	2.198	2.198	1	1	1
57374-49-9	57374499	4553	**methyl 3-acetoxy-2-pentyl-2-cyclopentene-1-acetate**	3_REACH		2-Cyclopentene-1-acetic acid, 3-(acetyloxy)-2-pentyl-, methyl ester			268.35	CCCCCC1=C(CCC1CC(=O)OC)OC(=O)C	InChI=1S/C15H24O4/c1-4-5-6-7-13-12(10-15(17)18-3)8-9-14(13)19-11(2)16/h12H,4-10H2,1-3H3			1	1	1
576-26-1	576261	723	**2,6-xylenol**	3_REACH	Phenol, 2,6-dimethyl-	2,6-Dimethylphenol	C8H10O	C8H10O	122.17	Cc1cccc(C)c1O	InChI=1/C8H10O/c1-6-4-3-5-7(2)8(6)9/h3-5,9H,1-2H3	2.56	2.56	1	1	1
5766-67-6	5766676	3236	**ethylenediaminetetraacetonitrile**	3_REACH		ethylenediaminetetraacetonitrile		C10H12N6	216.25	NC(CC#N)(CC#N)C(N)(CC#N)CC#N	InChI=1/C10H12N6/c11-5-1-9(15,2-6-12)10(16,3-7-13)4-8-14/h1-4,15-16H2	-1.792	-1.792	1	1	1
57843-53-5	57843535	3238	**N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide**	3_REACH		N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide		C18H36N2O6	376.5	CC(O)CN(CC(C)O)C(=O)CCCCC(=O)N(CC(C)O)CC(C)O	InChI=1/C18H36N2O6/c1-13(21)9-19(10-14(2)22)17(25)7-5-6-8-18(26)20(11-15(3)23)12-16(4)24/h1 16,21-24H,5-12H2,1-4H3	-0.527	-0.527	1	1	1
58190-57-1	58190571	3242	**2-Propanone, 2,2',2''-(O,O',O''-(ethylsilylidyne)trioxime)**	3_REACH		2-Propanone, 2,2',2''-(O,O',O''-(ethylsilylidyne)trioxime)		C11H23N3O3Si	273.41	CC[Si](ON=C(C)C)(ON=C(C)C)ON=C(C)C	InChI=1S/C11H23N3O3Si/c1-8-18(15-12-9(2)3,16-13-10(4)5)17-14-11(6)7/h8H2,1-7H3			1	1	1
583-39-1	583391	3244	**benzimidazole-2-thiol**	3_REACH		benzimidazole-2-thiol		C7H6N2S	150.21	Sc1nc2ccccc2[nH]1	InChI=1/C7H6N2S/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H2,8,9,10)	2.247	2.211	1	1	1
583-78-8	583788	728	**2,5-dichlorophenol**	3_REACH	Phenol, 2,5-dichloro-	2,5-Dichlorophenol	C6H4Cl2O	C6H4Cl2O	163	Oc1cc(Cl)ccc1Cl	InChI=1/C6H4Cl2O/c7-4-1-2-5(8)6(9)3-4/h1-3,9H	2.916	2.744	1	1	1
58430-94-7	58430947	3247	**3,5,5-trimethylhexyl acetate**	3_REACH	3,5,5-Trimethylhexyl acetate	3,5,5-trimethylhexyl acetate	C11H22O2	C11H22O2	186.29	CC(CCOC(=O)C)CC(C)(C)C	InChI=1/C11H22O2/c1-9(6-7-13-10(2)12)8-11(3,4)5/h9H,6-8H2,1-5H3	2.972	2.972	1	1	1
584-84-9	584849	729	**4-methyl-m-phenylene diisocyanate**	3_REACH	Benzene, 2,4-diisocyanato-1-methyl-	2,4-Diisocyanate-1-methylbenzene	C9H6N2O2	C9H6N2O2	174.16	Cc1ccc(cc1N=C=O)N=C=O	InChI=1/C9H6N2O2/c1-7-2-3-8(10-5-12)4-9(7)11-6-13/h2-4H,1H3	2.036	2.036	1	1	1
58567-11-6	58567116	3249	**(ethoxymethoxy)cyclododecane**	3_REACH		(ethoxymethoxy)cyclododecane		C15H30O2	242.4	CCOCOC1CCCCCCCCCCC1	InChI=1/C15H30O2/c1-2-16-14-17-15-12-10-8-6-4-3-5-7-9-11-13-15/h15H,2-14H2,1H3	4.846	4.846	1	1	1
586-62-9	586629	731	**p-mentha-1,4(8)-diene**	3_REACH	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	1-Methyl-4-(1-methylethylidene)-cyclohexene	C10H16	C10H16	136.24	CC(=C1CCC(=CC1)C)C	InChI=1/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4H,5-7H2,1-3H3	3.643	3.643	1	1	1
58670-89-6	58670896	3252	**2-decyltetradecanol**	3_REACH		2-decyltetradecanol		C24H50O	354.66	CCCCCCCCCCCCC(CO)CCCCCCCCCC	InChI=1/C24H50O/c1-3-5-7-9-11-13-14-16-18-20-22-24(23-25)21-19-17-15-12-10-8-6-4-2/h24-25H,3-23H2,1-2H3	9.957	9.957	0	0	1
5888-33-5	5888335	3257	**exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate**	3_REACH		exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate		C13H20O2	208.3	CC1(C)[C@H]2CC[C@]1(C)[C@H](C2)OC(=O)C=C	InChI=1/C13H20O2/c1-5-11(14)15-10-8-9-6-7-13(10,4)12(9,2)3/h5,9-10H,1,6-8H2,2-4H3/t9-,10-,13+/m0/s1	3.051	3.051	1	1	1
5888-87-9	5888879	3258	**N,N'-hexane-1,6-diylbis(hexahydro-2-oxo-1H-azepine-1-carboxamide)**	3_REACH		N,N'-hexane-1,6-diylbis(hexahydro-2-oxo-1H-azepine-1-carboxamide)		C20H34N4O4	394.52	O=C(NCCCCCCNC(=O)N1CCCCCC1=O)N2CCCCCC2=O	InChI=1/C20H34N4O4/c25-17-11-5-3-9-15-23(17)19(27)21-13-7-1-2-8-14-22-20(28)24-16-10-4-6-1 18(24)26/h1-16H2,(H,21,27)(H,22,28)	2.428	2.428	1	1	1
591-27-5	591275	734	**3-aminophenol**	3_REACH	Phenol, 3-amino-	3-Aminophenol	C6H7NO	C6H7NO	109.13	Nc1cccc(O)c1	InChI=1/C6H7NO/c7-5-2-1-3-6(8)4-5/h1-4,8H,7H2	0.841	0.841	1	1	1
59227-88-2	59227882	4300	**1-octylazepin-2-one**	3_REACH		1-octylazepin-2-one			225.38	CCCCCCCCN1CCCCCC1=O	InChI=1S/C14H27NO/c1-2-3-4-5-6-9-12-15-13-10-7-8-11-14(15)16/h2-13H2,1H3			1	1	1
59447-55-1	59447551	3278	**(pentabromophenyl)methyl acrylate**	3_REACH		(pentabromophenyl)methyl acrylate		C10H5Br5O2	556.7	Brc1c(Br)c(Br)c(COC(=O)C=C)c(Br)c1Br	InChI=1/C10H5Br5O2/c1-2-5(16)17-3-4-6(11)8(13)10(15)9(14)7(4)12/h2H,1,3H2	6.044	6.044	1	1	1
59487-23-9	59487239	3279	**4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide**	3_REACH		4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide		C34H27ClN5O7	654.08	COc1cc(OC)c(NC(=O)c2cc3ccccc3c(N=Nc4cc(ccc4OC)C(=O)Nc5ccc(cc5)C(=O)N)c2[O-])cc1Cl	InChI=1/C34H28ClN5O7/c1-45-27-13-10-20(33(43)37-21-11-8-18(9-12-21)32(36)42)15-26(27)39-4 30-22-7-5-4-6-19(22)14-23(31(30)41)34(44)38-25-16-24(35)28(46-2)17-29(25)47-3/h4-17,41H,1-3H3,(H2,36,42)(H,37,43)(H,38,44)/p-1	5.349	6.044	1	1	1
59-50-7	59507	737	**chlorocresol**	3_REACH	Phenol, 4-chloro-3-methyl-	4-chloro-3-methylphenol	C7H7ClO	C7H7ClO	142.59	Cc1cc(O)ccc1Cl	InChI=1/C7H7ClO/c1-5-4-6(9)2-3-7(5)8/h2-4,9H,1H3	2.738	2.736	1	1	1
59719-67-4	59719674	3284	**bis[2-[2-(1-methylethyl)-3-oxazolidinyl]ethyl] hexan-1,2-diylbiscarbamate**	3_REACH		bis[2-[2-(1-methylethyl)-3-oxazolidinyl]ethyl] hexan-1,2-diylbiscarbamate		C24H48N4O6	486.66	CCCCC(CNC(=O)OCC[NH+]1CCOC1C(C)C)NC(=O)OCC[NH+]2CCOC2C(C)C	InChI=1/C24H46N4O6/c1-6-7-8-20(26-24(30)34-16-12-28-10-14-32-22(28)19(4)5)17-25-23(29)33-1 11-27-9-13-31-21(27)18(2)3/h18-22H,6-17H2,1-5H3,(H,25,29)(H,26,30)/p+2	0.721	2.087	1	1	1
5989-27-5	5989275	743	**(R)-p-mentha-1,8-diene**	3_REACH	(+)-Limonene	(4R)-1-Methyl-4-(1-methylethenyl)cyclohexene	C10H16	C10H16	136.24	CC(=C)[C@@H]1CCC(=CC1)C	InChI=1/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3/t10-/m0/s1	3.502	3.502	1	1	1
5989-54-8	5989548	744	**(S)-p-mentha-1,8-diene**	3_REACH	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-	(4S)-1-Methyl-4-(1-methylethenyl)cyclohexene	C10H16	C10H16	136.24	CC(=C)[C@H]1CCC(=CC1)C	InChI=1/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3/t10-/m1/s1	3.502	3.502	1	1	1
599-04-2	599042	3296	**2,4-dihydroxy-3,3-dimethylbutyric acid gamma-lactone**	3_REACH	Pantolactone	a-hydroxy-ß,ß-dimethyl-¿-butyrolactone	C6H10O3	C6H10O3	130.14	CC1(C)COC(=O)C1O	InChI=1/C6H10O3/c1-6(2)3-9-5(8)4(6)7/h4,7H,3H2,1-2H3	0.217	0.217	1	1	1
599-61-1	599611	3298	**3,3'-sulphonyldianiline**	3_REACH	Benzenamine, 3,3'-sulfonylbis-	3,3'-sulphonyldianiline	C12H12N2O2S	C12H12N2O2S	248.31	Nc1cccc(c1)S(=O)(=O)c2cccc(N)c2	InChI=1/C12H12N2O2S/c13-9-3-1-5-11(7-9)17(15,16)12-6-2-4-10(14)8-12/h1-8H,13-14H2	1.439	1.439	1	1	1
599-64-4	599644	3299	**P-Cumylphenol**	3_REACH	p-α-Cumylphenol	4-(a,a-dimethylbenzyl)phenol	C15H16O	C15H16O	212.29	CC(C)(c1ccccc1)c2ccc(O)cc2	InChI=1/C15H16O/c1-15(2,12-6-4-3-5-7-12)13-8-10-14(16)11-9-13/h3-11,16H,1-2H3	4.02	4.02	1	1	1
60-00-4	60004	71	**edetic acid**	3_REACH	N,N'-1,2-Ethane diylbis-(N-(carboxymethyl)glycine)	N,N'-1,2-Ethanediylbis[N-(carboxymethyl)glycine	C10H16N2O8	C10H13N2O8	292.25	[O-]C(=O)CN(CC[NH+](CC(=O)[O-])CC(=O)[O-])CC(=O)[O-]	InChI=1/C10H16N2O8/c13-7(14)3-11(4-8(15)16)1-2-12(5-9(17)18)6-10(19)20/h1-6H2,(H,13,14)(H,15,16)(H,17,18)(H,19,20)/p-3	-9.072	-8.443	1	1	1
60-09-3	60093	746	**4-aminoazobenzene**	3_REACH	Benzenamine, 4-(phenylazo)-	4-(Phenylazo)benzenamine	C12H11N3	C12H11N3	197.24	Nc1ccc(cc1)N=Nc2ccccc2	InChI=1/C12H11N3/c13-10-6-8-12(9-7-10)15-14-11-4-2-1-3-5-11/h1-9H,13H2/b15-14+	3.452	3.452	1	1	1
60111-54-8	60111548	3304	**3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-divinyltrisiloxane**	3_REACH		3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-divinyltrisiloxane		C16H36O4Si5	432.89	C[Si](C)(O[Si](O[Si](C)(C)C=C)(O[Si](C)(C)C=C)O[Si](C)(C)C=C)C=C	InChI=1/C16H36O4Si5/c1-13-21(5,6)17-25(18-22(7,8)14-2,19-23(9,10)15-3)20-24(11,12)16-4/h13-16H,1-4H2,5-12H3	9.158	9.158	1	1	1
60-12-8	60128	3306	**2-phenylethanol**	3_REACH	Benzeneethanol	2-phenylethanol	C8H10O	C8H10O	122.17	OCCc1ccccc1	InChI=1/C8H10O/c9-7-6-8-4-2-1-3-5-8/h1-5,9H,6-7H2	1.546	1.546	1	1	1
603-35-0	603350	751	**triphenylphosphine**	3_REACH	Phosphine, triphenyl-	Triphenylphosphine	C18H15P	C18H15P	262.29	c1ccc(cc1)P(c2ccccc2)c3ccccc3	InChI=1/C18H15P/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H	5.707	5.707	1	1	1
6041-94-7	6041947	3310	**4-[(2,5-dichlorophenyl)azo]-3-hydroxy-N-phenylnaphthalene-2-carboxamide**	3_REACH		4-[(2,5-dichlorophenyl)azo]-3-hydroxy-N-phenylnaphthalene-2-carboxamide		C23H14Cl2N3O2	436.3	[O-]c1c(cc2ccccc2c1N=Nc3cc(Cl)ccc3Cl)C(=O)Nc4ccccc4	InChI=1/C23H15Cl2N3O2/c24-15-10-11-19(25)20(13-15)27-28-21-17-9-5-4-6-14(17)12-18(22(21)29)23(30)26-16-7-2-1-3-8-16/h1-13,29H,(H,26,30)/p-1	6.276	6.979	1	1	1
60658-04-0	60658040	4438	**Ethyl 2-(3-benzoylphenyl)propanoate**	3_REACH		K002			282.34	CCOC(=O)C(C)C1=CC=CC(=C1)C(=O)C2=CC=CC=C2	InChI=1S/C18H18O3/c1-3-21-18(20)13(2)15-10-7-11-16(12-15)17(19)14-8-5-4-6-9-14/h4-13H,3H2,1-2H3			1	1	1
608-25-3	608253	3317	**2-methylresorcinol**	3_REACH	1,3-Benzenediol, 2-methyl-	2-methylresorcinol	C7H8O2	C7H8O2	124.14	Cc1c(O)cccc1O	InChI=1/C7H8O2/c1-5-6(8)3-2-4-7(5)9/h2-4,8-9H,1H3	1.832	1.83	1	1	1
611-06-3	611063	755	**1,3-dichloro-4-nitrobenzene**	3_REACH	Benzene, 2,4-dichloro-1-nitro-	2,4-Dichloro-1-nitrobenzene	C6H3Cl2NO2	C6H3Cl2NO2	192	[O-][N+](=O)c1ccc(Cl)cc1Cl	InChI=1/C6H3Cl2NO2/c7-4-1-2-6(9(10)11)5(8)3-4/h1-3H	3.053	3.053	1	1	1
611-19-8	611198	3326	**2-Chlorobenzyl chloride**	3_REACH	Benzene, 1-chloro-2-(chloromethyl	a,2-dichlorotoluene	C7H6Cl2	C7H6Cl2	161.03	ClCc1ccccc1Cl	InChI=1/C7H6Cl2/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2	3.094	3.094	1	1	1
611-70-1	611701	3328	**isobutyrophenone**	3_REACH	Isopropyl phenyl ketone	isobutyrophenone	C10H12O	C10H12O	148.21	CC(C)C(=O)c1ccccc1	InChI=1/C10H12O/c1-8(2)10(11)9-6-4-3-5-7-9/h3-8H,1-2H3	2.699	2.699	1	1	1
61260-55-7	61260557	3330	**N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine**	3_REACH		N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine		C24H54N4	394.7	CC1(C)CC(CC(C)(C)[NH2+]1)[NH2+]CCCCCC[NH2+]C2CC(C)(C)[NH2+]C(C)(C)C2	InChI=1/C24H50N4/c1-21(2)15-19(16-22(3,4)27-21)25-13-11-9-10-12-14-26-20-17-23(5,6)28-24(7,8)18-20/h19-20,25-28H,9-18H2,1-8H3/p+4	-2.502	0.074	1	1	1
613-62-7	613627	4310	**2-(phenylmethoxy)naphthalene**	3_REACH	Naphthalene, 2-(phenylmethoxy)-	2-(phenylmethoxy)naphthalene	C17H14O		234.3	C1=CC=C(C=C1)COC2=CC3=CC=CC=C3C=C2	InChI=1S/C17H14O/c1-2-6-14(7-3-1)13-18-17-11-10-15-8-4-5-9-16(15)12-17/h1-12H,13H2			1	1	1
614-45-9	614459	3334	**tert-butyl perbenzoate**	3_REACH	tert-Butyl peroxybenzoate	tert-butyl perbenzoate	C11H14O3	C11H14O3	194.23	CC(C)(C)OOC(=O)c1ccccc1	InChI=1/C11H14O3/c1-11(2,3)14-13-10(12)9-7-5-4-6-8-9/h4-8H,1-3H3	2.276	2.276	1	1	1
615-20-3	615203	3338	**2-chlorobenzothiazole**	3_REACH	Benzothiazole, 2-chloro-	2-chlorobenzothiazole	C7H4ClNS	C7H4ClNS	169.63	Clc1nc2ccccc2s1	InChI=1/C7H4ClNS/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H	2.79	2.789	1	1	1
615-60-1	615601	3339	**4-chloro-o-xylene**	3_REACH	Benzene, 4-chloro-1,2-dimethyl-	4-chloro-o-xylene	C8H9Cl	C8H9Cl	140.61	Cc1ccc(Cl)cc1C	InChI=1/C8H9Cl/c1-6-3-4-8(9)5-7(6)2/h3-5H,1-2H3	3.466	3.466	1	1	1
61597-98-6	61597986	3340	**L-Menthyl lactate**	3_REACH		Propanoic acid, 2-hydroxy-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester, (2S)			228.33	CC1CCC(C(C1)OC(=O)C(C)O)C(C)C	InChI=1S/C13H24O3/c1-8(2)11-6-5-9(3)7-12(11)16-13(15)10(4)14/h8-12,14H,5-7H2,1-4H3/t9-,10+,11+,12-/m1/s1			1	1	1
616-45-5	616455	757	**2-pyrrolidone**	3_REACH	2-Pyrrolidinone	2-Pyrrolidinone	C4H7NO	C4H7NO	85.107	O=C1CCCN1	InChI=1/C4H7NO/c6-4-2-1-3-5-4/h1-3H2,(H,5,6)	-0.371	-0.371	1	1	1
616-47-7	616477	3346	**1-methylimidazole**	3_REACH	1H-Imidazole, 1-methyl-	1-methylimidazole	C4H6N2	C4H6N2	82.108	Cn1ccnc1	InChI=1/C4H6N2/c1-6-3-2-5-4-6/h2-4H,1H3	-0.077	0.559	1	1	1
6166-86-5	6166865	3347	**2,4,6,8,10-pentamethylcyclopentasiloxane**	3_REACH	2,4,6,8,10-Pentamethylcyclopentasiloxane	2,4,6,8,10-pentamethylcyclopentasiloxane	C5H20O5Si5	C5H20O5Si5	295.6	C[SiH]1O[SiH](C)O[SiH](C)O[SiH](C)O[SiH](C)O1	InChI=1/C5H20O5Si5/c1-11-6-12(2)8-14(4)10-15(5)9-13(3)7-11/h11-15H,1-5H3	10.695	10.695	1	1	1
61826-76-4	61826764	4625	**(S)-2-Hydroxy-2-(3-phenoxyphenyl)acetonitrile**	3_REACH		SCMB			225.25	C1=CC=C(C=C1)OC2=CC=CC(=C2)C(C#N)O	InChI=1S/C14H11NO2/c15-10-14(16)11-5-4-8-13(9-11)17-12-6-2-1-3-7-12/h1-9,14,16H/t14-/m1/s1			1	1	1
61847-48-1	61847481	3356	**methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-[[2-hydroxy-3-[[(2-methoxyphenyl)amino]carbonyl]-1-naphthyl]azo]benzoate**	3_REACH		methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-[[2-hydroxy-3-[[(2-methoxyphenyl)amino]carbonyl]-1-naphthyl]azo]benzoate		C33H23Cl2N4O6	643.49	COC(=O)c1ccc(cc1N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4ccccc4OC)C(=O)Nc5cc(Cl)ccc5Cl	InChI=1/C33H24Cl2N4O6/c1-44-28-10-6-5-9-25(28)36-32(42)23-15-18-7-3-4-8-21(18)29(30(23)40) 38-26-16-19(11-13-22(26)33(43)45-2)31(41)37-27-17-20(34)12-14-24(27)35/h3-17,40H,1-2H3,(H,36,42)(H,37,41)/p-1	6.899	7.602	1	1	1
618-62-2	618622	759	**3,5-dichloronitrobenzene**	3_REACH	3,5-Dichloronitrobenzene	1,3-Dichloro-5-nitrobenzene	C6H3Cl2NO2	C6H3Cl2NO2	192	[O-][N+](=O)c1cc(Cl)cc(Cl)c1	InChI=1/C6H3Cl2NO2/c7-4-1-5(8)3-6(2-4)9(10)11/h1-3H	3.053	3.053	1	1	1
618-88-2	618882	3358	**5-nitroisophthalic acid**	3_REACH		5-nitroisophthalic acid		C8H3NO6	211.13	[O-]C(=O)c1cc(cc(c1)[N+](=O)[O-])C(=O)[O-]	InChI=1/C8H5NO6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)(H,12,13)/p-2	-1.964	-1.961	1	1	1
6197-30-4	6197304	3360	**octocrilene**	3_REACH		octocrilene		C24H27NO2	361.49	CCCCC(CC)COC(=O)C(=C(c1ccccc1)c2ccccc2)C#N	InChI=1/C24H27NO2/c1-3-5-12-19(4-2)18-27-24(26)22(17-25)23(20-13-8-6-9-14-20)21-15-10-7-11-16-21/h6-11,13-16,19H,3-5,12,18H2,1-2H3	6.487	6.487	1	1	1
621-29-4	621294	3362	**m-tolyl isocyanate**	3_REACH	Benzene, 1-isocyanato-3-methyl-	m-tolyl isocyanate	C8H7NO	C8H7NO	133.15	Cc1cccc(c1)N=C=O	InChI=1/C8H7NO/c1-7-3-2-4-8(5-7)9-6-10/h2-5H,1H3	2.176	2.176	1	1	1
62-23-7	62237	761	**4-nitrobenzoic acid**	3_REACH	Benzoic acid, 4-nitro-	4-Nitrobenzoic acid	C7H5NO4	C7H4NO4	167.12	[O-]C(=O)c1ccc(cc1)[N+](=O)[O-]	InChI=1/C7H5NO4/c9-7(10)5-1-3-6(4-2-5)8(11)12/h1-4H,(H,9,10)/p-1	-0.12	-0.119	1	1	1
622-40-2	622402	762	**2-morpholinoethanol**	3_REACH	4-Morpholineethanol	Hydroxyethylmorpholine	C6H13NO2	C6H13NO2	131.18	OCCN1CCOCC1	InChI=1/C6H13NO2/c8-4-1-7-2-5-9-6-3-7/h8H,1-6H2	-0.532	-0.688	1	1	1
622-58-2	622582	3365	**p-tolyl isocyanate**	3_REACH	Benzene, 1-isocyanato-4-methyl-	p-tolyl isocyanate	C8H7NO	C8H7NO	133.15	Cc1ccc(cc1)N=C=O	InChI=1/C8H7NO/c1-7-2-4-8(5-3-7)9-6-10/h2-5H,1H3	2.176	2.176	1	1	1
623-03-0	623030	763	**4-chlorobenzonitrile**	3_REACH	4-Chlorobenzoic acid nitrile	4-Chlorobenzonitrile	C7H4ClN	C7H4ClN	137.57	Clc1ccc(cc1)C#N	InChI=1/C7H4ClN/c8-7-3-1-6(5-9)2-4-7/h1-4H	2.373	2.373	1	1	1
623-40-5	623405	4785	**2-Pentanone oxime**	3_REACH	2-Pentanone oxime	2-Pentanone oxime		C5H11NO	101.15	CCCC(=NO)C	InChI=1S/C5H11NO/c1-3-4-5(2)6-7/h7H,3-4H2,1-2H3/b6-5-			1	1	1
624-54-4	624544	3370	**pentyl propionate**	3_REACH	Amyl propionate	pentyl propionate	C8H16O2	C8H16O2	144.21	CCCCCOC(=O)CC	InChI=1/C8H16O2/c1-3-5-6-7-10-8(9)4-2/h3-7H2,1-2H3	2.472	2.472	1	1	1
62-53-3	62533	765	**aniline**	3_REACH	Aniline	Aniline	C6H7N	C6H7N	93.13	Nc1ccccc1	InChI=1/C6H7N/c7-6-4-2-1-3-5-6/h1-5H,7H2	1.083	1.083	1	1	1
62-56-6	62566	767	**thiourea**	3_REACH	Thiourea	Thiourea	CH4N2S	CH4N2S	76.123	NC(=S)N	InChI=1/CH4N2S/c2-1(3)4/h(H4,2,3,4)	-0.206	-0.206	1	1	1
6259-76-3	6259763	3375	**hexyl salicylate**	3_REACH	n-Hexyl salicylate	hexyl salicylate	C13H18O3	C13H18O3	222.28	CCCCCCOC(=O)c1ccccc1O	InChI=1/C13H18O3/c1-2-3-4-7-10-16-13(15)11-8-5-6-9-12(11)14/h5-6,8-9,14H,2-4,7,10H2,1H3	3.684	3.612	1	1	1
626-43-7	626437	768	**3,5-dichloroaniline**	3_REACH	Benzenamine, 3,5-dichloro-	3,5-Dichloroaniline	C6H5Cl2N	C6H5Cl2N	162.02	Nc1cc(Cl)cc(Cl)c1	InChI=1/C6H5Cl2N/c7-4-1-5(8)3-6(9)2-4/h1-3H,9H2	2.412	2.412	1	1	1
6284-40-8	6284408	770	**meglumine**	3_REACH	N-methylglucamine	1-Deoxy-1-(methylamino)-D-glucitol	C7H17NO5	C7H18NO5	195.22	C[NH2+]C[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	InChI=1/C7H17NO5/c1-8-2-4(10)6(12)7(13)5(11)3-9/h4-13H,2-3H2,1H3/p+1/t4-,5+,6+,7+/m0/s1	-4.029	-3.971	1	1	1
62889-66-1	62889661	3379	**613-099-6**	3_REACH		2-Propanol, 1,1'-(tridecylimino)bis-			315.54	CCCCCCCCCCCCCN(CC(C)O)CC(C)O	InChI=1S/C19H41NO2/c1-4-5-6-7-8-9-10-11-12-13-14-15-20(16-18(2)21)17-19(3)22/h18-19,21-22H,4-17H2,1-3H3			1	1	1
628-89-7	628897	3380	**2-(2-chloroethoxy)ethanol**	3_REACH	Ethanol, 2-(2-chloroethoxy)-	2-(2-chloroethoxy)ethanol	C4H9ClO2	C4H9ClO2	124.57	OCCOCCCl	InChI=1/C4H9ClO2/c5-1-3-7-4-2-6/h6H,1-4H2	0.176	0.176	1	1	1
628-96-6	628966	3382	**ethylene dinitrate**	3_REACH	1,2-Ethanediol, dinitrate	ethylene dinitrate	C2H4N2O6	C2H4N2O6	152.06	[O-][N+](=O)OCCO[N+](=O)[O-]	InChI=1/C2H4N2O6/c5-3(6)9-1-2-10-4(7)8/h1-2H2	3.923	3.923	1	1	1
629-11-8	629118	3385	**hexane-1,6-diol**	3_REACH	1,6-Hexanediol	hexane-1,6-diol	C6H14O2	C6H14O2	118.18	OCCCCCCO	InChI=1/C6H14O2/c7-5-3-1-2-4-6-8/h7-8H,1-6H2	0.657	0.657	1	1	1
6291-95-8	6291958	4276	**1,3,5-tris(2-methyl-2-propenyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione**	3_REACH		1,3,5-tris(2-methyl-2-propenyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione			291.35	CC(=C)CN1C(=O)N(C(=O)N(C1=O)CC(=C)C)CC(=C)C	InChI=1S/C15H21N3O3/c1-10(2)7-16-13(19)17(8-11(3)4)15(21)18(14(16)20)9-12(5)6/h1,3,5,7-9H2,2,4,6H3			1	1	1
629-40-3	629403	771	**suberonitrile**	3_REACH	Octanedinitrile	Octanedinitrile	C8H12N2	C8H12N2	136.2	N#CCCCCCCC#N	InChI=1/C8H12N2/c9-7-5-3-1-2-4-6-8-10/h1-6H2	1.963	1.963	1	1	1
629-50-5	629505	3389	**tridecane**	3_REACH	Tridecane	tridecane	C13H28	C13H28	184.37	CCCCCCCCCCCCC	InChI=1/C13H28/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-13H2,1-2H3	6.302	6.302	1	1	1
629-59-4	629594	3390	**tetradecane**	3_REACH	Tetradecane	tetradecane	C14H30	C14H30	198.39	CCCCCCCCCCCCCC	InChI=1/C14H30/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-14H2,1-2H3	6.758	6.758	1	1	1

629-62-9	629629	772	**pentadecane**	3_REACH	Pentadecane	Pentadecane	C15H32	C15H32	212.42	CCCCCCCCCCCCCCC	InChI=1/C15H32/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h3-15H2,1-2H3	7.214	7.214	1	1	1
629-73-2	629732	3391	**hexadec-1-ene**	3_REACH	1-Hexadecene	hexadec-1-ene	C16H32	C16H32	224.43	CCCCCCCCCCCCCCC=C	InChI=1/C16H32/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3H,1,4-16H2,2H3	7.28	7.28	1	1	1
629-82-3	629823	3392	**dioctyl ether**	3_REACH	Octane, 1,1'-oxybis-	dioctyl ether	C16H34O	C16H34O	242.45	CCCCCCCCOCCCCCCCC	InChI=1/C16H34O/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3-16H2,1-2H3	6.357	6.357	1	1	1
63-05-8	63058	75	**androst-4-ene-3,17-dione**	3_REACH	Androst-4-ene-3,17-dione	Androst-4-ene-3,17-dione	C19H26O2	C19H26O2	286.42	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CCC2=O	InChI=1/C19H26O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)18/h11,14-16H,3-10H2,1-2H3/t14-,15-,16-,18-,19-/m0/s1	3.573	3.573	1	1	1
6309-51-9	6309519	3394	**isopentyl laurate**	3_REACH	Isoamyl laurate	isopentyl laurate	C17H34O2	C17H34O2	270.46	CCCCCCCCCCCC(=O)OCCC(C)C	InChI=1/C17H34O2/c1-4-5-6-7-8-9-10-11-12-13-17(18)19-15-14-16(2)3/h16H,4-15H2,1-3H3	6.374	6.374	1	1	1
6331-96-0	6331960	3399	**2-amino-4,5-dichlorobenzenesulfonic acid**	3_REACH		2-amino-4,5-dichlorobenzenesulfonic acid			242.08	C1=C(C(=CC(=C1Cl)Cl)S(=O)(=O)O)N	InChI=1S/C6H5Cl2NO3S/c7-3-1-5(9)6(2-4(3)8)13(10,11)12/h1-2H,9H2,(H,10,11,12)			1	1	1
63562-34-5	63562345	3405	**bis(2-hydroxyethyl) (6H-dibenz[c,e][1,2]oxaphosphorin-6-ylmethyl)succinate P-oxide**	3_REACH		bis(2-hydroxyethyl) (6H-dibenz[c,e][1,2]oxaphosphorin-6-ylmethyl)succinate P-oxide		C21H23O8P	434.38	OCCOC(=O)CC(CP1(=O)Oc2ccccc2c3ccccc13)C(=O)OCCO	InChI=1/C21H23O8P/c22-9-11-27-20(24)13-15(21(25)28-12-10-23)14-30(26)19-8-4-2-6-17(19)16-5-3-7-18(16)29-30/h1-8,15,22-23H,9-14H2	1.42	1.42	1	1	1
6358-30-1	6358301	3406	**8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3',2'-m]triphenodioxazine**	3_REACH		8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3',2'-m]triphenodioxazine		C34H24Cl2N4O2	589.49	CC[NH+]1c2ccccc2c3cc4N=C5C(=C6Oc7cc8[NH+](CC)c9ccccc9c8cc7N=C6C(=C5Oc4cc13)Cl)Cl	InChI=1/C34H22Cl2N4O2/c1-3-39-23-11-7-5-9-17(23)19-13-21-27(15-25(19)39)41-33-29(35)32-34(30(36)31(33)37-21)42-28-16-26-20(14-22(28)38-32)18-10-6-8-12-24(18)40(26)4-2/h5-16H,3-4H2,1-2H3/p+2	4.208	4.805	1	1	1
6358-37-8	6358378	3408	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-methylphenyl)-3-oxobutyramide]**	3_REACH		2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-methylphenyl)-3-oxobutyramide]		C34H30Cl2N6O4	657.56	CC(=O)C(N=Nc1ccc(cc1Cl)c2ccc(N=NC(C(=O)C)C(=O)Nc3ccc(C)cc3)c(Cl)c2)C(=O)Nc4ccc(C)cc4	InChI=1/C34H30Cl2N6O4/c1-19-5-11-25(12-6-19)37-33(45)31(21(3)43)41-39-29-15-9-23(17-27(29)35)24-10-16-30(28(36)18-24)40-42-32(22(4)44)34(46)38-26-13-7-20(2)8-14-26/h5-18,31-32H,1-4H3,(H,37,45)(H,38,46)	8.369	8.369	1	1	1
6358-64-1	6358641	3409	**4-chloro-2,5-dimethoxyaniline**	3_REACH	Aniline, 4-chloro-2,5-dimethoxy-	4-chloro-2,5-dimethoxyaniline	C8H10ClNO2	C8H10ClNO2	187.63	COc1cc(Cl)c(OC)cc1N	InChI=1/C8H10ClNO2/c1-11-7-4-6(10)8(12-2)3-5(7)9/h3-4H,10H2,1-2H3	1.714	1.714	1	1	1
6358-85-6	6358856	3410	**2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]**	3_REACH		2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]		C32H26Cl2N6O4	629.51	CC(=O)C(N=Nc1ccc(cc1Cl)c2ccc(N=NC(C(=O)C)C(=O)Nc3ccccc3)c(Cl)c2)C(=O)Nc4ccccc4	InChI=1/C32H26Cl2N6O4/c1-19(41)29(31(43)35-23-9-5-3-6-10-23)39-37-27-15-13-21(17-25(27)33)22-14-16-28(26(34)18-22)38-40-30(20(2)42)32(44)36-24-11-7-4-8-12-24/h3-18,29-30H,1-2H3,(H,35,43)(H,36,44)	7.397	7.397	1	1	1
636-30-6	636306	774	**2,4,5-trichloroaniline**	3_REACH	Benzenamine, 2,4,5-trichloro-	2,4,5-Trichlorobenzenamine	C6H4Cl3N	C6H4Cl3N	196.47	Nc1cc(Cl)c(Cl)cc1Cl	InChI=1/C6H4Cl3N/c7-3-1-5(9)6(10)2-4(3)8/h1-2H,10H2	3.076	3.076	1	1	1
6386-38-5	6386385	3420	**methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate**	3_REACH		methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate		C18H28O3	292.42	COC(=O)CCc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C	InChI=1/C18H28O3/c1-17(2,3)13-10-12(8-9-15(19)21-7)11-14(16(13)20)18(4,5)6/h10-11,20H,8-9H2,1-7H3	4.735	4.735	1	1	1
6410-32-8	6410328	3424	**3-hydroxy-4-[(2-methyl-4-nitrophenyl)azo]-N-(o-tolyl)naphthalene-2-carboxamide**	3_REACH		3-hydroxy-4-[(2-methyl-4-nitrophenyl)azo]-N-(o-tolyl)naphthalene-2-carboxamide		C25H19N4O4	440.46	Cc1ccccc1NC(=O)c2cc3ccccc3c(N=Nc4ccc(cc4C)[N+](=O)[O-])c2[O-]	InChI=1/C25H20N4O4/c1-15-7-3-6-10-21(15)26-25(31)20-14-17-8-4-5-9-19(17)23(24(20)30)28-27-22-12-11-18(29(32)33)13-16(22)2/h3-14,30H,1-2H3,(H,26,31)/p-1	5.814	6.517	1	1	1
6410-41-9	6410419	3425	**N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulphonyl]-2-methoxyphenyl]azo]-3-hydroxynaphthalene-2-carboxamide**	3_REACH		N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulphonyl]-2-methoxyphenyl]azo]-3-hydroxynaphthalene-2-carboxamide		C30H30ClN4O7S	627.12	CCN(CC)S(=O)(=O)c1ccc(OC)c(c1)N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4cc(Cl)c(OC)cc4OC	InChI=1/C30H31ClN4O7S/c1-6-35(7-2)43(38,39)19-12-13-25(40-3)24(15-19)33-34-28-20-11-9-8-10-18(20)14-21(29(28)36)30(37)32-23-16-22(31)26(41-4)17-27(23)42-5/h8-17,36H,6-7H2,1-5H3,(H,32,37)/p-1	5.377	6.08	1	1	1
6419-19-8	6419198	3429	**nitrilotrimethylenetris(phosphonic acid)**	3_REACH		nitrilotrimethylenetris(phosphonic acid)		C3H10NO9P3	299.05	OP(=O)([O-])C[NH+](CP(=O)(O)[O-])CP(=O)(O)[O-]	InChI=1/C3H12NO9P3/c5-14(6,7)1-4(2-15(8,9)10)3-16(11,12)13/h1-3H2,(H2,5,6,7)(H2,8,9,10)(H2,11,12,13)/p-2	-8.009	-8.859	1	1	1
6422-86-2	6422862	3430	**bis(2-ethylhexyl) terephthalate**	3_REACH		bis(2-ethylhexyl) terephthalate		C24H38O4	390.56	CCCCC(CC)COC(=O)c1ccc(cc1)C(=O)OCC(CC)CCCC	InChI=1/C24H38O4/c1-5-9-11-19(7-3)17-27-23(25)21-13-15-22(16-14-21)24(26)28-18-20(8-4)12-10-6-2/h13-16,19-20H,5-12,17-18H2,1-4H3	7.574	7.574	1	1	1
6425-39-4	6425394	3432	**2,2'-dimorpholinyldiethyl ether**	3_REACH		2,2'-dimorpholinyldiethyl ether		C12H24N2O3	244.34	C(CN1CCOCC1)OCCN2CCOCC2	InChI=1/C12H24N2O3/c1-7-15-8-2-13(1)5-11-17-12-6-14-3-9-16-10-4-14/h1-12H2	-0.297	-0.416	1	1	1
64354-92-3	64354923	3434	**3-(isodecyloxy)propiononitrile**	3_REACH		3-(isodecyloxy)propiononitrile		C13H25NO	211.35	CC(C)CCCCCCCOCCC#N	InChI=1/C13H25NO/c1-13(2)9-6-4-3-5-7-11-15-12-8-10-14/h13H,3-9,11-12H2,1-2H3	3.89	3.89	1	1	1
6440-58-0	6440580	779	**1,3-bis(hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione**	3_REACH		1,3-bis(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione		C7H12N2O4	188.19	CC1(C)N(CO)C(=O)N(CO)C1=O	InChI=1/C7H12N2O4/c1-7(2)5(12)8(3-10)6(13)9(7)4-11/h10-11H,3-4H2,1-2H3	-1.067	-1.067	0	1	1
6448-95-9	6448959	3436	**3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthalene-2-carboxamide**	3_REACH		3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthalene-2-carboxamide		C24H17N4O4	426.44	Cc1ccc(cc1N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4ccccc4)[N+](=O)[O-]	InChI=1/C24H18N4O4/c1-15-11-12-18(28(31)32)14-21(15)26-27-22-19-10-6-5-7-16(19)13-20(23(22)29)24(30)25-17-8-3-2-4-9-17/h2-14,29H,1H3,(H,25,30)/p-1	5.327	6.031	1	1	1
645-62-5	645625	3438	**2-ethylhex-2-enal**	3_REACH	2-Hexenal, 2-ethyl-	2-ethylhex-2-enal	C8H14O	C8H14O	126.2	CCCC=C(CC)C=O	InChI=1/C8H14O/c1-3-5-6-8(4-2)7-9/h6-7H,3-5H2,1-2H3	2.732	2.732	1	1	1
646-24-2	646242	3439	**nonamethylenediamine**	3_REACH	1,9-Diaminononane	nonamethylenediamine	C9H22N2	C9H24N2	158.29	[NH3+]CCCCCCCCC[NH3+]	InChI=1/C9H22N2/c10-8-6-4-2-1-3-5-7-9-11/h1-11H2/p+2	-0.563	-0.557	1	1	1
6485-40-1	6485401	781	**l-p-mentha-1(6),8-dien-2-one**	3_REACH	Carvone	(5R)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	C10H14O	C10H14O	150.22	CC(=C)C1CC=C(C)C(=O)C1	InChI=1/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3	2.501	2.501	1	1	1
6485-55-8	6485558	3445	**cis-2,6-dimethylmorpholine**	3_REACH		cis-2,6-dimethylmorpholine		C6H14NO	115.18	C[C@@H]1C[NH2+]C[C@H](C)O1	InChI=1/C6H13NO/c1-5-3-7-4-6(2)8-5/h5-7H,3-4H2,1-2H3/p+1/t5-,6+	-1.004	-0.977	1	1	1
6485-67-2	6485672	4453	**(2R)-2-amino-2-phenylacetamide**	3_REACH		D-PHENYLGLYCINE-AMIDE			150.18	C1=CC=C(C=C1)C(C(=O)N)N	InChI=1S/C8H10N2O/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H,9H2,(H2,10,11)/t7-/m1/s1			1	1	1
6486-23-3	6486233	3446	**2-[(4-chloro-2-nitrophenyl)azo]-N-(2-chlorophenyl)-3-oxobutyramide**	3_REACH		2-[(4-chloro-2-nitrophenyl)azo]-N-(2-chlorophenyl)-3-oxobutyramide		C16H12Cl2N4O4	395.21	CC(=O)C(N=Nc1ccc(Cl)cc1[N+](=O)[O-])C(=O)Nc2ccccc2Cl	InChI=1/C16H12Cl2N4O4/c1-9(23)15(16(24)19-12-5-3-2-4-11(12)18)21-20-13-7-6-10(17)8-14(13)22(25)26/h2-8,15H,1H3,(H,19,24)	4.413	4.413	1	1	1
6528-34-3	6528343	3450	**2-[(4-methoxy-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide**	3_REACH		2-[(4-methoxy-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide		C18H18N4O6	386.37	COc1ccc(N=NC(C(=O)C)C(=O)Nc2ccccc2OC)c(c1)[N+](=O)[O-]	InChI=1/C18H18N4O6/c1-11(23)17(18(24)19-14-6-4-5-7-16(14)28-3)21-20-13-9-8-12(27-2)10-15(13)22(25)26/h4-10,17H,1-3H3,(H,19,24)	3.051	3.051	1	1	1
65405-77-8	65405778	3452	**(Z)-3-hexenyl salicylate**	3_REACH	cis-3-Hexenyl salicylate	(Z)-3-hexenyl salicylate	C13H16O3	C13H16O3	220.27	CC\C=C/CCOC(=O)c1ccccc1O	InChI=1/C13H16O3/c1-2-3-4-7-10-16-13(15)11-8-5-6-9-12(11)14/h3-6,8-9,14H,2,7,10H2,1H3/b4-3-	3.239	3.168	1	1	1
65-45-2	65452	784	**salicylamide**	3_REACH	Benzamide, 2-hydroxy-	2-Hydroxybenzamide	C7H7NO2	C7H7NO2	137.14	NC(=O)c1ccccc1O	InChI=1/C7H7NO2/c8-7(10)5-3-1-2-4-6(5)9/h1-4,9H,(H2,8,10)	0.59	0.555	1	1	1
65520-46-9	65520469	3455	**bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] adipate**	3_REACH		bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] adipate		C26H50O10	522.68	CCCCOCCOCCOCCOC(=O)CCCCC(=O)OCCOCCOCCOCCCC	InChI=1/C26H50O10/c1-3-5-11-29-13-15-31-17-19-33-21-23-35-25(27)9-7-8-10-26(28)36-24-22-34-20-18-32-16-14-30-12-6-4-2/h3-24H2,1-2H3	2.876	2.876	1	1	1
65-85-0	65850	785	**benzoic acid**	3_REACH	Benzoic acid	Benzoic acid	C7H6O2	C7H5O2	122.12	[O-]C(=O)c1ccccc1	InChI=1/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)/p-1	-0.015	-0.013	1	1	1
65855-02-9	65855029	4291	**1-benzyl-5-ethoxyimidazolidine-2,4-dione**	3_REACH		1-benzyl-5-ethoxyimidazolidine-2,4-dione			234.26	CCOC1C(=O)NC(=O)N1CC2=CC=CC=C2	InChI=1S/C12H14N2O3/c1-2-17-11-10(15)13-12(16)14(11)8-9-6-4-3-5-7-9/h3-7,11H,2,8H2,1H3,(H,13,15,16)			1	1	1
6600-31-3	6600313	3458	**3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane**	3_REACH		3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane		C19H28O4	320.43	C1CC(CC=C1)C2OCC3(COC(OC3)C4CCC=CC4)CO2	InChI=1/C19H28O4/c1-3-7-15(8-4-1)17-20-11-19(12-21-17)13-22-18(23-14-19)16-9-5-2-6-10-16/h1-3,5,15-18H,4,6-14H2	2.735	2.735	1	1	1
66063-15-8	66063158	3459	**4-chloro-N-cyclopentylbenzylamine**	3_REACH		4-chloro-N-cyclopentylbenzylamine		C12H17ClN	209.72	Clc1ccc(C[NH2+]C2CCCC2)cc1	InChI=1/C12H16ClN/c13-11-7-5-10(6-8-11)9-14-12-3-1-2-4-12/h5-8,12,14H,1-4,9H2/p+1	2.203	2.243	1	1	1
66068-84-6	66068846	3460	**4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol**	3_REACH		4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol		C16H28O	236.4	CC1C2CC(CC2C3CCC(O)CC3)C1(C)C	InChI=1/C16H28O/c1-10-14-8-12(16(10,2)3)9-15(14)11-4-6-13(17)7-5-11/h10-15,17H,4-9H2,1-3H3	3.842	3.842	1	1	1
6610-29-3	6610293	3462	**4-methylthiosemicarbazide**	3_REACH		4-methylthiosemicarbazide		C2H7N3S	105.17	CNC(=S)NN	InChI=1/C2H7N3S/c1-4-2(6)5-3/h3H2,1H3,(H2,4,5,6)	-0.112	-0.112	1	1	1
66423-13-0	66423130	3473	**octyl (R)-2-(4-chloro-2-methylphenoxy)propionate**	3_REACH		octyl (R)-2-(4-chloro-2-methylphenoxy)propionate		C18H27ClO3	326.86	CCCCCCCCOC(=O)[C@@H](C)Oc1ccc(Cl)cc1C	InChI=1/C18H27ClO3/c1-4-5-6-7-8-9-12-21-18(20)15(3)22-17-11-10-16(19)13-14(17)2/h10-11,13,15H,4-9,12H2,1-3H3/t15-/m1/s1	6.309	6.309	1	1	1
66492-51-1	66492511	3475	**(5-ethyl-1,3-dioxan-5-yl)methyl acrylate**	3_REACH		(5-ethyl-1,3-dioxan-5-yl)methyl acrylate		C10H16O4	200.23	CCC1(COC(=O)C=C)COCOC1	InChI=1/C10H16O4/c1-3-9(11)14-7-10(4-2)5-12-8-13-6-10/h3H,1,4-8H2,2H3	1.076	1.076	1	1	1
6674-22-2	6674222	3481	**1,8-diazabicyclo[5.4.0]undec-7-ene**	3_REACH	1,8-diazabicyclo [5.4.0]undec-7-ene	1,8-diazabicyclo[5.4.0]undec-7-ene	C9H16N2	C9H17N2	152.24	C1CCN2CCC[NH+]=C2CC1	InChI=1/C9H16N2/c1-2-5-9-10-6-4-8-11(9)7-3-1/h1-8H2/p+1	0.785	0.786	1	1	1
67075-37-0	67075370	3484	**2,9-bis(2-phenylethyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone**	3_REACH		2,9-bis(2-phenylethyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone		C40H26N2O4	598.66	O=C1N(CCc2ccccc2)C(=O)c3ccc4c5ccc6C(=O)N(CCc7ccccc7)C(=O)c8ccc(c9ccc1c3c49)c5c68	InChI=1/C40H26N2O4/c43-37-29-15-11-25-27-13-17-31-36-32(40(46)42(39(31)45)22-20-24-9-5-2-6-10-24)18-14-28(34(27)36)26-12-16-30(35(29)33(25)26)38(44)41(37)21-19-23-7-3-1-4-8-23/h1-18H,19-22H2	6.727	6.727	1	1	1
6711-48-4	6711484	3485	**N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamine**	3_REACH	1,3-Propanediamine, N'-[3-(dimethylamino)propyl]-N,N-dimethyl-	N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamine	C10H25N3	C10H26N3	187.33	CN(C)CCC[NH2+]CCCN(C)C	InChI=1/C10H25N3/c1-12(2)9-5-7-11-8-6-10-13(3)4/h11H,5-10H2,1-4H3/p+1	-1.045	-1.132	1	1	1
6712-98-7	6712987	3486	**1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol**	3_REACH	2-Propanol, 1-[bis(2-hydroxyethyl)amino]-	1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol	C7H17NO3	C7H18NO3	163.22	CC(O)C[NH+](CCO)CCO	InChI=1/C7H17NO3/c1-7(11)6-8(2-4-9)3-5-10/h7,9-11H,2-6H2,1H3/p+1	-2.482	-1.615	1	1	1
67151-63-7	67151637	3487	**1-[bis[3-(dimethylamino)propyl]amino]propan-2-ol**	3_REACH		1-[bis[3-(dimethylamino)propyl]amino]propan-2-ol		C13H33N3O	245.41	CC(O)CN(CCC[NH+](C)C)CCC[NH+](C)C	InChI=1/C13H31N3O/c1-13(17)12-16(10-6-8-14(2)3)11-7-9-15(4)5/h13,17H,6-12H2,1-5H3/p+2	-2.561	-2.568	1	1	1
6731-36-8	6731368	3488	**di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide**	3_REACH		di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide		C17H34O4	302.45	CC1CC(C)(C)CC(C1)(OOC(C)(C)C)OOC(C)(C)C	InChI=1/C17H34O4/c1-13-10-16(8,9)12-17(11-13,20-18-14(2,3)4)21-19-15(5,6)7/h13H,10-12H2,1-9H3	3.673	3.673	1	1	1
67-43-6	67436	82	**N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)**	3_REACH	N,N-Bis(2-(bis-(carboxymethyl)amino)ethyl)-glycine	N,N-bis[2-[bisCarboxymethyl)amino]ethyl]-glycine	C14H23N3O10	C14H20N3O10	393.35	[O-]C(=O)CN(CC[NH+](CC(=O)[O-])CC(=O)[O-])CC[NH+](CC(=O)[O-])CC(=O)[O-]	InChI=1/C14H23N3O10/c18-10(19)5-15(1-3-16(6-11(20)21)7-12(22)23)2-4-17(8-13(24)25)9-14(26)27/h1-9H2,(H,18,19)(H,20,21)(H,22,23)(H,24,25)(H,26,27)/p-3	-12.487	-10.798	1	1	1
674-82-8	674828	3493	**but-3-en-3-olide**	3_REACH	2-Oxetanone, 4-methylene-	but-3-en-3-olide	C4H4O2	C4H4O2	84.074	C=C1CC(=O)O1	InChI=1/C4H4O2/c1-3-2-4(5)6-3/h1-2H2	0.204	0.204	1	1	1
67801-15-4	67801154	3500	**3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one**	3_REACH		3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one		C14H22O	206.33	CC(C=CC1CC=C(C)C1(C)C)C(=O)C	InChI=1/C14H22O/c1-10(12(3)15)6-8-13-9-7-11(2)14(13,4)5/h6-8,10,13H,9H2,1-5H3	3.201	3.201	1	1	1
6786-83-0	6786830	3502	**alpha,alpha-Bis[4-(dimethylamino)phenyl]-4-(phenylamino)naphthalene-1-methanol**	3_REACH		a,a-bis[4-(dimethylamino)phenyl]-4-(phenylamino)naphthalene-1-methanol		C33H34N3O	487.65	CN(C)c1ccc(cc1)C(O)(c2ccc(cc2)[NH+](C)C)c3ccc(Nc4ccccc4)c5ccccc35	InChI=1/C33H33N3O/c1-35(2)27-18-14-24(15-19-27)33(37,25-16-20-28(21-17-25)36(3)4)31-22-23-32(30-13-9-8-12-29(30)31)34-26-10-6-5-7-11-26/h5-23,34,37H,1-4H3/p+1	5.404	5.395	1	1	1
67990-05-0	67990050	3504	**N-(5-chloro-2-methoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide**	3_REACH		N-(5-chloro-2-methoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide		C32H24ClN4O5	581.03	COc1ccc(Cl)cc1NC(=O)c2cc3ccccc3c(N=Nc4cc(ccc4OC)C(=O)Nc5ccccc5)c2[O-]	InChI=1/C32H25ClN4O5/c1-41-27-15-13-21(33)18-25(27)35-32(40)24-16-19-8-6-7-11-23(19)29(30(24)38)37-36-26-17-20(12-14-28(26)42-2)31(39)34-22-9-4-3-5-10-22/h3-18,38H,1-2H3,(H,34,39)(H,35,40)/p-1	6.363	7.066	1	1	1
68-11-1	68111	798	**mercaptoacetic acid**	3_REACH	Acetic acid, mercapto-	Mercaptoacetic acid	C2H4O2S	C2H3O2S	92.116	[O-]C(=O)CS	InChI=1/C2H4O2S/c3-2(4)1-5/h5H,1H2,(H,3,4)/p-1	-1.38	-1.377	1	1	1
68134-22-5	68134225	3507	**N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo-2-[[2-(trifluoromethyl)phenyl]azo]butyramide**	3_REACH		N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo-2-[[2-(trifluoromethyl)phenyl]azo]butyramide		C18H14F3N5O3	405.34	CC(=O)C(N=Nc1ccccc1C(F)(F)F)C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C18H14F3N5O3/c1-9(27)15(26-25-12-5-3-2-4-11(12)18(19,20)21)16(28)22-10-6-7-13-14(8-10)24-17(29)23-13/h2-8,15H,1H3,(H,22,28)(H2,23,24,29)	3.947	3.947	1	1	1
682-01-9	682019	3509	**tetrapropyl orthosilicate**	3_REACH	Tetrapropyl silicate	tetrapropyl orthosilicate	C12H28O4Si	C12H28O4Si	264.44	CCCO[Si](OCCC)(OCCC)OCCC	InChI=1/C12H28O4Si/c1-5-9-13-17(14-10-6-2,15-11-7-3)16-12-8-4/h5-12H2,1-4H3	5.547	5.547	1	1	1
682-09-7	682097	3510	**2,2-bis(allyloxymethyl)butan-1-ol**	3_REACH		2,2-bis(allyloxymethyl)butan-1-ol		C12H22O3	214.31	CCC(CO)(COCC=C)COCC=C	InChI=1/C12H22O3/c1-4-7-14-10-12(6-3,9-13)11-15-8-5-2/h4-5,13H,1-2,6-11H2,3H3	1.432	1.432	1	1	1
682-11-1	682111	3511	**2-allyloxymethyl-2-ethylpropanediol**	3_REACH		2-allyloxymethyl-2-ethylpropanediol		C9H18O3	174.24	CCC(C)(COCC=C)C(O)O	InChI=1/C9H18O3/c1-4-6-12-7-9(3,5-2)8(10)11/h4,8,10-11H,1,5-7H2,2-3H3	1.158	1.158	1	1	1
68227-78-1	68227781	3512	**N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide**	3_REACH		N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide		C32H24ClN4O4	565.03	COc1ccc(cc1N=Nc2c([O-])c(cc3ccccc23)C(=O)Nc4cc(Cl)ccc4C)C(=O)Nc5ccccc5	InChI=1/C32H25ClN4O4/c1-19-12-14-22(33)18-26(19)35-32(40)25-16-20-8-6-7-11-24(20)29(30(25)38)37-36-27-17-21(13-15-28(27)41-2)31(39)34-23-9-4-3-5-10-23/h3-18,38H,1-2H3,(H,34,39)(H,35,40)/p-1	6.866	7.569	1	1	1
68-26-8	68268	3514	**retinol**	3_REACH	Retinol	retinol	C20H30O	C20H30O	286.46	C\C(=C/CO)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C	InChI=1/C20H30O/c1-16(8-6-9-17(2)13-15-21)11-12-19-18(3)10-7-14-20(19,4)5/h6,8-9,11-13,21H,7,10,14-15H2,1-5H3/b9-6+,12-11+,16-8+,17-13+	5.316	5.316	1	1	1
6842-62-2	6842622	3515	**614-477-3**	3_REACH		Benzene, 1-chloro-3-(4-chlorophenoxy)-			239.1	C1=CC(=CC(=C1)Cl)OC2=CC=C(C=C2)Cl	InChI=1S/C12H8Cl2O/c13-9-4-6-11(7-5-9)15-12-3-1-2-10(14)8-12/h1-8H			1	1	1
6843-66-9	6843669	3516	**dimethoxydiphenylsilane**	3_REACH	Silane, dimethoxydiphenyl-	dimethoxydiphenylsilane	C14H16O2Si	C14H16O2Si	244.37	CO[Si](OC)(c1ccccc1)c2ccccc2	InChI=1/C14H16O2Si/c1-15-17(16-2,13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12H,1-2H3	5.145	5.145	1	1	1
6850-63-1	6850631	801	**2,6-dimethylcyclohexylamine**	3_REACH		2,6-dimethylcyclohexylamine		C8H18N	127.23	CC1CCCC(C)C1[NH3+]	InChI=1/C8H17N/c1-6-4-3-5-7(2)8(6)9/h6-8H,3-5,9H2,1-2H3/p+1	0.844	0.846	1	1	1
68516-73-4	68516734	3518	**tetramethyl 2,2'-[1,4-phenylenebis[imino(1-acetyl-2-oxoethane-1,2-diyl)azo]]bisterephthalate**	3_REACH		tetramethyl 2,2'-[1,4-phenylenebis[imino(1-acetyl-2-oxoethane-1,2-diyl)azo]]bisterephthalate		C34H32N6O12	716.67	COC(=O)c1ccc(C(=O)OC)c(c1)N=NC(=O)C(Nc2ccc(NC(C(=O)C)C(=O)N=Nc3cc(ccc3C(=O)OC)C(=O)OC)cc2)C(=O)C	InChI=1/C34H32N6O12/c1-17(41)27(29(43)39-37-25-15-19(31(45)49-3)7-13-23(25)33(47)51-5)35-21-9-11-22(12-10-21)36-28(18(2)42)30(44)40-38-26-16-20(32(46)50-4)8-14-24(26)34(48)52-6/h7-16,27,28,35-36H,1-6H3	4.916	4.918	1	1	1
68610-86-6	68610866	3522	**Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-**	3_REACH		Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(o-anisyl			687.59	CC1=CC(=C(C=C1)NC(=O)C(C(=O)C)N=NC2=C(C=C(C=C2)C3=CC(=C(C=C3)N=NC(C(=O)C)C(=O)NC4=CC=CC=C4	InChI=1S/C35H32Cl2N6O5/c1-19-10-13-27(20(2)16-19)38-34(46)32(21(3)44)42-40-28-14-11-23(17-25(28)36)24-12-15-29			1	1	1
687-47-8	687478	3526	**ethyl (S)-2-hydroxypropionate**	3_REACH	Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	ethyl (S)-2-hydroxypropionate	C5H10O3	C5H10O3	118.13	CCOC(=O)[C@H](C)O	InChI=1/C5H10O3/c1-3-8-5(7)4(2)6/h4,6H,3H2,1-2H3/t4-/m0/s1	0.182	0.182	1	1	1
68855-18-5	68855185	3527	**(3-Hydroxy-2,2-dimethylpropyl) heptanoate**	3_REACH		Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol			216.32	CCCCCCC(=O)OCC(C)(C)CO	InChI=1S/C12H24O3/c1-4-5-6-7-8-11(14)15-10-12(2,3)9-13/h13H,4-10H2,1-3H3			1	1	1
688-84-6	688846	3529	**2-ethylhexyl methacrylate**	3_REACH	Octyl methacrylate	2-ethylhexyl methacrylate	C12H22O2	C12H22O2	198.31	CCCCC(CC)COC(=O)C(=C)C	InChI=1/C12H22O2/c1-5-7-8-11(6-2)9-14-12(13)10(3)4/h11H,3,5-9H2,1-2,4H3	4.181	4.181	1	1	1
69045-84-7	69045847	4322	**2,3-dichloro-5-trifluoromethylpyridine**	3_REACH		2,3-dichloro-5-trifluoromethylpyridine			215.99	C1=C(C=NC(=C1Cl)Cl)C(F)(F)F	InChI=1S/C6H2Cl2F3N/c7-4-1-3(6(9,10)11)2-12-5(4)8/h1-2H			1	1	1
6925-69-5	6925695	3537	**12H-phthaloperin-12-one**	3_REACH		12H-phthaloperin-12-one		C18H10N2O	270.29	O=C1N2C(=Nc3cccc4cccc2c34)c5ccccc15	InChI=1/C18H10N2O/c21-18-13-8-2-1-7-12(13)17-19-14-9-3-5-11-6-4-10-15(16(11)14)20(17)18/h1-10H	3.354	3.255	1	1	1
693-21-0	693210	804	**oxydiethylene dinitrate**	3_REACH	Ethanol, 2,2'-oxybis-, dinitrate	2,2'-Oxybisethanol, Dinitrate	C4H8N2O7	C4H8N2O7	196.12	[O-][N+](=O)OCCOCCO[N+](=O)[O-]	InChI=1/C4H8N2O7/c7-5(8)12-3-1-11-2-4-13-6(9)10/h1-4H2	3.792	3.792	1	1	1
693-23-2	693232	3538	**dodecanedioic acid**	3_REACH	Dodecanedioic acid	dodecanedioic acid	C12H22O4	C12H20O4	230.3	[O-]C(=O)CCCCCCCCCCC(=O)[O-]	InChI=1/C12H22O4/c13-11(14)9-7-5-3-1-2-4-6-8-10-12(15)16/h1-10H2,(H,13,14)(H,15,16)/p-2	0.342	0.393	1	1	1
693-36-7	693367	3539	**dioctadecyl 3,3'-thiodipropionate**	3_REACH		dioctadecyl 3,3'-thiodipropionate		C42H82O4S	683.18	CCCCCCCCCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCCCCCCCC	InChI=1/C42H82O4S/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-37-45-41(43)35-39-47-40-36-42(44)46-38-34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h3-40H2,1-2H3	16.136	16.136	0	0	1
693-57-2	693572	3540	**12-aminododecanoic acid**	3_REACH		12-aminododecanoic acid		C12H25NO2	215.34	[NH3+]CCCCCCCCCCCC(=O)[O-]	InChI=1/C12H25NO2/c13-11-9-7-5-3-1-2-4-6-8-10-12(14)15/h1-11,13H2,(H,14,15)	0.574	0.599	1	1	1
6938-94-9	6938949	3541	**diisopropyl adipate**	3_REACH	Hexanedioic acid, bis(1-methylethyl) ester	diisopropyl adipate	C12H22O4	C12H22O4	230.3	CC(C)OC(=O)CCCCC(=O)OC(C)C	InChI=1/C12H22O4/c1-9(2)15-11(13)7-5-6-8-12(14)16-10(3)4/h9-10H,5-8H2,1-4H3	2.456	2.456	1	1	1
693-98-1	693981	806	**2-methylimidazole**	3_REACH	1H-Imidazole, 2-methyl-	2-Methylimidazole	C4H6N2	C4H7N2	82.108	Cc1[nH+]cc[nH]1	InChI=1/C4H6N2/c1-4-5-2-3-6-4/h2-3H,1H3,(H,5,6)/p+1	0.345	0.25	1	1	1
6940-53-0	6940530	3543	**1-chloro-2,5-dimethoxy-4-nitrobenzene**	3_REACH		1-chloro-2,5-dimethoxy-4-nitrobenzene		C8H8ClNO4	217.61	COc1cc(c(OC)cc1Cl)[N+](=O)[O-]	InChI=1/C8H8ClNO4/c1-13-7-4-6(10(11)12)8(14-2)3-5(7)9/h3-4H,1-2H3	2.355	2.355	1	1	1
694-83-7	694837	807	**cyclohex-1,2-ylenediamine**	3_REACH	1,2-Cyclohexanediamine	cyclohex-1,2-ylenediamine	C6H14N2	C6H15N2	114.19	NC1CCCCC1[NH3+]	InChI=1/C6H14N2/c7-5-3-1-2-4-6(5)8/h5-6H,1-4,7-8H2/p+1	-1.051	-1.056	1	1	1
700-13-0	700130	3554	**2,3,5-trimethylhydroquinone**	3_REACH	Trimethylhydroquinone	2,3,5-trimethylhydroquinone	C9H12O2	C9H12O2	152.19	Cc1cc(O)c(C)c(C)c1O	InChI=1/C9H12O2/c1-5-4-8(10)6(2)7(3)9(5)11/h4,10-11H,1-3H3	2.804	2.804	1	1	1
70356-09-1	70356091	3560	**1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-1,3-dione**	3_REACH		1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-1,3-dione		C20H21O3	310.39	COc1ccc(cc1)C(=O)[CH-]C(=O)c2ccc(cc2)C(C)(C)C	InChI=1/C20H21O3/c1-20(2,3)16-9-5-14(6-10-16)18(21)13-19(22)15-7-11-17(23-4)12-8-15/h5-13H,4H3/q-1	4.538	4.552	1	1	1
70445-33-9	70445339	4370	**3-(2-ethylhexyloxy)propane-1,2-diol**	3_REACH		3-(2-ethylhexyloxy)propane-1,2-diol			204.31	CCCCC(CC)COCC(CO)O	InChI=1S/C11H24O3/c1-3-5-6-10(4-2)8-14-9-11(13)7-12/h10-13H,3-9H2,1-2H3			1	1	1
70516-41-5	70516415	3563	**2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one**	3_REACH		2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one		C34H34N2O3	518.66	CCN(CCC(C)C)c1ccc2c(Oc3cc(C)c(Nc4ccccc4)cc3C25OC(=O)c6ccccc56)c1	InChI=1/C34H34N2O3/c1-5-36(18-17-22(2)3)25-15-16-28-32(20-25)38-31-19-23(4)30(35-24-11-7-6-12-24)21-29(31)34(28)27-14-10-9-13-26(27)33(37)39-34/h6-16,19-22,35H,5,17-18H2,1-4H3	8.348	7.731	1	1	1
70-55-3	70553	85	**toluene-4-sulphonamide**	3_REACH	4-Methylbenzenesulfonamide	toluene-4-sulphonamide	C7H9NO2S	C7H9NO2S	171.22	Cc1ccc(cc1)S(=O)(=O)N	InChI=1/C7H9NO2S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)	1.021	1.021	1	1	1
706-14-9	706149	813	**decan-4-olide**	3_REACH	2(3H)-Furanone, 5-hexyldihydro-	gamma-Decanolactone	C10H18O2	C10H18O2	170.25	CCCCCCC1CCC(=O)O1	InChI=1/C10H18O2/c1-2-3-4-5-6-9-7-8-10(11)12-9/h9H,2-8H2,1H3	3.002	3.002	1	1	1
7069-42-3	7069423	3567	**retinyl propionate**	3_REACH		retinyl propionate		C23H32O3	342.52	CCC(=O)OC(=O)\C=C(/C)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C	InChI=1/C23H32O3/c1-7-21(24)26-22(25)16-18(3)11-8-10-17(2)13-14-20-19(4)12-9-15-23(20,5,6)/h8,10-11,13-14,16H,7,9,12,15H2,1-6H3/b11-8+,14-13+,17-10+,18-16+	6.227	6.227	1	1	1
70969-58-3	70969583	815	**diisobutyl hexahydrophthalate**	3_REACH		diisobutyl hexahydrophthalate		C16H28O4	284.4	CC(C)COC(=O)C1CCCCC1C(=O)OCC(C)C	InChI=1/C16H28O4/c1-11(2)9-19-15(17)13-7-5-6-8-14(13)16(18)20-10-12(3)4/h11-14H,5-10H2,1-4H3	3.941	3.941	1	1	1
71048-82-3	71048823	3577	**(2E)-1-[(1R,2S)-2,6,6-Trimethylcyclohex-3-en-1-yl]but-2-en-1-one**	3_REACH		[1a(E),2ß]-1-(2,6,6-trimethylcyclohex-3-en-1-yl)but-2-en-1-one		C13H20O	192.3	C\C=C\C(=O)C1C(C)C=CCC1(C)C	InChI=1/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-8,10,12H,9H2,1-4H3/b7-5+	3.387	3.387	1	1	1
712-50-5	712505	818	**cyclohexyl phenyl ketone**	3_REACH	Phenyl cyclohexyl ketone	cyclohexyl phenyl ketone	C13H16O	C13H16O	188.27	O=C(C1CCCCC1)c2ccccc2	InChI=1/C13H16O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10H2	3.696	3.696	1	1	1
713-95-1	713951	3581	**dodecan-5-olide**	3_REACH	2H-Pyran-2-one, 6-	dodecan-5-olide	C12H22O2	C12H22O2	198.31	CCCCCCCC1CCCC(=O)O1	InChI=1/C12H22O2/c1-2-3-4-5-6-8-11-9-7-10-12(13)14-11/h11H,2-10H2,1H3	3.914	3.914	1	1	1
71604-74-5	71604745	3586	**m-(2,3-epoxypropoxy)-N,N-bis(2,3-**	3_REACH		m-(2,3-epoxypropoxy)-N,N-bis(2,3-		C15H19NO4	277.32	C(Oc1cccc(c1)N(CC2CO2)CC3CO3)C4CO4	InChI=1/C15H19NO4/c1-2-11(4-12(3-1)17-9-15-10-20-15)16(5-13-7-18-13)6-14-8-19-14/h1-4,13-15H,5-10H2	1.125	1.116	1	1	1
71617-10-2	71617102	3587	**isopentyl p-methoxycinnamate**	3_REACH		isopentyl p-methoxycinnamate		C15H20O3	248.32	COc1ccc(\C=C\C(=O)OCCC(C)C)cc1	InChI=1/C15H20O3/c1-12(2)10-11-18-15(16)9-6-13-4-7-14(17-3)8-5-13/h4-9,12H,10-11H2,1-3H3/b9-6+	3.717	3.717	1	1	1
71735-74-5	71735745	3588	**ethyl 3-[[bis(1-methylethoxy)phosphinothioyl]thio]propionate**	3_REACH		ethyl 3-[[bis(1-methylethoxy)phosphinothioyl]thio]propionate		C11H23O4PS2	314.4	CCOC(=O)CCSP(=S)(OC(C)C)OC(C)C	InChI=1/C11H23O4PS2/c1-6-13-11(12)7-8-18-16(17,14-9(2)3)15-10(4)5/h9-10H,6-8H2,1-5H3	3.049	3.049	1	1	1
7173-62-8	7173628	3589	**(Z)-N-9-octadecenylpropane-1,3-diamine**	3_REACH		(Z)-N-9-octadecenylpropane-1,3-diamine		C21H46N2	324.6	CCCCCCCC\C=C\CCCCCCCC[NH2+]CCC[NH3+]	InChI=1/C21H44N2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-21-18-19-22/h9-10,23H,2-8,11-22H2,1H3/p+2/b10-9+	4.052	4.496	1	1	1
71902-23-3	71902233	3594	**6-[(1-oxomethyloctyl)amino]hexanoic acid**	3_REACH		6-[(1-oxomethyloctyl)amino]hexanoic acid		C15H29NO3	271.4	CCCCCCCC([NH2+]CCCCCC(=O)[O-])C=O	InChI=1/C15H29NO3/c1-2-3-4-5-7-10-14(13-17)16-12-9-6-8-11-15(18)19/h13-14,16H,2-12H2,1H3,(H,18,19)	0.835	0.861	1	1	1
7195-44-0	7195440	3595	**bis(2,3-epoxypropyl) terephthalate**	3_REACH		bis(2,3-epoxypropyl) terephthalate		C14H14O6	278.26	O=C(OCC1CO1)c2ccc(cc2)C(=O)OCC3CO3	InChI=1/C14H14O6/c15-13(19-7-11-5-17-11)9-1-2-10(4-3-9)14(16)20-8-12-6-18-12/h1-4,11-12H,5-8H2	0.973	0.973	1	1	1
72361-35-4	72361354	3603	**triisotridecyl benzene-1,2,4-tricarboxylate**	3_REACH		triisotridecyl benzene-1,2,4-tricarboxylate		C48H84O6	757.19	CC(C)CCCCCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCC(C)C)c(c1)C(=O)OCCCCCCCCCCC(C)C	InChI=1/C48H84O6/c1-40(2)31-25-19-13-7-10-16-22-28-36-52-46(49)43-34-35-44(47(50)53-37-29-17-11-8-14-20-26-32-41(3)4)45(39-43)48(51)54-38-30-24-18-12-9-15-21-27-33-42(5)6/h34-35,39-42H,7-33,36-38H2,1-6H3	17.086	17.086	1	1	1
7300-34-7	7300347	3612	**3,3'-[butane-1,4-diylbis(oxy)]bispropanamine**	3_REACH	4,9-Dioxa-1,12-dodecanediamine	3,3'-[butane-1,4-diylbis(oxy)]bispropanamine	C10H24N2O2	C10H26N2O2	204.32	[NH3+]CCCOCCCCOCCC[NH3+]	InChI=1/C10H24N2O2/c11-5-3-9-13-7-1-2-8-14-10-4-6-12/h1-12H2/p+2	-2.981	-2.939	1	1	1
7305-71-7	7305717	4342	**2-amino-5-methylthiazole**	3_REACH	Thiazole, 2-amino-5-methyl-	2-amino-5-methylthiazole	C4H6N2S		114.17					1	1	1
732-26-3	732263	829	**2,4,6-tri-tert-butylphenol**	3_REACH	Phenol, 2,4,6-tris(1,1-dimethylethyl)-	2,4,6-tris(1,1-Dimethylethyl)phenol	C18H30O	C18H30O	262.44	CC(C)(C)c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C	InChI=1/C18H30O/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11,19H,1-9H3	5.789	5.789	1	1	1
7328-22-5	7328225	3618	**2-(2-butoxyethoxy)ethyl methacrylate**	3_REACH		2-(2-butoxyethoxy)ethyl methacrylate		C12H22O4	230.3	CCCCOCCOCCOC(=O)C(=C)C	InChI=1/C12H22O4/c1-4-5-6-14-7-8-15-9-10-16-12(13)11(2)3/h2,4-10H2,1,3H3	2.231	2.231	1	1	1
7381-13-7	7381137	3627	**1,1'-(1,3-Phenylenedicarbonyl)diazepan-2-one**	3_REACH		1,1'-(1,3-Phenylenedicarbonyl)diazepan-2-one			356.42	C1CCC(=O)N(CC1)C(=O)C2=CC(=CC=C2)C(=O)N3CCCCCC3=O	InChI=1S/C20H24N2O4/c23-17-10-3-1-5-12-21(17)19(25)15-8-7-9-16(14-15)20(26)22-13-6-2-4-11-18(22)24/h7-9,14H,1-6			1	1	1
7396-58-9	7396589	3629	**N-methyldidecylamine**	3_REACH		N-methyldidecylamine		C21H46N	311.6	CCCCCCCCCC[NH+](C)CCCCCCCCCC	InChI=1/C21H45N/c1-4-6-8-10-12-14-16-18-20-22(3)21-19-17-15-13-11-9-7-5-2/h4-21H2,1-3H3/p+1	6.891	6.955	1	1	1
7397-62-8	7397628	3630	**butyl glycollate**	3_REACH	Butyl glycolate	butyl glycollate	C6H12O3	C6H12O3	132.16	CCCCOC(=O)CO	InChI=1/C6H12O3/c1-2-3-4-9-6(8)5-7/h7H,2-5H2,1H3	0.677	0.677	1	1	1
74338-72-0	74338720	4323	**2,4,4,7-tetramethyl-6-octen-3-one**	3_REACH		2,4,4,7-tetramethyl-6-octen-3-one			182.31	CC(C)C(=O)C(C)(C)CC=C(C)C	InChI=1S/C12H22O/c1-9(2)7-8-12(5,6)11(13)10(3)4/h7,10H,8H2,1-6H3			1	1	1
74441-05-7	74441057	3635	**N-[4-(aminocarbonyl)phenyl]-4-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzamide**	3_REACH		N-[4-(aminocarbonyl)phenyl]-4-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzamide		C25H21N7O5	499.49	CC(=O)C(N=Nc1ccc(cc1)C(=O)Nc2ccc(cc2)C(=O)N)C(=O)Nc3ccc4[nH]c(O)nc4c3	InChI=1/C25H21N7O5/c1-13(33)21(24(36)28-18-10-11-19-20(12-18)30-25(37)29-19)32-31-17-8-4-15(5-9-17)23(35)27-16-6-2-14(3-7-16)22(26)34/h2-12,21H,1H3,(H2,26,34)(H,27,35)(H,28,36)(H2,29,30,37)	2.792	2.8	1	1	1
7473-98-5	7473985	3642	**2-hydroxy-2-methylpropiophenone**	3_REACH		2-hydroxy-2-methylpropiophenone		C10H12O2	164.2	CC(C)(O)C(=O)c1ccccc1	InChI=1/C10H12O2/c1-10(2,12)9(11)8-6-4-3-5-7-8/h3-7,12H,1-2H3	1.693	1.693	1	1	1
75-12-7	75127	851	**formamide**	3_REACH	Formamide	Formamide	CH3NO	CH3NO	45.042	NC=O	InChI=1/CH3NO/c2-1-3/h1H,(H2,2,3)	-0.911	-0.911	1	1	1
7526-26-3	7526263	3659	**diphenyl methylphosphonate**	3_REACH	Phosphonic acid, methyl-, diphenyl ester	diphenyl methylphosphonate	C13H13O3P	C13H13O3P	248.22	CP(=O)(Oc1ccccc1)Oc2ccccc2	InChI=1/C13H13O3P/c1-17(14,15-12-8-4-2-5-9-12)16-13-10-6-3-7-11-13/h2-11H,1H3	3.021	3.021	1	1	1
7534-94-3	7534943	3668	**exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate**	3_REACH		exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate		C14H22O2	222.33	CC(=C)C(=O)O[C@H]1C[C@@H]2CC[C@@]1(C)C2(C)C	InChI=1/C14H22O2/c1-9(2)12(15)16-11-8-10-6-7-14(11,5)13(10,3)4/h10-11H,1,6-8H2,2-5H3/t10-,11 ,14+/m0/s1	3.498	3.498	1	1	1
75490-39-0	75490390	4313	**2,2,4-trimethyl-4-phenyl-butane-nitrile**	3_REACH		2,2,4-trimethyl-4-phenyl-butane-nitrile			187.29	CC(CC(C)(C)C#N)C1=CC=CC=C1	InChI=1S/C13H17N/c1-11(9-13(2,3)10-14)12-7-5-4-6-8-12/h4-8,11H,9H2,1-3H3			1	1	1
756-80-9	756809	864	**O,O-dimethyl hydrogen dithiophosphate**	3_REACH		O,O-Dimethyl ester, Phosphorodithioic acid		C2H7O2PS2	158.18	COP(=S)(S)OC	InChI=1/C2H7O2PS2/c1-3-5(6,7)4-2/h1-2H3,(H,6,7)	1.11	1.11	1	1	1
75-75-2	75752	3683	**methanesulphonic acid**	3_REACH	CH3SO3H	methanesulphonic acid	CH4O3S	CH3O3S	96.104	CS(=O)(=O)[O-]	InChI=1/CH4O3S/c1-5(2,3)4/h1H3,(H,2,3,4)/p-1	-2.659	-2.659	1	1	1
7575-23-7	7575237	3684	**pentaerythritol tetrakis(3-mercaptopropionate)**	3_REACH		pentaerythritol tetrakis(3-mercaptopropionate)		C17H28O8S4	488.66	SCCC(=O)OCC(COC(=O)CCS)(COC(=O)CCS)COC(=O)CCS	InChI=1/C17H28O8S4/c18-13(1-5-26)22-9-17(10-23-14(19)2-6-27,11-24-15(20)3-7-28)12-25-16(21)4-8-29/h26-29H,1-12H2	1.541	1.623	1	1	1
75980-60-8	75980608	3692	**diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide**	3_REACH		diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide		C22H21O2P	348.38	Cc1cc(C)c(C(=O)P(=O)(c2ccccc2)c3ccccc3)c(C)c1	InChI=1/C22H21O2P/c1-16-14-17(2)21(18(3)15-16)22(23)25(24,19-10-6-4-7-11-19)20-12-8-5-9-13-20/h4-15H,1-3H3	6.307	6.307	1	1	1
75-98-9	75989	868	**pivalic acid**	3_REACH	Pivalic acid	2,2-Dimethylpropionic acid	C5H10O2	C5H9O2	102.13	CC(C)(C)C(=O)[O-]	InChI=1/C5H10O2/c1-5(2,3)4(6)7/h1-3H3,(H,6,7)/p-1	-0.133	-0.073	1	1	1
76-03-9	76039	90	**trichloroacetic acid**	3_REACH	Acetic acid, trichloro-	Trichloroacetic acid	C2HCl3O2	C2Cl3O2	163.39	[O-]C(=O)C(Cl)(Cl)Cl	InChI=1/C2HCl3O2/c3-2(4,5)1(6)7/h(H,6,7)/p-1	-0.001	-0.001	1	1	1
7605-52-9	7605529	3696	**methyl cis-3-methylcyclohexanecarboxylate**	3_REACH		methyl cis-3-methylcyclohexanecarboxylate			156.22	CC1CCCC(C1)C(=O)OC	InChI=1S/C9H16O2/c1-7-4-3-5-8(6-7)9(10)11-2/h7-8H,3-6H2,1-2H3/t7-,8+/m0/s1			1	1	1
760-67-8	760678	3697	**2-ethylhexanoyl chloride**	3_REACH	Hexanoyl chloride, 2-ethyl-	2-ethylhexanoyl chloride	C8H15ClO	C8H15ClO	162.66	CCCCC(CC)C(=O)Cl	InChI=1/C8H15ClO/c1-3-5-6-7(4-2)8(9)10/h7H,3-6H2,1-2H3	3.326	3.326	1	1	1
76114-73-3	76114733	3699	**2-Propynyl butylcarbamate**	3_REACH		Carbamic acid, N-butyl-, 2-propyn-1-yl ester			155.2	CCCCNC(=O)OCC#C	InChI=1S/C8H13NO2/c1-3-5-6-9-8(10)11-7-4-2/h2H,3,5-7H2,1H3,(H,9,10)			1	1	1
76201-56-4	76201564	3704	**3-[dimethyl(3-{[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino}propyl)ammonio]-2-hydroxypropane-1-sulfonate**	3_REACH		3-[dimethyl(3-{[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino}propyl)ammonio]-2-hydroxypropane-1-sulfonate			650.47					1	1	1
762-04-9	762049	3705	**diethyl phosphonate**	3_REACH	Phosphonic acid, diethyl ester	diethyl phosphonate	C4H11O3P	C4H11O3P	138.1	CCOP(=O)OCC	InChI=1/C4H11O3P/c1-3-6-8(5)7-4-2/h8H,3-4H2,1-2H3	-0.33	-0.33	1	1	1
76-22-2	76222	872	**bornan-2-one**	3_REACH	Camphor	Camphor	C10H16O	C10H16O	152.24	CC1(C)C2CCC1(C)C(=O)C2	InChI=1/C10H16O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7H,4-6H2,1-3H3	2.075	2.075	1	1	1
763-69-9	763699	3710	**ethyl 3-ethoxypropionate**	3_REACH	Propionic acid, 3-ethoxy-, ethyl ester	ethyl 3-ethoxypropionate	C7H14O3	C7H14O3	146.19	CCOCCC(=O)OCC	InChI=1/C7H14O3/c1-3-9-6-5-7(8)10-4-2/h3-6H2,1-2H3	0.703	0.703	1	1	1
764-99-8	764998	3714	**1,1'-[oxybis(ethyleneoxy)]diethylene**	3_REACH	Ethene, 1,1'-[oxybis(2,1-ethanediyloxy)]bis-	1,1'-[oxybis(ethyleneoxy)]diethylene	C8H14O3	C8H14O3	158.2	C=COCCOCCOC=C	InChI=1/C8H14O3/c1-3-9-5-7-11-8-6-10-4-2/h3-4H,1-2,5-8H2	0.33	0.33	1	1	1
76524-94-2	76524942	3715	**N-[3-(Triethoxysilyl)propyl]formamide**	3_REACH		N-[3-(Triethoxysilyl)propyl]formamide			249.38	CCO[Si](CCCNC=O)(OCC)OCC	InChI=1S/C10H23NO4Si/c1-4-13-16(14-5-2,15-6-3)9-7-8-11-10-12/h10H,4-9H2,1-3H3,(H,11,12)			1	1	1
7659-86-1	7659861	3721	**2-ethylhexyl mercaptoacetate**	3_REACH		2-ethylhexyl mercaptoacetate		C10H20O2S	204.33	CCCCC(CC)COC(=O)CS	InChI=1/C10H20O2S/c1-3-5-6-9(4-2)7-12-10(11)8-13/h9,13H,3-8H2,1-2H3	3.337	3.341	1	1	1
76855-69-1	76855691	4234	**Azetidon**	3_REACH		(2R,3R)-3-((R)-1-(tert-butyldimethylsiloxy)ethyl)-4-oxoazetidin-2-yl acetate			287.43	CC(C1C(NC1=O)OC(=O)C)O[Si](C)(C)C(C)(C)C	InChI=1S/C13H25NO4Si/c1-8(18-19(6,7)13(3,4)5)10-11(16)14-12(10)17-9(2)15/h8,10,12H,1-7H3,(H,14,16)/t8-,10+,12-/m			1	1	1
768-94-5	768945	878	**amantadine**	3_REACH	Tricyclo[3.3.1.13,7]decane-1-amine	Tricyclo[3.3.1.1 3,7]decan-1-amine	C10H17N	C10H18N	151.25	[NH3+]C12CC3CC(CC(C3)C1)C2	InChI=1/C10H17N/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H,1-6,11H2/p+1	0.49	0.492	1	1	1
7695-91-2	7695912	3727	**3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-yl acetate**	3_REACH	Vitamin E acetate	3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-yl acetate	C31H52O3	C31H52O3	472.75	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2c(C)c(OC(=O)C)c(C)c(C)c2O1	InChI=1/C31H52O3/c1-21(2)13-10-14-22(3)15-11-16-23(4)17-12-19-31(9)20-18-28-26(7)29(33-27(8)32)24(5)25(6)30(28)34-31/h21-23H,10-20H2,1-9H3	10.45	10.45	0	0	1
770-35-4	770354	3730	**1-phenoxypropan-2-ol**	3_REACH	1-Phenoxy-2-propanol	1-phenoxypropan-2-ol	C9H12O2	C9H12O2	152.19	CC(O)COc1ccccc1	InChI=1/C9H12O2/c1-8(10)7-11-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3	1.651	1.651	1	1	1

77-09-8	77098	879	**phenolphthalein**	3_REACH	Phenolphthalein	3,3-Bis(4-hydroxyphenyl)-1(3H)-isobenzofuranone	C20H14O4	C20H14O4	318.33	Oc1ccc(cc1)C2(OC(=O)c3ccccc23)c4ccc(O)cc4	InChI=1/C20H14O4/c21-15-9-5-13(6-10-15)20(14-7-11-16(22)12-8-14)18-4-2-1-3-17(18)19(23)24-20/h1-12,21-22H	4.006	3.993	1	1	1
7747-35-5	7747355	880	**7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole**	3_REACH		7a-Ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole		C7H14NO2	143.19	CCC12COC[NH+]1COC2	InChI=1/C7H13NO2/c1-2-7-3-9-5-8(7)6-10-4-7/h2-6H2,1H3/p+1	-1.144	-0.103	1	1	1
77501-63-4	77501634	882	**Lactofen**	3_REACH		Lactofen			461.78	CCOC(=O)C(C)OC(=O)C1=C(C=CC(=C1)OC2=C(C=C(C=C2)C(F)(F)F)Cl)[N+](=O)[O-]	InChI=1S/C19H15ClF3NO7/c1-3-29-17(25)10(2)30-18(26)13-9-12(5-6-15(13)24(27)28)31-16-7-4-11(8-14(16)20)19(21,22			1	1	1
77-71-4	77714	883	**5,5-dimethylhydantoin**	3_REACH	2,4-Imidazolidinedione, 5,5-dimethyl-	5,5-Dimethylhydantoin	C5H8N2O2	C5H8N2O2	128.13	CC1(C)NC(=O)NC1=O	InChI=1/C5H8N2O2/c1-5(2)3(8)6-4(9)7-5/h1-2H3,(H2,6,7,8,9)	-0.365	-0.363	1	1	1
77-73-6	77736	884	**3a,4,7,7a-tetrahydro-4,7-methanoindene**	3_REACH	4,7-Methano-1H-indene, 3a,4,7,7a-tetrahydro-	3a,4,7,7a-Tetrahydro-4,7-methano-1H-indene	C10H12	C10H12	132.21	C1C=CC2C3CC(C=C3)C12	InChI=1/C10H12/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,4-5,7-10H,3,6H2	2.111	2.111	1	1	1
77-78-1	77781	886	**dimethyl sulphate**	3_REACH	Sulfuric acid, dimethyl ester	Dimethyl sulfate	C2H6O4S	C2H6O4S	126.13	COS(=O)(=O)OC	InChI=1/C2H6O4S/c1-5-7(3,4)6-2/h1-2H3	-0.529	-0.529	1	1	1
77804-81-0	77804810	3736	**2,2'-[ethylenebis(oxyphenyl-2,1-eneazo)]bis[N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide**	3_REACH		2,2'-[ethylenebis(oxyphenyl-2,1-eneazo)]bis[N(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide		C36H32N10O8	732.72	CC(=O)C(N=Nc1ccccc1OCCOc2ccccc2N=NC(C(=O)C)C(=O)Nc3ccc4[nH]c(O)nc4c3)C(=O)Nc5ccc6[nH]c(O)nc6c5	InChI=1/C36H32N10O8/c1-19(47)31(33(49)37-21-11-13-23-27(17-21)41-35(51)39-23)45-43-25-7-3-9-29(25)53-15-16-54-30-10-6-4-8-26(30)44-46-32(20(2)48)34(50)38-22-12-14-24-28(18-22)42-36(52)40-24/h3-14,17-18,31-32H,15-16H2,1-2H3,(H,37,49)(H,38,50)(H2,39,41,51)(H2,40,42,52)/b45-43+,46-44+	5.796	5.093	1	1	1
77-83-8	77838	3738	**ethyl 2,3-epoxy-3-phenylbutyrate**	3_REACH	Glycidic acid, 3-methyl-3-phenyl, ethyl ester	ethyl 2,3-epoxy-3-phenylbutyrate	C12H14O3	C12H14O3	206.24	CCOC(=O)C1OC1(C)c2ccccc2	InChI=1/C12H14O3/c1-3-14-11(13)10-12(2,15-10)9-7-5-4-6-8-9/h4-8,10H,3H2,1-2H3	1.877	1.877	1	1	1
7785-26-4	7785264	887	**(-)-pin-2(3)-ene**	3_REACH	(1s)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	(1S,5S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	C10H16	C10H16	136.24	CC1=CC[C@H]2C[C@@H]1C2(C)C	InChI=1/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-6H2,1-3H3/t8-,9-/m0/s1	2.872	2.872	1	1	1
7785-70-8	7785708	888	**(+)-pin-2(3)-ene**	3_REACH	α-Pinene(dextro)	(1R,5R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	C10H16	C10H16	136.24	CC1=CC[C@@H]2C[C@H]1C2(C)C	InChI=1/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-6H2,1-3H3/t8-,9-/m1/s1	2.872	2.872	1	1	1
77-86-1	77861	3739	**trometamol**	3_REACH	1,3-Propanediol, 2-amino-2-(hydroxymethyl)-	trometamol	C4H11NO3	C4H12NO3	121.14	[NH3+]C(CO)(CO)CO	InChI=1/C4H11NO3/c5-4(1-6,2-7)3-8/h6-8H,1-3,5H2/p+1	-3.386	-2.975	1	1	1
7787-93-1	7787931	3741	**dichloro(3-chloropropyl)methylsilane**	3_REACH		dichloro(3-chloropropyl)methylsilane		C4H9Cl3Si	191.56	C[Si](Cl)(Cl)CCCCl	InChI=1/C4H9Cl3Si/c1-8(6,7)4-2-3-5/h2-4H2,1H3	3.681	3.681	1	1	1
778-94-9	778949	3743	**2-nitro-4-(trifluoromethyl)benzonitrile**	3_REACH	4-Cyano-3-nitrobenzotrifluoride	2-nitro-4-(trifluoromethyl)benzonitrile	C8H3F3N2O2	C8H3F3N2O2	216.12	[O-][N+](=O)c1cc(ccc1C#N)C(F)(F)F	InChI=1/C8H3F3N2O2/c9-8(10,11)6-2-1-5(4-12)7(3-6)13(14)15/h1-3H	2.545	2.545	1	1	1
77-90-7	77907	3744	**tributyl O-acetylcitrate**	3_REACH	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester	tributyl O-acetylcitrate	C20H34O8	C20H34O8	402.48	CCCCOC(=O)CC(CC(=O)OCCCC)(OC(=O)C)C(=O)OCCCC	InChI=1/C20H34O8/c1-5-8-11-25-17(22)14-20(28-16(4)21,19(24)27-13-10-7-3)15-18(23)26-12-9-6-2/h5-15H2,1-4H3	3.723	3.723	1	1	1
77-92-9	77929	889	**citric acid**	3_REACH	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	2-Hydroxy-1,2,3-propanetricarboxylic acid	C6H8O7	C6H6O7	192.12	OC(=O)CC(O)(CC(=O)[O-])C(=O)[O-]	InChI=1/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/p-2	-4.267	-3.85	1	1	1
77-93-0	77930	92	**triethyl citrate**	3_REACH	Ethyl citrate	triethyl citrate	C12H20O7	C12H20O7	276.29	CCOC(=O)CC(O)(CC(=O)OCC)C(=O)OCC	InChI=1/C12H20O7/c1-4-17-9(13)7-12(16,11(15)19-6-3)8-10(14)18-5-2/h16H,4-8H2,1-3H3	0.404	0.404	1	1	1
77-94-1	77941	3745	**tributyl citrate**	3_REACH	Butyl citrate	tributyl citrate	C18H32O7	C18H32O7	360.45	CCCCOC(=O)CC(O)(CC(=O)OCCCC)C(=O)OCCCC	InChI=1/C18H32O7/c1-4-7-10-23-15(19)13-18(22,17(21)25-12-9-6-3)14-16(20)24-11-8-5-2/h22H,4-14H2,1-3H3	3.344	3.344	1	1	1
77-99-6	77996	890	**propylidynetrimethanol**	3_REACH	1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-	2-Ethyl-2-hydroxymethyl-1,3-propanediol	C6H14O3	C6H14O3	134.18	CCC(CO)(CO)CO	InChI=1/C6H14O3/c1-2-6(3-7,4-8)5-9/h7-9H,2-5H2,1H3	-0.618	-0.618	1	1	1
780-69-8	780698	891	**triethoxy(phenyl)silane**	3_REACH	Triethoxyphenylsilane	(Triethoxysilyl)benzene	C12H20O3Si	C12H20O3Si	240.38	CCO[Si](OCC)(OCC)c1ccccc1	InChI=1/C12H20O3Si/c1-4-13-16(14-5-2,15-6-3)12-10-8-7-9-11-12/h7-11H,4-6H2,1-3H3	4.648	4.648	1	1	1
78-08-0	78080	3746	**triethoxy(vinyl)silane**	3_REACH	Silane, ethenyltriethoxy-	triethoxy(vinyl)silane	C8H18O3Si	C8H18O3Si	190.32	CCO[Si](OCC)(OCC)C=C	InChI=1/C8H18O3Si/c1-5-9-12(8-4,10-6-2)11-7-3/h8H,4-7H2,1-3H3	3.155	3.155	1	1	1
78-11-5	78115	892	**pentaerithrityl tetranitrate**	3_REACH	Pentaerythritol, tetranitrate	Pentaerythritol tetranitrate	C5H8N4O12	C5H8N4O12	316.14	[O-][N+](=O)OCC(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-]	InChI=1/C5H8N4O12/c10-6(11)18-1-5(2-19-7(12)13,3-20-8(14)15)4-21-9(16)17/h1-4H2	7.476	7.476	1	1	1
78-27-3	78273	893	**1-ethynylcyclohexanol**	3_REACH	Cyclohexanol, 1-ethynyl-	1-Ethynyl cyclohexanol	C8H12O	C8H12O	124.18	OC1(CCCCC1)C#C	InChI=1/C8H12O/c1-2-8(9)6-4-3-5-7-8/h1,9H,3-7H2	2.548	2.548	1	1	1
78-40-0	78400	894	**triethyl phosphate**	3_REACH	Triethyl phosphate	Triethyl phosphate	C6H15O4P	C6H15O4P	182.16	CCOP(=O)(OCC)OCC	InChI=1/C6H15O4P/c1-4-8-11(7,9-5-2)10-6-3/h4-6H2,1-3H3	0.695	0.695	1	1	1
78-42-2	78422	895	**tris(2-ethylhexyl) phosphate**	3_REACH	2-Ethylhexanol phosphate (3:1)	tris(2-Ethylhexyl)ester phosphoric acid	C24H51O4P	C24H51O4P	434.64	CCCCC(CC)COP(=O)(OCC(CC)CCCC)OCC(CC)CCCC	InChI=1/C24H51O4P/c1-7-13-16-22(10-4)19-26-29(25,27-20-23(11-5)17-14-8-2)28-21-24(12-6)18-15-9-3/h22-24H,7-21H2,1-6H3	8.698	8.698	1	1	1
78-51-3	78513	93	**tris(2-butoxyethyl) phosphate**	3_REACH	Phosphoric acid, tri-(2-butoxyethyl) ester	2-Butoxyethanol, Phosphate (3:1)	C18H39O7P	C18H39O7P	398.48	CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC	InChI=1/C18H39O7P/c1-4-7-10-20-13-16-23-26(19,24-17-14-21-11-8-5-2)25-18-15-22-12-9-6-3/h4-18H2,1-3H3	3.242	3.242	1	1	1
78521-39-8	78521398	3751	**6-[[(4-methylphenyl)sulphonyl]amino]hexanoic acid**	3_REACH		6-[[(4-methylphenyl)sulphonyl]amino]hexanoic acid		C13H18NO4S	285.36	Cc1ccc(cc1)S(=O)(=O)NCCCCCC(=O)[O-]	InChI=1/C13H19NO4S/c1-11-6-8-12(9-7-11)19(17,18)14-10-4-2-3-5-13(15)16/h6-9,14H,2-5,10H2,1H3,(H,15,16)/p-1	0.716	0.742	1	1	1
78531-61-0	78531610	4400	**4-(trans-4-propylcyclohexyl)acetophenone**	3_REACH		4-(trans-4-propylcyclohexyl)acetophenone			244.38	CCCC1CCC(CC1)C2=CC=C(C=C2)C(=O)C	InChI=1S/C17H24O/c1-3-4-14-5-7-16(8-6-14)17-11-9-15(10-12-17)13(2)18/h9-12,14,16H,3-8H2,1-2H3			1	1	1
78-59-1	78591	897	**3,5,5-trimethylcyclohex-2-enone**	3_REACH	2-Cyclohexen-1-one, 3,5,5-trimethyl-	Isophorone	C9H14O	C9H14O	138.21	CC1=CC(=O)CC(C)(C)C1	InChI=1/C9H14O/c1-7-4-8(10)6-9(2,3)5-7/h4H,5-6H2,1-3H3	2.195	2.195	1	1	1
78605-96-6	78605966	3752	**alpha-Amylcinnamaldehyde**	3_REACH		Heptanal, 2-(phenylmethylene)-, (2E)-			202.3	CCCCCC(=CC1=CC=CC=C1)C=O	InChI=1S/C14H18O/c1-2-3-5-10-14(12-15)11-13-8-6-4-7-9-13/h4-9,11-12H,2-3,5,10H2,1H3/b14-11+			1	1	1
78-63-7	78637	3753	**di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide**	3_REACH		di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide		C16H34O4	290.44	CC(C)(C)OOC(C)(C)CCC(C)(C)OOC(C)(C)C	InChI=1/C16H34O4/c1-13(2,3)17-19-15(7,8)11-12-16(9,10)20-18-14(4,5)6/h11-12H2,1-10H3	3.281	3.281	1	1	1
78-67-1	78671	3754	**2,2'-dimethyl-2,2'-azodipropiononitrile**	3_REACH	2,2'-Azo-bis-isobutyronitrile	2,2'-dimethyl-2,2'-azodipropiononitrile	C8H12N4	C8H12N4	164.22	CC(C)(N=NC(C)(C)C#N)C#N	InChI=1/C8H12N4/c1-7(2,5-9)11-12-8(3,4)6-10/h1-4H3/b12-11+	2.099	2.099	1	1	1
78-69-3	78693	3755	**3,7-dimethyloctan-3-ol**	3_REACH	3,7-Dimethyl-3-octanol	3,7-dimethyloctan-3-ol	C10H22O	C10H22O	158.29	CCC(C)(O)CCCC(C)C	InChI=1/C10H22O/c1-5-10(4,11)8-6-7-9(2)3/h9,11H,5-8H2,1-4H3	3.241	3.241	1	1	1
78-70-6	78706	899	**linalool**	3_REACH	2,6-Dimethylocta-2,7-dien-6-ol	3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	C10H18O	154.25	CC(=CCCC(C)(O)C=C)C	InChI=1/C10H18O/c1-5-10(4,11)8-6-7-9(2)3/h5,7,11H,1,6,8H2,2-4H3	2.735	2.735	1	1	1
78850-37-0	78850370	5023	**methyl (3aR,4R,7aR)-2-methyl-4-(1S,2R,3-triacetoxypropyl)-3a,7a-dihydro-4H-pyrano[3,4-d]oxazole-6-carboxylate**	3_REACH		methyl (3aR,4R,7aR)-2-methyl-4-(1S,2R,3-triacetoxypropyl)-3a,7a-dihydro-4H-pyrano[3,4-d]oxazole-6-carboxylate			413.38	CC1=NC2C(O1)C=C(OC2C(C(COC(=O)C)OC(=O)C)OC(=O)C)C(=O)OC	InChI=1S/C18H23NO10/c1-8-19-15-12(26-8)6-13(18(23)24-5)29-17(15)16(28-11(4)22)14(27-10(3)21)7-25-9(2)20/h6,12,1			1	1	1
78-97-7	78977	3762	**lactonitrile**	3_REACH	Propanenitrile, 2-hydroxy-	lactonitrile	C3H5NO	C3H5NO	71.08	CC(O)C#N	InChI=1/C3H5NO/c1-3(5)2-4/h3,5H,1H3	-0.144	-0.144	1	1	1
79-06-1	79061	911	**acrylamide**	3_REACH	Acrylamide	2-Propenamide	C3H5NO	C3H5NO	71.08	NC(=O)C=C	InChI=1/C3H5NO/c1-2-3(4)5/h2H,1H2,(H2,4,5)	-0.135	-0.135	1	1	1
79-07-2	79072	3765	**2-chloroacetamide**	3_REACH	Acetamide, 2-chloro-	2-chloroacetamide	C2H4ClNO	C2H4ClNO	93.514	NC(=O)CCl	InChI=1/C2H4ClNO/c3-1-2(4)5/h1H2,(H2,4,5)	-0.3	-0.3	1	1	1
79-08-3	79083	912	**bromoacetic acid**	3_REACH	Acetic acid, bromo-	Bromoacetic acid	C2H3BrO2	C2H2BrO2	138.95	[O-]C(=O)CBr	InChI=1/C2H3BrO2/c3-1-2(4)5/h1H2,(H,4,5)/p-1	-1.002	-1.002	1	1	1
79-11-8	79118	915	**chloroacetic acid**	3_REACH	Acetic acid, chloro-	Chloroacetic acid	C2H3ClO2	C2H2ClO2	94.497	[O-]C(=O)CCl	InChI=1/C2H3ClO2/c3-1-2(4)5/h1H2,(H,4,5)/p-1	-1.146	-1.146	1	1	1
791-28-6	791286	95	**triphenylphosphine oxide**	3_REACH	(C6H5)3PO	Triphenylphosphine oxide	C18H15OP	C18H15OP	278.29	O=P(c1ccccc1)(c2ccccc2)c3ccccc3	InChI=1/C18H15OP/c19-20(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H	4.977	4.977	1	1	1
79-14-1	79141	3766	**glycollic acid**	3_REACH	Acetic acid, hydroxy-	glycollic acid	C2H4O3	C2H3O3	76.051	OCC(=O)[O-]	InChI=1/C2H4O3/c3-1-2(4)5/h3H,1H2,(H,4,5)/p-1	-2.351	-2.348	1	1	1
79-16-3	79163	3767	**N-methylacetamide**	3_REACH	Acetamide, N-methyl-	N-methylacetamide	C3H7NO	C3H7NO	73.096	CNC(=O)C	InChI=1/C3H7NO/c1-3(5)4-2/h1-2H3,(H,4,5)	-0.627	-0.627	1	1	1
793-24-8	793248	3771	**N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine**	3_REACH		N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine		C18H24N2	268.41	CC(C)CC(C)Nc1ccc(Nc2ccccc2)cc1	InChI=1/C18H24N2/c1-14(2)13-15(3)19-17-9-11-18(12-10-17)20-16-7-5-4-6-8-16/h4-12,14-15,19-20H,13H2,1-3H3	5.146	4.709	1	1	1
79-33-4	79334	920	**L-(+)-lactic acid**	3_REACH	(s)-2-Hydroxypropanoic acid	(2S)-2-Hydroxypropanoic acid	C3H6O3	C3H5O3	90.078	C[C@H](O)C(=O)[O-]	InChI=1/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)/p-1/t2-/m0/s1	-1.867	-1.863	1	1	1
79-41-4	79414	3776	**methacrylic acid**	3_REACH	2-Propenoic acid, 2-methyl-	methacrylic acid	C4H6O2	C4H5O2	86.09	CC(=C)C(=O)[O-]	InChI=1/C4H6O2/c1-3(2)4(5)6/h1H2,2H3,(H,5,6)/p-1	-0.535	-0.513	1	1	1
79456-26-1	79456261	4391	**3-chloro-5-trifluoromethyl-2-pyridylamine**	3_REACH		3-chloro-5-trifluoromethyl-2-pyridylamine			196.56	C1=C(C=NC(=C1Cl)N)C(F)(F)F	InChI=1S/C6H4ClF3N2/c7-4-1-3(6(8,9)10)2-12-5(4)11/h1-2H,(H2,11,12)			1	1	1
79-74-3	79743	3781	**2,5-di-tert-pentylhydroquinone**	3_REACH	1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-	2,5-di-tert-pentylhydroquinone	C16H26O2	C16H26O2	250.38	CCC(C)(C)c1cc(O)c(cc1O)C(C)(C)CC	InChI=1/C16H26O2/c1-7-15(3,4)11-9-14(18)12(10-13(11)17)16(5,6)8-2/h9-10,17-18H,7-8H2,1-6H3	5.059	5.059	1	1	1
79-77-6	79776	926	**(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one**	3_REACH	3-Buten-2-one, 4-(2,6,6-trimethyl-1 cyclohexen-1-yl)-, (E)-	beta-Ionone	C13H20O	C13H20O	192.3	CC(=O)\C=C\C1=C(C)CCCC1(C)C	InChI=1/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8H,5-6,9H2,1-4H3/b8-7+	3.355	3.355	1	1	1
79815-20-6	79815206	4252	**(S)-2,3-dihydro-1H-indole-2-carboxylic acid**	3_REACH		(S)-2,3-dihydro-1H-indole-2-carboxylic acid			163.18	C1C(NC2=CC=CC=C21)C(=O)O	InChI=1S/C9H9NO2/c11-9(12)8-5-6-3-1-2-4-7(6)10-8/h1-4,8,10H,5H2,(H,11,12)/t8-/m0/s1			1	1	1
79-94-7	79947	929	**2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol**	3_REACH	Phenol, 4,4'-(2,2-propanediyl) bis[2,6-dibromo]-	Tetrabromobisphenol-A	C15H12Br4O2	C15H11Br4O2	543.9	CC(C)(c1cc(Br)c(O)c(Br)c1)c2cc(Br)c([O-])c(Br)c2	InChI=1/C15H12Br4O2/c1-15(2,7-3-9(16)13(20)10(17)4-7)8-5-11(18)14(21)12(19)6-8/h3-6,20-21H,1-2H3/p-1	6.068	6.07	1	1	1
80-04-6	80046	931	**4,4'-isopropylidenedicyclohexanol**	3_REACH		4,4'-isopropylidenedicyclohexanol		C15H28O2	240.39	CC(C)(C1CCC(O)CC1)C2CCC(O)CC2	InChI=1/C15H28O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h11-14,16-17H,3-10H2,1-2H3	3.134	3.134	1	1	1
80-05-7	80057	96	**4,4'-isopropylidenediphenol**	3_REACH	Phenol, 4,4'-(1-methylethylidene)bis-	Bisphenol-A	C15H16O2	C15H16O2	228.29	CC(C)(c1ccc(O)cc1)c2ccc(O)cc2	InChI=1/C15H16O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h3-10,16-17H,1-2H3	3.778	3.776	1	1	1
80-07-9	80079	3786	**bis(4-chlorophenyl) sulphone**	3_REACH	4,4'-Dichlorodiphenyl sulphone	bis(4-chlorophenyl) sulphone	C12H8Cl2O2S	C12H8Cl2O2S	287.16	Clc1ccc(cc1)S(=O)(=O)c2ccc(Cl)cc2	InChI=1/C12H8Cl2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H	4.261	4.261	1	1	1
80-10-4	80104	3788	**dichloro(diphenyl)silane**	3_REACH	Diphenyldichlorosilane	dichloro(diphenyl)silane	C12H10Cl2Si	C12H10Cl2Si	253.2	Cl[Si](Cl)(c1ccccc1)c2ccccc2	InChI=1/C12H10Cl2Si/c13-15(14,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	5.847	5.847	1	1	1
80-15-9	80159	932	**Cumene hydroperoxide**	3_REACH	Hydroperoxide, 1-methyl-1-phenylethyl	Cumene hydroperoxide	C9H12O2	C9H12O2	152.19	CC(C)(OO)c1ccccc1	InChI=1/C9H12O2/c1-9(2,11-10)8-6-4-3-5-7-8/h3-7,10H,1-2H3	2.023	2.023	1	1	1
80-26-2	80262	934	**p-menth-1-en-8-yl acetate**	3_REACH	α-Terpenyl acetate	alpha,alpha,4-Trimethyl-3-cyclohexene-1-methanol acetate	C12H20O2	C12H20O2	196.29	CC(=O)OC(C)(C)C1CCC(=CC1)C	InChI=1/C12H20O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h5,11H,6-8H2,1-4H3	2.794	2.794	1	1	1
80-43-3	80433	3791	**Dicumyl peroxide**	3_REACH		bis(a,a-dimethylbenzyl) peroxide		C18H22O2	270.37	CC(C)(OOC(C)(C)c1ccccc1)c2ccccc2	InChI=1/C18H22O2/c1-17(2,15-11-7-5-8-12-15)19-20-18(3,4)16-13-9-6-10-14-16/h5-14H,1-4H3	4.228	4.228	1	1	1
80-46-6	80466	936	**p-(1,1-dimethylpropyl)phenol**	3_REACH	Phenol, 4-(1,1-dimethylpropyl)-	4-tert-Pentylphenol	C11H16O	C11H16O	164.25	CCC(C)(C)c1ccc(O)cc1	InChI=1/C11H16O/c1-4-11(2,3)9-5-7-10(12)8-6-9/h5-8,12H,4H2,1-3H3	3.444	3.444	1	1	1
80-51-3	80513	3792	**4,4'-oxydi(benzenesulphonohydrazide)**	3_REACH	4,4'-Oxydibenzenesulfonyl hydrazide	4,4'-oxydi(benzenesulphonohydrazide)	C12H14N4O5S2	C12H14N4O5S2	358.4	NNS(=O)(=O)c1ccc(Oc2ccc(cc2)S(=O)(=O)NN)cc1	InChI=1/C12H14N4O5S2/c13-15-22(17,18)11-5-1-9(2-6-11)21-10-3-7-12(8-4-10)23(19,20)16-14/h1-8,15-16H,13-14H2	-0.184	-0.184	1	1	1
80-54-6	80546	3794	**2-(4-tert-butylbenzyl)propionaldehyde**	3_REACH	Lilial	2-(4-tert-butylbenzyl)propionaldehyde	C14H20O	C14H20O	204.31	CC(Cc1ccc(cc1)C(C)(C)C)C=O	InChI=1/C14H20O/c1-11(10-15)9-12-5-7-13(8-6-12)14(2,3)4/h5-8,10-11H,9H2,1-4H3	3.835	3.835	1	1	1
80-56-8	80568	937	**pin-2(3)-ene**	3_REACH	α-Pinene	alpha-Pinene	C10H16	C10H16	136.24	CC1=CCC2CC1C2(C)C	InChI=1/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-6H2,1-3H3	2.872	2.872	1	1	1
80-73-9	80739	3797	**1,3-dimethylimidazolidin-2-one**	3_REACH	1,3-Dimethyl-2-imidazolidinone	1,3-dimethylimidazolidin-2-one	C5H10N2O	C5H10N2O	114.15	CN1CCN(C)C1=O	InChI=1/C5H10N2O/c1-6-3-4-7(2)5(6)8/h3-4H2,1-2H3	-0.4	-0.4	1	1	1
81-07-2	81072	98	**1,2-benzisothiazol-3(2H)-one 1,1-dioxide**	3_REACH	Saccharin	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	C7H5NO3S	C7H4NO3S	183.19	O=C1[N-]S(=O)(=O)c2ccccc12	InChI=1/C7H5NO3S/c9-7-5-3-1-2-4-6(5)12(10,11)8-7/h1-4H,(H,8,9)/p-1	0.463	0.463	1	1	1
81-19-6	81196	939	**1,3-Dichloro-2-(dichloromethyl)benzene**	3_REACH	Benzene, 1,3-dichloro-2-(dichloromethyl)-	1,3-Dichloro-2-(dichloromethyl)benzene	C7H4Cl4	C7H4Cl4	229.92	ClC(Cl)c1c(Cl)cccc1Cl	InChI=1/C7H4Cl4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,7H	4.202	4.202	1	1	1
81-25-4	81254	100	**cholic acid**	3_REACH	Cholic acid	cholic acid	C24H40O5	C24H39O5	408.58	C[C@H](CCC(=O)[O-])[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C	InChI=1/C24H40O5/c1-13(4-7-21(28)29)16-5-6-17-22-18(12-20(27)24(16,17)3)23(2)9-8-15(25)10-14(23)11-19(22)26/h13-20,22,25-27H,4-12H2,1-3H3,(H,28,29)/p-1/t13-,14+,15-,16-,17+,18+,19-,20+,22+,23+,24-/m1/s1	1.438	1.634	1	1	1
81-33-4	81334	3804	**perylene-3,4:9,10-tetracarboxydiimide**	3_REACH		perylene-3,4:9,10-tetracarboxydiimide		C24H8N2O4	390.36	O=C1[N-]C(=O)c2ccc3c4ccc5C(=O)[N-]C(=O)c6ccc(c7ccc1c2c37)c4c56	InChI=1/C24H10N2O4/c27-21-13-5-1-9-10-2-6-15-20-16(24(30)26-23(15)29)8-4-12(18(10)20)11-3-7-14(22(28)25-21)19(13)17(9)11/h1-8H,(H2,25,26,27,28,29,30)/p-2	2.713	2.713	1	1	1
81782-77-6	81782776	3814	**4-methyl-3-decen-5-ol**	3_REACH		4-methyl-3-decen-5-ol		C11H22O	170.3	CCCCCC(O)C(=CCC)C	InChI=1/C11H22O/c1-4-6-7-9-11(12)10(3)8-5-2/h8,11-12H,4-7,9H2,1-3H3	3.833	3.833	1	1	1
818-61-1	818611	943	**2-hydroxyethyl acrylate**	3_REACH	2-Propenoic acid, 2-hydroxyethyl ester	2-Hydroxyethyl acrylate	C5H8O3	C5H8O3	116.12	OCCOC(=O)C=C	InChI=1/C5H8O3/c1-2-5(7)8-4-3-6/h2,6H,1,3-4H2	0.179	0.179	1	1	1
82199-12-0	82199120	3820	**N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(2-methoxyphenyl)azo]-3-oxobutyramide**	3_REACH		N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(2-methoxyphenyl)azo]-3-oxobutyramide		C18H17N5O4	367.37	COc1ccccc1N=NC(C(=O)C)C(=O)Nc2ccc3[nH]c(O)nc3c2	InChI=1/C18H17N5O4/c1-10(24)16(23-22-13-5-3-4-6-15(13)27-2)17(25)19-11-7-8-12-14(9-11)21-18(26)20-12/h3-9,16H,1-2H3,(H,19,25)(H2,20,21,26)	2.988	2.988	1	1	1
822-06-0	822060	3822	**hexamethylene diisocyanate**	3_REACH	1,6-Hexamethylene diisocyanate	hexamethylene diisocyanate	C8H12N2O2	C8H14N2O2	168.2	O=C=[NH+]CCCCCC[NH+]=C=O	InChI=1/C8H12N2O2/c11-7-9-5-3-1-2-4-6-10-8-12/h1-6H2/p+2	1.393	1.393	1	1	1
826-36-8	826368	3834	**2,2,6,6-tetramethyl-4-piperidone**	3_REACH	4-Piperidinone, 2,2,6,6-tetramethyl-	2,2,6,6-tetramethyl-4-piperidone	C9H17NO	C9H18NO	155.24	CC1(C)CC(=O)CC(C)(C)[NH2+]1	InChI=1/C9H17NO/c1-8(2)5-7(11)6-9(3,4)10-8/h10H,5-6H2,1-4H3/p+1	-0.518	0.168	1	1	1
82985-35-1	82985351	3839	**bis(trimethoxysilylpropyl)amine**	3_REACH		bis(trimethoxysilylpropyl)amine		C12H32NO6Si2	341.55	CCC([NH2+]C(CC)[Si](OC)(OC)OC)[Si](OC)(OC)OC	InChI=1/C12H31NO6Si2/c1-9-11(20(14-3,15-4)16-5)13-12(10-2)21(17-6,18-7)19-8/h11-13H,9-10H2	4.385	4.387	1	1	1
830-13-7	830137	3840	**cyclododecanone**	3_REACH	Cyclododecanone	cyclododecanone	C12H22O	C12H22O	182.31	O=C1CCCCCCCCCCC1	InChI=1/C12H22O/c13-12-10-8-6-4-2-1-3-5-7-9-11-12/h1-11H2	4.051	4.051	1	1	1
83066-88-0	83066880	950	**(2R)-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoic acid**	3_REACH		(2R)-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoic acid			327.26	CC(C(=O)O)OC1=CC=C(C=C1)OC2=NC=C(C=C2)C(F)(F)F	InChI=1S/C15H12F3NO4/c1-9(14(20)21)22-11-3-5-12(6-4-11)23-13-7-2-10(8-19-13)15(16,17)18/h2-9H,1H3,(H,20,21)/t9-/			1	1	1
83261-15-8	83261158	3844	**isobutyl (S)-2-chloropropionate**	3_REACH		isobutyl (S)-2-chloropropionate		C7H13ClO2	164.63	CC(C)COC(=O)[C@H](C)Cl	InChI=1/C7H13ClO2/c1-5(2)4-10-7(9)6(3)8/h5-6H,4H2,1-3H3/t6-/m0/s1	2.229	2.229	1	1	1
83-32-9	83329	952	**acenaphthene**	3_REACH	Acenaphthene	Acenaphthene	C12H10	C12H10	154.21	C1Cc2cccc3cccc1c23	InChI=1/C12H10/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-6H,7-8H2	3.339	3.339	1	1	1
83-42-1	83421	954	**2-chloro-6-nitrotoluene**	3_REACH	Benzene, 1-chloro-2-methyl-3-nitro	2-Chloro-6-nitrotoluene	C7H6ClNO2	C7H6ClNO2	171.58	Cc1c(Cl)cccc1[N+](=O)[O-]	InChI=1/C7H6ClNO2/c1-5-6(8)3-2-4-7(5)9(10)11/h2-4H,1H3	2.875	2.875	1	1	1
83524-75-8	83524758	3848	**2,9-bis(p-methoxybenzyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone**	3_REACH		2,9-bis(p-methoxybenzyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)tetrone		C40H26N2O6	630.66	COc1ccc(CN2C(=O)c3ccc4c5ccc6C(=O)N(Cc7ccc(OC)cc7)C(=O)c8ccc(c9ccc(C2=O)c3c49)c5c68)cc1	InChI=1/C40H26N2O6/c1-47-23-7-3-21(4-8-23)19-41-37(43)29-15-11-25-27-13-17-31-36-32(40(46)42(39(31)45)20-22-5-9-24(48-2)10-6-22)18-14-28(34(27)36)26-12-16-30(38(41)44)35(29)33(25)26/h3-18H,19-20H2,1-2H3	6.052	6.052	1	1	1
83-73-8	83738	3850	**diiodohydroxyquinoline**	3_REACH	5,7-Diiodo-8-hydroxyquinoline	diiodohydroxyquinoline	C9H5I2NO	C9H5I2NO	396.95	Oc1c(I)cc(I)c2cccnc12	InChI=1/C9H5I2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H	2.93	2.721	1	1	1
83926-73-2	83926732	4796	**4-cyclohexyl-2-methyl-2-butanol**	3_REACH		4-cyclohexyl-2-methyl-2-butanol			170.3	CC(C)(CCC1CCCCC1)O	InChI=1S/C11H22O/c1-11(2,12)9-8-10-6-4-3-5-7-10/h10,12H,3-9H2,1-2H3			1	1	1
84170-74-1	84170741	3857	**(2,2-Dimethyl-1,3-propanediyl)bis(oxy-3,1-propanediyl) bisacrylate**	3_REACH		Poly[oxy(methyl-1,2-ethanediyl)], a,a'-(2,2-dimethyl-1,3-propanediyl)bis[?-[(1-oxo-2-propen-1-yl)oxy]-			328.4	CC(C)(COCCCOC(=O)C=C)COCCCOC(=O)C=C	InChI=1S/C17H28O6/c1-5-15(18)22-11-7-9-20-13-17(3,4)14-21-10-8-12-23-16(19)6-2/h5-6H,1-2,7-14H2,3-4H3			1	1	1
84281-74-3	84281743	3859	**1,3-Benzenediamine, coupled with diazotized m-phenylenediamine, acetates**	3_REACH		1,3-Benzenediamine, coupled with diazotized m-phenylenediamine, acetates			346.41	CC([O-])=O.CC([O-])=O.CC([O-])=O.CC([O-])=O.[NH3+]C1=CC([NH3+])=C(C=C1)\N=N\C1=CC(=CC=C1)\N=N\C1=CC=C([NH3+])C=C1[NH3+]				1	1	1
84418-63-3	84418633	3863	**Isononanoic acid, mixed esters with dipentaerythritol, heptanoic acid and pentaerythritol**	3_REACH		Isononanoic acid, mixed esters with dipentaerythritol, heptanoic acid and pentaerythritol			328.4					1	1	1
84434-11-7	84434117	3864	**ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate**	3_REACH		ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate		C18H21O3P	316.34	CCOP(=O)(C(=O)c1c(C)cc(C)cc1C)c2ccccc2	InChI=1/C18H21O3P/c1-5-21-22(20,16-9-7-6-8-10-16)18(19)17-14(3)11-13(2)12-15(17)4/h6-12H,5H2,1-4H3	4.481	4.481	1	1	1
84583-68-6	84583686	3868	**2-Butenoic acid, 4-oxo-4-(tridecylamino)-, (Z)-, branched**	3_REACH		2-Butenoic acid, 4-oxo-4-(tridecylamino)-, (Z)-branched			297.44	CCCCCCCCCCCCCNC(=O)C=CC(=O)O	InChI=1S/C17H31NO3/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-16(19)13-14-17(20)21/h13-14H,2-12,15H2,1H3,(H,18,19)(H,20			1	1	1
84-65-1	84651	960	**anthraquinone**	3_REACH	9,10-Anthraquinone	Anthraquinone	C14H8O2	C14H8O2	208.22	O=C1c2ccccc2C(=O)c3ccccc13	InChI=1/C14H8O2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H	2.808	2.808	1	1	1
84-66-2	84662	961	**diethyl phthalate**	3_REACH	Diethyl phthalate	Diethyl phthalate	C12H14O4	C12H14O4	222.24	CCOC(=O)c1ccccc1C(=O)OCC	InChI=1/C12H14O4/c1-3-15-11(13)9-7-5-6-8-10(9)12(14)16-4-2/h5-8H,3-4H2,1-2H3	2.238	2.238	1	1	1
84-69-5	84695	962	**diisobutyl phthalate**	3_REACH	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	1,2-Benzenedicarboxylic acid, bis(2-Methylpropyl) ester	C16H22O4	C16H22O4	278.35	CC(C)COC(=O)c1ccccc1C(=O)OCC(C)C	InChI=1/C16H22O4/c1-11(2)9-19-15(17)13-7-5-6-8-14(13)16(18)20-10-12(3)4/h5-8,11-12H,9-10H2,1-4H3	3.924	3.924	1	1	1
84713-17-7	84713177	3874	**2,2,4(or 2,4,4)-trimethylhexanedinitrile**	3_REACH		2,2,4(or 2,4,4)-trimethylhexanedinitrile		C9H14N2	150.23	CC(CC#N)CC(C)(C)C#N	InChI=1/C9H14N2/c1-8(4-5-10)6-9(2,3)7-11/h8H,4,6H2,1-3H3	2.182	2.182	1	1	1
84-74-2	84742	963	**dibutyl phthalate**	3_REACH	Dibutyl phthalate	Di-n-butylorthophthalate	C16H22O4	C16H22O4	278.35	CCCCOC(=O)c1ccccc1C(=O)OCCCC	InChI=1/C16H22O4/c1-3-5-11-19-15(17)13-9-7-8-10-14(13)16(18)20-12-6-4-2/h7-10H,3-6,11-12H2,1-2H3	4.198	4.198	1	1	1
84852-15-3	84852153	964	**Phenol, 4-nonyl-, branched**	3_REACH		4-Nonylphenol, Branched			220.36	CCCCCCCCCC1=CC=CC=C1O	InChI=1S/C15H24O/c1-2-3-4-5-6-7-8-11-14-12-9-10-13-15(14)16/h9-10,12-13,16H,2-8,11H2,1H3			1	1	1
84852-53-9	84852539	3878	**1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]**	3_REACH		1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]		C14H4Br10	971.29	Brc1c(Br)c(Br)c(CCc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c1Br	InChI=1/C14H4Br10/c15-5-3(6(16)10(20)13(23)9(5)19)1-2-4-7(17)11(21)14(24)12(22)8(4)18/h1-2H2	11.744	11.744	0	0	1
85-41-6	85416	965	**phthalimide**	3_REACH	Phthalimide	Phthalimide	C8H5NO2	C8H5NO2	147.13	O=C1NC(=O)c2ccccc12	InChI=1/C8H5NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-4H,(H,9,10,11)	0.656	0.669	1	1	1
85-42-7	85427	3889	**cyclohexane-1,2-dicarboxylic anhydride**	3_REACH	1,2-Cyclohexane dicarboxylic anhydride	cyclohexane-1,2-dicarboxylic anhydride	C8H10O3	C16H20O7	154.16	[O-]C(=O)C1CCCCC1C(=O)OC(=O)C2CCCCC2C(=O)[O-]	InChI=1/C16H22O7/c17-13(18)9-5-1-3-7-11(9)15(21)23-16(22)12-8-4-2-6-10(12)14(19)20/h9-12H,1-8H2,(H,17,18)(H,19,20)/p-2	-0.521	-0.509	1	1	1
85-68-7	85687	968	**benzyl butyl phthalate**	3_REACH	Phthalic acid, benzyl butyl ester	1,2-Benzenedicarboxylic acid, Butylphenylmethyl ester	C19H20O4	C19H20O4	312.37	CCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2	InChI=1/C19H20O4/c1-2-3-13-22-18(20)16-11-7-8-12-17(16)19(21)23-14-15-9-5-4-6-10-15/h4-12H,2-3,13-14H2,1H3	4.452	4.452	1	1	1
85702-79-0	85702790	3896	**6-(isononanoylamino)hexanoic acid, compound with 2,2',2''-nitrilotriethanol (1:1)**	3_REACH		6-(isononanoylamino)hexanoic acid, compound with 2,2',2''-nitrilotriethanol (1:1)			271.4	CC(C)CCCCCC(=O)NCCCCCC(=O)O.C(CO)N(CCO)CCO	InChI=1S/C15H29NO3.C6H15NO3/c1-13(2)9-5-3-6-10-14(17)16-12-8-4-7-11-15(18)19;8-4-1-7(2-5-9)3-6-10/h13H,3-12H2,1-2H3,(H,16,17)(H,18,19);8-10H,1-6H2			1	1	1
85-73-4	85734	3897	**phthalylsulfathiazole**	3_REACH	Phthalylsulfathiazole	phthalylsulfathiazole	C17H13N3O5S2	C17H11N3O5S2	403.44	[O-]C(=O)c1ccccc1C(=O)Nc2ccc(cc2)S(=O)(=O)[N-]c3nccs3	InChI=1/C17H13N3O5S2/c21-15(13-3-1-2-4-14(13)16(22)23)19-11-5-7-12(8-6-11)27(24,25)20-17-18-9-10-26-17/h1-10H,(H,18,19,20,21,22,23)/p-2	0.358	0.359	1	1	1
86261-90-7	86261907	3902	**2-(2-oxoimidazolidin-1-yl)ethyl methacrylate**	3_REACH		2-(2-oxoimidazolidin-1-yl)ethyl methacrylate		C9H14N2O3	198.22	CC(=C)C(=O)OCCN1CCNC1=O	InChI=1/C9H14N2O3/c1-7(2)8(12)14-6-5-11-4-3-10-9(11)13/h1,3-6H2,2H3,(H,10,13)	0.377	0.377	1	1	1
867-13-0	867130	3910	**triethyl phosphonoacetate**	3_REACH		triethyl phosphonoacetate		C8H17O5P	224.19	CCOC(=O)CP(=O)(OCC)OCC	InChI=1/C8H17O5P/c1-4-11-8(9)7-14(10,12-5-2)13-6-3/h4-7H2,1-3H3	0.248	0.248	1	1	1
86-73-7	86737	973	**fluorene**	3_REACH	Fluorene	9H-Fluorene	C13H10	C13H10	166.22	C1c2ccccc2c3ccccc13	InChI=1/C13H10/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)12/h1-8H,9H2	3.492	3.492	1	1	1
86-74-8	86748	974	**carbazole**	3_REACH	Carbazole	Carbazole	C12H9N	C12H9N	167.21	c1ccc2c(c1)[nH]c3ccccc23	InChI=1/C12H9N/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8,13H	3.323	3.323	1	1	1
868-77-9	868779	975	**2-hydroxyethyl methacrylate**	3_REACH	2-Hydroxyethyl methacrylate	2-Methyl-2-propenoic acid, 2-Hydroxyethyl ester	C6H10O3	C6H10O3	130.14	CC(=C)C(=O)OCCO	InChI=1/C6H10O3/c1-5(2)6(8)9-4-3-7/h7H,1,3-4H2,2H3	0.625	0.625	1	1	1
86960-46-5	86960465	3914	**4-(decanoyloxy)benzoic acid**	3_REACH		4-(decanoyloxy)benzoic acid			292.38	CCCCCCCCCC(=O)OC1=CC=C(C=C1)C(=O)O	InChI=1S/C17H24O4/c1-2-3-4-5-6-7-8-9-16(18)21-15-12-10-14(11-13-15)17(19)20/h10-13H,2-9H2,1H3,(H,19,2			1	1	1
872-05-9	872059	3921	**dec-1-ene**	3_REACH	1-Decene	dec-1-ene	C10H20	C10H20	140.27	CCCCCCCCC=C	InChI=1/C10H20/c1-3-5-7-9-10-8-6-4-2/h3H,1,4-10H2,2H3	4.542	4.542	1	1	1
872-36-6	872366	3923	**vinylene carbonate**	3_REACH	1,3-Dioxol-2-one	vinylene carbonate	C3H2O3	C3H2O3	86.046	O=C1OC=CO1	InChI=1/C3H2O3/c4-3-5-1-2-6-3/h1-2H	-0.115	-0.115	1	1	1
872-50-4	872504	977	**1-methyl-2-pyrrolidone**	3_REACH	2-Pyrrolidinone, 1-methyl-	1-Methyl-2-pyrrolidinone	C5H9NO	C5H9NO	99.134	CN1CCCC1=O	InChI=1/C5H9NO/c1-6-4-2-3-5(6)7/h2-4H2,1H3	-0.165	-0.165	1	1	1
87305-03-1	87305031	3924	**(1R,4R,5S)-6,6-Dimethyl-4-(tribromomethyl)-3-oxabicyclo[3.1.0]hexan-2-one**	3_REACH		(1R,4R,5S)-6,6-dimethyl-4-(tribromomethyl)-3-oxabicyclo[3.1.0]hexan-2-one			376.89	CC1([C@@H]2[C@H]1C(=O)O[C@H]2C(Br)(Br)Br)C	InChI=1S/C8H9Br3O2/c1-7(2)3-4(7)6(12)13-5(3)8(9,10)11/h3-5H,1-2H3/t3-,4+,5-/m1/s1			1	1	1
873-32-5	873325	3927	**2-chlorobenzonitrile**	3_REACH	2-Chlorobenzoic acid nitrile	2-chlorobenzonitrile	C7H4ClN	C7H4ClN	137.57	Clc1ccccc1C#N	InChI=1/C7H4ClN/c8-7-4-2-1-3-6(7)5-9/h1-4H	2.373	2.373	1	1	1
87333-22-0	87333220	4632	**methyl 2-(acetylamino)-3-chloropropionate**	3_REACH		NACA			195.599	CC(=O)NC(C(O)Cl)C(=O)OC	InChI=1S/C6H10ClNO4/c1-3(9)8-4(5(7)10)6(11)12-2/h4-5,10H,1-2H3,(H,8,9)/t4-,5?/m0/s1			1	1	1
87-59-2	87592	978	**2,3-xylidine**	3_REACH	Benzenamine, 2,3-dimethyl-	2,3-Dimethylbenzenamine	C8H11N	C8H11N	121.18	Cc1cccc(N)c1C	InChI=1/C8H11N/c1-6-4-3-5-8(9)7(6)2/h3-5H,9H2,1-2H3	2.055	2.055	1	1	1
87-61-6	87616	979	**1,2,3-trichlorobenzene**	3_REACH	Benzene, 1,2,3-trichloro-	1,2,3-Trichlorobenzene	C6H3Cl3	C6H3Cl3	181.45	Clc1cccc(Cl)c1Cl	InChI=1/C6H3Cl3/c7-4-2-1-3-5(8)6(4)9/h1-3H	3.823	3.823	1	1	1
87-62-7	87627	980	**2,6-xylidine**	3_REACH	Benzenamine, 2,6-dimethyl-	2,6-Xylidine	C8H11N	C8H11N	121.18	Cc1cccc(C)c1N	InChI=1/C8H11N/c1-6-4-3-5-7(2)8(6)9/h3-5H,9H2,1-2H3	2.055	2.055	1	1	1
87-99-0	87990	3944	**xylitol**	3_REACH	Xylitol	xylitol	C5H12O5	C5H12O5	152.15	OC[C@@H](O)[C@H](O)[C@@H](O)CO	InChI=1/C5H12O5/c6-1-3(8)5(10)4(9)2-7/h3-10H,1-2H2/t3-,4+,5+	-2.43	-2.43	1	1	1
88-12-0	88120	3948	**1-vinyl-2-pyrrolidone**	3_REACH	N-Vinylpyrrolidone	1-vinyl-2-pyrrolidone	C6H9NO	C6H9NO	111.15	C=CN1CCCC1=O	InChI=1/C6H9NO/c1-2-7-5-3-4-6(7)8/h2H,1,3-5H2	-0.081	-0.081	1	1	1
88150-62-3	88150623	4393	**3-ethyl 5-methyl 4-(2-chlorophenyl)-1,4-dihydro-2-[2-(1,3-dihydro-1,3-dioxo-(2H)isoindol-2-yl)-ethoxymethyl]-6-methyl-3,5-pyridinedicarboxylate**	3_REACH		3-ethyl 5-methyl 4-(2-chlorophenyl)-1,4-dihydro-2-[2-(1,3-dihydro-1,3-dioxo-(2H)isoindol-2-yl)-ethoxymethyl]-6-methyl-3,5-pyridinedicarboxylate			538.99	CCOC(=O)C1=C(NC(=C(C1C2=CC=CC=C2Cl)C(=O)OC)C)COCCN3C(=O)C4=CC=CC=C4C3=O	InChI=1S/C28H27ClN2O7/c1-4-38-28(35)24-21(15-37-14-13-31-25(32)17-9-5-6-10-18(17)26(31)33)30-16(2)22(27(34)36-			1	1	1
88-18-6	88186	983	**2-tert-butylphenol**	3_REACH	Phenol, 2-(1,1-dimethylethyl)-	2-(1,1-Dimethylethyl)phenol	C10H14O	C10H14O	150.22	CC(C)(C)c1ccccc1O	InChI=1/C10H14O/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7,11H,1-3H3	2.988	2.988	1	1	1
88-27-7	88277	3954	**2,6-Di-Tert-butyl-4-(dimethylaminomethyl)phenol**	3_REACH	2,6-Di-tert-butyl-alpha-dimethylamino-p-cresol	2,6-di-tert-butyl-a-dimethylamino-p-cresol	C17H29NO	C17H29NO	263.43	CN(C)Cc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C	InChI=1/C17H29NO/c1-16(2,3)13-9-12(11-18(7)8)10-14(15(13)19)17(4,5)6/h9-10,19H,11H2,1-8H3	4.462	4.437	1	1	1
88374-05-4	88374054	3955	**2-(2-Fluorophenyl)-2-(4-fluorophenyl)oxirane**	3_REACH		Oxirane, 2-(2-fluorophenyl)-2-(4-fluorophenyl)-			232.23	C1C(O1)(C2=CC=C(C=C2)F)C3=CC=CC=C3F	InChI=1S/C14H10F2O/c15-11-7-5-10(6-8-11)14(9-17-14)12-3-1-2-4-13(12)16/h1-8H,9H2			1	1	1
88-44-8	88448	3956	**4-aminotoluene-3-sulphonic acid**	3_REACH		4-aminotoluene-3-sulphonic acid		C7H8NO3S	187.22	Cc1ccc(N)c(c1)S(=O)(=O)[O-]	InChI=1/C7H9NO3S/c1-5-2-3-6(8)7(4-5)12(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)/p-1	-1.343	-1.343	1	1	1
88-45-9	88459	3957	**2,5-diaminobenzenesulphonic acid**	3_REACH		2,5-diaminobenzenesulphonic acid		C6H7N2O3S	188.21	Nc1ccc(N)c(c1)S(=O)(=O)[O-]	InChI=1/C6H8N2O3S/c7-4-1-2-5(8)6(3-4)12(9,10)11/h1-3H,7-8H2,(H,9,10,11)/p-1	-2.576	-2.605	1	1	1
88-51-7	88517	3959	**4-amino-6-chlorotoluene-3-sulphonic acid**	3_REACH		4-amino-6-chlorotoluene-3-sulphonic acid		C7H7ClNO3S	221.66	Cc1cc(c(N)cc1Cl)S(=O)(=O)[O-]	InChI=1/C7H8ClNO3S/c1-4-2-7(13(10,11)12)6(9)3-5(4)8/h2-3H,9H2,1H3,(H,10,11,12)/p-1	-0.679	-0.678	1	1	1
88-60-8	88608	3961	**6-tert-butyl-m-cresol**	3_REACH	Phenol, 2-(1,1-dimethylethyl)-5-methyl-	6-tert-butyl-m-cresol	C11H16O	C11H16O	164.25	Cc1ccc(c(O)c1)C(C)(C)C	InChI=1/C11H16O/c1-8-5-6-9(10(12)7-8)11(2,3)4/h5-7,12H,1-4H3	3.474	3.474	1	1	1
88-72-2	88722	985	**2-nitrotoluene**	3_REACH	Benzene, 1-methyl-2-nitro-	1-Methyl-2-nitrobenzene	C7H7NO2	C7H7NO2	137.14	Cc1ccccc1[N+](=O)[O-]	InChI=1/C7H7NO2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3	2.21	2.21	1	1	1
88-73-3	88733	986	**1-chloro-2-nitrobenzene**	3_REACH	Benzene, 1-chloro-2-nitro-	1-Chloro-2-nitrobenzene	C6H4ClNO2	C6H4ClNO2	157.56	[O-][N+](=O)c1ccccc1Cl	InChI=1/C6H4ClNO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H	2.388	2.388	1	1	1
88-74-4	88744	987	**2-nitroaniline**	3_REACH	o-Nitroaniline	2-Nitroaniline	C6H6N2O2	C6H6N2O2	138.13	Nc1ccccc1[N+](=O)[O-]	InChI=1/C6H6N2O2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H,7H2	0.977	0.977	1	1	1
88-75-5	88755	988	**2-nitrophenol**	3_REACH	Phenol, 2-nitro-	2-Nitrophenol	C6H5NO3	C6H4NO3	139.11	[O-]c1ccccc1[N+](=O)[O-]	InChI=1/C6H5NO3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H/p-1	0.779	1.199	1	1	1
88-85-7	88857	989	**dinoseb**	3_REACH	2-Sec-butyl-4,6-dinitrophenol	Dinoseb	C10H12N2O5	C10H11N2O5	240.22	CCC(C)c1cc(cc(c1[O-])[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C10H12N2O5/c1-3-6(2)8-4-7(11(14)15)5-9(10(8)13)12(16)17/h4-6,13H,3H2,1-2H3/p-1	2.323	2.326	1	1	1
88-99-3	88993	990	**phthalic acid**	3_REACH	1,2-Benzenedicarboxylic acid	Phthalic acid	C8H6O4	C8H4O4	166.13	[O-]C(=O)c1ccccc1C(=O)[O-]	InChI=1/C8H6O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H,(H,9,10)(H,11,12)/p-2	-1.859	-1.661	1	1	1
89182-60-5	89182605	3969	**D-Glucitol, 1-deoxy-1-(formylamino)-**	3_REACH		D-Glucitol, 1-deoxy-1-(formylamino)-			209.2	C(C(C(C(C(CO)O)O)O)O)NC=O	InChI=1S/C7H15NO6/c9-2-5(12)7(14)6(13)4(11)1-8-3-10/h3-7,9,11-14H,1-2H2,(H,8,10)/t4-,5+,6+,7+/m0/s1			1	1	1
89-48-5	89485	3976	**menthyl acetate**	3_REACH	Menthyl acetate	menthyl acetate	C12H22O2	C12H22O2	198.31	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)C	InChI=1/C12H22O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3/t9-,11+,12-/m1/s1	3.158	3.158	1	1	1
89604-91-1	89604911	4680	**3-[2-(1,3-benzothiazol-2-ylsulfanyl)-1-(methoxyimino)-2-oxoethyl]-1,2,4-thiadiazol-5-amine**	3_REACH		[Name not available]			351.43	CON=C(C1=NSC(=N1)N)C(=O)SC2=NC3=CC=CC=C3S2	InChI=1S/C12H9N5O2S3/c1-19-16-8(9-15-11(13)22-17-9)10(18)21-12-14-6-4-2-3-5-7(6)20-12/h2-5H,1H3,(H2,13,15,17)/			1	1	1
89-62-3	89623	991	**2-nitro-p-toluidine**	3_REACH	3-Nitro-4-aminotoluene	4-Methyl-2-nitro-benzenamine	C7H8N2O2	C7H8N2O2	152.16	Cc1ccc(N)c(c1)[N+](=O)[O-]	InChI=1/C7H8N2O2/c1-5-2-3-6(8)7(4-5)9(10)11/h2-4H,8H2,1H3	1.463	1.463	1	1	1
89-63-4	89634	992	**4-chloro-2-nitroaniline**	3_REACH	Aniline, 4-chloro-2-nitro-	4-Chloro-2-nitroaniline	C6H5ClN2O2	C6H5ClN2O2	172.57	Nc1ccc(Cl)cc1[N+](=O)[O-]	InChI=1/C6H5ClN2O2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H,8H2	1.642	1.642	1	1	1
89-72-5	89725	993	**2-sec-butylphenol**	3_REACH	Phenol, 2-(1-methylpropyl)-	o-sec-Butylphenol	C10H14O	C10H14O	150.22	CCC(C)c1ccccc1O	InChI=1/C10H14O/c1-3-8(2)9-6-4-5-7-10(9)11/h4-8,11H,3H2,1-2H3	3.238	3.238	1	1	1
89-83-8	89838	996	**thymol**	3_REACH	Phenol, 5-methyl-2-(1-methylethyl)-	5-Methyl-2-(1-methylethyl)phenol	C10H14O	C10H14O	150.22	CC(C)c1ccc(C)cc1O	InChI=1/C10H14O/c1-7(2)9-5-4-8(3)6-10(9)11/h4-7,11H,1-3H3	3.268	3.267	1	1	1
89-98-5	89985	997	**2-chlorobenzaldehyde**	3_REACH	Benzaldehyde, 2-chloro-	o-Chlorobenzaldehyde	C7H5ClO	C7H5ClO	140.57	Clc1ccccc1C=O	InChI=1/C7H5ClO/c8-7-4-2-1-3-6(7)5-9/h1-5H	2.253	2.253	1	1	1
90-02-8	90028	998	**salicylaldehyde**	3_REACH	Benzaldehyde, 2-hydroxy-	Salicylaldehyde	C7H6O2	C7H6O2	122.12	Oc1ccccc1C=O	InChI=1/C7H6O2/c8-5-6-3-1-2-4-7(6)9/h1-5,9H	1.347	1.326	1	1	1
90-04-0	90040	999	**o-anisidine**	3_REACH	Benzenamine, 2-methoxy-	2-Methoxybenzeneamine	C7H9NO	C7H9NO	123.16	COc1ccccc1N	InChI=1/C7H9NO/c1-9-7-5-3-2-4-6(7)8/h2-5H,8H2,1H3	1.066	1.066	1	1	1
90-05-1	90051	3990	**guaiacol**	3_REACH	Phenol, 2-methoxy-	guaiacol	C7H8O2	C7H8O2	124.14	COc1ccccc1O	InChI=1/C7H8O2/c1-9-7-5-3-2-4-6(7)8/h2-5,8H,1H3	1.571	1.57	1	1	1
90-12-0	90120	1000	**1-methylnaphthalene**	3_REACH	Naphthalene, 1-methyl-	1-Methylnaphthalene	C11H10	C11H10	142.2	Cc1cccc2ccccc12	InChI=1/C11H10/c1-9-5-4-7-10-6-2-3-8-11(9)10/h2-8H,1H3	3.224	3.224	1	1	1
901-44-0	901440	3991	**2,2'-isopropylidenebis(p-phenyleneoxy)diethanol**	3_REACH		2,2'-isopropylidenebis(p-phenyleneoxy)diethanol		C19H24O4	316.4	CC(C)(c1ccc(OCCO)cc1)c2ccc(OCCO)cc2	InChI=1/C19H24O4/c1-19(2,15-3-7-17(8-4-15)22-13-11-20)16-5-9-18(10-6-16)23-14-12-21/h3-10,20-21H,11-14H2,1-2H3	3.151	3.151	1	1	1
9016-45-9	9016459	1001	**Nonylphenol, ethoxylated**	3_REACH		alpha-(Nonylphenyl)-omega-hydroxypoly(oxy-1,2-ethanediyl)			308.462	CCCCCCCCCC1=CC=C(C=C1)OCCOCCO	InChI=1S/C19H32O3/c1-2-3-4-5-6-7-8-9-18-10-12-19(13-11-18)22-17-16-21-15-14-20/h10-13,20H,2-9,14-17H2,1H3			1	1	1
90-17-5	90175	3992	**2,2,2-trichloro-1-phenylethyl acetate**	3_REACH	Benzenemethanol, .alpha.-(trichloromethyl)-, acetate	2,2,2-trichloro-1-phenylethyl acetate	C10H9Cl3O2	C10H9Cl3O2	267.54	CC(=O)OC(c1ccccc1)C(Cl)(Cl)Cl	InChI=1/C10H9Cl3O2/c1-7(14)15-9(10(11,12)13)8-5-3-2-4-6-8/h2-6,9H,1H3	3.23	3.23	1	1	1
90268-23-8	90268238	3995	**Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(p-anisyl and Ph) derivs.**	3_REACH		Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(p-anisyl and Ph) derivs.			659.54	CC(=O)C(C(=O)NC1=CC=CC=C1)N=NC2=C(C=C(C=C2)C3=CC(=C(C=C3)N=NC(C(=O)C)C(=O)NC4=CC=C(C=C4)OC	InChI=1S/C33H28Cl2N6O5/c1-19(42)30(32(44)36-23-7-5-4-6-8-23)40-38-28-15-9-21(17-26(28)34)22-10-16-29(27(35)18-			1	1	1
90268-24-9	90268249	3996	**Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxyphenyl and 2,4-xylyl) derivs.**	3_REACH		Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxyphenyl and 2,4-xylyl) derivs.			752.06	CC1=CC(=C(C=C1)NC(=O)C(C(=O)C)N=NC2=C(C=C(C=C2)C3=CC(=C(C=C3)N=NC(C(=O)C)C(=O)NC4=CC(=C(C=C	InChI=1S/C36H33Cl3N6O6/c1-18-7-10-27(19(2)13-18)40-35(48)33(20(3)46)44-42-28-11-8-22(14-24(28)37)23-9-12-29(25			1	1	1
90-30-2	90302	1002	**N-1-naphthylaniline**	3_REACH	1-Naphthyl phenyl amine	N-Phenyl-1-naphthylamine	C16H13N	C16H13N	219.29	N(c1ccccc1)c2cccc3ccccc23	InChI=1/C16H13N/c1-2-9-14(10-3-1)17-16-12-6-8-13-7-4-5-11-15(13)16/h1-12,17H	4.288	4.288	1	1	1
90-43-7	90437	106	**biphenyl-2-ol**	3_REACH	o-Hydroxybiphenyl	1,1'-Biphenyl-2-ol	C12H10O	C12H10O	170.21	Oc1ccccc1c2ccccc2	InChI=1/C12H10O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9,13H	3.106	3.105	1	1	1
90474-13-8	90474138	4000	**diethyl 1,2-cyclopentanedicarboxylate**	3_REACH		diethyl 1,2-cyclopentanedicarboxylate		C11H18O4	214.26	CCOC(=O)C1CCCC1C(=O)OCC	InChI=1/C11H18O4/c1-3-14-10(12)8-6-5-7-9(8)11(13)15-4-2/h8-9H,3-7H2,1-2H3	1.799	1.799	1	1	1
90498-90-1	90498901	4387	**3,9-bis(2-(3-(3-tert-butyl-4-hydroxy-5-methylphenyl)propionyloxy-1,1-**	3_REACH		3,9-bis(2-(3-(3-tert-butyl-4-hydroxy-5-methylphenyl)propionyloxy-1,1-dimethylethyl)-			740.98	CC1=C(C(=CC(=C1)CCC(=O)OCC(C)(C)C2OCC3(CO2)COC(OC3)C(C)(C)COC(=O)CCC4=CC(=C(C(=C4)C(C)(C)C)O	InChI=1S/C43H64O10/c1-27-17-29(19-31(35(27)46)39(3,4)5)13-15-33(44)48-21-41(9,10)37-50-23-43(24-51-37)25-52-38(			1	1	1
90-51-7	90517	4001	**6-amino-4-hydroxynaphthalene-2-sulphonic acid**	3_REACH		6-amino-4-hydroxynaphthalene-2-sulphonic acid		C10H8NO4S	239.25	Nc1ccc2cc(cc(O)c2c1)S(=O)(=O)[O-]	InChI=1/C10H9NO4S/c11-7-2-1-6-3-8(16(13,14)15)5-10(12)9(6)4-7/h1-5,12H,11H2,(H,13,14,15)/p-1	-1.163	-1.163	1	1	1

90-72-2	90722	4003	**2,4,6-tris(dimethylaminomethyl)phenol**	3_REACH	Phenol, 2,4,6-tris[(dimethylamino)methyl]-	2,4,6-tris(dimethylaminomethyl)phenol	C15H27N3O	C15H27N3O	265.4	CN(C)Cc1cc(CN(C)C)c(O)c(CN(C)C)c1	InChI=1/C15H27N3O/c1-16(2)9-12-7-13(10-17(3)4)15(19)14(8-12)11-18(5)6/h7-8,19H,9-11H2,1-6H3	1.808	1.729	1	1	1
90-80-2	90802	4006	**D-glucono-1,5-lactone**	3_REACH	D-Gluconic acid, δ-lactone	D-glucono-1,5-lactone	C6H10O6	C6H10O6	178.14	OC[C@H]1OC(=O)[C@H](O)[C@@H](O)[C@@H]1O	InChI=1/C6H10O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-5,7-10H,1H2/t2-,3-,4+,5-/m1/s1	-2.23	-2.23	0	1	1
91-15-6	91156	1004	**phthalonitrile**	3_REACH	Phthalonitrile	Phthalonitrile	C8H4N2	C8H4N2	128.14	N#Cc1ccccc1C#N	InChI=1/C8H4N2/c9-5-7-3-1-2-4-8(7)6-10/h1-4H	1.587	1.587	1	1	1
91-17-8	91178	1005	**decahydronaphthalene**	3_REACH	Naphthalene, decahydro-	Decalin	C10H18	C10H18	138.25	C1CCC2CCCCC2C1	InChI=1/C10H18/c1-2-6-10-8-4-3-7-9(10)5-1/h9-10H,1-8H2	3.781	3.781	1	1	1
91-20-3	91203	107	**naphthalene**	3_REACH	Naphthalene	Naphthalene	C10H8	C10H8	128.17	c1ccc2ccccc2c1	InChI=1/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H	2.738	2.738	1	1	1
91-22-5	91225	1006	**quinoline**	3_REACH	Quinoline	Quinoline	C9H7N	C9H7N	129.16	c1ccc2ncccc2c1	InChI=1/C9H7N/c1-2-6-9-8(4-1)5-3-7-10-9/h1-7H	2.016	2.017	1	1	1
91273-04-0	91273040	4271	**1-(N,N-bis(2-ethylhexyl)aminomethyl)-1,2,4-triazole**	3_REACH		1-(N,N-bis(2-ethylhexyl)aminomethyl)-1,2,4-triazole			322.55	CCCCC(CC)CN(CC(CC)CCCC)CN1C=NC=N1	InChI=1S/C19H38N4/c1-5-9-11-18(7-3)13-22(17-23-16-20-15-21-23)14-19(8-4)12-10-6-2/h15-16,18-19H,5-14,17H2,1-4H3			1	1	1
91-57-6	91576	1007	**2-methylnaphthalene**	3_REACH	Naphthalene, 2-methyl-	2-Methylnaphthalene	C11H10	C11H10	142.2	Cc1ccc2ccccc2c1	InChI=1/C11H10/c1-9-6-7-10-4-2-3-5-11(10)8-9/h2-8H,1H3	3.224	3.224	1	1	1
91-64-5	91645	1008	**coumarin**	3_REACH	Coumarin	2H-1-Benzopyran-2-one	C9H6O2	C9H6O2	146.15	O=C1Oc2ccccc2C=C1	InChI=1/C9H6O2/c10-9-6-5-7-3-1-2-4-8(7)11-9/h1-6H	1.899	1.899	1	1	1
91-66-7	91667	1009	**N,N-diethylaniline**	3_REACH	Benzenamine, N,N-diethyl-	N,N-Diethyl-aniline	C10H15N	C10H15N	149.24	CCN(CC)c1ccccc1	InChI=1/C10H15N/c1-3-11(4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3	2.689	2.632	1	1	1
91-68-9	91689	4019	**3-diethylaminophenol**	3_REACH	Phenol, 3-(diethylamino)-	3-diethylaminophenol	C10H15NO	C10H15NO	165.24	CCN(CC)c1cccc(O)c1	InChI=1/C10H15NO/c1-3-11(4-2)9-6-5-7-10(12)8-9/h5-8,12H,3-4H2,1-2H3	2.447	2.441	1	1	1
91-76-9	91769	4021	**6-phenyl-1,3,5-triazine-2,4-diyldiamine**	3_REACH	1,3,5-Triazine-2,4-diamine, 6-phenyl-	6-phenyl-1,3,5-triazine-2,4-diyldiamine	C9H9N5	C9H9N5	187.21	Nc1nc(N)nc(n1)c2ccccc2	InChI=1/C9H9N5/c10-8-12-7(13-9(11)14-8)6-4-2-1-3-5-6/h1-5H,(H4,10,11,12,13,14)	1.114	1.114	1	1	1
919-30-2	919302	4023	**3-aminopropyltriethoxysilane**	3_REACH	1-Propanamine, 3-(triethoxysilyl)-	3-aminopropyltriethoxysilane	C9H23NO3Si	C9H24NO3Si	221.37	CCO[Si](CCC[NH3+])(OCC)OCC	InChI=1/C9H23NO3Si/c1-4-11-14(12-5-2,13-6-3)9-7-8-10/h4-10H2,1-3H3/p+1	1.558	1.561	1	1	1
91-97-4	91974	4025	**3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate**	3_REACH		3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate		C16H12N2O2	264.29	Cc1cc(ccc1N=C=O)c2ccc(N=C=O)c(C)c2	InChI=1/C16H12N2O2/c1-11-7-13(3-5-15(11)17-9-19)14-4-6-16(18-10-20)12(2)8-14/h3-8H,1-2H3	4.041	4.041	1	1	1
923-02-4	923024	4030	**N-(hydroxymethyl)methacrylamide**	3_REACH		N-(hydroxymethyl)methacrylamide		C5H9NO2	115.13	CC(=C)C(=O)NCO	InChI=1/C5H9NO2/c1-4(2)5(8)6-3-7/h7H,1,3H2,2H3,(H,6,8)	-0.04	-0.04	1	1	1
925-21-3	925213	4038	**butyl hydrogen maleate**	3_REACH	2-Butenedioic acid (Z)-, monobutyl ester	butyl hydrogen maleate	C8H12O4	C8H11O4	172.18	CCCCOC(=O)\C=C/C(=O)[O-]	InChI=1/C8H12O4/c1-2-3-6-12-8(11)5-4-7(9)10/h4-5H,2-3,6H2,1H3,(H,9,10)/p-1/b5-4-	0.119	0.119	1	1	1
92-52-4	92524	1012	**biphenyl**	3_REACH	Biphenyl	1,1'-Biphenyl	C12H10	C12H10	154.21	c1ccc(cc1)c2ccccc2	InChI=1/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H	3.348	3.348	1	1	1
92-69-3	92693	1013	**biphenyl-4-ol**	3_REACH	p-Hydroxybiphenyl	4-Biphenylol	C12H10O	C12H10O	170.21	Oc1ccc(cc1)c2ccccc2	InChI=1/C12H10O/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9,13H	3.106	3.103	1	1	1
92-70-6	92706	4045	**3-hydroxy-2-naphthoic acid**	3_REACH	2-Naphthalenecarboxylic acid, 3-hydroxy-	3-hydroxy-2-naphthoic acid	C11H8O3	C11H7O3	188.18	Oc1cc2ccccc2cc1C(=O)[O-]	InChI=1/C11H8O3/c12-10-6-8-4-2-1-3-7(8)5-9(10)11(13)14/h1-6,12H,(H,13,14)/p-1	0.652	0.652	1	1	1
927-07-1	927071	4046	**tert-butyl peroxypivalate**	3_REACH		tert-butyl peroxypivalate		C9H18O3	174.24	CC(C)(C)OOC(=O)C(C)(C)C	InChI=1/C9H18O3/c1-8(2,3)7(10)11-12-9(4,5)6/h1-6H3	2.158	2.158	1	1	1
92-84-2	92842	4051	**phenothiazine**	3_REACH	Phenothiazine	phenothiazine	C12H9NS	C12H9NS	199.28	N1c2ccccc2Sc3ccccc13	InChI=1/C12H9NS/c1-3-7-11-9(5-1)13-10-6-2-4-8-12(10)14-11/h1-8,13H	3.668	3.668	1	1	1
92-88-6	92886	1015	**biphenyl-4,4'-diol**	3_REACH	p,p'-Biphenol	[1,1'-Biphenyl]-4,4'-diol	C12H10O2	C12H10O2	186.21	Oc1ccc(cc1)c2ccc(O)cc2	InChI=1/C12H10O2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8,13-14H	2.864	2.859	1	1	1
928-96-1	928961	1016	**cis-hex-3-en-1-ol**	3_REACH	3-Hexen-1-ol, (Z)-	(Z)-3-Hexen-1-ol	C6H12O	C6H12O	100.16	CC\C=C/CCO	InChI=1/C6H12O/c1-2-3-4-5-6-7/h3-4,7H,2,5-6H2,1H3/b4-3-	1.438	1.438	1	1	1
929-06-6	929066	4053	**2-(2-aminoethoxy)ethanol**	3_REACH	Ethanol, 2-(2-aminoethoxy)-	2-(2-aminoethoxy)ethanol	C4H11NO2	C4H12NO2	105.14	[NH3+]CCOCCO	InChI=1/C4H11NO2/c5-1-3-7-4-2-6/h6H,1-5H2/p+1	-2.323	-2.186	1	1	1
92952-81-3	92952813	4412	**4-[(3-hydroxypropyl)amino]-3-nitrophenol**	3_REACH		4-[(3-hydroxypropyl)amino]-3-nitrophenol			212.21	C1=CC(=C(C=C1O)[N+](=O)[O-])NCCCO	InChI=1S/C9H12N2O4/c12-5-1-4-10-8-3-2-7(13)6-9(8)11(14)15/h2-3,6,10,12-13H,1,4-5H2			1	1	1
93-04-9	93049	1017	**methyl 2-naphthyl ether**	3_REACH	Naphthalene, 2-methoxy-	2-Methoxynaphthalene	C11H10O	C11H10O	158.2	COc1ccc2ccccc2c1	InChI=1/C11H10O/c1-12-11-7-6-9-4-2-3-5-10(9)8-11/h2-8H,1H3	2.722	2.722	1	1	1
931-36-2	931362	4059	**2-ethyl-4-methylimidazole**	3_REACH	1H-Imidazole, 2-ethyl-4-methyl-	2-ethyl-4-methylimidazole	C6H10N2	C6H11N2	110.16	CCc1[nH+]c(C)c[nH]1	InChI=1/C6H10N2/c1-3-6-7-4-5(2)8-6/h4H,3H2,1-2H3,(H,7,8)/p+1	1.158	1.149	1	1	1
93-17-4	93174	4063	**3,4-dimethoxyphenylacetonitrile**	3_REACH	Benzeneacetonitrile, 3,4-dimethoxy	3,4-dimethoxyphenylacetonitrile	C10H11NO2	C10H11NO2	177.2	COc1ccc(CC#N)cc1OC	InChI=1/C10H11NO2/c1-12-9-4-3-8(5-6-11)7-10(9)13-2/h3-4,7H,5H2,1-2H3	1.71	1.71	1	1	1
93-20-9	93209	4065	**2-(2-naphthyloxy)ethanol**	3_REACH	2-(2-Naphthoxy)ethanol	2-(2-naphthyloxy)ethanol	C12H12O2	C12H12O2	188.23	OCCOc1ccc2ccccc2c1	InChI=1/C12H12O2/c13-7-8-14-12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9,13H,7-8H2	2.182	2.182	1	1	1
932-64-9	932649	4066	**1,2-dihydro-5-nitro-3H-1,2,4-triazol-3-one**	3_REACH	3H-1,2,4-Triazol-3-one, 1,2-dihydro-5-nitro-	1,2-dihydro-5-nitro-3H-1,2,4-triazol-3-one	C2H2N4O3	C2H2N4O3	130.07	Oc1nc(n[nH]1)[N+](=O)[O-]	InChI=1/C2H2N4O3/c7-2-3-1(4-5-2)6(8)9/h(H2,3,4,5,7)	0.305	0.305	1	1	1
93413-62-8	93413628	4069	**4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol**	3_REACH		4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol			263.38	CN(C)CC(C1=CC=C(C=C1)O)C2(CCCCC2)O	InChI=1S/C16H25NO2/c1-17(2)12-15(13-6-8-14(18)9-7-13)16(19)10-4-3-5-11-16/h6-9,15,18-19H,3-5,10-12H2,1-2H3			1	1	1
93-58-3	93583	4073	**methyl benzoate**	3_REACH	Benzoic acid, methyl ester	methyl benzoate	C8H8O2	C8H8O2	136.15	COC(=O)c1ccccc1	InChI=1/C8H8O2/c1-10-8(9)7-5-3-2-4-6-7/h2-6H,1H3	1.685	1.685	1	1	1
936-49-2	936492	4076	**2-phenyl-2-imidazoline**	3_REACH		2-phenyl-2-imidazoline		C9H11N2	146.19	C1CN=C([NH2+]1)c2ccccc2	InChI=1/C9H10N2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-5H,6-7H2,(H,10,11)/p+1	1.013	1.013	1	1	1
93-69-6	93696	4079	**1-o-tolylbiguanide**	3_REACH		1-o-tolylbiguanide		C9H13N5	191.24	Cc1ccccc1\N=C(/N)\N=C(N)N	InChI=1/C9H13N5/c1-6-4-2-3-5-7(6)13-9(12)14-8(10)11/h2-5H,1H3,(H6,10,11,12,13,14)	0.469	0.449	1	1	1
93-70-9	93709	4080	**2'-chloroacetoacetanilide**	3_REACH		2'-chloroacetoacetanilide		C10H10ClNO2	211.65	CC(=O)CC(=O)Nc1ccccc1Cl	InChI=1/C10H10ClNO2/c1-7(13)6-10(14)12-9-5-3-2-4-8(9)11/h2-5H,6H2,1H3,(H,12,14)	1.525	1.525	1	1	1
93-92-5	93925	4093	**1-phenylethyl acetate**	3_REACH	Benzenemethanol, .alpha.-methyl-, acetate	1-phenylethyl acetate	C10H12O2	C10H12O2	164.2	CC(OC(=O)C)c1ccccc1	InChI=1/C10H12O2/c1-8(12-9(2)11)10-6-4-3-5-7-10/h3-8H,1-2H3	1.982	1.982	1	1	1
93957-50-7	93957507	4490	**3-[3-(4-fluorophenyl)-1-(1-methylethyl)-1H-indol-2-yl]-(E)-2-propenal**	3_REACH		2-Propenal, 3-[3-(4-fluorophenyl)-1-(1-methylethyl)-1H-indol-2-yl]-, (2E)-			307.37	CC(C)N1C2=CC=CC=C2C(=C1C=CC=O)C3=CC=C(C=C3)F	InChI=1S/C20H18FNO/c1-14(2)22-18-7-4-3-6-17(18)20(19(22)8-5-13-23)15-9-11-16(21)12-10-15/h3-14H,1-2H3/b8-5+			1	1	1
939-97-9	939979	4095	**4-tert-butylbenzaldehyde**	3_REACH		4-tert-butylbenzaldehyde		C11H14O	162.23	CC(C)(C)c1ccc(C=O)cc1	InChI=1/C11H14O/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-8H,1-3H3	2.989	2.989	1	1	1
94-04-2	94042	4096	**vinyl 2-ethylhexanoate**	3_REACH	Vinyl 2-ethylhexanoate	vinyl 2-ethylhexanoate	C10H18O2	C10H18O2	170.25	CCCCC(CC)C(=O)OC=C	InChI=1/C10H18O2/c1-4-7-8-9(5-2)10(11)12-6-3/h6,9H,3-5,7-8H2,1-2H3	3.059	3.059	1	1	1
94050-90-5	94050905	4248	**(R)-2-(4-hydroxyphenoxy)propanoic acid**	3_REACH		(R)-2-(4-hydroxyphenoxy)propanoic acid			182.18	CC(C(=O)O)OC1=CC=C(C=C1)O	InChI=1S/C9H10O4/c1-6(9(11)12)13-8-4-2-7(10)3-5-8/h2-6,10H,1H3,(H,11,12)/t6-/m1/s1			1	1	1
94-13-3	94133	109	**propyl 4-hydroxybenzoate**	3_REACH	N-propyl-p-hydroxy-benzoate	propyl 4-hydroxybenzoate	C10H12O3	C10H12O3	180.2	CCCOC(=O)c1ccc(O)cc1	InChI=1/C10H12O3/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h3-6,11H,2,7H2,1H3	2.315	2.286	1	1	1
941-69-5	941695	4098	**N-phenylmaleimide**	3_REACH	N-Phenylmaleimide	N-phenylmaleimide	C10H7NO2	C10H7NO2	173.17	O=C1C=CC(=O)N1c2ccccc2	InChI=1/C10H7NO2/c12-9-6-7-10(13)11(9)8-4-2-1-3-5-8/h1-7H	1.388	1.388	1	1	1
947-04-6	947046	4110	**dodecane-12-lactam**	3_REACH		dodecane-12-lactam		C12H23NO	197.32	O=C1CCCCCCCCCCCN1	InChI=1/C12H23NO/c14-12-10-8-6-4-2-1-3-5-7-9-11-13-12/h1-11H2,(H,13,14)	3.278	3.278	1	1	1
947-19-3	947193	4112	**hydroxycyclohexyl phenyl ketone**	3_REACH		hydroxycyclohexyl phenyl ketone		C13H16O2	204.27	OC1(CCCCC1)C(=O)c2ccccc2	InChI=1/C13H16O2/c14-12(11-7-3-1-4-8-11)13(15)9-5-2-6-10-13/h1,3-4,7-8,15H,2,5-6,9-10H2	2.825	2.825	1	1	1
94723-86-1	94723861	4485	**2-butanoyl-3-hydroxy-5-(thian-3-yl)cyclohex-2-en-1-one**	3_REACH		625-TRIKETON			282.4	CCCC(=O)C1=C(O)CC(CC1=O)C1CCCSC1	InChI=1/C15H22O3S/c1-2-4-12(16)15-13(17)7-11(8-14(15)18)10-5-3-6-19-9-10/h10-11,17H,2-9H2,1H3 AuxInfo=1/0/N:19,			1	1	1
947753-66-4	947753664	4115	**2-Ethylhexyl-2-cyano-3-(4-methoxyphenyl)-3-phenylprop-2-enoate**	3_REACH		2-Ethylhexyl-2-cyano-3-(4-methoxyphenyl)-3-phenylprop-2-enoate			391.51	CCCCC(CC)COC(=O)C(=C(C1=CC=CC=C1)C2=CC=C(C=C2)OC)C#N	InChI=1S/C25H29NO3/c1-4-6-10-19(5-2)18-29-25(27)23(17-26)24(20-11-8-7-9-12-20)21-13-15-22(28-3)16-14-21/h7-9,11			1	1	1
94-91-7	94917	4116	**N,N'-Bis(salicylidene)-1,2-propanediamine**	3_REACH		a,a'-propylenedinitrilodi-o-cresol		C17H19N2O2	282.35	CC(CN=Cc1ccccc1O)[NH+]=Cc2ccccc2O	InChI=1/C17H18N2O2/c1-13(19-12-15-7-3-5-9-17(15)21)10-18-11-14-6-2-4-8-16(14)20/h2-9,11-13,20-21H,10H2,1H3/p+1	3.308	2.558	1	1	1
94-96-2	94962	1024	**2-ethylhexane-1,3-diol**	3_REACH	1,3-Hexanediol, 2-ethyl-	2-Ethyl-1,3-hexanediol	C8H18O2	C8H18O2	146.23	CCCC(O)C(CC)CO	InChI=1/C8H18O2/c1-3-5-8(10)7(4-2)6-9/h7-10H,3-6H2,1-2H3	1.427	1.427	1	1	1
95-14-7	95147	112	**benzotriazole**	3_REACH	1H-Benzotriazole	benzotriazol	C6H5N3	C6H5N3	119.13	c1ccc2[nH]nnc2c1	InChI=1/C6H5N3/c1-2-4-6-5(3-1)7-9-8-6/h1-4H,(H,7,8,9)	1.434	1.434	1	1	1
95-16-9	95169	113	**benzothiazole**	3_REACH	Benzothiazole	Benzothiazole	C7H5NS	C7H5NS	135.19	c1ccc2scnc2c1	InChI=1/C7H5NS/c1-2-4-7-6(3-1)8-5-9-7/h1-5H	1.913	1.914	1	1	1
95235-30-6	95235306	4398	**4-(4-isopropoxyphenylsulfonyl)phenol**	3_REACH		4-(4-isopropoxyphenylsulfonyl)phenol			292.35	CC(C)OC1=CC=C(C=C1)S(=O)(=O)C2=CC=C(C=C2)O	InChI=1S/C15H16O4S/c1-11(2)19-13-5-9-15(10-6-13)20(17,18)14-7-3-12(16)4-8-14/h3-11,16H,1-2H3			1	1	1
95-31-8	95318	4124	**N-tert-butylbenzothiazole-2-sulphenamide**	3_REACH	2-Benzothiazolesulfenamide, n-(1,1-dimethylethyl)-	N-tert-butylbenzothiazole-2-sulphenamide	C11H14N2S2	C11H14N2S2	238.38	CC(C)(C)NSc1nc2ccccc2s1	InChI=1/C11H14N2S2/c1-11(2,3)13-15-10-12-8-6-4-5-7-9(8)14-10/h4-7,13H,1-3H3	3.436	3.436	1	1	1
95-33-0	95330	4125	**N-cyclohexylbenzothiazole-2-sulfenamide**	3_REACH		N-cyclohexylbenzothiazole-2-sulfenamide		C13H16N2S2	264.42	C1CCC(CC1)NSc2nc3ccccc3s2	InChI=1/C13H16N2S2/c1-2-6-10(7-3-1)15-17-13-14-11-8-4-5-9-12(11)16-13/h4-5,8-10,15H,1-3,6-7H2	4.363	4.363	1	1	1
95-38-5	95385	4126	**2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol**	3_REACH		2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol		C22H42N2O	350.59	CCCCCCCCC=CCCCCCCCC1=NCCN1CCO	InChI=1/C22H42N2O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-23-18-19-24(22)20-21-25/h9-10,25H,2-8,11-21H2,1H3	6.184	6.184	1	1	1
95-48-7	95487	1029	**o-cresol**	3_REACH	Phenol, 2-methyl-	2-Methylphenol	C7H8O	C7H8O	108.14	Cc1ccccc1O	InChI=1/C7H8O/c1-6-4-2-3-5-7(6)8/h2-5,8H,1H3	2.074	2.073	1	1	1
95-49-8	95498	1030	**2-chlorotoluene**	3_REACH	Benzene, 1-chloro-2-methyl-	1-Chloro-2-methylbenzene	C7H7Cl	C7H7Cl	126.59	Cc1ccccc1Cl	InChI=1/C7H7Cl/c1-6-4-2-3-5-7(6)8/h2-5H,1H3	2.98	2.98	1	1	1
95-51-2	95512	1031	**2-chloroaniline**	3_REACH	o-Chloroaniline	2-Chloroaniline	C6H6ClN	C6H6ClN	127.58	Nc1ccccc1Cl	InChI=1/C6H6ClN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2	1.747	1.747	1	1	1
95-53-4	95534	1032	**o-toluidine**	3_REACH	Benzenamine, 2-methyl-	2-Methylbenzenamine	C7H9N	C7H9N	107.16	Cc1ccccc1N	InChI=1/C7H9N/c1-6-4-2-3-5-7(6)8/h2-5H,8H2,1H3	1.569	1.569	1	1	1
95-54-5	95545	1033	**o-phenylenediamine**	3_REACH	1,2-Benzenediamine	1,2-Benzenediamine	C6H8N2	C6H8N2	108.15	Nc1ccccc1N	InChI=1/C6H8N2/c7-5-3-1-2-4-6(5)8/h1-4H,7-8H2	0.336	0.334	1	1	1
95-63-6	95636	1035	**1,2,4-trimethylbenzene**	3_REACH	Benzene, 1,2,4-trimethyl-	1,2,4-Trimethylbenzene	C9H12	C9H12	120.19	Cc1ccc(C)c(C)c1	InChI=1/C9H12/c1-7-4-5-8(2)9(3)6-7/h4-6H,1-3H3	3.288	3.288	1	1	1
95-68-1	95681	1036	**2,4-xylidine**	3_REACH	Benzenamine, 2,4-dimethyl-	2,4-Dimethylaniline	C8H11N	C8H11N	121.18	Cc1ccc(N)c(C)c1	InChI=1/C8H11N/c1-6-3-4-8(9)7(2)5-6/h3-5H,9H2,1-2H3	2.055	2.054	1	1	1
95-74-9	95749	1037	**3-chloro-p-toluidine**	3_REACH	Benzenamine, 3-chloro-4-methyl-	3-Chloro-4-methylbenzenamine	C7H8ClN	C7H8ClN	141.6	Cc1ccc(N)cc1Cl	InChI=1/C7H8ClN/c1-5-2-3-6(9)4-7(5)8/h2-4H,9H2,1H3	2.233	2.233	1	1	1
95-80-7	95807	1039	**4-methyl-m-phenylenediamine**	3_REACH	1,3-Benzenediamine, 4-methyl-	4-Methyl-1,3-benzenediamine	C7H10N2	C7H10N2	122.17	Cc1ccc(N)cc1N	InChI=1/C7H10N2/c1-5-2-3-6(8)4-7(5)9/h2-4H,8-9H2,1H3	0.822	0.566	1	1	1
95-82-9	95829	1040	**2,5-dichloroaniline**	3_REACH	Benzenamine, 2,5-dichloro-	2,5-Dichloroaniline	C6H5Cl2N	C6H5Cl2N	162.02	Nc1cc(Cl)ccc1Cl	InChI=1/C6H5Cl2N/c7-4-1-2-5(8)6(9)3-4/h1-3H,9H2	2.412	2.412	1	1	1
95962-14-4	95962144	4305	**2-(2-(4-methyl-3-cyclohexen-1-yl)propyl)cyclopentanone**	3_REACH		2-(2-(4-methyl-3-cyclohexen-1-yl)propyl)cyclopentanone			220.36	CC1=CCC(CC1)C(C)CC2CCCC2=O	InChI=1S/C15H24O/c1-11-6-8-13(9-7-11)12(2)10-14-4-3-5-15(14)16/h6,12-14H,3-5,7-10H2,1-2H3			1	1	1
95-96-5	95965	4140	**dilactide**	3_REACH	1,4-Dioxane-2,5-dione, 3,6-dimethyl-	dilactide	C6H8O4	C6H8O4	144.13	CC1OC(=O)C(C)OC1=O	InChI=1/C6H8O4/c1-3-5(7)10-4(2)6(8)9-3/h3-4H,1-2H3	0.382	0.382	1	1	1
96-09-3	96093	1044	**(epoxyethyl)benzene**	3_REACH	Oxirane, phenyl-	Phenyloxirane	C8H8O	C8H8O	120.15	C1OC1c2ccccc2	InChI=1/C8H8O/c1-2-4-7(5-3-1)8-6-9-8/h1-5,8H,6H2	1.481	1.481	1	1	1
96-12-8	96128	1045	**1,2-dibromo-3-chloropropane**	3_REACH	Propane, 1,2-dibromo-3-chloro-	Nemagon	C3H5Br2Cl	C3H5Br2Cl	236.35	ClCC(Br)CBr	InChI=1/C3H5Br2Cl/c4-1-3(5)2-6/h3H,1-2H2	2.494	2.494	1	1	1
96-18-4	96184	1047	**1,2,3-trichloropropane**	3_REACH	Propane, 1,2,3-trichloro-	1,2,3-Trichloropropane	C3H5Cl3	C3H5Cl3	147.43	ClCC(Cl)CCl	InChI=1/C3H5Cl3/c4-1-3(6)2-5/h3H,1-2H2	2.205	2.205	1	1	1
96-23-1	96231	1049	**1,3-dichloropropan-2-ol**	3_REACH	2-Propanol, 1,3-dichloro-	1,3-Dichloro-2-propanol	C3H6Cl2O	C3H6Cl2O	128.99	OC(CCl)CCl	InChI=1/C3H6Cl2O/c4-1-3(6)2-5/h3,6H,1-2H2	1.001	1.001	1	1	1
96-24-2	96242	1050	**3-chloropropane-1,2-diol**	3_REACH	1,2-Propanediol, 3-chloro-	3-Chloro-1,2-propanediol	C3H7ClO2	C3H7ClO2	110.54	OCC(O)CCl	InChI=1/C3H7ClO2/c4-1-3(6)2-5/h3,5-6H,1-2H2	-0.204	-0.204	1	1	1
96-29-7	96297	1051	**butanone oxime**	3_REACH	2-Butanone, oxime	2-Butanone, Oxime	C4H9NO	C4H9NO	87.123	CC\C(=N\O)\C	InChI=1/C4H9NO/c1-3-4(2)5-6/h6H,3H2,1-2H3/b5-4+	0.63	0.63	1	1	1
96-31-1	96311	1052	**1,3-dimethylurea**	3_REACH	Urea, N,N'-dimethyl-	1,3-Dimethylurea	C3H8N2O	C3H8N2O	88.112	CNC(=O)NC	InChI=1/C3H8N2O/c1-4-3(6)5-2/h1-2H3,(H2,4,5,6)	-0.631	-0.631	1	1	1
96-45-7	96457	1054	**imidazolidine-2-thione**	3_REACH	2-Imidazolidinethione	Ethylene thiourea	C3H6N2S	C3H6N2S	102.16	S=C1NCCN1	InChI=1/C3H6N2S/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)	0.476	0.476	1	1	1
96-48-0	96480	4148	**Butyrolactone**	3_REACH	γ-Butyrolactone	γ-butyrolactone	C4H6O2	C4H6O2	86.09	O=C1CCCO1	InChI=1/C4H6O2/c5-4-2-1-3-6-4/h1-3H2	0.276	0.276	1	1	1
96-49-1	96491	4149	**ethylene carbonate**	3_REACH	Ethylene carbonate	ethylene carbonate	C3H4O3	C3H4O3	88.062	O=C1OCCO1	InChI=1/C3H4O3/c4-3-5-1-2-6-3/h1-2H2	0.482	0.482	1	1	1
96-67-3	96673	4151	**3-amino-2-hydroxy-5-nitrobenzenesulphonic acid**	3_REACH		3-amino-2-hydroxy-5-nitrobenzenesulphonic acid		C6H4N2O6S	234.19	Nc1cc(cc(c1[O-])S(=O)(=O)[O-])[N+](=O)[O-]	InChI=1/C6H6N2O6S/c7-4-1-3(8(10)11)2-5(6(4)9)15(12,13)14/h1-2,9H,7H2,(H,12,13,14)/p-2	-2.88	-2.185	1	1	1
96-69-5	96695	4152	**6,6'-di-tert-butyl-4,4'-thiodi-m-cresol**	3_REACH	4,4'-Thiobis(3-methyl-6-t-butylphenol)	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	C22H30O2S	C22H30O2S	358.54	Cc1cc(O)c(cc1Sc2cc(c(O)cc2C)C(C)(C)C)C(C)(C)C	InChI=1/C22H30O2S/c1-13-9-17(23)15(21(3,4)5)11-19(13)25-20-12-16(22(6,7)8)18(24)10-14(20)2/h9-12,23-24H,1-8H3	7.237	7.237	1	1	1
96-76-4	96764	4153	**2,4-di-tert-butylphenol**	3_REACH	Phenol, 2,4-bis(1,1-dimethylethyl)-	2,4-di-tert-butylphenol	C14H22O	C14H22O	206.33	CC(C)(C)c1ccc(O)c(c1)C(C)(C)C	InChI=1/C14H22O/c1-13(2,3)10-7-8-12(15)11(9-10)14(4,5)6/h7-9,15H,1-6H3	4.388	4.388	1	1	1
96-93-5	96935	4156	**3-amino-4-hydroxy-5-nitrobenzenesulphonic acid**	3_REACH		3-amino-4-hydroxy-5-nitrobenzenesulphonic acid		C6H4N2O6S	234.19	Nc1cc(cc(c1[O-])[N+](=O)[O-])S(=O)(=O)[O-]	InChI=1/C6H6N2O6S/c7-4-1-3(15(12,13)14)2-5(6(4)9)8(10)11/h1-2,9H,7H2,(H,12,13,14)/p-2	-2.88	-2.175	1	1	1
96-96-8	96968	4157	**2-nitro-p-anisidine**	3_REACH	Benzenamine, 4-methoxy-2-nitro-	2-nitro-p-anisidine	C7H8N2O3	C7H8N2O3	168.15	COc1ccc(N)c(c1)[N+](=O)[O-]	InChI=1/C7H8N2O3/c1-12-5-2-3-6(8)7(4-5)9(10)11/h2-4H,8H2,1H3	0.961	0.961	1	1	1
96-97-9	96979	4158	**5-nitrosalicylic acid**	3_REACH		5-nitrosalicylic acid		C7H3NO5	183.12	[O-]C(=O)c1cc(ccc1[O-])[N+](=O)[O-]	InChI=1/C7H5NO5/c9-6-2-1-4(8(12)13)3-5(6)7(10)11/h1-3,9H,(H,10,11)/p-2	-1.066	-0.364	1	1	1
97-00-7	97007	1056	**1-chloro-2,4-dinitrobenzene**	3_REACH	Benzene, 1-chloro-2,4-dinitro-	1-Chloro-2,4-dinitrobenzene	C6H3ClN2O4	C6H3ClN2O4	202.56	[O-][N+](=O)c1ccc(Cl)c(c1)[N+](=O)[O-]	InChI=1/C6H3ClN2O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H	2.283	2.283	1	1	1
97-39-2	97392	4164	**1,3-di-o-tolylguanidine**	3_REACH	Guanidine, 1,3-di-o-tolyl-	1,3-di-o-tolylguanidine	C15H17N3	C15H19N3	239.32	Cc1ccccc1[NH2+]C(=N)[NH2+]c2ccccc2C	InChI=1/C15H17N3/c1-11-7-3-5-9-13(11)17-15(16)18-14-10-6-4-8-12(14)2/h3-10H,1-2H3,(H3,16,17,18)/p+2	3.588	3.577	1	1	1
97-52-9	97529	4165	**4-nitro-o-anisidine**	3_REACH	Benzenamine, 2-methoxy-4-nitro-	4-nitro-o-anisidine	C7H8N2O3	C7H8N2O3	168.15	COc1cc(ccc1N)[N+](=O)[O-]	InChI=1/C7H8N2O3/c1-12-7-4-5(9(10)11)2-3-6(7)8/h2-4H,8H2,1H3	0.961	0.961	1	1	1
97-53-0	97530	1057	**eugenol**	3_REACH	Eugenol	2-Methoxy-4-(2-propenyl)phenol	C10H12O2	C10H12O2	164.2	COc1cc(CC=C)ccc1O	InChI=1/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3,5-7,11H,1,4H2,2H3	2.579	2.578	1	1	1
97-65-4	97654	4168	**itaconic acid**	3_REACH	Butanedioic acid, methylene-	itaconic acid	C5H6O4	C5H4O4	130.1	[O-]C(=O)CC(=C)C(=O)[O-]	InChI=1/C5H6O4/c1-3(5(8)9)2-4(6)7/h1-2H2,(H,6,7)(H,8,9)/p-2	-2.831	-1.602	1	1	1
976-71-6	976716	4170	**canrenone**	3_REACH		canrenone		C22H28O3	340.46	C[C@]12CCC(=O)C=C1C=C[C@@H]3[C@@H]2CC[C@@]4(C)[C@H]3CC[C@@]45CCC(=O)O5	InChI=1/C22H28O3/c1-20-9-5-15(23)13-14(20)3-4-16-17(20)6-10-21(2)18(16)7-11-22(21)12-8-19(24)25-22/h3-4,13,16-18H,5-12H2,1-2H3/t16-,17+,18+,20+,21+,22-/m1/s1	3.519	3.519	1	1	1
97-74-5	97745	1059	**tetramethylthiuram monosulphide**	3_REACH	Tetramethylthiuram monosulfide	bis(Dimethylthiocarbamyl)sulfide	C6H12N2S3	C6H12N2S3	208.37	CN(C)C(=S)SC(=S)N(C)C	InChI=1/C6H12N2S3/c1-7(2)5(9)11-6(10)8(3)4/h1-4H3	3.614	3.614	1	1	1
97-78-9	97789	4172	**N-lauroylsarcosine**	3_REACH		N-lauroylsarcosine		C15H28NO3	271.4	CCCCCCCCCCCC(=O)N(C)CC(=O)[O-]	InChI=1/C15H29NO3/c1-3-4-5-6-7-8-9-10-11-12-14(17)16(2)13-15(18)19/h3-13H2,1-2H3,(H,18,19)/p-1	2.359	2.368	1	1	1
97-88-1	97881	1061	**butyl methacrylate**	3_REACH	Butyl methacrylate	Butyl methacrylate	C8H14O2	C8H14O2	142.2	CCCCOC(=O)C(=C)C	InChI=1/C8H14O2/c1-4-5-6-10-8(9)7(2)3/h2,4-6H2,1,3H3	2.493	2.493	1	1	1
97-90-5	97905	4175	**ethylene dimethacrylate**	3_REACH	2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester	ethylene dimethacrylate	C10H14O4	C10H14O4	198.22	CC(=C)C(=O)OCCOC(=O)C(=C)C	InChI=1/C10H14O4/c1-7(2)9(11)13-5-6-14-10(12)8(3)4/h1,3,5-6H2,2,4H3	2.148	2.148	1	1	1
98-00-0	98000	1063	**furfuryl alcohol**	3_REACH	2-Furanmethanol	Furfuryl alcohol	C5H6O2	C5H6O2	98.101	OCc1occc1	InChI=1/C5H6O2/c6-4-5-2-1-3-7-5/h1-3,6H,4H2	0.407	0.407	1	1	1
980-26-7	980267	4177	**5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione**	3_REACH		5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione		C22H16N2O2	340.38	Cc1ccc2nc3cc4c(O)c5cc(C)ccc5nc4cc3c(O)c2c1	InChI=1/C22H16N2O2/c1-11-3-5-17-13(7-11)21(25)15-9-20-16(10-19(15)23-17)22(26)14-8-12(2)4-6-18(14)24-20/h3-10H,1-2H3,(H,23,25)(H,24,26)	5.364	5.011	1	1	1
98-07-7	98077	1065	**benzotrichloride**	3_REACH	Benzene, (trichloromethyl)-	(Trichloromethyl)benzene	C7H5Cl3	C7H5Cl3	195.48	ClC(Cl)(Cl)c1ccccc1	InChI=1/C7H5Cl3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H	3.362	3.362	1	1	1
98-09-9	98099	1066	**benzenesulphonyl chloride**	3_REACH	Benzenesulfonyl chloride	Benzenesulfonyl chloride	C6H5ClO2S	C6H5ClO2S	176.62	ClS(=O)(=O)c1ccccc1	InChI=1/C6H5ClO2S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H	1.739	1.739	1	1	1
98-13-5	98135	1067	**trichloro(phenyl)silane**	3_REACH	Phenyl trichlorosilane	Trichlorophenylsilane	C6H5Cl3Si	C6H5Cl3Si	211.55	Cl[Si](Cl)(Cl)c1ccccc1	InChI=1/C6H5Cl3Si/c7-10(8,9)6-4-2-1-3-5-6/h1-5H	4.654	4.654	1	1	1
98-16-8	98168	1068	**3-Trifluoromethylaniline**	3_REACH	Benzenamine, 3-(trifluoromethyl)-	3-Trifluoromethylbenzenamine	C7H6F3N	C7H6F3N	161.13	Nc1cccc(c1)C(F)(F)F	InChI=1/C7H6F3N/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4H,11H2	2.025	2.025	1	1	1
98-17-9	98179	1069	**3-(Trifluoromethyl)phenol**	3_REACH	Phenol, 3-(trifluoromethyl)-	3-(Trifluoromethyl)phenol	C7H5F3O	C7H5F3O	162.11	Oc1cccc(c1)C(F)(F)F	InChI=1/C7H5F3O/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4,11H	2.53	2.486	1	1	1
98-29-3	98293	4181	**4-tert-butylpyrocatechol**	3_REACH	1,2-Benzenediol, 4-(1,1-dimethylethyl)-	4-tert-butylpyrocatechol	C10H14O2	C10H14O2	166.22	CC(C)(C)c1ccc(O)c(O)c1	InChI=1/C10H14O2/c1-10(2,3)7-4-5-8(11)9(12)6-7/h4-6,11-12H,1-3H3	2.746	2.743	1	1	1
98-37-3	98373	4183	**3-amino-4-hydroxybenzenesulphonic acid**	3_REACH		3-amino-4-hydroxybenzenesulphonic acid		C6H6NO4S	189.19	Nc1cc(ccc1O)S(=O)(=O)[O-]	InChI=1/C6H7NO4S/c7-5-3-4(12(9,10)11)1-2-6(5)8/h1-3,8H,7H2,(H,9,10,11)/p-1	-2.071	-2.071	1	1	1
98377-35-6	98377356	4501	**1-(2-chlorophenyl)-1,2-dihydro-5H-tetrazol-5-one**	3_REACH		CPT			196.6	C1=CC=C(C(=C1)N2C(=O)N=NN2)Cl	InChI=1S/C7H5ClN4O/c8-5-3-1-2-4-6(5)12-7(13)9-10-11-12/h1-4H,(H,9,11,13)			1	1	1
98-44-2	98442	4185	**2-aminobenzene-1,4-disulphonic acid**	3_REACH		2-aminobenzene-1,4-disulphonic acid		C6H5NO6S2	253.25	Nc1cc(ccc1S(=O)(=O)[O-])S(=O)(=O)[O-]	InChI=1/C6H7NO6S2/c7-5-3-4(14(8,9)10)1-2-6(5)15(11,12)13/h1-3H,7H2,(H,8,9,10)(H,11,12,13)/p-2	-4.741	-3.876	1	1	1
98-51-1	98511	1071	**4-tert-butyltoluene**	3_REACH	4-Tert-butyltoluene	1-(1,1-Dimethylethyl)-4-methylbenzene	C11H16	C11H16	148.25	Cc1ccc(cc1)C(C)(C)C	InChI=1/C11H16/c1-9-5-7-10(8-6-9)11(2,3)4/h5-8H,1-4H3	3.716	3.716	1	1	1
98-52-2	98522	1072	**4-tert-butylcyclohexanol**	3_REACH	Cyclohexanol, 4-(1,1-dimethylethyl)	4-tert-butylcyclohexanol	C10H20O	C10H20O	156.27	CC(C)(C)C1CCC(O)CC1	InChI=1/C10H20O/c1-10(2,3)8-4-6-9(11)7-5-8/h8-9,11H,4-7H2,1-3H3	2.666	2.666	1	1	1
98-53-3	98533	4186	**4-tert-butylcyclohexanone**	3_REACH	Cyclohexanone, 4-(1,1-dimethylethyl)-	4-tert-butylcyclohexanone	C10H18O	C10H18O	154.25	CC(C)(C)C1CCC(=O)CC1	InChI=1/C10H18O/c1-10(2,3)8-4-6-9(11)7-5-8/h8H,4-7H2,1-3H3	2.48	2.48	1	1	1
98-54-4	98544	1073	**4-tert-butylphenol**	3_REACH	Phenol, p-tert-butyl-	4-(1,1-Dimethylethyl)phenol	C10H14O	C10H14O	150.22	CC(C)(C)c1ccc(O)cc1	InChI=1/C10H14O/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7,11H,1-3H3	2.988	2.987	1	1	1
98-55-5	98555	1074	**p-menth-1-en-8-ol**	3_REACH	3-Cyclohexene-1-methanol, α,α4-trimethyl-	alpha-Terpineol	C10H18O	C10H18O	154.25	CC1=CCC(CC1)C(C)(C)O	InChI=1/C10H18O/c1-8-4-6-9(7-5-8)10(2,3)11/h4,9,11H,5-7H2,1-3H3	2.415	2.415	1	1	1
98-59-9	98599	4188	**tosyl chloride**	3_REACH	Benzenesulfonyl chloride, 4-methyl-	tosyl chloride	C7H7ClO2S	C7H7ClO2S	190.65	Cc1ccc(cc1)S(=O)(=O)Cl	InChI=1/C7H7ClO2S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3	2.225	2.225	1	1	1
98730-04-2	98730042	4191	**2,2-Dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)ethanone**	3_REACH		2,2-Dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)ethanone			260.12	CC1COC2=CC=CC=C2N1C(=O)C(Cl)Cl	InChI=1S/C11H11Cl2NO2/c1-7-6-16-9-5-3-2-4-8(9)14(7)11(15)10(12)13/h2-5,7,10H,6H2,1H3			1	1	1
98-73-7	98737	1075	**4-tert-butylbenzoic acid**	3_REACH	Benzoic acid, p-tert-butyl-	p-tert-Butylbenzoic acid	C11H14O2	C11H13O2	178.23	CC(C)(C)c1ccc(cc1)C(=O)[O-]	InChI=1/C11H14O2/c1-11(2,3)9-6-4-8(5-7-9)10(12)13/h4-7H,1-3H3,(H,12,13)/p-1	1.386	2.491	1	1	1
98-82-8	98828	1076	**cumene**	3_REACH	Benzene, (1-methylethyl)-	Cumene	C9H12	C9H12	120.19	CC(C)c1ccccc1	InChI=1/C9H12/c1-8(2)9-6-4-3-5-7-9/h3-8H,1-2H3	3.024	3.024	1	1	1
98-83-9	98839	4193	**2-phenylpropene**	3_REACH	α-Methylstyrene	2-phenylpropene	C9H10	C9H10	118.18	CC(=C)c1ccccc1	InChI=1/C9H10/c1-8(2)9-6-4-3-5-7-9/h3-7H,1H2,2H3	2.828	2.828	1	1	1
98-85-1	98851	4194	**1-phenylethanol**	3_REACH	Benzenemethanol, α-methyl-	1-phenylethanol	C8H10O	C8H10O	122.17	CC(O)c1ccccc1	InChI=1/C8H10O/c1-7(9)8-5-3-2-4-6-8/h2-7,9H,1H3	1.602	1.602	1	1	1
98-86-2	98862	1077	**acetophenone**	3_REACH	Acetophenone	Acetophenone	C8H8O	C8H8O	120.15	CC(=O)c1ccccc1	InChI=1/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3	1.569	1.569	1	1	1
98967-40-9	98967409	1081	**N-(2,6-difluorophenyl)-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine-2-sulfonamide | Flumetsulam**	3_REACH		Flumetsulam			325.3	CC1=NC2=NC(=NN2C=C1)S(=O)(=O)NC3=C(C=CC=C3F)F	InChI=1S/C12H9F2N5O2S/c1-7-5-6-19-11(15-7)16-12(17-19)22(20,21)18-10-8(13)3-2-4-9(10)14/h2-6,18H,1H3			1	1	1
99-08-1	99081	1082	**3-nitrotoluene**	3_REACH	Benzene, 1-methyl-3-nitro-	1-Methyl-3-nitrobenzene	C7H7NO2	C7H7NO2	137.14	Cc1cccc(c1)[N+](=O)[O-]	InChI=1/C7H7NO2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3	2.21	2.21	1	1	1
99189-60-3	99189603	4198	**2-[1-(2-Amino-2-oxoethyl)cyclohexyl]acetic acid**	3_REACH		Cyclohexaneacetic acid, 1-(2-amino-2-oxoethyl)-			199.25	C1CCC(CC1)(CC(=O)N)CC(=O)O	InChI=1S/C10H17NO3/c11-8(12)6-10(7-9(13)14)4-2-1-3-5-10/h1-7H2,(H2,11,12)(H,13,14)			1	1	1
993-13-5	993135	4203	**methylphosphonic acid**	3_REACH	Methylphosphonic acid	methylphosphonic acid	CH5O3P	CH4O3P	96.022	CP(=O)(O)[O-]	InChI=1/CH5O3P/c1-5(2,3)4/h1H3,(H2,2,3,4)/p-1	-2.057	-2.128	1	1	1
99-34-3	99343	4204	**3,5-dinitrobenzoic acid**	3_REACH	Benzoic acid, 3,5-dinitro-	3,5-dinitrobenzoic acid	C7H4N2O6	C7H3N2O6	212.12	[O-]C(=O)c1cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-]	InChI=1/C7H4N2O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)/p-1	-0.226	-0.226	1	1	1
99-54-7	99547	1087	**1,2-dichloro-4-nitrobenzene**	3_REACH	Benzene, 1,2-dichloro-4-nitro-	1,2-Dichloro-4-nitrobenzene	C6H3Cl2NO2	C6H3Cl2NO2	192	[O-][N+](=O)c1ccc(Cl)c(Cl)c1	InChI=1/C6H3Cl2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H	3.053	3.053	1	1	1
99-55-8	99558	1088	**5-nitro-o-toluidine**	3_REACH	Benzenamine, 2-methyl-5-nitro-	2-Methyl-5-nitrobenzenamine	C7H8N2O2	C7H8N2O2	152.16	Cc1ccc(cc1N)[N+](=O)[O-]	InChI=1/C7H8N2O2/c1-5-2-3-6(9(10)11)4-7(5)8/h2-4H,8H2,1H3	1.463	1.463	1	1	1
99-57-0	99570	4206	**2-amino-4-nitrophenol**	3_REACH		2-amino-4-nitrophenol		C6H6N2O3	154.13	Nc1cc(ccc1O)[N+](=O)[O-]	InChI=1/C6H6N2O3/c7-5-3-4(8(10)11)1-2-6(5)9/h1-3,9H,7H2	0.735	0.734	1	1	1
99591-74-9	99591749	4207	**1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide**	3_REACH		1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide			188.18	C1OS(=O)(=O)CS(=O)(=O)O1	InChI=1S/C2H4O6S2/c3-9(4)2-10(5,6)8-1-7-9/h1-2H2			1	1	1
99607-70-2	99607702	1089	**Heptan-2-yl [(5-chloroquinolin-8-yl)oxy]acetate**	3_REACH		cloquintoceet			335.83	CCCCCC(C)OC(=O)COC1=C2C(=C(C=C1)Cl)C=CC=N2	InChI=1S/C18H22ClNO3/c1-3-4-5-7-13(2)23-17(21)12-22-16-10-9-15(19)14-8-6-11-20-18(14)16/h6,8-11,13H,3-5,7,12H2,			1	1	1
99-62-7	99627	4210	**1,3-diisopropylbenzene**	3_REACH	Benzene, 1,3-bis(1-methylethyl)-	1,3-diisopropylbenzene	C12H18	C12H18	162.28	CC(C)c1cccc(c1)C(C)C	InChI=1/C12H18/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-10H,1-4H3	4.218	4.218	1	1	1
99-63-8	99638	4214	**isophthaloyl dichloride**	3_REACH	1,3-Benzenedicarbonyl dichloride	isophthaloyl dichloride	C8H4Cl2O2	C8H4Cl2O2	203.02	ClC(=O)c1cccc(c1)C(=O)Cl	InChI=1/C8H4Cl2O2/c9-7(11)5-2-1-3-6(4-5)8(10)12/h1-4H	2.242	2.242	1	1	1
99-75-2	99752	4215	**methyl p-toluate**	3_REACH	Benzoic acid, 4-methyl-, methyl ester	methyl p-toluate	C9H10O2	C9H10O2	150.18	COC(=O)c1ccc(C)cc1	InChI=1/C9H10O2/c1-7-3-5-8(6-4-7)9(10)11-2/h3-6H,1-2H3	2.171	2.171	1	1	1
99-76-3	99763	4216	**methyl 4-hydroxybenzoate**	3_REACH	Benzoic acid, 4-hydroxy-, methyl ester	methyl 4-hydroxybenzoate	C8H8O3	C8H8O3	152.15	COC(=O)c1ccc(O)cc1	InChI=1/C8H8O3/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5,9H,1H3	1.443	1.415	1	1	1
99817-36-4	99817364	4328	**2,4-dichloro-3-ethyl-6-nitrophenol**	3_REACH		2,4-dichloro-3-ethyl-6-nitrophenol			236.06	CCC1=C(C=C(C(=C1Cl)O)[N+](=O)[O-])Cl	InChI=1S/C8H7Cl2NO3/c1-2-4-5(9)3-6(11(13)14)8(12)7(4)10/h3,12H,2H2,1H3			1	1	1
99-87-6	99876	1092	**p-cymene**	3_REACH	Benzene, 1-methyl-4-(1-methylethyl)-	1-Methyl-4-(1-methylethyl)benzene	C10H14	C10H14	134.22	CC(C)c1ccc(C)cc1	InChI=1/C10H14/c1-8(2)10-6-4-9(3)5-7-10/h4-8H,1-3H3	3.51	3.51	1	1	1
99-88-7	99887	4221	**4-isopropylaniline**	3_REACH	4-Isopropylaniline	4-isopropylaniline	C9H13N	C9H13N	135.21	CC(C)c1ccc(N)cc1	InChI=1/C9H13N/c1-7(2)8-3-5-9(10)6-4-8/h3-7H,10H2,1-2H3	2.277	2.276	1	1	1
99-93-4	99934	4222	**4'-hydroxyacetophenone**	3_REACH	Acetophenone, 4'-hydroxy-	4'-hydroxyacetophenone	C8H8O2	C8H8O2	136.15	CC(=O)c1ccc(O)cc1	InChI=1/C8H8O2/c1-6(9)7-2-4-8(10)5-3-7/h2-5,10H,1H3	1.327	1.259	1	1	1
99-96-7	99967	1093	**4-hydroxybenzoic acid**	3_REACH	Benzoic acid, 4-hydroxy-	4-Hydroxybenzoic acid	C7H6O3	C7H5O3	138.12	Oc1ccc(cc1)C(=O)[O-]	InChI=1/C7H6O3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H,(H,9,10)/p-1	-0.257	-0.236	1	1	1
99-97-8	99978	1094	**N,N-dimethyl-p-toluidine**	3_REACH	Benzenamine, N,N,4-trimethyl-	N,N-Dimethyl-p-toluidine	C9H13N	C9H13N	135.21	CN(C)c1ccc(C)cc1	InChI=1/C9H13N/c1-8-4-6-9(7-5-8)10(2)3/h4-7H,1-3H3	2.478	2.471	1	1	1
99-99-0	99990	1095	**4-nitrotoluene**	3_REACH	Benzene, 1-methyl-4-nitro-	1-Methyl-4-nitrobenzene	C7H7NO2	C7H7NO2	137.14	Cc1ccc(cc1)[N+](=O)[O-]	InChI=1/C7H7NO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3	2.21	2.21	1	1	1

CAS	CAS_NR	ID	Compound	MW	Emissions	NO(A)EL [mg/kg/day], mixed animal & human	NO(A)EL [mg/kg/day], corrected to animal	Missing Tox?	Genotox alert	Genotox NOEL [mg/kg/day]	Cramer Class	CC NOEL [mg/kg/day]	DDD [mg/kg/day]	TOXTREE & DDD [mg/kg/day]	Final NO(A)EL [mg/kg/day]	TTC derived? [1=Yes]	Drinking water intake [ug/l]	fish uptake [ug/kg]
100986-85-4	100986854	139	Levofloxacin	361.38	1_Pharma			1	0	0	3	0.15	7.142857143	7.142857143	7.14285714	0	25000	434782.6
10238-21-8	10238218	152	Glibenklamid	494.01	1_Pharma			1	0	0	3	0.15	0.1	0.1	0.1	0	350	6087.0
103-90-2	103902	165	paracetamol	151.17	1_Pharma	120	120	0	1	0.00025	1	3	42.85714286	42.85714286	120	0	420000	7304347.8
114-07-8	114078	336	erythromycin	733.94	1_Pharma			1	0	0	3	0.15	14.28571429	14.28571429	14.2857143	0	50000	869565.2
114798-26-4	114798264	1626	Losartan	422.93	1_Pharma	0.005	0.5	0	0	0	3	0.15	0.714285714	0.714285714	0.5	0	1750	30434.8
120-51-4	120514	359	benzyl benzoate	212.25	1_Pharma			1	0	0	1	3	0	3	3	1	10500	182608.7
121-75-5	121755	374	Malathion	330.36	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
123-99-9	123999	1782	azelaic acid	188.22	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
126-07-8	126078	1144	Griseofulvin	352.77	1_Pharma			1	1	0.00025	3	0.15	7.142857143	7.142857143	7.14285714	0	25000	434782.6
127-07-1	127071	411	Hydroxikarbamid	76.057	1_Pharma	0.000266667	0.026666667	0	0	0	3	0.15	0	0.15	0.02666667	0	93.33333333	1623.2
128-13-2	128132	1816	Ursodiol	392.58	1_Pharma			1	0	0	3	0.15	10.71428571	10.71428571	10.7142857	0	37500	652173.9
130-26-7	130267	1834	Clioquinol	305.5	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
13311-84-7	13311847	427	Flutamid	276.22	1_Pharma			1	1	0.00025	3	0.15	10.71428571	10.71428571	10.7142857	0	37500	652173.9
134523-00-5	134523005	431	Atorvastatin	558.65	1_Pharma			1	0	0	3	0.15	0.285714286	0.285714286	0.28571429	0	1000	17391.3
137862-53-4	137862534	442	Valsartan	435.53	1_Pharma			1	0	0	3	0.15	1.142857143	1.142857143	1.14285714	0	4000	69565.2
138402-11-6	138402116	444	Irbesartan	428.55	1_Pharma	4580	4580	0	0	0	3	0.15	2.142857143	2.142857143	4580	0	16030000	278782608.7
139481-59-7	139481597	447	Candesartan	440.47	1_Pharma	3200	3200	0	0	0	3	0.15	0.114285714	0.114285714	3200	0	11200000	194782608.7
15307-86-5	15307865	31	diclofenac	296.15	1_Pharma	2250	2250	0	0	0	3	0.15	1.428571429	1.428571429	2250	0	7875000	136956521.7
15687-27-1	15687271	493	ibuprofen	206.29	1_Pharma			1	0	0	1	3	0.428571429	0.428571429	0.42857143	0	1500	26087.0
20830-75-5	20830755	529	Digoxin	780.95	1_Pharma			1	0	0	3	0.15	0.003571429	0.003571429	0.00357143	0	12.5	217.4
22204-53-1	22204531	539	Naproxen	230.26	1_Pharma			1	0	0	3	0.15	7.142857143	7.142857143	7.14285714	0	25000	434782.6
23593-75-1	23593751	553	Klotrimazol	344.85	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
25812-30-0	25812300	570	Gemfibrozil	250.34	1_Pharma			1	0	0	1	3	17.14285714	17.14285714	17.1428571	0	60000	1043478.3
26787-78-0	26787780	574	amoxicillin	365.41	1_Pharma			1	0	0	3	0.15	14.28571429	14.28571429	14.2857143	0	50000	869565.2
29122-68-7	29122687	44	Atenolol	266.34	1_Pharma			1	0	0	3	0.15	1.071428571	1.071428571	1.07142857	0	3750	65217.4
298-46-4	298464	45	Carbamazepine	236.28	1_Pharma			1	0	0	3	0.15	14.28571429	14.28571429	14.2857143	0	50000	869565.2
3380-34-5	3380345	48	triclosan	289.55	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
37350-58-6	37350586	50	Metoprolol	267.37	1_Pharma	1.6	1.6	0	0	0	3	0.15	0.28	0.28	1.6	0	5600	97391.3
3930-20-9	3930209	51	Sotalol	272.37	1_Pharma			1	0	0	3	0.15	2.285714286	2.285714286	2.28571429	0	8000	139130.4
41859-67-0	41859670	53	Bezafibrat	361.83	1_Pharma			1	0	0	3	0.15	8.571428571	8.571428571	8.57142857	0	30000	521739.1
42200-33-9	42200339	1154	Nadolol	309.41	1_Pharma			1	0	0	3	0.15	2.285714286	2.285714286	2.28571429	0	8000	139130.4
439-14-5	439145	640	Diazepam	284.75	1_Pharma			1	0	0	3	0.15	0.142857143	0.142857143	0.14285714	0	500	8695.7
443-48-1	443481	642	Metronidazol	171.16	1_Pharma			1	1	0.00025	3	0.15	28.57142857	28.57142857	28.5714286	0	100000	1739130.4
49562-28-9	49562289	649	fenofibrate	360.84	1_Pharma	1000	1000	0	0	0	3	0.15	2.857142857	2.857142857	1000	0	3500000	60869565.2
50-02-2	50022	652	Dexametason	392.47	1_Pharma			1	1	0.00025	3	0.15	0.021428571	0.021428571	0.02142857	0	75	1304.3
50-06-6	50066	4945	phenobarbital	232.24	1_Pharma			1	0	0	3	0.15	1.428571429	1.428571429	1.42857143	0	5000	86956.5
50-18-0	50180	1131	Cyclophosphamid	261.09	1_Pharma	375	375	0	1	0.00025	3	0.15	0.714285714	0.714285714	375	0	1312500	22826087.0
50-24-8	50248	656	prednisolone	360.45	1_Pharma			1	1	0.00025	3	0.15	0.142857143	0.142857143	0.14285714	0	500	8695.7
50-28-2	50282	55	estradiol	272.39	1_Pharma	16	16	0	0	0	2	0.91	0.028571429	0.028571429	16	0	56000	973913.0
50-78-2	50782	666	O-acetylsalicylic acid	180.16	1_Pharma	200	200	0	0	0	1	3	42.85714286	42.85714286	200	0	700000	12173913.0
51-21-8	51218	668	fluorouracil	130.08	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
51481-61-9	51481619	1129	Cimetidin	252.35	1_Pharma			1	0	0	3	0.15	11.42857143	11.42857143	11.4285714	0	40000	695652.2
51-52-5	51525	5108	propylthiouracil	170.24	1_Pharma			1	0	0	3	0.15	1.428571429	1.428571429	1.42857143	0	5000	86956.5
525-66-6	525666	59	Propranolol	259.35	1_Pharma			1	0	0	3	0.15	2.285714286	2.285714286	2.28571429	0	8000	139130.4
52645-53-1	52645531	676	Permethrin	391.29	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
53-86-1	53861	1101	Indometacin	357.79	1_Pharma	8000	8000	0	0	0	3	0.15	1.428571429	1.428571429	8000	0	28000000	486956521.7
54-11-5	54115	5067	nicotine	162.24	1_Pharma	25	25	0	0	0	3	0.15	0.428571429	0.428571429	25	0	87500	1521739.1
54-31-9	54319	62	Furosemid	330.75	1_Pharma	50	50	0	0	0	3	0.15	0.571428571	0.571428571	50	0	175000	3043478.3
54739-18-3	54739183	689	Fluvoxamin	318.34	1_Pharma			1	0	0	3	0.15	1.428571429	1.428571429	1.42857143	0	5000	86956.5
54-85-3	54853	691	Isoniazid	137.15	1_Pharma	250	250	0	0	0	3	0.15	4.285714286	4.285714286	250	0	875000	15217391.3
54910-89-3	54910893	692	Fluoxetin	309.33	1_Pharma			1	0	0	3	0.15	0.285714286	0.285714286	0.28571429	0	1000	17391.3
55-56-1	55561	3175	chlorhexidine	505.47	1_Pharma	73.25	73.25	0	0	0	3	0.15	0.428571429	0.428571429	73.25	0	256375	4458695.7
55-63-0	55630	702	glycerol trinitrate	227.09	1_Pharma	0.476666667	0.476666667	0	0	0	3	0.15	0.071428571	0.071428571	0.47666667	0	1668.333333	29014.5
56-75-7	56757	64	Chloramphenicol	323.13	1_Pharma	0.009666667	0.966666667	0	1	0.00025	3	0.15	42.85714286	42.85714286	0.96666667	0	3383.333333	58840.6
56-81-5	56815	716	glycerol	92.094	1_Pharma			1	0	0	1	3	0	3	3	1	10500	182608.7
56-86-0	56860	3214	glutamic acid	147.13	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
57-13-6	57136	719	urea	60.058	1_Pharma			1	0	0	1	3	0	3	3	1	10500	182608.7
57-63-6	57636	724	Etinylestradiol	296.41	1_Pharma	25	25	0	0	0	1	3	0.000357143	0.000357143	25	0	87500	1521739.1
58-08-2	58082	66	caffeine	194.2	1_Pharma	192	192	0	0	0	3	0.15	5.714285714	5.714285714	192	0	672000	11686956.5
58-22-0	58220	67	testosterone	288.43	1_Pharma	40	40	0	1	0.00025	3	0.15	1.714285714	1.714285714	40	0	140000	2434782.6
58-55-9	58559	730	theophylline	180.17	1_Pharma			1	0	0	3	0.15	5.714285714	5.714285714	5.71428571	0	20000	347826.1
59-05-2	59052	732	Metotrexat	454.45	1_Pharma			1	1	0.00025	3	0.15	0.035714286	0.035714286	0.03571429	0	125	2173.9
59277-89-3	59277893	735	Aciklovir	225.21	1_Pharma			1	1	0.00025	3	0.15	57.14285714	57.14285714	57.1428571	0	200000	3478260.9
59467-70-8	59467708	736	Midazolam	325.78	1_Pharma			1	0	0	3	0.15	0.214285714	0.214285714	0.21428571	0	750	13043.5
59-67-6	59676	739	Niacin	123.11	1_Pharma			1	0	0	3	0.15	2.857142857	2.857142857	2.85714286	0	10000	173913.0
59-92-7	59927	745	Levodopa	197.19	1_Pharma			1	0	0	3	0.15	50	50	50	0	175000	3043478.3
60-54-8	60548	754	Tetracycline	444.44	1_Pharma	170	170	0	1	0.00025	3	0.15	14.28571429	14.28571429	170	0	595000	10347826.1
61-68-7	61687	1150	Mefenamic acid	241.29	1_Pharma			1	0	0	3	0.15	14.28571429	14.28571429	14.2857143	0	50000	869565.2
61869-08-7	61869087	760	Paroxetin	329.37	1_Pharma			1	0	0	3	0.15	0.285714286	0.285714286	0.28571429	0	1000	17391.3
62571-86-2	62571862	1103	Captopril	217.29	1_Pharma			1	0	0	3	0.15	0.714285714	0.714285714	0.71428571	0	2500	43478.3
657-24-9	657249	79	Metformin	129.17	1_Pharma			1	0	0	3	0.15	28.57142857	28.57142857	28.5714286	0	100000	1739130.4
66357-35-5	66357355	789	ranitidine	314.41	1_Pharma			1	0	0	3	0.15	4.285714286	4.285714286	4.28571429	0	15000	260869.6
67-20-9	67209	791	Nitrofurantoin	238.16	1_Pharma			1	1	0.00025	3	0.15	2.857142857	2.857142857	2.85714286	0	10000	173913.0
68-35-9	68359	1165	Sulfadiazin	250.28	1_Pharma			1	1	0.00025	3	0.15	8.571428571	8.571428571	8.57142857	0	30000	521739.1
69-53-4	69534	808	ampicillin	349.41	1_Pharma			1	0	0	3	0.15	28.57142857	28.57142857	28.5714286	0	100000	1739130.4
69-72-7	69727	84	salicylic acid	138.12	1_Pharma			1	0	0	1	3	1.428571429	1.428571429	1.42857143	0	5000	86956.5
70458-96-7	70458967	812	Norfloxacin	319.34	1_Pharma	5	5	0	0	0	3	0.15	11.42857143	11.42857143	5	0	17500	304347.8
723-46-6	723466	86	Sulfametoxazol	253.28	1_Pharma			1	1	0.00025	3	0.15	28.57142857	28.57142857	28.5714286	0	100000	1739130.4
72956-09-3	72956093	826	Carvedilol	406.48	1_Pharma			1	1	0.00025	3	0.15	0.535714286	0.535714286	0.53571429	0	1875	32608.7
73334-07-3	73334073	4988	Iopromide	791.11	1_Pharma			1	0	0	3	0.15	714.2857143	714.2857143	714.285714	0	2500000	43478260.9
738-70-5	738705	89	Trimetoprim	290.33	1_Pharma			1	1	0.00025	3	0.15	5.714285714	5.714285714	5.71428571	0	20000	347826.1
76824-35-6	76824356	1100	Famotidine	337.45	1_Pharma			1	0	0	3	0.15	0.571428571	0.571428571	0.57142857	0	2000	34782.6
78439-06-2	78439062	896	Ceftazidim	546.59	1_Pharma			1	1	0.00025	3	0.15	57.14285714	57.14285714	57.1428571	0	200000	3478260.9
79-57-2	79572	923	Oxitetracyklin	460.44	1_Pharma			1	1	0.00025	3	0.15	14.28571429	14.28571429	14.2857143	0	50000	869565.2
79617-96-2	79617962	924	Sertraline	306.24	1_Pharma			1	0	0	3	0.15	0.714285714	0.714285714	0.71428571	0	2500	43478.3
80-08-0	80080	3787	dapsone	248.31	1_Pharma			1	1	0.00025	3	0.15	0.714285714	0.714285714	0.71428571	0	2500	43478.3
81103-11-9	81103119	99	Claritromycin	747.97	1_Pharma			1	0	0	3	0.15	7.142857143	7.142857143	7.14285714	0	25000	434782.6
81-13-0	81130	3802	dexpanthenol	205.26	1_Pharma			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
81-81-2	81812	942	warfarin	308.33	1_Pharma			1	0	0	3	0.15	0.107142857	0.107142857	0.10714286	0	375	6521.7
82419-36-1	82419361	945	Ofloxacin	361.38	1_Pharma			1	0	0	3	0.15	5.714285714	5.714285714	5.71428571	0	20000	347826.1
83799-24-0	83799240	956	Fexofenadine	501.67	1_Pharma			1	0	0	3	0.15	1.714285714	1.714285714	1.71428571	0	6000	104347.8
83905-01-5	83905015	957	Azithromycin	749	1_Pharma			1	0	0	3	0.15	4.285714286	4.285714286	4.28571429	0	15000	260869.6
84057-84-1	84057841	102	Lamotrigin	256.1	1_Pharma			1	1	0.00025	3	0.15	4.285714286	4.285714286	4.28571429	0	15000	260869.6
85721-33-1	85721331	969	Ciprofloxacin	331.35	1_Pharma			1	0	0	3	0.15	0.285714286	0.285714286	0.28571429	0	1000	17391.3
86386-73-4	86386734	970	Fluconazole	306.28	1_Pharma			1	0	0	3	0.15	2.857142857	2.857142857	2.85714286	0	10000	173913.0
88150-42-9	88150429	982	Amlodipine	408.88	1_Pharma			1	0	0	3	0.15	0.071428571	0.071428571	0.07142857	0	250	4347.8
89-57-6	89576	3980	Mesalamine	153.14	1_Pharma			1	1	0.00025	1	3	21.42857143	21.42857143	21.4285714	0	75000	1304347.8
89-78-1	89781	994	menthol	156.27	1_Pharma			1	0	0	1	3	0	3	3	1	10500	182608.7
90-82-4	90824	4008	pseudoephedrine	165.24	1_Pharma			1	0	0	3	0.15	3.428571429	3.428571429	3.42857143	0	12000	208695.7
93413-69-5	93413695	1019	Venlafaxine	277.41	1_Pharma			1	0	0	1	3	1.428571429	1.428571429	1.42857143	0	5000	86956.5
94-09-7	94097	1020	Bensokain	165.19	1_Pharma			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
94-36-0	94360	4103	dibenzoyl peroxide	242.23	1_Pharma			1	0	0	1	3	0	3	3	1	10500	182608.7
97-77-8	97778	1060	disulfiram	296.54	1_Pharma			1	0	0	3	0.15	2.857142857	2.857142857	2.85714286	0	10000	173913.0
98-92-0	98920	1079	nicotinamide	122.13	1_Pharma			1	0	0	1	3	2.142857143	2.142857143	2.14285714	0	7500	130434.8
99-66-1	99661	1091	Valproic acid	144.21	1_Pharma			1	0	0	3	0.15	21.42857143	21.42857143	21.4285714	0	75000	1304347.8
2164-08-1	2164081	114	Lenacil	234.3	2_Pest	12	12	0	0	0	3	0.15	0	0.15	12	0	42000	730434.8
2439-01-2	2439012	5114	Quinomethionate	234.3	2_Pest	0.6	0.6	0	1	0.00025	3	0.15	0	0.00025	0.6	0	2100	36521.7
3813-05-6	3813056	116	Benazolin	243.67	2_Pest	300	300	0	0	0	3	0.15	0	0.15	300	0	1050000	18260869.6
10004-44-1	10004441	121	Hymexazol	99.09	2_Pest	17	17	0	0	0	3	0.15	0	0.15	17	0	59500	1034782.6
100646-51-3	100646513	5117	Quizalofop-P-ethyl	372.81	2_Pest	0.9	0.9	0	0	0	3	0.15	0	0.15	0.9	0	3150	54782.6
101-05-3	101053	141	Anilazine	275.53	2_Pest	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
101200-48-0	101200480	142	Tribenuron-methyl	395.4	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
101205-02-1	101205021	144	Cycloxydim	325.47	2_Pest	7	7	0	1	0.00025	3	0.15	0	0.00025	7	0	24500	426087.0
101-21-3	101213	145	Chlorpropham	213.66	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
101-42-8	101428	147	Fenuron	164.21	2_Pest	500	500	0	0	0	1	3	0	3	500	0	1750000	30434782.6
101463-69-8	101463698	148	Flufenoxuron	488.77	2_Pest	3.8	3.8	0	0	0	3	0.15	0	0.15	3.8	0	13300	231304.3
1014-69-3	1014693	149	Desmetryn	213.31	2_Pest	20	20	0	1	0.00025	3	0.15	0	0.00025	20	0	70000	1217391.3
10265-92-6	10265926	153	Methamidophos	141.13	2_Pest	0.3	0.3	0	0	0	3	0.15	0	0.15	0.3	0	1050	18260.9
102851-06-9	102851069	157	Tau-fluvalinate	502.92	2_Pest	0.5	0.5	0	0	0	3	0.15	0	0.15	0.5	0	1750	30434.8
103055-07-8	103055078	158	Lufenuron	511.15	2_Pest	1.5	1.5	0	0	0	3	0.15	0	0.15	1.5	0	5250	91304.3
10311-84-9	10311849	4894	Dialifos	393.85	2_Pest	3.333333333	3.333333333	0	1	0.00025	3	0.15	0	0.00025	3.33333333	0	11666.66667	202898.6
104040-78-0	104040780	166	Flazasulfuron	407.33	2_Pest	1.3	1.3	0	0	0	3	0.15	0	0.15	1.3	0	4550	79130.4
104206-82-8	104206828	167	Mesotrione	339.32	2_Pest	0.3	0.3	0	1	0.00025	3	0.15	0	0.00025	0.3	0	1050	18260.9
10453-86-8	10453868	1114	Resmethrin	338.45	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
10552-74-6	10552746	176	Nitrothal-isopropyl	295.29	2_Pest			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
10605-21-7	10605217	3	Carbendazim	191.19	2_Pest	2.5	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
1071-83-6	1071836	212	Glyphosate	169.07	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
107534-96-3	107534963	221	Tebuconazole	307.83	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
1085-98-9	1085989	241	Dichlofluanid	333.23	2_Pest	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
110488-70-5	110488705	4906	Dimethomorph	387.86	2_Pest	4.9	4.9	0	0	0	3	0.15	0	0.15	4.9	0	17150	298260.9
1113-02-6	1113026	295	Omethoate	213.19	2_Pest	0.03	0.03	0	0	0	3	0.15	0	0.15	0.03	0	105	1826.1
111479-05-1	111479051	303	Propaquizafop	443.89	2_Pest	1.5	1.5	0	0	0	3	0.15	0	0.15	1.5	0	5250	91304.3
111988-49-9	111988499	6	Thiacloprid	252.73	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
111991-09-4	111991094	319	Nicosulfuron	410.42	2_Pest	199	199	0	0	0	3	0.15	0	0.15	199	0	696500	12113043.5
112281-77-3	112281773	323	Tetraconazole	372.15	2_Pest	0.4	0.4	0	0	0	3	0.15	0	0.15	0.4	0	1400	24347.8
112410-23-8	112410238	328	Tebufenozide	352.48	2_Pest	2	2	0	1	0.00025	3	0.15	0	0.00025	2	0	7000	121739.1
113136-77-9	113136779	334	Cyclanilide	274.1	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
113158-40-0	113158400	335	Fenoxaprop-P	333.73	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
1134-23-2	1134232	4878	Cycloate	215.36	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
114-26-1	114261	337	Propoxur	209.25	2_Pest	3	3	0	0	0	1	3	0	3	3	0	10500	182608.7
114369-43-6	114369436	338	Fenbuconazole	336.83	2_Pest	0.62	0.62	0	0	0	3	0.15	0	0.15	0.62	0	2170	37739.1
115-29-7	115297	4921	Endosulfan	406.93	2_Pest	0.57	0.57	0	0	0	3	0.15	0	0.15	0.57	0	1995	34695.7
115-32-2	115322	340	Dicofol	370.49	2_Pest	15	15	0	0	0	3	0.15	0	0.15	15	0	52500	913043.5
116-06-3	116063	342	Aldicarb	190.27	2_Pest	0.025	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
116255-48-2	116255482	343	Bromuconazole	377.08	2_Pest	0.88	0.88	0	0	0	3	0.15	0	0.15	0.88	0	3080	53565.2
116-29-0	116290	344	Tetradifon	356.05	2_Pest	200	200	0	0	0	3	0.15	0	0.15	200	0	700000	12173913.0
118134-30-8	118134308	347	Spiroxamine	297.48	2_Pest	2.5	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
119168-77-3	119168773	350	Tebufenpyrad	333.87	2_Pest	0.7	0.7	0	0	0	3	0.15	0	0.15	0.7	0	2450	42608.7
119446-68-3	119446683	351	Difenoconazole	406.27	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
1194-65-6	1194656	352	dichlobenil	172.01	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
120068-37-3	120068373	11	Fipronil	437.15	2_Pest	0.02	0.02	0	1	0.00025	3	0.15	0	0.00025	0.02	0	70	1217.4
120-36-5	120365	4895	Dichlorprop	235.07	2_Pest	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
120928-09-8	120928098	366	Fenazaquin	306.41	2_Pest	0.46	0.46	0	0	0	3	0.15	0	0.15	0.46	0	1610	28000.0
121552-61-2	121552612	371	Cyprodinil	225.3	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
122-14-5	122145	378	Fenitrothion	277.24	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
122-34-9	122349	15	Simazine	201.67	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
122-42-9	122429	5107	Propham	179.22	2_Pest	80	80	0	0	0	1	3	0	3	80	0	280000	4869565.2
122453-73-0	122453730	380	Chlorfenapyr	407.63	2_Pest	2.8	2.8	0	0	0	3	0.15	0	0.15	2.8	0	9800	170434.8
122931-48-0	122931480	383	Rimsulfuron	431.45	2_Pest	9.63	9.63	0	0	0	3	0.15	0	0.15	9.63	0	33705	586173.9
123312-89-0	123312890	387	Pymetrozine	217.24	2_Pest	0.57	0.57	0	1	0.00025	3	0.15	0	0.00025	0.57	0	1995	34695.7
123-33-1	123331	389	Maleic hydrazide	112.09	2_Pest	25	25	0	0	0	3	0.15	0	0.15	25	0	87500	1521739.1
125116-23-6	125116236	405	Metconazole	319.84	2_Pest	4	4	0	0	0	3	0.15	0	0.15	4	0	14000	243478.3
126833-17-8	126833178	409	Fenhexamid	302.2	2_Pest	19.2	19.2	0	0	0	3	0.15	0	0.15	19.2	0	67200	1168695.7
13071-79-9	13071799	416	Terbufos	288.43	2_Pest	0.2	0.2	0	0	0	3	0.15	0	0.15	0.2	0	700	12173.9
13121-70-5	13121705	419	Cyhexatin	385.16	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
131341-86-1	131341861	420	Fludioxonil	248.19	2_Pest	37	37	0	0	0	3	0.15	0	0.15	37	0	129500	2252173.9
13171-21-6	13171216	5093	Phosphamidon	299.69	2_Pest	0.05	0.05	0	1	0.00025	3	0.15	0	0.00025	0.05	0	175	3043.5
131807-57-3	131807573	421	Famoxadone	374.4	2_Pest	1.2	1.2	0	1	0.00025	3	0.15	0	0.00025	1.2	0	4200	73043.5
13181-17-4	13181174	422	Bromofenoxim	461.04	2_Pest	0.63	0.63	0	1	0.00025	3	0.15	0	0.00025	0.63	0	2205	38347.8
131860-33-8	131860338	423	Azoxystrobin	403.4	2_Pest	18	18	0	0	0	3	0.15	0	0.15	18	0	63000	1095652.2
13194-48-4	13194484	4930	Ethoprophos	242.34	2_Pest	0.04	0.04	0	0	0	3	0.15	0	0.15	0.04	0	140	2434.8
131983-72-7	131983727	424	Triticonazole	317.82	2_Pest	2.5	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
132-66-1	132661	5059	Naptalam	291.31	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
133-06-2	133062	425	Captan	300.59	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
133-07-3	133073	426	Folpet	296.56	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
13360-45-7	13360457	428	Chlorbromuron	293.56	2_Pest	21	21	0	0	0	3	0.15	0	0.15	21	0	73500	1278260.9
134098-61-6	134098616	429	Fenpyroximate	421.5	2_Pest	0.97	0.97	0	0	0	3	0.15	0	0.15	0.97	0	3395	59043.5
13457-18-6	13457186	432	Pyrazophos	373.37	2_Pest	0.4	0.4	0	0	0	3	0.15	0	0.15	0.4	0	1400	24347.8
13593-03-8	13593038	437	Quinalphos	298.3	2_Pest	0.05	0.05	0	0	0	3	0.15	0	0.15	0.05	0	175	3043.5
136426-54-5	136426545	438	Fluquinconazole	376.18	2_Pest	0.2	0.2	0	0	0	3	0.15	0	0.15	0.2	0	700	12173.9

13684-56-5	13684565	439	Desmedipham	300.32	2_Pest	3.2	3.2	0	0	0	1	3	0	3	3.2	0	11200	194782.6
13684-63-4	13684634	440	Phenmedipham	300.32	2_Pest	25	25	0	0	0	1	3	0	3	25	0	87500	1521739.1
137-26-8	137268	441	thiram	240.43	2_Pest	0.84	0.84	0	0	0	3	0.15	0	0.15	0.84	0	2940	51130.4
138261-41-3	138261413	443	Imidacloprid	255.67	2_Pest	5.7	5.7	0	0	0	3	0.15	0	0.15	5.7	0	19950	346956.5
139-40-2	139402	446	propazine	229.72	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
139528-85-1	139528851	1922	Metosulam	419.27	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
140923-17-7	140923177	453	Iprovalicarb	320.44	2_Pest	1	1	0	1	0.00025	1	3	0	0.00025	1	0	3500	60869.6
141517-21-7	141517217	5178	Trifloxystrobine	408.38	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
141776-32-1	141776321	457	Sulfosulfuron	470.49	2_Pest	24.4	24.4	0	0	0	3	0.15	0	0.15	24.4	0	85400	1485217.4
1420-07-1	1420071	4911	Dinoterb	240.22	2_Pest	0.375	0.375	0	1	0.00025	3	0.15	0	0.00025	0.375	0	1312.5	22826.1
14214-32-5	14214325	4902	Difenoxuron	286.33	2_Pest	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
142459-58-3	142459583	461	Flufenacet	363.34	2_Pest	1.3	1.3	0	0	0	3	0.15	0	0.15	1.3	0	4550	79130.4
143390-89-0	143390890	470	Kresoxim-Methyl	313.35	2_Pest	36	36	0	0	0	3	0.15	0	0.15	36	0	126000	2191304.3
145701-23-1	145701231	473	Florasulam	359.283	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
14816-18-3	14816183	475	Phoxim	298.3	2_Pest	0.38	0.38	0	0	0	3	0.15	0	0.15	0.38	0	1330	23130.4
148-79-8	148798	476	Thiabendazole	201.25	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
149961-52-4	149961524	481	Dimoxystrobin	326.4	2_Pest	4	4	0	0	0	3	0.15	0	0.15	4	0	14000	243478.3
149979-41-9	149979419	5148	Tepraloxydim	341.84	2_Pest	5	5	0	1	0.00025	3	0.15	0	0.00025	5	0	17500	304347.8
150-68-5	150685	482	Monuron	198.66	2_Pest	250	250	0	0	0	3	0.15	0	0.15	250	0	875000	15217391.3
15165-67-0	15165670	4896	Dichlorprop-P	235.07	2_Pest	6	6	0	0	0	3	0.15	0	0.15	6	0	21000	365217.4
15299-99-7	15299997	5058	Napropamide	271.36	2_Pest	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
153719-23-4	153719234	487	Thiamethoxam	291.72	2_Pest	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
15457-05-3	15457053	4958	Fluorodifen	328.2	2_Pest	10	10	0	1	0.00025	3	0.15	0	0.00025	10	0	35000	608695.7
15545-48-9	15545489	32	Chlorotoluron	212.68	2_Pest	4	4	0	0	0	3	0.15	0	0.15	4	0	14000	243478.3
156052-68-5	156052685	490	Zoxamide	336.65	2_Pest	50	50	0	1	0.00025	3	0.15	0	0.00025	50	0	175000	3043478.3
1563-66-2	1563662	491	Carbofuran	221.26	2_Pest	0.01	0.01	0	0	0	3	0.15	0	0.15	0.01	0	35	608.7
1582-09-8	1582098	496	Trifluralin	335.29	2_Pest	2.6	2.6	0	1	0.00025	3	0.15	0	0.00025	2.6	0	9100	158260.9
15972-60-8	15972608	497	Alachlor	269.77	2_Pest	1	1	0	1	0.00025	3	0.15	0	0.00025	1	0	3500	60869.6
161050-58-4	161050584	5021	Methoxyfenozide	368.48	2_Pest	9.8	9.8	0	1	0.00025	3	0.15	0	0.00025	9.8	0	34300	596521.7
161326-34-7	161326347	499	Fenamidone	311.41	2_Pest	3.9	3.9	0	1	0.00025	3	0.15	0	0.00025	3.9	0	13650	237391.3
163515-14-8	163515148	502	Dimethenamid-P	275.8	2_Pest	25	25	0	1	0.00025	3	0.15	0	0.00025	25	0	87500	1521739.1
16672-87-0	16672870	505	Ethephon	144.49	2_Pest	6	6	0	1	0.00025	3	0.15	0	0.00025	6	0	21000	365217.4
16752-77-5	16752775	506	Methomyl	162.21	2_Pest	0.25	0.25	0	0	0	3	0.15	0	0.15	0.25	0	875	15217.4
1689-83-4	1689834	507	Ioxynil	370.91	2_Pest	0.5	0.5	0	0	0	3	0.15	0	0.15	0.5	0	1750	30434.8
1689-84-5	1689845	34	Bromoxynil	276.93	2_Pest	0.3	0.3	0	0	0	3	0.15	0	0.15	0.3	0	1050	18260.9
1698-60-8	1698608	35	Chloridazon	221.65	2_Pest	13	13	0	1	0.00025	3	0.15	0	0.00025	13	0	45500	791304.3
1702-17-6	1702176	509	Clopyralid	192	2_Pest	15	15	0	0	0	3	0.15	0	0.15	15	0	52500	913043.5
173159-57-4	173159574	510	Foramsulfuron	452.45	2_Pest	25	25	0	1	0.00025	3	0.15	0	0.00025	25	0	87500	1521739.1
1746-81-2	1746812	511	Monolinuron	214.65	2_Pest	500	500	0	0	0	3	0.15	0	0.15	500	0	1750000	30434782.6
175013-18-0	175013180	512	Pyraclostrobin	387.83	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
17804-35-2	17804352	513	Benomyl	290.33	2_Pest	13	13	0	0	0	3	0.15	0	0.15	13	0	45500	791304.3
18181-80-1	18181801	4865	Bromopropylate	428.13	2_Pest	3.7	3.7	0	0	0	3	0.15	0	0.15	3.7	0	12950	225217.4
1861-40-1	1861401	514	Benfluralin	335.29	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
18691-97-9	18691979	515	Methabenzthiazuron	221.29	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
188425-85-6	188425856	36	Boscalid	343.21	2_Pest	8	8	0	0	0	3	0.15	0	0.15	8	0	28000	486956.5
1897-45-6	1897456	516	Chlorothalonil	265.92	2_Pest	1.5	1.5	0	0	0	3	0.15	0	0.15	1.5	0	5250	91304.3
19044-88-3	19044883	517	Oryzalin	346.37	2_Pest	5	5	0	1	0.00025	3	0.15	0	0.00025	5	0	17500	304347.8
1912-24-9	1912249	37	atrazine	215.69	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
1918-00-9	1918009	519	Dicamba	221.04	2_Pest	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
1918-16-7	1918167	520	Propachlor	211.69	2_Pest	58	58	0	1	0.00025	3	0.15	0	0.00025	58	0	203000	3530434.8
1929-77-7	1929777	521	Vernolate	203.35	2_Pest	32	32	0	1	0.00025	3	0.15	0	0.00025	32	0	112000	1947826.1
19666-30-9	19666309	526	Oxadiazon	345.23	2_Pest	0.36	0.36	0	0	0	3	0.15	0	0.15	0.36	0	1260	21913.0
1967-16-4	1967164	4870	Chlorbufam	223.66	2_Pest	400	400	0	0	0	3	0.15	0	0.15	400	0	1400000	24347826.1
19937-59-8	19937598	527	Metoxuron	228.68	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2032-65-7	2032657	528	Methiocarb	225.31	2_Pest	1.33	1.33	0	0	0	3	0.15	0	0.15	1.33	0	4655	80956.5
208465-21-8	208465218	5020	Mesosulfuron-methyl	503.51	2_Pest	103	103	0	0	0	3	0.15	0	0.15	103	0	360500	6269565.2
21087-64-9	21087649	531	Metribuzin	214.29	2_Pest	1.3	1.3	0	1	0.00025	3	0.15	0	0.00025	1.3	0	4550	79130.4
2164-17-2	2164172	534	Fluometuron	232.21	2_Pest	0.55	0.55	0	0	0	3	0.15	0	0.15	0.55	0	1925	33478.3
21725-46-2	21725462	535	Cyanazine	240.7	2_Pest	30	30	0	1	0.00025	3	0.15	0	0.00025	30	0	105000	1826087.0
2212-67-1	2212671	537	Molinate	187.31	2_Pest	10	10	0	1	0.00025	3	0.15	0	0.00025	10	0	35000	608695.7
22224-92-6	22224926	540	Fenamiphos	303.36	2_Pest	0.08	0.08	0	0	0	3	0.15	0	0.15	0.08	0	280	4869.6
2275-23-2	2275232	543	Vamidothion	287.34	2_Pest	0.08	8	0	0	0	3	0.15	0	0.15	8	0	28000	486956.5
22781-23-3	22781233	544	Bendiocarb	223.23	2_Pest	0.125	0.125	0	0	0	3	0.15	0	0.15	0.125	0	437.5	7608.7
2303-17-5	2303175	545	Tri-allate	304.67	2_Pest	2.5	2.5	0	1	0.00025	3	0.15	0	0.00025	2.5	0	8750	152173.9
2310-17-0	2310170	546	Phosalone	367.81	2_Pest	0.9	0.9	0	0	0	3	0.15	0	0.15	0.9	0	3150	54782.6
23103-98-2	23103982	547	Pirimicarb	238.29	2_Pest	3.5	3.5	0	1	0.00025	3	0.15	0	0.00025	3.5	0	12250	213043.5
23135-22-0	23135220	549	Oxamyl	219.27	2_Pest	0.1	0.1	0	0	0	3	0.15	0	0.15	0.1	0	350	6087.0
23560-59-0	23560590	551	Heptenophos	250.62	2_Pest	1	1	0	1	0.00025	3	0.15	0	0.00025	1	0	3500	60869.6
23564-05-8	23564058	552	Thiophanate-methyl	342.4	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
23947-60-6	23947606	555	Ethirimol	209.3	2_Pest	3.5	3.5	0	1	0.00025	3	0.15	0	0.00025	3.5	0	12250	213043.5
23950-58-5	23950585	556	Propyzamide	256.13	2_Pest	4.5	4.5	0	0	0	3	0.15	0	0.15	4.5	0	15750	273913.0
24017-47-8	24017478	557	Triazophos	313.32	2_Pest	0.0125	1.25	0	0	0	3	0.15	0	0.15	1.25	0	4375	76087.0
24579-73-5	24579735	5105	Propamocarb	188.27	2_Pest	11.1	11.1	0	1	0.00025	3	0.15	0	0.00025	11.1	0	38850	675652.2
24934-91-6	24934916	564	Chlormephos	234.7	2_Pest			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
25057-89-0	25057890	39	Bentazone	240.28	2_Pest	3.2	3.2	0	0	0	3	0.15	0	0.15	3.2	0	11200	194782.6
25311-71-1	25311711	567	Isofenphos	345.4	2_Pest	0.5	0.5	0	0	0	3	0.15	0	0.15	0.5	0	1750	30434.8
2540-82-1	2540821	569	Formothion	257.27	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
2593-15-9	2593159	571	Etridiazole	247.53	2_Pest	3.1	3.1	0	0	0	3	0.15	0	0.15	3.1	0	10850	188695.7
26225-79-6	26225796	573	Ethofumesate	286.35	2_Pest	60.9	60.9	0	0	0	1	3	0	3	60.9	0	213150	3706956.5
2642-71-9	2642719	40	Azinphos-ethyl	345.38	2_Pest	0.02	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
26644-46-2	26644462	5180	Triforine	434.97	2_Pest	3.4	3.4	0	0	0	3	0.15	0	0.15	3.4	0	11900	206956.5
27314-13-2	27314132	5073	Norflurazon	303.67	2_Pest	1.58	1.58	0	1	0.00025	3	0.15	0	0.00025	1.58	0	5530	96173.9
2764-72-9	2764729	4912	Diquat	184.24	2_Pest	0.19	0.19	0	0	0	3	0.15	0	0.15	0.19	0	665	11565.2
2797-51-5	2797515	5113	Quinoclamine	207.62	2_Pest	0.21	0.21	0	1	0.00025	3	0.15	0	0.00025	0.21	0	735	12782.6
28249-77-6	28249776	580	Thiobencarb	257.78	2_Pest	25	25	0	1	0.00025	3	0.15	0	0.00025	25	0	87500	1521739.1
28434-01-7	28434017	581	Bioresmethrin	338.45	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
29091-05-2	29091052	4910	Dinitramine	322.25	2_Pest	15	15	0	1	0.00025	3	0.15	0	0.00025	15	0	52500	913043.5
29104-30-1	29104301	4847	Benzoximate	363.8	2_Pest	20	20	0	0	0	3	0.15	0	0.15	20	0	70000	1217391.3
2921-88-2	2921882	585	Chlorpyrifos	350.59	2_Pest	0.1	0.1	0	0	0	3	0.15	0	0.15	0.1	0	350	6087.0
29232-93-7	29232937	586	Pirimiphos-Methyl	305.34	2_Pest	0.4	0.4	0	1	0.00025	3	0.15	0	0.00025	0.4	0	1400	24347.8
298-00-0	298000	5086	Parathion-Methyl	263.21	2_Pest	0.25	0.25	0	1	0.00025	3	0.15	0	0.00025	0.25	0	875	15217.4
298-02-2	298022	589	Phorate	260.38	2_Pest	0.3	0.3	0	0	0	3	0.15	0	0.15	0.3	0	1050	18260.9
298-04-4	298044	590	Disulfoton	274.4	2_Pest	0.3	0.3	0	0	0	3	0.15	0	0.15	0.3	0	1050	18260.9
29973-13-5	29973135	593	Ethiofencarb	225.31	2_Pest	10	10	0	0	0	1	3	0	3	10	0	35000	608695.7
300-76-5	300765	594	Naled	380.8	2_Pest	0.2	0.2	0	1	0.00025	3	0.15	0	0.00025	0.2	0	700	12173.9
301-12-2	301122	595	Oxydemeton-methyl	246.28	2_Pest	0.03	0.03	0	0	0	3	0.15	0	0.15	0.03	0	105	1826.1
30560-19-1	30560191	596	Acephate	183.17	2_Pest	0.25	25	0	0	0	3	0.15	0	0.15	25	0	87500	1521739.1
3060-89-7	3060897	598	Metobromuron	259.11	2_Pest	0.8	0.8	0	0	0	3	0.15	0	0.15	0.8	0	2800	48695.7
314-40-9	314409	4864	Bromacil	261.13	2_Pest	12.5	12.5	0	0	0	3	0.15	0	0.15	12.5	0	43750	760869.6
330-54-1	330541	46	diuron	233.1	2_Pest	0.66	0.66	0	0	0	3	0.15	0	0.15	0.66	0	2310	40173.9
330-55-2	330552	602	Linuron	249.1	2_Pest	0.208333333	0.208333333	0	0	0	3	0.15	0	0.15	0.20833333	0	729.1666667	12681.2
33089-61-1	33089611	603	Amitraz	293.42	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
333-41-5	333415	47	Diazinon	304.35	2_Pest	0.02	0.02	0	0	0	3	0.15	0	0.15	0.02	0	70	1217.4
3347-22-6	3347226	604	Dithianon	296.33	2_Pest	1	1	0	1	0.00025	3	0.15	0	0.00025	1	0	3500	60869.6
33629-47-9	33629479	605	Butralin	295.34	2_Pest	6	6	0	1	0.00025	3	0.15	0	0.00025	6	0	21000	365217.4
33693-04-8	33693048	606	Terbumeton	225.3	2_Pest	7.5	7.5	0	1	0.00025	3	0.15	0	0.00025	7.5	0	26250	456521.7
33820-53-0	33820530	4982	Isopropalin	309.37	2_Pest	15	15	0	1	0.00025	3	0.15	0	0.00025	15	0	52500	913043.5
34014-18-1	34014181	607	Tebuthiuron	228.32	2_Pest	20	20	0	0	0	3	0.15	0	0.15	20	0	70000	1217391.3
34123-59-6	34123596	49	Isoproturon	206.29	2_Pest	3.1	3.1	0	0	0	1	3	0	3	3.1	0	10850	188695.7
34256-82-1	34256821	608	Acetochlor	269.77	2_Pest	0.333333333	0.333333333	0	1	0.00025	3	0.15	0	0.00025	0.33333333	0	1166.666667	20289.9
34681-10-2	34681102	610	Butocarboxim	190.27	2_Pest	33.33333333	33.33333333	0	0	0	3	0.15	0	0.15	33.3333333	0	116666.6667	2028985.5
35367-38-5	35367385	612	Diflubenzuron	310.69	2_Pest	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
35554-44-0	35554440	614	Imazalil	297.19	2_Pest	2.5	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
36734-19-7	36734197	616	Iprodione	330.17	2_Pest	2.033333333	2.033333333	0	0	0	3	0.15	0	0.15	2.03333333	0	7116.666667	123768.1
3689-24-5	3689245	5137	Sulfotep	322.32	2_Pest	0.1	0.1	0	0	0	3	0.15	0	0.15	0.1	0	350	6087.0
3878-19-1	3878191	622	Fuberidazole	184.2	2_Pest	0.72	0.72	0	0	0	3	0.15	0	0.15	0.72	0	2520	43826.1
39515-41-8	39515418	624	Fenpropathrin	349.43	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
39807-15-3	39807153	626	Oxadiargyl	341.2	2_Pest	0.8	0.8	0	0	0	3	0.15	0	0.15	0.8	0	2800	48695.7
40487-42-1	40487421	628	Pendimethalin	281.32	2_Pest	12.5	12.5	0	1	0.00025	3	0.15	0	0.00025	12.5	0	43750	760869.6
41083-11-8	41083118	630	Azocyclotin	436.21	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
41394-05-2	41394052	632	Metamitron	202.22	2_Pest	3	3	0	1	0.00025	3	0.15	0	0.00025	3	0	10500	182608.7
41483-43-6	41483436	633	Bupirimate	316.43	2_Pest	5	5	0	1	0.00025	3	0.15	0	0.00025	5	0	17500	304347.8
42576-02-3	42576023	4851	Bifenox	342.13	2_Pest	16	16	0	1	0.00025	3	0.15	0	0.00025	16	0	56000	973913.0
42874-03-3	42874033	638	Oxyfluorfen	361.7	2_Pest	2.17	2.17	0	1	0.00025	3	0.15	0	0.00025	2.17	0	7595	132087.0
43121-43-3	43121433	639	Triadimefon	293.76	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
4685-14-7	4685147	5085	Paraquat	186.26	2_Pest	0.5	0.5	0	0	0	3	0.15	0	0.15	0.5	0	1750	30434.8
470-90-6	470906	1098	Chlorfenvinphos	359.57	2_Pest	0.05	0.05	0	1	0.00025	3	0.15	0	0.00025	0.05	0	175	3043.5
49866-87-7	49866877	4903	Difenzoquat	249.34	2_Pest	25	25	0	0	0	3	0.15	0	0.15	25	0	87500	1521739.1
50471-44-8	50471448	661	Vinclozolin	286.12	2_Pest	6	6	0	0	0	3	0.15	0	0.15	6	0	21000	365217.4
50563-36-5	50563365	663	Dimethachlor	255.75	2_Pest	10	10	0	1	0.00025	3	0.15	0	0.00025	10	0	35000	608695.7
50594-66-6	50594666	4828	Acifluorfen	361.66	2_Pest	1	1	0	1	0.00025	3	0.15	0	0.00025	1	0	3500	60869.6
51218-45-2	51218452	56	Metolachlor	283.8	2_Pest	15	15	0	1	0.00025	3	0.15	0	0.00025	15	0	52500	913043.5
51276-47-2	51276472	4969	Glufosinate	181.13	2_Pest	0.4	0.4	0	0	0	3	0.15	0	0.15	0.4	0	1400	24347.8
51630-58-1	51630581	1111	Fenvalerate	419.91	2_Pest	1.7	1.7	0	0	0	3	0.15	0	0.15	1.7	0	5950	103478.3
51707-55-2	51707552	5158	Thidiazuron	220.26	2_Pest	25	25	0	0	0	3	0.15	0	0.15	25	0	87500	1521739.1
52315-07-8	52315078	1099	Cypermethrin	416.31	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
5234-68-4	5234684	673	Carboxin	235.31	2_Pest	0.82	0.82	0	1	0.00025	3	0.15	0	0.00025	0.82	0	2870	49913.0
52-68-6	52686	677	Trichlorfon	257.44	2_Pest	13.2	13.2	0	1	0.00025	3	0.15	0	0.00025	13.2	0	46200	803478.3
52888-80-9	52888809	60	Prosulfocarb	251.39	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
52918-63-5	52918635	679	Deltamethrin	505.22	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
53112-28-0	53112280	681	Pyrimethanil	199.26	2_Pest	5.4	5.4	0	0	0	3	0.15	0	0.15	5.4	0	18900	328695.7
55179-31-2	55179312	693	Bitertanol	337.43	2_Pest	0.1	0.1	0	0	0	3	0.15	0	0.15	0.1	0	350	6087.0
55219-65-3	55219653	694	Triadimenol	295.77	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
55283-68-6	55283686	695	Ethalfluralin	333.27	2_Pest	4.2	4.2	0	1	0.00025	3	0.15	0	0.00025	4.2	0	14700	255652.2
55285-14-8	55285148	696	Carbosulfan	380.55	2_Pest	0.1	0.1	0	0	0	3	0.15	0	0.15	0.1	0	350	6087.0
55335-06-3	55335063	698	Triclopyr	256.47	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
55-38-9	55389	699	Fenthion	278.33	2_Pest	0.09	0.09	0	0	0	3	0.15	0	0.15	0.09	0	315	5478.3
55512-33-9	55512339	701	Pyridate	378.92	2_Pest	3.6	3.6	0	0	0	3	0.15	0	0.15	3.6	0	12600	219130.4
555-37-3	555373	5063	Neburon	275.18	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5598-13-0	5598130	709	Chlorpyrifos-Methyl	322.54	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
563-12-2	563122	711	Ethion	384.48	2_Pest	0.2	0.2	0	0	0	3	0.15	0	0.15	0.2	0	700	12173.9
56-38-2	56382	713	Parathion	291.26	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
57018-04-9	57018049	718	Tolclofos-methyl	301.13	2_Pest	6.4	6.4	0	0	0	3	0.15	0	0.15	6.4	0	22400	389565.2
57646-30-7	57646307	725	Furalaxyl	301.34	2_Pest	1.8	1.8	0	0	0	3	0.15	0	0.15	1.8	0	6300	109565.2
57837-19-1	57837191	726	Metalaxyl	279.34	2_Pest	8	8	0	0	0	1	3	0	3	8	0	28000	486956.5
57966-95-7	57966957	727	Cymoxanil	198.19	2_Pest	1.3	1.3	0	0	0	3	0.15	0	0.15	1.3	0	4550	79130.4
58138-08-2	58138082	5176	Tridiphane	320.43	2_Pest	3	3	0	1	0.00025	3	0.15	0	0.00025	3	0	10500	182608.7
58-89-9	58899	68	Lindane	290.83	2_Pest	0.47	0.47	0	0	0	3	0.15	0	0.15	0.47	0	1645	28608.7
5902-51-2	5902512	5149	Terbacil	216.67	2_Pest	6.25	6.25	0	0	0	3	0.15	0	0.15	6.25	0	21875	380434.8
5915-41-3	5915413	70	Terbuthylazine	229.72	2_Pest	0.35	0.35	0	1	0.00025	3	0.15	0	0.00025	0.35	0	1225	21304.3
60168-88-9	60168889	747	Fenarimol	331.2	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
60207-90-1	60207901	748	Propiconazole	342.23	2_Pest	1.25	1.25	0	0	0	3	0.15	0	0.15	1.25	0	4375	76087.0
60-51-5	60515	753	Dimethoate	229.26	2_Pest	0.04	0.04	0	0	0	3	0.15	0	0.15	0.04	0	140	2434.8
61213-25-0	61213250	4960	Flurochloridone	312.12	2_Pest	3.9	3.9	0	1	0.00025	3	0.15	0	0.00025	3.9	0	13650	237391.3
62-73-7	62737	4897	Dichlorvos	220.98	2_Pest			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
62850-32-2	62850322	4946	Fenothiocarb	253.37	2_Pest	0.75	0.75	0	1	0.00025	3	0.15	0	0.00025	0.75	0	2625	45652.2
63-25-2	63252	76	Carbaryl	201.23	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
63284-71-9	63284719	773	Nuarimol	314.75	2_Pest	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
640-15-3	640153	775	Thiometon	246.35	2_Pest	0.35	0.35	0	0	0	3	0.15	0	0.15	0.35	0	1225	21304.3
64902-72-3	64902723	783	Chlorsulfuron	357.78	2_Pest	20	20	0	0	0	3	0.15	0	0.15	20	0	70000	1217391.3
66215-27-8	66215278	4881	Cypromazine	166.19	2_Pest	5.74	5.74	0	1	0.00025	3	0.15	0	0.00025	5.74	0	20090	349391.3
66230-04-4	66230044	786	Esfenvalerate	419.91	2_Pest	1.75	1.75	0	0	0	3	0.15	0	0.15	1.75	0	6125	106521.7
66246-88-6	66246886	787	Penconazole	284.19	2_Pest	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
66332-96-5	66332965	4961	Flutolanil	323.32	2_Pest	8.7	8.7	0	0	0	3	0.15	0	0.15	8.7	0	30450	529565.2
668-34-8	668348	790	Fentin	350.01	2_Pest	0.4	0.4	0	0	0	3	0.15	0	0.15	0.4	0	1400	24347.8
66841-25-6	66841256	5167	Tralomethrin	665.04	2_Pest	0.75	0.75	0	1	0.00025	3	0.15	0	0.00025	0.75	0	2625	45652.2
67129-08-2	67129082	81	Metazachlor	277.76	2_Pest	8.5	8.5	0	1	0.00025	3	0.15	0	0.00025	8.5	0	29750	517391.3
67306-00-7	67306007	792	Fenpropidin	273.46	2_Pest	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
67375-30-8	67375308	1108	alpha-Cypermethrin	416.31	2_Pest	1.5	1.5	0	0	0	3	0.15	0	0.15	1.5	0	5250	91304.3
67564-91-4	67564914	4949	Fenpropimorph	303.49	2_Pest	0.3	0.3	0	0	0	3	0.15	0	0.15	0.3	0	1050	18260.9
67747-09-5	67747095	797	Prochloraz	376.67	2_Pest	0.9	0.9	0	0	0	3	0.15	0	0.15	0.9	0	3150	54782.6
68694-11-1	68694111	802	Triflumizole	345.76	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
6923-22-4	6923224	803	Monocrotophos	223.17	2_Pest	0.006	0.6	0	1	0.00025	3	0.15	0	0.00025	0.6	0	2100	36521.7
69377-81-7	69377817	805	Fluroxypyr	255.03	2_Pest	26.66666667	26.66666667	0	0	0	3	0.15	0	0.15	26.6666667	0	93333.33333	1623188.4
69806-34-4	69806344	810	Haloxyfop	361.7	2_Pest	0.03	0.03	0	0	0	3	0.15	0	0.15	0.03	0	105	1826.1
7003-89-6	7003896	4871	Chlormequat	122.62	2_Pest	4.7	4.7	0	1	0.00025	3	0.15	0	0.00025	4.7	0	16450	286087.0
70124-77-5	70124775	811	Flucythrinate	451.47	2_Pest	2.5	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
70630-17-0	70630170	1113	Metalaxyl-M	279.34	2_Pest	8	8	0	0	0	1	3	0	3	8	0	28000	486956.5
709-98-8	709988	816	Propanil	218.08	2_Pest	1.666666667	1.666666667	0	0	0	3	0.15	0	0.15	1.66666667	0	5833.333333	101449.3
71626-11-4	71626114	823	Benalaxyl	325.41	2_Pest	4.42	4.42	0	0	0	3	0.15	0	0.15	4.42	0	15470	269043.5
71751-41-2	71751412	1097	Abamectin	873.09	2_Pest	0.12	0.12	0	0	0	3	0.15	0	0.15	0.12	0	420	7304.3

72178-02-0	72178020	824	Fomesafen	438.77	2_Pest	2.5	2.5	0	1	0.00025	3	0.15	0	0.00025	2.5	0	8750	152173.9
72490-01-8	72490018	825	Fenoxycarb	301.34	2_Pest	1.766666667	1.766666667	0	1	0.00025	3	0.15	0	0.00025	1.76666667	0	6183.333333	107536.2
7287-19-6	7287196	87	Prometryn	241.37	2_Pest	3.75	3.75	0	0	0	3	0.15	0	0.15	3.75	0	13125	228260.9
731-27-1	731271	827	Tolylfluanid	347.26	2_Pest	12	12	0	0	0	3	0.15	0	0.15	12	0	42000	730434.8
732-11-6	732116	828	Phosmet	317.32	2_Pest	0.333333333	0.333333333	0	0	0	3	0.15	0	0.15	0.33333333	0	1166.666667	20289.9
74051-80-2	74051802	834	Sethoxydim	327.49	2_Pest	8.86	8.86	0	1	0.00025	3	0.15	0	0.00025	8.86	0	31010	539304.3
74070-46-5	74070465	835	Aclonifen	264.67	2_Pest	7	7	0	1	0.00025	3	0.15	0	0.00025	7	0	24500	426087.0
74223-64-6	74223646	836	Metsulfuron-methyl	381.37	2_Pest	22.4	22.4	0	0	0	3	0.15	0	0.15	22.4	0	78400	1363478.3
74738-17-3	74738173	4948	Fenpiclonil	237.09	2_Pest	1.2	1.2	0	0	0	3	0.15	0	0.15	1.2	0	4200	73043.5
75-99-0	75990	4884	Dalapon	142.97	2_Pest	15	15	0	0	0	3	0.15	0	0.15	15	0	52500	913043.5
759-94-4	759944	869	EPTC	189.32	2_Pest	2.5	2.5	0	1	0.00025	3	0.15	0	0.00025	2.5	0	8750	152173.9
76578-12-6	76578126	5116	Quizalofop	344.76	2_Pest	128	128	0	0	0	3	0.15	0	0.15	128	0	448000	7791304.3
76674-21-0	76674210	875	Flutriafol	301.3	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
76738-62-0	76738620	5082	Paclobutrazol	293.8	2_Pest	2.2	2.2	0	0	0	3	0.15	0	0.15	2.2	0	7700	133913.0
76-87-9	76879	1110	Fentin hydroxide	367.01	2_Pest	0.1	0.1	0	0	0	3	0.15	0	0.15	0.1	0	350	6087.0
77732-09-3	77732093	5080	Oxadixyl	278.31	2_Pest	5	5	0	1	0.00025	3	0.15	0	0.00025	5	0	17500	304347.8
7786-34-7	7786347	5035	Mevinphos	224.15	2_Pest	0.016	1.6	0	1	0.00025	3	0.15	0	0.00025	1.6	0	5600	97391.3
78587-05-0	78587050	4974	Hexythiazox	352.89	2_Pest	2.87	2.87	0	0	0	3	0.15	0	0.15	2.87	0	10045	174695.7
786-19-6	786196	898	carbophenothion	342.87	2_Pest	0.5	0.5	0	0	0	3	0.15	0	0.15	0.5	0	1750	30434.8
79241-46-6	79241466	4954	Fluazifop-P-butyl	383.37	2_Pest	0.9	0.9	0	0	0	3	0.15	0	0.15	0.9	0	3150	54782.6
79277-27-3	79277273	918	Thifensulfuron-methyl	387.4	2_Pest	1.3	1.3	0	0	0	3	0.15	0	0.15	1.3	0	4550	79130.4
79538-32-2	79538322	922	Tefluthrin	418.74	2_Pest	0.5	0.5	0	1	0.00025	3	0.15	0	0.00025	0.5	0	1750	30434.8
79622-59-6	79622596	925	Fluazinam	465.1	2_Pest	1	1	0	1	0.00025	3	0.15	0	0.00025	1	0	3500	60869.6
79983-71-4	79983714	930	Hexaconazole	314.22	2_Pest	0.47	0.47	0	0	0	3	0.15	0	0.15	0.47	0	1645	28608.7
80-33-1	80331	935	Chlorfenson	303.16	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
81335-37-7	81335377	4977	Imazaquin	311.34	2_Pest	25	25	0	0	0	3	0.15	0	0.15	25	0	87500	1521739.1
81777-89-1	81777891	941	Clomazone	239.7	2_Pest	13.3	13.3	0	0	0	3	0.15	0	0.15	13.3	0	46550	809565.2
82097-50-5	82097505	944	Triasulfuron	401.83	2_Pest	50	50	0	1	0.00025	3	0.15	0	0.00025	50	0	175000	3043478.3
82558-50-7	82558507	946	Isoxaben	332.4	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
82560-54-1	82560541	947	Benfuracarb	410.54	2_Pest	0.63	0.63	0	0	0	3	0.15	0	0.15	0.63	0	2205	38347.8
82657-04-3	82657043	948	Bifenthrin	422.87	2_Pest	1.5	1.5	0	1	0.00025	3	0.15	0	0.00025	1.5	0	5250	91304.3
82-68-8	82688	5115	Quintozene	295.34	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
83055-99-6	83055996	949	Bensulfuron-methyl	410.41	2_Pest	19.9	19.9	0	0	0	3	0.15	0	0.15	19.9	0	69650	1211304.3
83121-18-0	83121180	5144	Teflubenzuron	381.11	2_Pest	0.7	0.7	0	0	0	3	0.15	0	0.15	0.7	0	2450	42608.7
83164-33-4	83164334	951	Diflufenican	394.3	2_Pest	19.47	19.47	0	0	0	3	0.15	0	0.15	19.47	0	68145	1185130.4
834-12-8	834128	953	ametryn	227.34	2_Pest	8.6	8.6	0	1	0.00025	3	0.15	0	0.00025	8.6	0	30100	523478.3
83657-24-3	83657243	955	Diniconazole	326.23	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
84087-01-4	84087014	958	Quinclorac	242.06	2_Pest	35	35	0	0	0	3	0.15	0	0.15	35	0	122500	2130434.8
841-06-5	841065	959	Methoprotryne	271.39	2_Pest	250	250	0	0	0	3	0.15	0	0.15	250	0	875000	15217391.3
85509-19-9	85509199	967	Flusilazole	315.4	2_Pest	0.2	0.2	0	0	0	3	0.15	0	0.15	0.2	0	700	12173.9
86479-06-3	86479063	971	Hexaflumuron	461.15	2_Pest	0.5	0.5	0	0	0	3	0.15	0	0.15	0.5	0	1750	30434.8
86-50-0	86500	972	Azinphos-methyl	317.33	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
87392-12-9	87392129	1115	S-Metolachlor	283.8	2_Pest	3.5	3.5	0	1	0.00025	3	0.15	0	0.00025	3.5	0	12250	213043.5
87674-68-8	87674688	1109	Dimethenamid	275.8	2_Pest	2	2	0	1	0.00025	3	0.15	0	0.00025	2	0	7000	121739.1
87820-88-0	87820880	981	Tralkoxydim	329.44	2_Pest	0.5	0.5	0	1	0.00025	1	3	0	0.00025	0.5	0	1750	30434.8
886-50-0	886500	104	Terbutryn	241.37	2_Pest	0.1	0.1	0	1	0.00025	3	0.15	0	0.00025	0.1	0	350	6087.0
88671-89-0	88671890	984	Myclobutanil	288.79	2_Pest	2.5	2.5	0	0	0	3	0.15	0	0.15	2.5	0	8750	152173.9
90717-03-6	90717036	1003	Quinmerac	221.64	2_Pest	7.9	7.9	0	0	0	3	0.15	0	0.15	7.9	0	27650	480869.6
91465-08-6	91465086	5001	Lambda-Cyhalothrin	449.86	2_Pest	0.25	0.25	0	1	0.00025	3	0.15	0	0.00025	0.25	0	875	15217.4
919-86-8	919868	1010	Demeton-S-methyl	230.29	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
93-65-2	93652	108	Mecoprop	214.65	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
94125-34-5	94125345	1021	Prosulfuron	419.39	2_Pest	1.7	1.7	0	0	0	3	0.15	0	0.15	1.7	0	5950	103478.3
94361-06-5	94361065	1022	Cyproconazole	291.79	2_Pest	1.4	1.4	0	0	0	3	0.15	0	0.15	1.4	0	4900	85217.4
944-22-9	944229	1023	Fonofos	246.33	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
94-74-6	94746	110	MCPA	200.62	2_Pest	0.15	0.15	0	0	0	3	0.15	0	0.15	0.15	0	525	9130.4
94-75-7	94757	111	2,4-D	221.04	2_Pest	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
94-81-5	94815	5015	MCPB	228.68	2_Pest	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
94-82-6	94826	4327	2,4-DB	249.09	2_Pest	2.04	2.04	0	0	0	3	0.15	0	0.15	2.04	0	7140	124173.9
950-37-8	950378	1025	Methidathion	302.33	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
95266-40-3	95266403	1026	Trinexapac-Ethyl	252.27	2_Pest	32	32	0	1	0.00025	3	0.15	0	0.00025	32	0	112000	1947826.1
95465-99-9	95465999	1027	Cadusafos	270.39	2_Pest	0.05	0.05	0	0	0	3	0.15	0	0.15	0.05	0	175	3043.5
95617-09-7	95617097	4947	Fenoxaprop	333.73	2_Pest			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
96489-71-3	96489713	1055	Pyridaben	364.94	2_Pest	0.81	0.81	0	0	0	3	0.15	0	0.15	0.81	0	2835	49304.3
99105-77-8	99105778	1083	Sulcotrione	328.77	2_Pest	0.013333333	0.013333333	0	0	0	3	0.15	0	0.15	0.01333333	0	46.66666667	811.6
99129-21-2	99129212	1084	Clethodim	359.92	2_Pest	16	16	0	1	0.00025	3	0.15	0	0.00025	16	0	56000	973913.0
99-30-9	99309	1085	Dicloran	207.02	2_Pest	2.5	2.5	0	1	0.00025	3	0.15	0	0.00025	2.5	0	8750	152173.9
2458-08-4	2458084	1246	12-Ketochenodeoxycholic acid	406.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2478-10-6	2478106	1247	4-hydroxybutyl acrylate	144.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2536-05-2	2536052	1249	2,2'-methylenediphenyl diisocyanat	250.26	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2550-02-9	2550029	1250	triethoxypropylsilane	206.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2550-06-3	2550063	1251	trichloro(3-chloropropyl)silane	211.98	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2554-06-5	2554065	1252	2,4,6,8-tetramethyl-2,4,6,8-tetraviny	344.66	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2643-07-4	2643074	1253	p-[(2-chloroethyl)ethylamino]benzal	211.69	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2680-03-7	2680037	1254	N,N-dimethylacrylamide	99.134	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3081-01-4	3081014	1257	N-(1,4-dimethylpentyl)-N'-phenylbe	282.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3302-10-1	3302101	1259	3,5,5-trimethylhexanoic acid	158.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3452-07-1	3452071	1261	icos-1-ene	280.54	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3913-02-8	3913028	1263	2-butyloctan-1-ol	186.34	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
4130-08-9	4130089	1265	triacetoxyvinylsilane	232.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4223-03-4	4223034	1266	N-(1,1,3,3-tetramethylbutyl)acrylam	183.3	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4292-10-8	4292108	1267	(carboxymethyl)dimethyl-3-[(1-oxod	342.53	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4719-04-4	4719044	117	2,2',2''-(hexahydro-1,3,5-triazine-1,:	219.29	3_REACH	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
5117-12-4	5117124	4397	4-(1-oxo-2-propenyl)-morpholine	141.17	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6318-09-8	6318098	1282	2,4,6-Tri(propan-2-yl)benzene-1,3-c	234.39	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
6992-11-6	6992116	1287	4-[(2,5-dichlorophenyl)azo]-N-(2,3-c	492.33	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
7027-11-4	7027114	4392	3-cyano-3,5,5-trimethylcyclohexanc	165.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7651-02-7	7651027	1289	N-[3-(dimethylamino)propyl]stearan	368.65	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
100-00-5	100005	119	1-chloro-4-nitrobenzene	157.56	3_REACH	1.666666667	1.666666667	0	1	0.00025	3	0.15	0	0.00025	1.66666667	0	5833.333333	101449.3
100-01-6	100016	120	4-nitroaniline	138.13	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
100-02-7	100027	1	4-nitrophenol	139.11	3_REACH	25	25	0	1	0.00025	3	0.15	0	0.00025	25	0	87500	1521739.1
1001354-72-8	1001354728	4779	3-Aminooctan-4-ol	145.25	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
10016-20-3	10016203	1295	cyclohexapentylose	972.85	3_REACH	10000	10000	0	0	0	3	0.15	0	0.15	10000	0	35000000	608695652.2
100-18-5	100185	1296	1,4-diisopropylbenzene	162.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
100-20-9	100209	1297	terephthaloyl dichloride	203.02	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
100-21-0	100210	122	terephthalic acid	166.13	3_REACH	240	240	0	0	0	1	3	0	3	240	0	840000	14608695.7
1003-52-7	1003527	1302	4-methyloxazole-5-carbonitrile	108.1	3_REACH	40	40	0	0	0	3	0.15	0	0.15	40	0	140000	2434782.6
100-37-8	100378	123	2-diethylaminoethanol	117.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
10042-59-8	10042598	1306	2-propylheptan-1-ol	158.29	3_REACH	30	30	0	0	0	1	3	0	3	30	0	105000	1826087.0
100-46-9	100469	127	benzylamine	107.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
100-47-0	100470	128	benzonitrile	103.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
100-51-6	100516	129	benzyl alcohol	108.14	3_REACH	143	143	0	0	0	1	3	0	3	143	0	500500	8704347.8
100-52-7	100527	130	benzaldehyde	106.12	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
100-54-9	100549	131	nicotinonitrile	104.11	3_REACH	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
100-61-8	100618	133	N-methylaniline	107.16	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
100-63-0	100630	134	phenylhydrazine	108.15	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
100-64-1	100641	135	cyclohexanone oxime	113.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
100-69-6	100696	1309	2-vinylpyridine	105.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
10081-67-1	10081671	1310	4-(1-methyl-1-phenylethyl)-N-[4-(1-	405.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
100-83-4	100834	138	3-hydroxybenzaldehyde	122.12	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
100-97-0	100970	2	methenamine	140.19	3_REACH	80	80	0	0	0	3	0.15	0	0.15	80	0	280000	4869565.2
10097-02-6	10097026	4315	2,2-bis(hydroxymethyl)butanoic aci	148.16	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
101-02-0	101020	140	triphenyl phosphite	310.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
101-14-4	101144	1315	4,4'-methylenebis[2-chloroaniline]	267.16	3_REACH	10	10	0	1	0.00025	3	0.15	0	0.00025	10	0	35000	608695.7
101-20-2	101202	143	triclocarban	315.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
101238-01-1	101238011	1317	2,2,6,6-Tetramethylpiperidin-4-yl dc	339.57	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
101-37-1	101371	1318	2,4,6-triallyloxy-1,3,5-triazine	249.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1013-88-3	1013883	4621	diphenylmethanimine	181.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
101-39-3	101393	1320	alpha-Methylcinnamaldehyde	146.19	3_REACH	220	220	0	0	0	1	3	0	3	220	0	770000	13391304.3
101-41-7	101417	1321	methyl phenylacetate	150.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
101-43-9	101439	1322	cyclohexyl methacrylate	168.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
101-54-2	101542	1323	N-(4-aminophenyl)aniline	184.24	3_REACH	50	50	0	1	0.00025	3	0.15	0	0.00025	50	0	175000	3043478.3
101-68-8	101688	1325	4,4'-methylenediphenyl diisocyanat	250.26	3_REACH	6000	6000	0	1	0.00025	3	0.15	0	0.00025	6000	0	21000000	365217391.3
1017183-70-8	1017183708	4503	3-(4-fluorophenyl)-2-methylpropion	200.64	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
101-72-4	101724	1326	N-isopropyl-N'-phenyl-p-phenylene	226.32	3_REACH	62.5	62.5	0	0	0	3	0.15	0	0.15	62.5	0	218750	3804347.8
101-77-9	101779	1328	4,4'-methylenedianiline	198.27	3_REACH	8.3	8.3	0	1	0.00025	3	0.15	0	0.00025	8.3	0	29050	505217.4
101-80-4	101804	1329	4,4'-oxydianiline	200.24	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
101-84-8	101848	150	diphenyl ether	170.21	3_REACH	15	15	0	0	0	3	0.15	0	0.15	15	0	52500	913043.5
101-96-2	101962	1331	N,N'-di-sec-butyl-p-phenylenediami	220.36	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
102-01-2	102012	1334	acetoacetanilide	177.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
102-06-7	102067	1335	1,3-diphenylguanidine	211.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102-08-9	102089	151	1,3-diphenyl-2-thiourea	228.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102-09-0	102090	1336	diphenyl carbonate	214.22	3_REACH	50	50	0	0	0	1	3	0	3	50	0	175000	3043478.3
10233-13-3	10233133	1339	isopropyl laurate	242.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
102-36-3	102363	1341	3,4-dichlorophenyl isocyanate	188.01	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
10254-57-6	10254576	1344	4,4'-methylene bis(dibutyldithiocarb	422.79	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
102-60-3	102603	1347	1,1',1'',1'''-ethylenedinitrilotetraprop:	292.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102-69-2	102692	154	tripropylamine	143.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102-71-6	102716	155	2,2',2''-nitrilotriethanol	149.19	3_REACH	120	120	0	0	0	3	0.15	0	0.15	120	0	420000	7304347.8
102-76-1	102761	1352	triacetin	218.21	3_REACH	1000	1000	0	0	0	1	3	0	3	1000	0	3500000	60869565.2
102-77-2	102772	1353	2-(morpholinothio)benzothiazole	252.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102-81-8	102818	1354	2-dibutylaminoethanol	173.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102-82-9	102829	156	tributylamine	185.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
102985-93-3	102985933	4723	2,2-dimethyl-3-oxopropyl dodecano	284.44	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
103-09-3	103093	1359	2-ethylhexyl acetate	172.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
103-11-7	103117	159	2-ethylhexyl acrylate	184.28	3_REACH	295.6666667	295.6666667	0	0	0	1	3	0	3	295.666667	0	1034833.333	17997101.4
103-23-1	103231	160	bis(2-ethylhexyl) adipate	370.57	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
103-26-4	103264	1362	methyl cinnamate	162.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
10326-41-7	10326417	161	(R)-lactic acid	90.078	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
103-45-7	103457	1367	phenethyl acetate	164.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
103-49-1	103491	1368	dibenzylamine	197.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
103-50-4	103504	1369	dibenzyl ether	198.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
103-60-6	103606	1374	2-phenoxyethyl isobutyrate	208.26	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
103694-68-4	103694684	4367	Trimethylbenzenepropanol	178.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
103-69-5	103695	162	N-ethylaniline	121.18	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
103-71-9	103719	1378	phenyl isocyanate	119.12	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
103-74-2	103742	163	2-(2-pyridyl)ethanol	123.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
103-83-3	103833	164	benzyldimethylamine	135.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
103-95-7	103957	1382	3-p-cumenyl-2-methylpropionaldeh	190.29	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
10411-92-4	10411924	1383	cis-4-tert-butylcyclohexyl acetate	198.31	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
10420-33-4	10420334	1387	dimethyl acetylsuccinate	188.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
104-23-4	104234	1388	4'-aminoazobenzene-4-sulphonic a	277.31	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
104-38-1	104381	1393	2,2'-p-phenylenedioxydiethanol	198.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
104468-21-5	104468215	4316	2,2-dimethyl 3-methyl-3-butenyl prc	170.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
104-55-2	104552	168	cinnamaldehyde	132.16	3_REACH	125	125	0	0	0	1	3	0	3	125	0	437500	7608695.7
104-61-0	104610	1395	nonan-4-olide	156.22	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
104-66-5	104665	1397	1,2-diphenoxyethane	214.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
104-67-6	104676	1398	undecan-4-olide	184.28	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
104-68-7	104687	1399	2-(2-phenoxyethoxy)ethanol	182.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1047-16-1	1047161	1400	5,12-dihydroquino[2,3-b]acridine-7,	312.33	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
104-75-6	104756	169	2-ethylhexylamine	129.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
104-76-7	104767	170	2-ethylhexan-1-ol	144.26	3_REACH	50	50	0	0	0	1	3	0	3	50	0	175000	3043478.3
104-88-1	104881	171	4-chlorobenzaldehyde	140.57	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
104-90-5	104905	172	5-ethyl-2-methylpyridine	121.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
104-93-8	104938	1403	4-methylanisole	122.17	3_REACH	100	100	0	0	0	1	3	0	3	100	0	350000	6086956.5
105-05-5	105055	1405	1,4-diethylbenzene	134.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
10543-57-4	10543574	175	N,N'-ethylenebis[N-acetylacetamide	228.25	3_REACH	90	90	0	0	0	3	0.15	0	0.15	90	0	315000	5478260.9
105-53-3	105533	177	diethyl malonate	160.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
105-55-5	105555	178	1,3-diethyl-2-thiourea	132.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
105-56-6	105566	1415	ethyl cyanoacetate	113.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
105-59-9	105599	1416	2,2'-methyliminodiethanol	119.17	3_REACH	300	300	0	0	0	3	0.15	0	0.15	300	0	1050000	18260869.6
105-60-2	105602	180	Caprolactam	113.16	3_REACH	750	750	0	0	0	3	0.15	0	0.15	750	0	2625000	45652173.9
10563-26-5	10563265	1417	N,N'-bis(3-aminopropyl)ethylenedia	174.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
10563-29-8	10563298	1418	N'-(3-aminopropyl)-N,N-dimethylprc	159.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
105-67-9	105679	181	2,4-xylenol	122.17	3_REACH	67	67	0	0	0	1	3	0	3	67	0	234500	4078260.9
105-75-9	105759	182	dibutyl fumarate	228.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
105-76-0	105760	183	dibutyl maleate	228.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
105812-81-5	105812815	4223	(-)-trans-4-(4'-fluorophenyl)-3-hydro	223.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
105827-91-6	105827916	4348	2-chloro-5-chloromethylthiazole	168.05	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
105-83-9	105839	1420	N,N-bis(3-aminopropyl)methylamin	145.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
105-95-3	105953	1422	1,4-dioxacycloheptadecane-5,17-di	270.37	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
105-99-7	105997	184	dibutyl adipate	258.36	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
106-02-5	106025	1425	pentadecan-15-olide	240.39	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
106-20-7	106207	1430	bis(2-ethylhexyl)amine	241.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4

106-21-8	106218	1431	3,7-dimethyloctan-1-ol	158.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
106-22-9	106229	185	citronellol	156.27	3_REACH	50	50	0	0	0	1	3	0	3	50	0	175000	3043478.3
106-23-0	106230	1432	citronellal	154.25	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
106-24-1	106241	186	geraniol	154.25	3_REACH	550	550	0	0	0	1	3	0	3	550	0	1925000	33478260.9
106-25-2	106252	187	nerol	154.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
106-26-3	106263	1433	(Z)-3,7-dimethylocta-2,6-dienal	152.24	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
106-43-4	106434	190	4-chlorotoluene	126.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
106-44-5	106445	191	p-cresol	108.14	3_REACH	67	67	0	0	0	1	3	0	3	67	0	234500	4078260.9
106461-41-0	106461410	4581	2,4-dihydro-4-(4-(4-(4-hydroxyphen	393.5	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
106-46-7	106467	192	1,4-dichlorobenzene	147	3_REACH	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
106-47-8	106478	193	4-chloroaniline	127.58	3_REACH	4.166666667	4.166666667	0	1	0.00025	3	0.15	0	0.00025	4.16666667	0	14583.33333	253623.2
106-48-9	106489	194	4-chlorophenol	128.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
106-49-0	106490	195	p-toluidine	107.16	3_REACH	40	40	0	1	0.00025	1	3	0	0.00025	40	0	140000	2434782.6
106-50-3	106503	196	p-phenylenediamine	108.15	3_REACH	4	4	0	1	0.00025	1	3	0	0.00025	4	0	14000	243478.3
106-51-4	106514	197	p-benzoquinone	108.1	3_REACH			1	1	0.00025	2	0.91	0	0.00025	0.00025	1	0.875	15.2
1067-33-0	1067330	199	dibutyltin di(acetate)	351.01	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
106-79-6	106796	1446	dimethyl sebacate	230.3	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
106797-53-9	106797539	4354	2-hydroxy-4'-hydroxyethoxy-2-meth	224.26	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
106-91-2	106912	1449	2,3-epoxypropyl methacrylate	142.15	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
1071-22-3	1071223	1455	3-(trichlorosilyl)propiononitrile	188.52	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1072-63-5	1072635	1457	1-vinylimidazole	94.119	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1073-69-4	1073694	1461	(4-chlorophenyl)hydrazine	142.59	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
107-41-5	107415	219	2-methylpentane-2,4-diol	118.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
107-56-2	107562	1465	O,O-diisopropyl hydrogen dithiophc	214.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
107-58-4	107584	1466	N-tert-butylacrylamide	127.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
107-66-4	107664	1467	dibutyl hydrogen phosphate	210.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
107737-97-3	107737973	4619	2,2-Dimethyl-3-(3-methylphenyl)prc	176.26	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
107-75-5	107755	1468	7-hydroxycitronellal	172.27	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
107-88-0	107880	1470	butane-1,3-diol	90.122	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
107898-54-4	107898544	4225	Supersantol	222.37	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
107-92-6	107926	224	butyric acid	88.106	3_REACH	120	120	0	0	0	3	0.15	0	0.15	120	0	420000	7304347.8
107-93-7	107937	225	trans-crotonic acid	86.09	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
107-96-0	107960	1473	3-mercaptopropionic acid	106.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
108-39-4	108394	237	m-cresol	108.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
108-42-9	108429	238	3-chloroaniline	127.58	3_REACH	3.333333333	3.333333333	0	1	0.00025	3	0.15	0	0.00025	3.33333333	0	11666.66667	202898.6
108-44-1	108441	239	m-toluidine	107.16	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
108-45-2	108452	1484	m-phenylenediamine	108.15	3_REACH	6	6	0	1	0.00025	1	3	0	0.00025	6	0	21000	365217.4
108-46-3	108463	240	resorcinol	110.11	3_REACH	36	36	0	0	0	1	3	0	3	36	0	126000	2191304.3
108-67-8	108678	242	mesitylene	120.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
108-68-9	108689	243	3,5-xylenol	122.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
108-69-0	108690	244	3,5-xylidine	121.18	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
108-78-1	108781	4	melamine	126.13	3_REACH	19	19	0	1	0.00025	3	0.15	0	0.00025	19	0	66500	1156521.7
108-80-5	108805	245	cyanuric acid	129.08	3_REACH	154	154	0	0	0	3	0.15	0	0.15	154	0	539000	9373913.0
108-83-8	108838	1490	2,6-dimethylheptan-4-one	142.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
108-93-0	108930	250	cyclohexanol	100.16	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
108-95-2	108952	252	phenol	94.113	3_REACH	0.6	0.6	0	0	0	1	3	0	3	0.6	0	2100	36521.7
108-98-5	108985	1491	benzenethiol	110.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
109-13-7	109137	1494	tert-butyl peroxyisobutyrate	160.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
109-16-0	109160	1495	2,2'-ethylenedioxydiethyl dimethacr	286.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
109-52-4	109524	256	valeric acid	102.13	3_REACH	120	120	0	0	0	3	0.15	0	0.15	120	0	420000	7304347.8
109-77-3	109773	266	malononitrile	66.065	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
110-15-6	110156	274	succinic acid	118.09	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
110-16-7	110167	275	maleic acid	116.07	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
110-25-8	110258	1515	(Z)-N-methyl-N-(1-oxo-9-octadecen	353.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
110-41-8	110418	1519	2-methylundecanal	184.32	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
110-42-9	110429	1520	methyl decanoate	186.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
110-44-1	110441	1521	hexa-2,4-dienoic acid	112.13	3_REACH	300	300	0	0	0	3	0.15	0	0.15	300	0	1050000	18260869.6
110-63-4	110634	1526	butane-1,4-diol	90.122	3_REACH	100	100	0	0	0	1	3	0	3	100	0	350000	6086956.5
110-64-5	110645	1527	but-2-ene-1,4-diol	88.106	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
110-65-6	110656	281	but-2-yne-1,4-diol	86.09	3_REACH	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
110-77-0	110770	283	2-(ethylthio)ethanol	106.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
110-93-0	110930	291	6-methylhept-5-en-2-one	126.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
110964-79-9	110964799	1534	4-(methylsulfonyl)-2-nitrobenzoic ac	245.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
110-97-4	110974	292	1,1'-iminodipropan-2-ol	133.19	3_REACH	100	100	0	0	0	3	0.15	0	0.15	100	0	350000	6086956.5
111-11-5	111115	1538	methyl octanoate	158.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-14-8	111148	293	heptanoic acid	130.19	3_REACH	120	120	0	0	0	3	0.15	0	0.15	120	0	420000	7304347.8
111-18-2	111182	1540	N,N,N',N'-tetramethylhexamethylen	172.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
111-21-7	111217	1542	2,2'-[ethane-1,2-diylbis(oxy)]bisethy	234.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-27-3	111273	294	hexan-1-ol	102.18	3_REACH	120	120	0	0	0	1	3	0	3	120	0	420000	7304347.8
111-30-8	111308	296	glutaral	100.12	3_REACH	4	4	0	1	0.00025	1	3	0	0.00025	4	0	14000	243478.3
111-40-0	111400	299	2,2'-iminodi(ethylamine)	103.17	3_REACH	80	80	0	0	0	3	0.15	0	0.15	80	0	280000	4869565.2
111-41-1	111411	1547	2-(2-aminoethylamino)ethanol	104.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
111-42-2	111422	300	2,2'-iminodiethanol	105.14	3_REACH	12.75	12.75	0	0	0	3	0.15	0	0.15	12.75	0	44625	776087.0
111-44-4	111444	301	bis(2-chloroethyl) ether	143.01	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
111-46-6	111466	302	2,2'-oxydiethanol	106.12	3_REACH	105	105	0	0	0	1	3	0	3	105	0	367500	6391304.3
111-64-8	111648	1551	octanoyl chloride	162.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
111-69-3	111693	307	adiponitrile	108.15	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
111-70-6	111706	308	heptan-1-ol	116.2	3_REACH	120	120	0	0	0	1	3	0	3	120	0	420000	7304347.8
1117-31-3	1117313	1555	1,3-butylene diacetate	174.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-75-1	111751	1556	2-butylaminoethanol	117.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
111-76-2	111762	309	2-butoxyethanol	118.18	3_REACH	3.166666667	3.166666667	0	0	0	1	3	0	3	3.16666667	0	11083.33333	192753.6
111-77-3	111773	310	2-(2-methoxyethoxy)ethanol	120.15	3_REACH	900	900	0	0	0	1	3	0	3	900	0	3150000	54782608.7
1117-86-8	1117868	1557	octane-1,2-diol	146.23	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
111-81-9	111819	1558	methyl undec-10-enoate	198.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-82-0	111820	1559	methyl laurate	214.35	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-85-3	111853	1561	1-chlorooctane	148.68	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
111-86-4	111864	313	octylamine	129.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
111-87-5	111875	314	octan-1-ol	130.23	3_REACH	120	120	0	0	0	1	3	0	3	120	0	420000	7304347.8
111-88-6	111886	1563	octane-1-thiol	146.3	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-90-0	111900	315	2-(2-ethoxyethoxy)ethanol	134.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
111-91-1	111911	316	bis(2-chloroethoxy)methane	173.04	3_REACH	10	10	0	1	0.00025	3	0.15	0	0.00025	10	0	35000	608695.7
111-92-2	111922	317	dibutylamine	129.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1120-21-4	1120214	1567	undecane	156.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1120-24-7	1120247	1568	decyldimethylamine	185.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-02-7	112027	7	cetrimonium chloride	320.01	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1120-36-1	1120361	1569	tetradec-1-ene	196.38	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-05-0	112050	320	nonanoic acid	158.24	3_REACH	120	120	0	0	0	3	0.15	0	0.15	120	0	420000	7304347.8
1120-71-4	1120714	1572	1,3-propanesultone	122.14	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
112-07-2	112072	1573	2-butoxyethyl acetate	160.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-15-2	112152	1577	2-(2-ethoxyethoxy)ethyl acetate	176.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-16-3	112163	1578	lauroyl chloride	218.77	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
112-18-5	112185	321	dodecyldimethylamine	213.41	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
112-25-4	112254	1580	2-hexyloxyethanol	146.23	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-27-6	112276	322	2,2'-(ethylenedioxy)diethanol	150.17	3_REACH	1	1	0	0	0	1	3	0	3	1	0	3500	60869.6
112-29-8	112298	324	1-bromodecane	221.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
112-30-1	112301	325	decan-1-ol	158.29	3_REACH	1000	1000	0	0	0	1	3	0	3	1000	0	3500000	60869565.2
112-31-2	112312	1581	decanal	156.27	3_REACH	120	120	0	1	0.00025	1	3	0	0.00025	120	0	420000	7304347.8
112-33-4	112334	1583	2-[2-(3-aminopropoxy)ethoxy]ethan	163.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-34-5	112345	326	2-(2-butoxyethoxy)ethanol	162.23	3_REACH	51	51	0	0	0	1	3	0	3	51	0	178500	3104347.8
112-35-6	112356	1584	2-(2-(2-methoxyethoxy)ethoxy)etha	164.2	3_REACH	300	300	0	0	0	1	3	0	3	300	0	1050000	18260869.6
112-36-7	112367	327	bis(2-ethoxyethyl) ether	162.23	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-38-9	112389	1585	undec-10-enoic acid	184.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-40-3	112403	1587	dodecane	170.34	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-41-4	112414	1588	dodec-1-ene	168.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-42-5	112425	329	undecan-1-ol	172.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-44-7	112447	1589	undecanal	170.3	3_REACH	120	120	0	1	0.00025	1	3	0	0.00025	120	0	420000	7304347.8
112-45-8	112458	1590	undec-10-enal	168.28	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
112-49-2	112492	330	1,2-bis(2-methoxyethoxy)ethane	178.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-50-5	112505	331	2-(2-(2-ethoxyethoxy)ethoxy)ethanc	178.23	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-53-8	112538	332	dodecan-1-ol	186.34	3_REACH	100	100	0	0	0	1	3	0	3	100	0	350000	6086956.5
112-54-9	112549	333	dodecanal	184.32	3_REACH	120	120	0	1	0.00025	1	3	0	0.00025	120	0	420000	7304347.8
112-55-0	112550	1592	dodecane-1-thiol	202.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-59-4	112594	1593	2-(2-hexyloxyethoxy)ethanol	190.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-67-4	112674	1597	palmitoyl chloride	274.88	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
112-69-6	112696	1598	hexadecyldimethylamine	269.52	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-72-1	112721	1599	tetradecanol	214.39	3_REACH	2000	2000	0	0	0	1	3	0	3	2000	0	7000000	121739130.4
112-73-2	112732	1600	bis(2-butoxyethyl) ether	218.34	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-75-4	112754	1601	dimethyl(tetradecyl)amine	241.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-76-5	112765	1602	stearoyl chloride	302.93	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
112-85-6	112856	1608	docosanoic acid	340.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
112-88-9	112889	1609	octadec-1-ene	252.49	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
112-92-5	112925	1611	octadecan-1-ol	270.5	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1134-94-7	1134947	4363	2-Phenylsulfanylaniline	201.29	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
114772-54-2	114772542	1625	4'-(Bromomethyl)-2-cyanobiphenyl	272.15	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
115-27-5	115275	1635	1,4,5,6,7,7-hexachloro-8,9,10-trinor	370.83	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1154308-86-7	1154308867	1636	N-(2-Hydroxyethyl)-3,5,5-trimethylh	201.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
115-70-8	115708	1638	2-amino-2-ethylpropanediol	119.17	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
115-77-5	115775	341	pentaerythritol	136.15	3_REACH	100	100	0	0	0	1	3	0	3	100	0	350000	6086956.5
115-86-6	115866	9	triphenyl phosphate	326.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
115-95-7	115957	1640	linalyl acetate	196.29	3_REACH	117	117	0	0	0	1	3	0	3	117	0	409500	7121739.1
115-96-8	115968	10	tris(2-chloroethyl) phosphate	285.49	3_REACH	22	22	0	1	0.00025	3	0.15	0	0.00025	22	0	77000	1339130.4
116-37-0	116370	1648	1,1'-isopropylidenebis(p-phenylene	344.45	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
116539-55-0	116539550	1651	(1S)-3-(methylamino)-1-(2-thienyl)p	171.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
116-75-6	116756	1653	1,4-bis(mesitylamino)anthraquinone	474.61	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
117-08-8	117088	1655	tetrachlorophthalic anhydride	285.9	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
117-21-5	117215	1657	3-chlorophthalic anhydride	182.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
117-61-3	117613	1661	benzidine-2,2'-disulphonic acid	344.37	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
117-81-7	117817	346	bis(2-ethylhexyl) phthalate	390.56	3_REACH	4.8	4.8	0	0	0	1	3	0	3	4.8	0	16800	292173.9
118135-28-7	118135287	1666	8-tert-Butyl-2-(chloromethyl)-1,4-dic	246.78	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
118-45-6	118456	1670	4-chlorophthalic anhydride	182.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
118-48-9	118489	1671	4H-3,1-benzoxazine-2,4(1H)-dione	163.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
118-58-1	118581	1674	benzyl salicylate	228.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
118-60-5	118605	1675	2-ethylhexyl salicylate	250.34	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
118-69-4	118694	1676	2,6-dichlorotoluene	161.03	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
118-75-2	118752	1677	tetrachloro-p-benzoquinone	245.88	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
118-79-6	118796	348	2,4,6-tribromophenol	330.82	3_REACH	100	100	0	0	0	3	0.15	0	0.15	100	0	350000	6086956.5
118-82-1	118821	1679	2,2',6,6'-tetra-tert-butyl-4,4'-methyle	424.67	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1189-08-8	1189088	1682	1-methyltrimethylene dimethacrylat	226.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
118-92-3	118923	1683	anthranilic acid	137.14	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
118-96-7	118967	349	2,4,6-trinitrotoluene	227.13	3_REACH	0.166666667	0.166666667	0	1	0.00025	3	0.15	0	0.00025	0.16666667	0	583.3333333	10144.9
119-17-5	119175	1686	m-(4,5-dihydro-3-methyl-5-oxo-1H-|	254.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
119313-12-1	119313121	4343	2-benzyl-2-dimethylamino-4'-morph	366.51	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
119462-56-5	119462565	4277	1,3-bis(3-methyl-2,5-dioxo-1H-pyrrc	324.34	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
119-53-9	119539	1694	benzoin	212.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
119-61-9	119619	354	benzophenone	182.22	3_REACH	3.1	3.1	0	0	0	3	0.15	0	0.15	3.1	0	10850	188695.7
119-64-2	119642	355	1,2,3,4-tetrahydronaphthalene	132.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
119-65-3	119653	356	isoquinoline	129.16	3_REACH	3	3	0	0	0	3	0.15	0	0.15	3	0	10500	182608.7
119-80-2	119802	357	2,2'-dithiodi(benzoic acid)	306.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
119851-28-4	119851284	1700	1-[2-Chloro-4-(4-chlorophenoxy)phe	281.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120068-79-3	120068793	4457	PYRAZOLE MB 45897	321.09	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
120100-77-8	120100778	1704	2-Chloro-4-(methylsulfonyl)-3-[(2,2,	346.71	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120-12-7	120127	358	anthracene	178.23	3_REACH	1000	1000	0	1	0.00025	3	0.15	0	0.00025	1000	0	3500000	60869565.2
120-18-3	120183	12	naphthalene-2-sulphonic acid	208.24	3_REACH	1000	1000	0	0	0	3	0.15	0	0.15	1000	0	3500000	60869565.2
120298-38-6	120298386	4257	(S,S)-trans-4-(acetylamino)-5,6-dih	338.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120-40-1	120401	13	N,N-bis(2-hydroxyethyl)dodecanam	287.44	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120-46-7	120467	1712	1,3-diphenylpropane-1,3-dione	224.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120-47-8	120478	14	ethyl 4-hydroxybenzoate	166.18	3_REACH	1043	1043	0	0	0	1	3	0	3	1043	0	3650500	63486956.5
120-55-8	120558	1714	oxydiethylene dibenzoate	314.34	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
120-57-0	120570	1715	piperonal	150.13	3_REACH	250	250	0	1	0.00025	3	0.15	0	0.00025	250	0	875000	15217391.3
120570-77-6	120570776	1716	2-(2-Formyloxyethoxy)ethyl formate	162.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
120578-03-2	120578032	4461	3-(2-(7-Chloroquinolin-2-yl)vinyl)bei	293.75	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
120-61-6	120616	1717	dimethyl terephthalate	194.19	3_REACH	240	240	0	0	0	1	3	0	3	240	0	840000	14608695.7
120-78-5	120785	360	di(benzothiazol-2-yl) disulphide	332.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120-80-9	120809	361	pyrocatechol	110.11	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
120-82-1	120821	362	1,2,4-trichlorobenzene	181.45	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
120-83-2	120832	363	2,4-dichlorophenol	163	3_REACH	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
120-93-4	120934	367	2-imidazolidone	86.096	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
121219-07-6	121219076	4298	1-Ethoxy-2,3-Difluorobenzene	158.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
121-32-4	121324	368	3-ethoxy-4-hydroxybenzaldehyde	166.18	3_REACH	500	500	0	1	0.00025	1	3	0	0.00025	500	0	1750000	30434782.6
121-33-5	121335	369	vanillin	152.15	3_REACH	400	400	0	1	0.00025	1	3	0	0.00025	400	0	1400000	24347826.1
121-57-3	121573	372	sulphanilic acid	173.19	3_REACH	1000	1000	0	0	0	1	3	0	3	1000	0	3500000	60869565.2
121-60-8	121608	1730	N-acetylsulphanilyl chloride	233.67	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2

121-69-7	121697	373	N,N-dimethylaniline	121.18	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
121-82-4	121824	375	perhydro-1,3,5-trinitro-1,3,5-triazine	222.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
121-86-8	121868	376	2-chloro-4-nitrotoluene	171.58	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
121-91-5	121915	1739	isophthalic acid	166.13	3_REACH	250	250	0	0	0	1	3	0	3	250	0	875000	15217391.3
122-00-9	122009	1740	4'-methylacetophenone	134.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
122-01-0	122010	1741	4-chlorobenzoyl chloride	175.01	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
122-03-2	122032	377	4-isopropylbenzaldehyde	148.21	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
122-20-3	122203	1743	1,1',1''-nitrilotripropan-2-ol	191.27	3_REACH	100	100	0	0	0	3	0.15	0	0.15	100	0	350000	6086956.5
12225-08-0	12225080	1744	N-(2,3-dihydro-2-oxo-1H-benzimida	576.59	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
12225-18-2	12225182	1745	N-(4-chloro-2,5-dimethoxyphenyl)-2	591.04	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
12236-62-3	12236623	1747	2-[(4-chloro-2-nitrophenyl)azo]-N-(2	416.79	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
12236-64-5	12236645	1748	N-[4-(acetylamino)phenyl]-4-[[5-(am	501.94	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
122-39-4	122394	379	diphenylamine	169.23	3_REACH	7.5	7.5	0	0	0	3	0.15	0	0.15	7.5	0	26250	456521.7
122-52-1	122521	1751	triethyl phosphite	166.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
122-57-6	122576	1752	4-phenylbutenone	146.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
122-62-3	122623	1755	bis(2-ethylhexyl) sebacate	426.68	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
122-99-6	122996	384	2-phenoxyethanol	138.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
123-04-6	123046	1760	3-(chloromethyl)heptane	148.68	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
123-05-7	123057	1761	2-ethylhexanal	128.22	3_REACH	50	50	0	1	0.00025	1	3	0	0.00025	50	0	175000	3043478.3
123-11-5	123115	1763	anisaldehyde	136.15	3_REACH	20	20	0	1	0.00025	1	3	0	0.00025	20	0	70000	1217391.3
123-17-1	123171	1764	2,6,8-trimethylnonan-4-ol	186.34	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
123-30-8	123308	386	4-aminophenol	109.13	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
123-31-9	123319	388	hydroquinone	110.11	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
123-39-7	123397	392	N-methylformamide	59.069	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
123-42-2	123422	393	4-hydroxy-4-methylpentan-2-one	116.16	3_REACH	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
123-68-2	123682	1773	allyl hexanoate	156.22	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
123-77-3	123773	1775	C,C'-azodi(formamide)	116.08	3_REACH	500	500	0	1	0.00025	3	0.15	0	0.00025	500	0	1750000	30434782.6
1238449-42-7	1238449427	1776	bis(2-propylheptyl) carbonate	342.56	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
123-96-6	123966	399	octan-2-ol	130.23	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
124-04-9	124049	400	adipic acid	146.14	3_REACH	750	750	0	0	0	3	0.15	0	0.15	750	0	2625000	45652173.9
124-07-2	124072	401	octanoic acid	144.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
124-09-4	124094	1783	hexamethylenediamine	116.21	3_REACH	500	500	0	0	0	3	0.15	0	0.15	500	0	1750000	30434782.6
124-13-0	124130	1786	octanal	128.22	3_REACH	120	120	0	1	0.00025	1	3	0	0.00025	120	0	420000	7304347.8
124-17-4	124174	1787	2-(2-butoxyethoxy)ethyl acetate	204.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
124-18-5	124185	402	decane	142.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1241-94-7	1241947	403	2-ethylhexyl diphenyl phosphate	362.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
124-19-6	124196	1788	nonanal	142.24	3_REACH	120	120	0	1	0.00025	1	3	0	0.00025	120	0	420000	7304347.8
124-26-5	124265	1789	stearamide	283.5	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
124-28-7	124287	1790	dimantine	297.57	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
124-30-1	124301	1791	octadecylamine	269.52	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
124655-09-0	124655090	4568	tert-butyl2-[(4R,6S)-6-(hydroxymeth	260.33	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
125-12-2	125122	1796	exo-1,7,7-trimethylbicyclo[2.2.1]hep	196.29	3_REACH	15	15	0	0	0	1	3	0	3	15	0	52500	913043.5
12542-30-2	12542302	1797	hexahydro-4,7-methano-1H-indenyl	204.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
125971-57-5	125971575	1800	(2Z)-2-Benzylidene-4-methyl-3-oxo	293.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
125971-96-2	125971962	4497	4-(4-F-PHENYL)-4-OXO-3-PHENYI	417.48	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
126-33-0	126330	406	tetrahydrothiophene 1,1-dioxide	120.17	3_REACH	2.9	2.9	0	0	0	3	0.15	0	0.15	2.9	0	10150	176521.7
126586-91-2	126586912	4597	N2-[1-(S)-ethoxycarbonyl-3-phenylp	414.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
126-71-6	126716	18	triisobutyl phosphate	266.32	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
126-73-8	126738	19	tributyl phosphate	266.32	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
127-47-9	127479	1812	retinyl acetate	328.5	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
128-37-0	128370	413	2,6-di-tert-butyl-p-cresol	220.36	3_REACH	25	25	0	0	0	2	0.91	0	0.91	25	0	87500	1521739.1
128-39-2	128392	1820	2,6-di-tert-butylphenol	206.33	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
128-69-8	128698	1822	perylene-3,4:9,10-tetracarboxylic di	392.32	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
129-00-0	129000	21	pyrene	202.26	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
129909-90-6	129909906	415	Amicarbazone	241.3	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13048-33-4	13048334	1837	hexamethylene diacrylate	226.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
130755-46-3	130755463	1842	4,4'-dithiobis[5-amino-3-cyano-1-[2,	704.3	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13076-17-0	13076170	1843	Lactide, D-	144.13	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
130841-23-5	130841235	1844	Benzene,1,4-dichloro-2-(1,1,2,3,3,3	358.02	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
131-11-3	131113	417	dimethyl phthalate	194.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
131-17-9	131179	418	diallyl phthalate	246.26	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
13122-18-4	13122184	1847	tert-butyl 3,5,5-trimethylperoxyhexa	230.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
13127-18-9	13127189	1848	Erythromycin oxime	748.95	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1315251-11-6	1315251116	1849	7,7,8,9,9-pentamethyl-6,7,8,9-tetral	242.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
131538-00-6	131538006	4321	2,3-bis((2-mercaptoethyl)thio)-1-prc	260.52	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
131-56-6	131566	1850	2,4-dihydroxybenzophenone	214.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
131-57-7	131577	22	oxybenzone	228.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
13170-23-5	13170235	1851	diacetoxydi-tert-butoxysilane	292.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
132694-65-6	132694656	4685	4-[4-[(1-Oxo-2-propenyl)oxy]butoxy	602.64	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1333-07-9	1333079	1866	toluenesulphonamide	171.22	3_REACH	214	214	0	0	0	3	0.15	0	0.15	214	0	749000	13026087.0
133467-41-1	133467411	4415	4-[4-(2-ethylhexyloxy)phenyl](1,4-th	339.5	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
13361-34-7	13361347	1870	2-ethylhexyl cyanoacetate	197.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
133636-82-5	133636825	4540	Spiro[bicyclo[3.1.1]heptane-3,1'-[2](	218.34	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
133-91-5	133915	1872	3,5-diiodosalicylic acid	389.91	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
13393-93-6	13393936	1873	tetradecahydro-7-isopropyl-1,4a-dir	292.51	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
13402-02-3	13402023	1875	hexadecyl acrylate	296.5	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
134605-64-4	134605644	433	1-(allyloxy)-2-methyl-1-oxopropan-2	474.82	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
134701-20-5	134701205	4329	2,4-dimethyl-6-(1-methyl-pentadecy	346.6	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
13472-08-7	13472087	1882	2,2'-azobis[2-methylbutyronitrile]	192.27	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13501-76-3	13501763	1885	(3-chloropropyl)diethoxymethylsilar	209.77	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13515-40-7	13515407	1887	2-[(4-chloro-2-nitrophenyl)azo]-N-(2	390.79	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
135-19-3	135193	435	2-naphthol	144.17	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
135590-91-9	135590919	436	1-(2,4-Dichlorophenyl)-4,5-dihydro-	373.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
136210-30-5	136210305	4527	1,4-diethyl 2-{[4-({4-[(1,4-diethoxy-1	554.73	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
136239-66-2	136239662	4294	1-butoxy-2,3-difluorobenzene	186.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
136465-81-1	136465811	4454	PHIQ	238.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1364731-90-7	1364731907	1900	2,6-dimethylphenyl 4-hydroxybenze	278.33	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
13674-84-5	13674845	24	tris(2-chloro-1-methylethyl) phospha	327.57	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13674-87-8	13674878	25	tris[2-chloro-1-(chloromethyl)ethyl]		430.91	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13749-61-6	13749616	1909	N-isopropylmethacrylamide	127.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
13752-51-7	13752517	1911	4-[(morpholinothio)thioxomethyl]mo	248.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
137863-20-8	137863208	1913	Valsartan benzyl ester	525.66	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
138564-59-7	138564597	4458	5-methyl-2-[(2-nitrophenyl)amino]-3	259.283	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
138-59-0	138590	445	(3R,4S,5R)-3,4,5-trihydroxycyclohe	174.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
139007-06-0	139007060	1915	(E)-2-Ethoxy-N-(2-methyl-1-phenylp	219.33	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
139122-17-1	139122171	4737	2-(3-chloro-2-oxo-2,3-dihydro-1H-in	315.76	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
139-13-9	139139	27	nitrilotriacetic acid	191.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
139189-30-3	139189303	4566	Phosphoric acid, P,P'-1,3-phenylen	686.68	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
139504-68-0	139504680	4286	1-[(2-tert-butylcyclohexyl)oxy]butan	228.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
140-11-4	140114	448	benzyl acetate	150.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
140-29-4	140294	1926	phenylacetonitrile	117.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
140-31-8	140318	449	2-piperazin-1-ylethylamine	129.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
14064-10-9	14064109	450	diethyl chloromalonate	194.61	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
140-66-9	140669	451	4-(1,1,3,3-tetramethylbutyl)phenol	206.33	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
14073-97-3	14073973	1929	L-menthan-3-one	154.25	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
14078-41-2	14078412	1930	3,3'-di-tert-butyl-5,5'-dimethoxybiph	358.48	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
141-05-9	141059	454	diethyl maleate	172.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
141-10-6	141106	1932	6,10-dimethylundeca-3,5,9-trien-2-(	192.3	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
141-17-3	141173	1933	bis(2-(2-butoxyethoxy)ethyl) adipate	434.57	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
141-18-4	141184	1934	bis(2-butoxyethyl) adipate	346.46	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
141-27-5	141275	1935	(E)-3,7-dimethylocta-2,6-dienal	152.24	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
141-62-8	141628	1939	decamethyltetrasiloxane	310.69	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
141-63-9	141639	1940	dodecamethylpentasiloxane	384.85	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
141-97-9	141979	459	ethyl acetoacetate	130.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
141-98-0	141980	460	O-isopropyl ethylthiocarbamate	147.24	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
142-16-5	142165	1948	bis(2-ethylhexyl) maleate	340.5	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
142-19-8	142198	1950	allyl heptanoate	170.25	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
14246-53-8	14246538	1956	N-(1-oxooctyl)glycine	201.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
142-62-1	142621	462	hexanoic acid	116.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
142-90-5	142905	465	dodecyl methacrylate	254.41	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
142-91-6	142916	1957	isopropyl palmitate	298.51	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
142-92-7	142927	466	hexyl acetate	144.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
143-07-7	143077	468	lauric acid	200.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
143-08-8	143088	469	nonan-1-ol	144.26	3_REACH	120	120	0	0	0	1	3	0	3	120	0	420000	7304347.8
143-22-6	143226	1959	2-(2-(2-butoxyethoxy)ethoxy)ethanc	206.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
143-24-8	143248	28	bis(2-(2-methoxyethoxy)ethyl) ether	222.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
143-28-2	143282	1962	(Z)-octadec-9-enol	268.49	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
14338-82-0	14338820	1965	dibutyl methylenedithiodi(acetate)	308.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
144-19-4	144194	1974	2,2,4-trimethylpentane-1,3-diol	146.23	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
14433-76-2	14433762	471	N,N-dimethyldecan-1-amide	199.34	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
144-62-7	144627	472	oxalic acid	90.034	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
144-83-2	144832	29	sulfapyridine	249.29	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
1453-58-3	1453583	1985	3-methylpyrazole	82.108	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
145783-14-8	145783148	1988	4,6-dichloro-5-nitro-2-(propylthio)py	268.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1459-93-4	1459934	1990	dimethyl isophthalate	194.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
146421-65-0	146421650	4455	URACROSS P 3307	400.52	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
14657-64-8	14657648	4379	3-(hydroxyphenylphosphinyl)propar	214.16	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
147315-50-2	147315502	4308	2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-	425.54	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
147504-92-5	147504925	4409	4,6-bis[2-(4-hydroxyphenyl)isopropy	378.47	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1477-55-0	1477550	1997	m-phenylenebis(methylamine)	136.2	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
147-85-3	147853	1999	L-proline	115.13	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
14814-09-6	14814096	2001	3-(triethoxysilyl)propanethiol	238.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
148528-05-6	148528056	2002	2-Methyloctane-1,8-diamine	158.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
14858-73-2	14858732	2004	bis(2-ethylhexyl) carbonate	286.46	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
14901-07-6	14901076	477	4-(2,6,6-trimethylcyclohex-1-ene-1-	192.3	3_REACH	10	10	0	1	0.00025	1	3	0	0.00025	10	0	35000	608695.7
149-30-4	149304	478	benzothiazole-2-thiol	167.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1493-13-6	1493136	2005	trifluoromethanesulphonic acid	150.07	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
149-57-5	149575	479	2-ethylhexanoic acid	144.21	3_REACH	200	200	0	0	0	3	0.15	0	0.15	200	0	700000	12173913.0
149-74-6	149746	2006	dichloro(methyl)(phenyl)silane	191.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
149850-30-6	149850306	5029	methyl N-[3-acetylamino)-4-(2-cyan	468.43	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
150-76-5	150765	483	mequinol	124.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
150-78-7	150787	484	1,4-dimethoxybenzene	138.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
150-84-5	150845	2012	citronellyl acetate	198.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
15214-89-8	15214898	2021	2-acrylamido-2-methylpropanesulpl	207.25	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
152402-98-7	152402987	2023	2-[[(3-Methyl-4-nitro-pyridin-2-yl)me	300.34	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
15267-95-5	15267955	2025	(chloromethyl)triethoxysilane	212.75	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
1530-32-1	1530321	2028	ethyltriphenylfosfonium bromide	371.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
15307-79-6	15307796	30	sodium [2-[(2,6-dichlorophenyl)amir	318.14	3_REACH	1.666666667	1.666666667	0	0	0	3	0.15	0	0.15	1.66666667	0	5833.333333	101449.3
15356-60-2	15356602	486	(+)-menthol	156.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
153719-38-1	153719381	4548	N-nitro-N-(3-methyl-3,6-dihydro-2H-	160.14	3_REACH	16	16	0	0	0	3	0.15	0	0.15	16	0	56000	973913.0
15396-00-6	15396006	2033	3-(trimethoxysilyl)propyl isocyanate	205.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
154279-60-4	154279604	2034	4,4'-methylenebis(N-sec-butylcyclol	322.58	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
15471-17-7	15471177	2039	1-(3-sulphonatopropyl)pyridinium	201.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
15520-10-2	15520102	2040	2-methylpentane-1,5-diamine	116.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
15625-89-5	15625895	2046	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1	296.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
156-43-4	156434	2048	p-phenetidine	137.18	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
1570-64-5	1570645	495	4-chloro-o-cresol	142.59	3_REACH	200	200	0	0	0	3	0.15	0	0.15	200	0	700000	12173913.0
15721-78-5	15721785	2055	bis(4-(1,1,3,3-tetramethylbutyl)pher	393.66	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
15827-60-8	15827608	2059	[[(phosphonomethyl)imino]bis[ethar	573.2	3_REACH	83	83	0	0	0	3	0.15	0	0.15	83	0	290500	5052173.9
15834-04-5	15834045	2060	2,2-bis[[(1-oxopentyl)oxy]methyl]prc	472.62	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
15848-49-4	15848494	2062	Ethyl 2-(cyclopent-2-EN-1-YL)aceta	154.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
15894-70-9	15894709	2065	N,N'''-1,6-hexanediylbis[N'-cyanogu	250.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
15993-42-7	15993427	2069	N-(5-chloro-2-methoxyphenyl)-2-[(2	420.81	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
16111-62-9	16111629	2079	bis(2-ethylhexyl) peroxydicarbonate	346.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
161462-35-7	161462357	4456	1-cyclopropyl-3-(2-methylthio-4-trifl	302.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
16219-75-3	16219753	2083	5-ethylidene-8,9,10-trinorborn-2-en	120.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
162208-27-7	162208277	4901	Diethyl thiophosphoril-(z)-(2-aminot	353.36	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
16298-38-7	16298387	4407	4,4'-methylenebis(2-isopropyl-6-me	310.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
16415-12-6	16415126	2092	hexadecyltrimethoxysilane	346.63	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
164578-11-4	164578114	4335	2,9-bis[N-[3-(diethylamino)propyl]su	696.9	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
165184-98-5	165184985	2096	alpha-Hexylcinnamaldehyde	216.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
16634-82-5	16634825	4584	2-Chloro-N-(4-methylphenyl)acetan	183.64	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
166524-65-8	166524658	2105	2-ethoxy-4,6-difluoropyrimidine	160.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
167004-78-6	167004786	2110	3-[butoxy(methyl)phosphoryl]-1-cya	261.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
16712-64-4	16712644	2111	6-hydroxy-2-naphthoic acid	188.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1696-20-4	1696204	2118	4-acetylmorpholine	129.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1704-62-7	1704627	2119	2-[2-(dimethylamino)ethoxy]ethanol	133.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1709-70-2	1709702	2121	Tris-bht mesitylene	775.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1724-39-6	1724396	2126	cyclododecanol	184.32	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3

172529-93-0	172529930	2128	1,3-dimethyl 2-[2-(2-amino-6-chloro	327.73	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
1738-25-6	1738256	2132	3-dimethylaminopropiononitrile	98.151	3_REACH	350	350	0	0	0	3	0.15	0	0.15	350	0	1225000	21304347.8
173904-11-5	173904115	2133	N,N'-[cyclohexane-1,3-diylbis(meth	250.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1739-84-0	1739840	2135	1,2-dimethylimidazole	96.135	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
174489-43-1	174489431	2137	1-(allyloxy)-2-methyl-1-oxopropan-2	297.74	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
174489-76-0	174489760	2138	1-(allyloxy)-2-methyl-1-oxopropan-2	327.72	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
1746-23-2	1746232	2139	p-tert-butylstyrene	160.26	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1760-24-3	1760243	2145	N-(3-(trimethoxysilyl)propyl)ethylen	222.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
17689-77-9	17689779	2148	triacetoxyethylsilane	234.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
176969-34-9	176969349	2150	3-(difluoromethyl)-1-methyl-1H-pyra	176.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
17796-82-6	17796826	2153	N-(cyclohexylthio)phthalimide	261.34	3_REACH	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
17832-28-9	17832289	2154	4-(vinyloxy)butan-1-ol	116.16	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
17865-07-5	17865075	2155	propyltriacetoxysilane	248.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
17928-28-8	17928288	2158	1,1,1,3,5,5,5-heptamethyl-3-[(trimet	310.69	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
18063-03-1	18063031	2163	2,6-difluorobenzamide	157.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1809-19-4	1809194	2164	dibutyl phosphonate	194.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
18127-01-0	18127010	2166	3-(4-tert-butylphenyl)propionaldehy	190.29	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
181587-01-9	181587019	4655	Ethiprole	397.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
18171-19-2	18171192	2172	(3-chloropropyl)dimethoxymethylsil	182.72	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
18379-25-4	18379254	2187	trichloro(2,4,4-trimethylpentyl)silane	247.67	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1843-03-4	1843034	2190	4,4',4''-(1-methylpropanyl-3-ylidene	544.82	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
18479-58-8	18479588	2192	2,6-dimethyloct-7-en-2-ol	156.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1852-17-1	1852171	2196	perhydropyrimidin-2-one	100.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
18600-59-4	18600594	4312	2,2-(1,4-phenylene)bis((4H-3,1-ben	368.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1860-26-0	1860260	2200	2-ethyl-N,N-bis(2-ethylhexyl)hexyla	353.68	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
186817-80-1	186817801	2203	Propanoic acid, 2-hydroxy-, 2-ethyll	202.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1879-09-0	1879090	2209	6-tert-butyl-2,4-xylenol	178.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
18835-33-1	18835331	2210	hexacos-1-ene	364.7	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
18835-34-2	18835342	2211	octacos-1-ene	392.76	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1889-67-4	1889674	2214	1,1'-(1,1,2,2-tetramethylethylene)di	238.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
19234-20-9	19234209	2228	2-(1-methylethoxy)ethyl acetate	146.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
19444-21-4	19444214	2233	allyl 2-hydroxy-2-methylpropanoate	144.17	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1948-33-0	1948330	523	2-tert-butylhydroquinone	166.22	3_REACH	72	72	0	0	0	1	3	0	3	72	0	252000	4382608.7
1955-46-0	1955460	2235	methyl 5-nitrohydrogen isophthalate	225.16	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
1962-75-0	1962750	525	dibutyl terephthalate	278.35	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
1975-78-6	1975786	2239	decanenitrile	153.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
1999-85-5	1999855	2247	alpha,alpha'-Dihydroxy-1,3-diisopro	194.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
20030-30-2	20030302	2248	2,5,6-trimethylcyclohex-2-en-1-one	138.21	3_REACH			1	1	0.00025	2	0.91	0	0.00025	0.00025	1	0.875	15.2
20120-33-6	20120336	2250	dimethyl [3-[(hydroxymethyl)amino]	211.16	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
20292-08-4	20292084	2257	2-ethylhexyl laurate	312.54	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
20298-69-5	20298695	2258	cis-2-tert-butylcyclohexyl acetate	198.31	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
2031-67-6	2031676	2259	triethoxy(methyl)silane	178.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2040-90-6	2040906	4576	2-chloro-6-fluoro-phenol	146.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2044-64-6	2044646	2265	N,N-dimethyl-3-oxobutyramide	129.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
204918-22-9	204918229	2267	1-(allyloxy)-2-methyl-1-oxopropan-2	323.73	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
20592-85-2	20592852	2271	[nitrilotris(methylene)]trisphosphoni	299.05	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
20749-68-2	20749682	2272	8,9,10,11-tetrachloro-12H-phthalop	408.07	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2082-81-7	2082817	2277	tetramethylene dimethacrylate	226.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
21282-97-3	21282973	2288	2-[(2-methyl-1-oxoallyl)oxy]ethyl ac	214.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2135-17-3	2135173	532	flumetasone	410.46	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2146-71-6	2146716	2295	vinyl laurate	226.36	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
21542-96-1	21542961	2298	N,N-dimethyldocosylamine	353.68	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2156-97-0	2156970	533	dodecyl acrylate	240.39	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2162-73-4	2162734	2299	2,4,6-triisopropyl-m-phenylene diisc	286.38	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
2162-74-5	2162745	2300	bis(2,6-diisopropylphenyl)carbodiim	362.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2163-00-0	2163000	2301	1,6-dichlorohexane	155.07	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2163-42-0	2163420	4357	2-methyl-1,3-propanediol	90.122	3_REACH	1000	1000	0	0	0	3	0.15	0	0.15	1000	0	3500000	60869565.2
21643-42-5	21643425	2302	tetradecyl acrylate	268.44	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
21743-27-1	21743271	4770	4-((Triethoxysilyl)methyl)morpholine	263.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2186-92-7	2186927	2308	p-(dimethoxymethyl)anisole	182.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
22047-49-0	22047490	2316	2-ethylhexyl stearate	396.7	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
220727-26-4	220727264	4596	S-(3-(triethoxysilyl)propyl)octanethi	364.616	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
22094-93-5	22094935	2317	2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphe	754.51	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2210-79-9	2210799	2319	2,3-epoxypropyl o-tolyl ether	164.2	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2216-51-5	2216515	538	L-menthol	156.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2224-33-1	2224331	2325	butan-2-one O,O',O''-(vinylsilylidyne	313.48	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2226-96-2	2226962	2327	4-hydroxy-2,2,6,6-tetramethylpiperi	173.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2235-00-9	2235009	2331	1-vinylhexahydro-2H-azepin-2-one	139.2	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
224049-04-1	224049041	2333	Isotianil	298.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2243-62-1	2243621	542	1,5-naphthylenediamine	158.21	3_REACH	43	43	0	1	0.00025	3	0.15	0	0.00025	43	0	150500	2617391.3
2280-49-1	2280491	2338	N-phenyl-N-[(trichloromethyl)thio]be	382.72	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
22871-58-5	22871585	2340	3-Amino-5-((2-hydroxyethyl)carbam	601.89	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
22984-54-9	22984549	2341	butan-2-one O,O',O''-(methylsilylidy	301.47	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2312-35-8	2312358	548	propargite	350.48	3_REACH	6.3	6.3	0	0	0	3	0.15	0	0.15	6.3	0	22050	383478.3
232938-43-1	232938431	4564	3-(3-Tosylureido)phenyl p-toluenes	460.53	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
23410-40-4	23410404	2351	N-[3-(dimethoxymethylsilyl)-2-meth	220.39	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2362-14-3	2362143	2353	4,4'-cyclohexylidenedi-o-cresol	296.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2370-88-9	2370889	2355	2,4,6,8-tetramethylcyclotetrasiloxan	236.48	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2372-82-9	2372829	554	N-(3-aminopropyl)-N-dodecylpropa	299.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
23779-32-0	23779320	2358	[3-(triethoxysilyl)propyl]urea	264.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
23783-42-8	23783428	2359	3,6,9,12-tetraoxotridecanol	208.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2380-86-1	2380861	4816	6-hydroxyindole	133.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
23847-08-7	23847087	2360	1,1'-dithiobis[hexahydro-2H-azepin	288.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2385-77-5	2385775	2361	(R)-3,7-dimethyloct-6-enal	154.25	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
2386-87-0	2386870	2362	7-oxabicyclo[4.1.0]hept-3-ylmethyl	252.31	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2402-79-1	2402791	2367	2,3,5,6-tetrachloropyridine	216.88	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2403-88-5	2403885	2368	2,2,6,6-tetramethylpiperidin-4-ol	157.26	3_REACH	20	20	0	0	0	3	0.15	0	0.15	20	0	70000	1217391.3
2403-89-6	2403896	2369	1,2,2,6,6-pentamethylpiperidin-4-ol	171.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
24085-06-1	24085061	2372	(5-Acetyl-2-acetyloxyphenyl)methyl	250.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2409-55-4	2409554	2373	2-tert-butyl-p-cresol	164.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2416-94-6	2416946	558	2,3,6-trimethylphenol	136.19	3_REACH	18.33333333	18.33333333	0	0	0	1	3	0	3	18.3333333	0	64166.66667	1115942.0
24199-46-0	24199460	2376	6-methyloct-5-en-2-one	140.23	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2421-28-5	2421285	2378	benzophenone-3,3':4,4'-tetracarbox	322.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2425-77-6	2425776	2381	2-hexyldecan-1-ol	242.45	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
24279-39-8	24279398	4333	2,6-dichloro-4-trifluoromethylaniline	230.02	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
24293-43-4	24293434	2384	bis(2-ethylhexyl) 2,2'-thiobisacetate	374.58	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2439-35-2	2439352	2391	2-(dimethylamino)ethyl acrylate	143.19	3_REACH	10	10	0	0	0	3	0.15	0	0.15	10	0	35000	608695.7
24424-99-5	24424995	2393	di(tert-butyl) carbonate	218.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
24468-13-1	24468131	2395	2-ethylhexyl chloroformate	192.69	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
24549-06-2	24549062	2397	6-ethyl-2-toluidine	135.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2461-15-6	2461156	561	[[(2-ethylhexyl)oxy]methyl]oxirane	186.29	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
24650-42-8	24650428	2400	2,2-dimethoxy-1,2-diphenylethan-1-	256.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
24800-44-0	24800440	2404	[(methylethylene)bis(oxy)]dipropanc	192.26	3_REACH	200	200	0	0	0	3	0.15	0	0.15	200	0	700000	12173913.0
24863-70-5	24863705	2405	1-Cyclopentene-1-acetic acid, 3-oxo	224.3	3_REACH			1	1	0.00025	2	0.91	0	0.00025	0.00025	1	0.875	15.2
2495-37-6	2495376	565	benzyl methacrylate	176.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2500-88-1	2500881	2411	dioctadecyl disulphide	571.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
25013-15-4	25013154	2412	vinyltoluene	118.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2512-29-0	2512290	2416	2-[(4-methyl-2-nitrophenyl)azo]-3-o:	340.34	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
25265-71-8	25265718	566	oxydipropanol	134.18	3_REACH	200	200	0	0	0	3	0.15	0	0.15	200	0	700000	12173913.0
25265-77-4	25265774	2426	isobutyric acid, monoester with 2,2,	216.32	3_REACH	100	100	0	0	0	2	0.91	0	0.91	100	0	350000	6086956.5
2526-62-7	2526627	2427	3-(trimethoxysilyl)propiononitrile	175.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2528-61-2	2528612	2428	heptanoyl chloride	148.63	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
25307-17-9	25307179	2429	2,2'-(octadec-9-enylimino)bisethanc	355.61	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2530-87-2	2530872	2430	3-chloropropyltrimethoxysilane	198.72	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
25322-69-4	25322694	568	Propane-1,2-diol, propoxylated	134.175	3_REACH	1000	1000	0	0	0	3	0.15	0	0.15	1000	0	3500000	60869565.2
25498-49-1	25498491	2436	[2-(2-methoxymethylethoxy)methyle	206.28	3_REACH	350	350	0	0	0	3	0.15	0	0.15	350	0	1225000	21304347.8
2550-26-7	2550267	2437	4-phenylbutan-2-one	148.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
25601-41-6	25601416	2440	Methyl 9-decenoate	184.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
256473-04-8	256473048	2441	2-Chloro-3-(2,2,2-trifluoroethoxy)py	211.57	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
256473-05-9	256473059	2442	2-(isopropylthio)-3-(2,2,2-trifluoroetl	251.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2568-90-3	2568903	2443	1,1'-[methylenebis(oxy)]dibutane	160.26	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2602-34-8	2602348	2449	[3-(2,3-epoxypropoxy)propyl]trietho	278.42	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2605-79-0	2605790	2452	N,N-dimethyldecylamine N-oxide	201.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2612-57-9	2612579	2455	2,4-dichlorophenyl isocyanate	188.01	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
26159-31-9	26159319	572	(±)-2-(6-methoxy-2-naphthyl)propio	230.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
26218-04-2	26218042	4353	2-ethylhexyl 4-aminobenzoate	249.35	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
26272-90-2	26272902	2460	hexadecyl chloroformate	304.9	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2627-86-3	2627863	2461	L-1-Phenylethylamine	121.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
26364-65-8	26364658	4511	2-thiazolidinylidenecyanamide	127.17	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
26399-02-0	26399020	2468	2-ethylhexyl oleate	394.68	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
26523-78-4	26523784	2474	tris(nonylphenyl) phosphite	689.02	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
26586-02-7	26586027	2480	(E)-3-formylbut-2-enyl acetate	142.15	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
26741-53-7	26741537	2485	3,9-bis(2,4-di-tert-butylphenoxy)-2,4	604.71	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
26761-45-5	26761455	2487	2,3-epoxypropyl neodecanoate	228.33	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
2687-91-4	2687914	2489	1-ethylpyrrolidin-2-one	113.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
26896-20-8	26896208	2491	neodecanoic acid	172.27	3_REACH	250	250	0	0	0	3	0.15	0	0.15	250	0	875000	15217391.3
2691-41-0	2691410	575	octahydro-1,3,5,7-tetranitro-1,3,5,7-	296.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2705-87-5	2705875	2493	allyl 3-cyclohexylpropionate	196.29	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
27458-94-2	27458942	2507	isononyl alcohol	144.26	3_REACH	144	144	0	0	0	1	3	0	3	144	0	504000	8765217.4
2752-17-2	2752172	2511	2,2'-oxydi(ethylamine)	104.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2778-42-9	2778429	2517	1,3-bis(1-isocyanato-1-methylethyl)	244.3	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
2786-76-7	2786767	2520	4-[[4-(aminocarbonyl)phenyl]azo]-N	454.49	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
27955-94-8	27955948	4403	4,4',4''-(ethan-1,1,1-triyl)triphenol	306.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2809-21-4	2809214	578	etidronic acid	206.03	3_REACH	30	30	0	0	0	3	0.15	0	0.15	30	0	105000	1826087.0
281-23-2	281232	579	tricyclo[3.3.1.13,7]decane	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
28219-61-6	28219616	2525	2-ethyl-4-(2,2,3-trimethyl-3-cyclope	208.35	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
28479-22-3	28479223	2533	3-chloro-p-tolyl isocyanate	167.6	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
28535-81-1	28535811	2535	Methyl 3alpha,7alpha-diacetoxy-12-	504.66	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2855-13-2	2855132	2536	3-aminomethyl-3,5,5-trimethylcyclo	170.3	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
28553-12-0	28553120	582	di-"isononyl" phthalate	418.62	3_REACH	15	15	0	0	0	1	3	0	3	15	0	52500	913043.5
2867-47-2	2867472	583	2-dimethylaminoethyl methacrylate	157.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
28768-32-3	28768323	2543	4,4'-methylenebis[N,N-bis(2,3-epox	422.53	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
288-13-1	288131	43	pyrazole	68.081	3_REACH	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
288-88-0	288880	584	1,2,4-triazole	69.07	3_REACH	17	17	0	0	0	3	0.15	0	0.15	17	0	59500	1034782.6
2896-70-0	2896700	2550	2,2,6,6-tetramethyl-4-oxopiperidino	171.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2915-57-3	2915573	2559	bis(2-ethylhexyl) succinate	342.52	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
29171-20-8	29171208	2560	3,7-dimethyloct-6-en-1-yn-3-ol	152.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2920-38-9	2920389	2561	p-phenylbenzonitrile	179.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2935-90-2	2935902	2563	methyl 3-mercaptopropionate	120.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
2942-59-8	2942598	2566	2-chloronicotinic acid	157.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
2943-75-1	2943751	2567	triethoxyoctylsilane	276.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
294-62-2	294622	587	cyclododecane	168.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
294-90-6	294906	4493	1,4,7,10-tetraazacyclododecane	172.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
29761-21-5	29761215	588	isodecyl diphenyl phosphate	390.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
298-06-6	298066	591	O,O-diethyl hydrogen phosphorodit	186.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
29806-73-3	29806733	2572	2-ethylhexyl palmitate	368.65	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
298-07-7	298077	592	bis(2-ethylhexyl) hydrogen phospha	322.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
298-12-4	298124	2573	glyoxylic acid	74.035	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
29911-28-2	29911282	2578	1-(2-butoxy-1-methylethoxy)propan	190.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
29920-31-8	29920318	2579	dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1	453.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
29964-84-9	29964849	2581	isodecyl methacrylate	226.36	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
2996-92-1	2996921	2582	trimethoxyphenylsilane	198.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3030-47-5	3030475	2590	bis(2-dimethylaminoethyl)(methyl)a	173.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3031-66-1	3031661	2591	hex-3-yne-2,5-diol	114.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3033-62-3	3033623	2592	N,N,N',N'-tetramethyl-2,2'-oxybis(et	160.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3047-32-3	3047323	2598	3-ethyloxetane-3-methanol	116.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3049-71-6	3049716	2600	2,9-bis[4-(phenylazo)phenyl]anthra	750.78	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3061-75-4	3061754	2604	docosanamide	339.61	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
30674-80-7	30674807	2606	2-isocyanatoethyl methacrylate	155.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3069-29-2	3069292	2608	N-[3-(dimethoxymethylsilyl)propyl]e	206.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3069-40-7	3069407	2609	trimethoxyoctylsilane	234.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3081-14-9	3081149	2612	N,N'-bis(1,4-dimethylpentyl)-p-pher	304.52	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3089-16-5	3089165	2614	4,11-dichloro-5,12-dihydroquino[2,3	381.22	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3089-17-6	3089176	2615	2,9-dichloro-5,12-dihydroquino[2,3-	381.22	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
31024-56-3	31024563	2617	N-[3-(trimethoxysilyl)propyl]butylam	235.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
31027-31-3	31027313	2618	p-isopropylphenyl isocyanate	161.21	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
3115-49-9	3115499	2619	(4-nonylphenoxy)acetic acid	278.39	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
31335-74-7	31335747	2625	2,2-dimethyl-1,3-propanediyl diocta	356.55	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3148-73-0	3148730	2627	N,N'-diacetylhydrazine	116.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2

3173-72-6	3173726	2631	1,5-naphthylene diisocyanate	210.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
31775-20-9	31775209	2632	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	717.62	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
31775-89-0	31775890	2633	3-[(3-sulfanylbutanoyl)oxy]-2,2-bis{[	544.77	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
31778-10-6	31778106	2634	butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-b	523.55	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3179-47-3	3179473	2635	decyl methacrylate	226.36	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3179-63-3	3179633	2636	3-dimethylaminopropan-1-ol	103.17	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3179-76-8	3179768	2637	3-(diethoxymethylsilyl)propylamine	191.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
31837-42-0	31837420	2639	2-[[1-[[(2,3-dihydro-2-oxo-1H-benzin	381.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
319002-92-1	319002921	4599	Propyl (2S)-2-(2-methylbutan-2-ylo:	202.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3209-22-1	3209221	600	1,2-dichloro-3-nitrobenzene	192	3_REACH	5	5	0	1	0.00025	3	0.15	0	0.00025	5	0	17500	304347.8
3234-85-3	3234853	2648	tetradecyl myristate	424.75	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
32388-55-9	32388559	2651	Acetyl cedrene	246.39	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
329-01-1	329011	2668	3-(Trifluoromethyl)phenyl isocyanat	187.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3290-92-4	3290924	2669	propylidynetrimethyl trimethacrylate	338.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3296-90-0	3296900	2671	2,2-bis(bromomethyl)propane-1,3-d	261.95	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3320-83-0	3320830	2677	2-chlorophenyl isocyanate	153.57	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3332-27-2	3332272	2679	N,N-dimethyltetradecylamine N-oxi	257.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
33329-35-0	33329350	2680	N,N-bis[3-(dimethylamino)propyl]-N	272.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
33704-61-9	33704619	2684	1,2,3,5,6,7-hexahydro-1,1,2,3,3-pe	206.33	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
337906-36-2	337906362	2686	2-(methoxymethyl)benzene-1,4-dia	152.2	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
3407-42-9	3407429	2689	3-(5,5,6-trimethylbicyclo[2.2.1]hept-	236.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
34090-76-1	34090761	2690	tetrahydro-4-methylphthalic anhydri	166.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
34206-40-1	34206401	2694	butan-2-one O,O',O'',O'''-silanetetra	372.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
342-25-6	342256	2695	2,4'-difluorobenzophenone	218.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
34316-64-8	34316648	2700	hexyl laurate	284.48	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3437-84-1	3437841	2701	bisisobutyryl peroxide	174.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
34396-03-7	34396037	2702	trimethoxy(2,4,4-trimethylpentyl)sila	234.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3452-97-9	3452979	609	3,5,5-trimethylhexan-1-ol	144.26	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
345-92-6	345926	2710	bis(4-fluorophenyl) ketone	218.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
34690-00-1	34690001	2714	[[(phosphonomethyl)imino]bis[hexa	685.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
34893-92-0	34893920	2717	1,3-dichloro-5-isocyanatobenzene	188.01	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
350-46-9	350469	611	1-fluoro-4-nitrobenzene	141.1	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3508-98-3	3508983	4362	2-phenylhexanenitrile	173.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
35265-04-4	35265044	2726	2-[(1-methylpropyl)amino]ethanol	117.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
35435-21-3	35435213	2734	triethoxy(2,4,4-trimethylpentyl)silan	276.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3547-33-9	3547339	613	2-(octylthio)ethanol	190.35	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
35636-63-6	35636636	2742	dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-'	453.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3576-88-3	3576883	2746	2,2'-iminobis[4,6-diamino-1,3,5-triaz	235.23	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
35836-72-7	35836727	2750	2-Pinene-10-methyl acetate	208.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
35948-25-5	35948255	2754	6H-dibenz[c,e][1,2]oxaphosphorin 6	216.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
36177-92-1	36177921	2761	N-butyl-2,2,6,6-tetramethylpiperidin	212.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3622-84-2	3622842	2763	N-butylbenzenesulphonamide	213.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3634-83-1	3634831	2766	1,3-bis(isocyanatomethyl)benzene	188.19	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
36443-68-2	36443682	2767	ethylenebis(oxyethylene) bis[3-(5-te	586.77	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
36483-57-5	36483575	2768	2,2-dimethylpropan-1-ol, tribromo d	324.86	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
36635-56-0	36635560	2772	N-[[(4-methylphenyl)sulfonyl]methyl	213.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
36727-29-4	36727294	2775	3,5,5-trimethylhexanoyl chloride	176.69	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
36768-62-4	36768624	2776	2,2,6,6-tetramethyl-4-piperidylamin	156.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3681-71-8	3681718	2779	(Z)-hex-3-enyl acetate	142.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3687-22-7	3687227	4777	2,4-Dinitro-6-(1-methylheptyl)phenc	296.32	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
369634-22-0	369634220	4583	Octalynol	140.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3699-54-5	3699545	2788	1-(2-hydroxyethyl)imidazolidin-2-on	130.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
37052-78-1	37052781	2789	1,3-dihydro-5-methoxy-2H-benzimic	180.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3710-84-7	3710847	2791	N,N-diethylhydroxylamine	89.139	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3717-40-6	3717406	2792	N,N-Dimethyladamantan-1-amine	179.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
372-09-8	372098	2794	cyanoacetic acid	85.063	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
373-44-4	373444	2796	octamethylenediamine	144.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3741-80-8	3741808	5041	N-(1,1-dimethylethyl)bis(2-benzothi	403.61	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3748-13-8	3748138	2798	m-bis(1-methylvinyl)benzene	158.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3749-87-9	3749879	2800	Methyl 3,7-di-O-acetylcholate	506.68	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3779-63-3	3779633	2809	(2,4,6-trioxotriazine-1,3,5(2H,4H,6H	504.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
37971-36-1	37971361	2811	2-phosphonobutane-1,2,4-tricarbox	270.13	3_REACH	424	424	0	0	0	3	0.15	0	0.15	424	0	1484000	25808695.7
38051-10-4	38051104	2812	2,2-bis(chloromethyl)trimethylene b	582.99	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
38083-17-9	38083179	620	climbazole	292.77	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3845-76-9	3845769	2822	N-[3-(dimethylamino)propyl]acrylam	156.23	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
3851-87-4	3851874	2823	bis(3,5,5-trimethylhexanoyl) peroxic	314.47	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
3855-32-1	3855321	2824	N-[3-(dimethylamino)propyl]-N,N',N	201.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
38668-48-3	38668483	2825	1,1'-(p-tolylimino)dipropan-2-ol	223.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
3886-69-9	3886699	2827	D-alpha-Methylbenzylamine	121.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
38888-98-1	38888981	2828	(phenylethyl)benzene	182.27	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
393509-79-0	393509790	4634	methyl 2-chlorosulfonyl-4-(methane	341.79	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
39515-51-0	39515510	625	m-phenoxybenzaldehyde	198.22	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
39670-09-2	39670092	2846	2-[2-(2-ethoxyethoxy)ethoxy]ethyl n	246.3	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
40306-75-0	40306750	2857	3-acetamido-5-amino-4-hydroxyber	246.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
40601-76-1	40601761	2859	1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6	699.94	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4065-45-6	4065456	52	sulisobenzone	308.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
4073-98-7	4073987	2864	4,4'-methylenebis(2,6-xylidine)	254.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
40758-65-4	40758654	2865	4,6-Dichloro-2-ethoxypyrimidine	193.04	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4083-64-1	4083641	629	p-toluenesulphonyl isocyanate	197.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4098-71-9	4098719	2867	3-isocyanatomethyl-3,5,5-trimethylc	222.29	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
41198-08-7	41198087	631	Profenofos	373.64	3_REACH	100	100	0	0	0	3	0.15	0	0.15	100	0	350000	6086956.5
41340-36-7	41340367	4309	2-(7-ethyl-1H-indol-3-yl)ethanol	189.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
41620-33-1	41620331	4337	2-[[2-(acetyloxy)-3-(1,1-dimethyleth	382.54	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4180-23-8	4180238	635	(E)-anethole	148.21	3_REACH	300	300	0	0	0	1	3	0	3	300	0	1050000	18260869.6
42019-78-3	42019783	2886	4-chloro-4'-hydroxybenzophenone	232.67	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
42125-46-2	42125462	2889	4-tert-butylcyclohexyl chloroformate	218.72	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4245-76-5	4245765	2892	610-029-6	118.1	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4246-51-9	4246519	2893	3,3'-oxybis(ethyleneoxy)bis(propyla	220.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4253-34-3	4253343	2896	methylsilanetriyl triacetate	220.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
43057-68-7	43057687	4478	2-Ethyl-2-methyl-1,3-dihydroperimic	212.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4378-61-4	4378614	2916	4,10-dibromodibenzo[def,mno]chrys	464.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4394-85-8	4394858	2918	4-morpholinecarbaldehyde	115.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4402-30-6	4402306	2919	1,1'-(methylimino)dipropan-2-ol	147.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4404-43-7	4404437	641	4,4'-bis[4-[bis(2-hydroxyethyl)aminc	917.01	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4431-83-8	4431838	2921	2,5,7,10-tetraoxaundecane	164.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4443-26-9	4443269	2925	1,3-dihydro-1,3-dioxo-2H-isoindole-	261.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4457-71-0	4457710	2927	3-methylpentane-1,5-diol	118.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
4488-57-7	4488577	2933	3a,4,5,6,7,7a-hexahydro-4,7-metha	134.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4500-29-2	4500292	2936	2,2'-(cyclohexylimino)bisethanol	187.28	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4511-42-6	4511426	2938	(3S-cis)-3,6-dimethyl-1,4-dioxane-2	144.13	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
4531-49-1	4531491	2939	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	689.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4559-86-8	4559868	2943	tetrabutylurea	284.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
461-58-5	461585	2948	cyanoguanidine	84.086	3_REACH	570	570	0	0	0	3	0.15	0	0.15	570	0	1995000	34695652.2
462-94-2	462942	2950	pentamethylenediamine	102.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4635-59-0	4635590	2951	4-chlorobutyryl chloride	141	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4651-67-6	4651676	2954	Nutriacholic acid	390.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4672-38-2	4672382	2957	propylphosphonic acid	124.08	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
470-82-6	470826	645	cineole	154.25	3_REACH	562.5	562.5	0	0	0	3	0.15	0	0.15	562.5	0	1968750	34239130.4
4724-48-5	4724485	2964	octylphosphonic acid	194.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
474-25-9	474259	2966	chenodeoxycholic acid	392.58	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
479-27-6	479276	646	1,8-naphthylenediamine	158.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
4813-57-4	4813574	2971	octadecyl acrylate	324.55	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
48145-04-6	48145046	2972	2-phenoxyethyl acrylate	192.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
482-89-3	482893	647	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	262.27	3_REACH	500	500	0	0	0	3	0.15	0	0.15	500	0	1750000	30434782.6
4904-61-4	4904614	648	cyclododeca-1,5,9-triene	162.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
4948-15-6	4948156	2983	2,9-bis(3,5-dimethylphenyl)anthra[2	598.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
497-18-7	497187	2989	carbonohydrazide	90.09	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
4979-32-2	4979322	2990	N,N-dicyclohexylbenzothiazole-2-su	346.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
50-21-5	50215	654	lactic acid	90.078	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
502-44-3	502443	2999	hexan-6-olide	114.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5026-74-4	5026744	3000	p-(2,3-epoxypropoxy)-N,N-bis(2,3-e	277.32	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5036-48-6	5036486	3003	1H-imidazole-1-propylamine	125.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
503-74-2	503742	657	isovaleric acid	102.13	3_REACH	2500	2500	0	0	0	3	0.15	0	0.15	2500	0	8750000	152173913.0
504-29-0	504290	658	2-pyridylamine	94.119	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
504-63-2	504632	660	propane-1,3-diol	76.095	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
506-30-9	506309	3012	icosanoic acid	312.54	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
507448-65-9	507448659	3018	ethyl (2Z)-4,4,4-trifluoro-3-(methyla	197.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5089-70-3	5089703	3022	(3-chloropropyl)triethoxysilane	240.8	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5102-83-0	5102830	3025	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	685.62	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
51-03-6	51036	667	2-(2-butoxyethoxy)ethyl 6-propylpip	338.44	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
51167-18-1	51167181	3028	2'-[2,4-dichloro-5-(1-methylethoxy)p	319.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5124-30-1	5124301	3030	4,4'-methylenedicyclohexyl diisocya	262.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
51-28-5	51285	57	2,4-dinitrophenol	184.11	3_REACH	59	59	0	1	0.00025	3	0.15	0	0.00025	59	0	206500	3591304.3
5131-66-8	5131668	3032	1-butoxypropan-2-ol	132.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
51920-12-8	51920128	3049	N-(2,3-dihydro-2-oxo-1H-benzimida	560.6	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5208-93-5	5208935	3052	3-methyl-1-(2,6,6-trimethylcyclohex	220.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
521-18-6	521186	672	androstanolone	290.45	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
52449-76-0	52449760	3059	Methyl 4-cyano-2-nitrobenzoate	206.16	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
52-51-7	52517	674	bronopol	200	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
52722-86-8	52722868	3072	4-hydroxy-2,2,6,6-tetramethylpiperi	201.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5280-68-2	5280682	3074	N-(4-chloro-2,5-dimethoxyphenyl)-3	611.06	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5280-80-8	5280808	3076	3,3'-[(2,5-dimethyl-p-phenylene)bis[	916.66	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
52829-07-9	52829079	3077	bis(2,2,6,6-tetramethyl-4-piperidyl) :	480.74	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5283-66-9	5283669	678	octyltrichlorosilane	247.67	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
52846-56-7	52846567	3078	N-(2,3-dihydro-2-oxo-1H-benzimida	382.34	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5292-45-5	5292455	680	dimethyl 2-nitroterephthalate	239.18	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5308-25-8	5308258	3087	1-ethylpiperazine	114.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
53-16-7	53167	61	estrone	270.37	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
53306-54-0	53306540	3094	bis(2-propylheptyl) phthalate	446.67	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5333-42-6	5333426	3096	2-octyldodecan-1-ol	298.56	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5333-84-6	5333846	3097	1,2,3,6-tetrahydro-3-methylphthalic	166.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
534-03-2	534032	3100	2-aminopropane-1,3-diol	91.111	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5343-92-0	5343920	3102	pentane-1,2-diol	104.15	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
53445-37-7	53445377	3103	2,2,4(or 2,4,4)-trimethyladipic acid	188.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
534-52-1	534521	682	2-methyl-4,6-dinitro-phenol | DNOC	198.14	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
53651-69-7	53651697	3107	Propanoic acid	132.16	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5372-81-6	5372816	683	dimethyl 2-aminoterephthalate	209.2	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
540-97-6	540976	3124	dodecamethylcyclohexasiloxane	444.93	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
541-02-6	541026	3125	decamethylcyclopentasiloxane	370.77	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5413-60-5	5413605	3128	3a,4,5,6,7,7a-hexahydro-4,7-metha	192.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
541-73-1	541731	685	1,3-dichlorobenzene	147	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
542-05-2	542052	3134	3-oxoglutaric acid	146.1	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5435-64-3	5435643	3140	3,5,5-trimethylhexanal	142.24	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
544-01-4	544014	3141	diisopentyl ether	158.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
54423-67-5	54423675	3143	vinyl neononanoate	184.28	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
5466-77-3	5466773	3151	2-ethylhexyl 4-methoxycinnamate	290.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5468-75-7	5468757	3152	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	657.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
54839-24-6	54839246	3154	2-ethoxy-1-methylethyl acetate	146.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
54914-37-3	54914373	3156	1,3,3-trimethyl-N-(2-methylpropylide	278.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5521-31-3	5521313	3163	2,9-dimethylanthra[2,1,9-def:6,5,10	418.41	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
55314-16-4	55314164	3166	611-255-8	176.22	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
553-86-6	553866	3169	(3H)-benzofuran-2-one	134.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
554-00-7	554007	700	2,4-dichloroaniline	162.02	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
556-67-2	556672	705	octamethylcyclotetrasiloxane	296.62	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5567-15-7	5567157	706	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	818.5	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
556-88-7	556887	707	1-nitroguanidine	104.07	3_REACH	316	316	0	0	0	3	0.15	0	0.15	316	0	1106000	19234782.6
5578-42-7	5578427	3177	dichlorocyclohexylmethylsilane	197.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
5580-57-4	5580574	3178	3,3'-[(2-chloro-5-methyl-p-phenylen	937.08	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5580-58-5	5580585	3179	3,3'-[(2,5-dichloro-p-phenylene)bis[i	957.49	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
55934-93-5	55934935	3182	[(butoxymethylethoxy)methylethoxy	248.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
561-41-1	561411	3187	4,4'-bis(dimethylamino)-4''-(methyla	375.52	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
56-18-8	56188	3188	3,3'-iminodi(propylamine)	131.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
56309-94-5	56309945	4472	4-(1,4-dioxa-spiro[4.5]dec-8-yl)-cyc	238.33	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
56358-17-9	56358179	3192	N-(2-ethylhexyl)naphthalen-2-amin	255.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
56-41-7	56417	3198	L-alanine	89.095	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
56519-71-2	56519712	3200	Propane-1,3-diyl dioctanoate	328.49	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
56539-66-3	56539663	3201	3-methoxy-3-methylbutan-1-ol	118.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
56677-60-2	56677602	3208	tetradecyl chloroformate	276.85	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
56706-10-6	56706106	3209	4,4,13,13-tetraethoxy-3,14-dioxa-8,	474.83	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4

56718-71-9	56718719	3211	p-(2-methoxyethyl)phenol	152.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
56-84-8	56848	3212	aspartic acid	133.1	3_REACH	700	700	0	0	0	3	0.15	0	0.15	700	0	2450000	42608695.7
56962-04-0	56962040	3217	3-Bromo-5-chlorophenol	207.46	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
56973-87-6	56973876	4267	1-(3,3-dimethylcyclohexyl)pent-4-er	194.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
57090-45-6	57090456	4249	(R)-3-chloropropane-1,2-diol	110.54	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5726-19-2	5726192	3228	2-methylcyclohexyl acetate	156.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
57374-49-9	57374499	4553	methyl 3-acetoxy-2-pentyl-2-cyclop	268.35	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
576-26-1	576261	723	2,6-xylenol	122.17	3_REACH	200	200	0	0	0	1	3	0	3	200	0	700000	12173913.0
5766-67-6	5766676	3236	ethylenediaminetetraacetonitrile	216.25	3_REACH	250	250	0	0	0	3	0.15	0	0.15	250	0	875000	15217391.3
57843-53-5	57843535	3238	N,N,N',N'-tetrakis(2-hydroxypropyl):	376.5	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
58190-57-1	58190571	3242	2-Propanone, 2,2',2''-(O,O',O''-(ethy	273.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
583-39-1	583391	3244	benzimidazole-2-thiol	150.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
583-78-8	583788	728	2,5-dichlorophenol	163	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
58430-94-7	58430947	3247	3,5,5-trimethylhexyl acetate	186.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
584-84-9	584849	729	4-methyl-m-phenylene diisocyanate	174.16	3_REACH	30	30	0	1	0.00025	1	3	0	0.00025	30	0	105000	1826087.0
58567-11-6	58567116	3249	(ethoxymethoxy)cyclododecane	242.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
586-62-9	586629	731	p-mentha-1,4(8)-diene	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
58670-89-6	58670896	3252	2-decyltetradecanol	354.66	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5888-33-5	5888335	3257	exo-1,7,7-trimethylbicyclo[2.2.1]hep	208.3	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
5888-87-9	5888879	3258	N,N'-hexane-1,6-diylbis(hexahydro-	394.52	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
591-27-5	591275	734	3-aminophenol	109.13	3_REACH	240	240	0	1	0.00025	1	3	0	0.00025	240	0	840000	14608695.7
59227-88-2	59227882	4300	1-octylazepin-2-one	225.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
59447-55-1	59447551	3278	(pentabromophenyl)methyl acrylate	556.7	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
59487-23-9	59487239	3279	4-[[5-[[[4-(aminocarbonyl)phenyl]am	654.08	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
59-50-7	59507	737	chlorocresol	142.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
59719-67-4	59719674	3284	bis[2-[2-(1-methylethyl)-3-oxazolidir	486.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
5989-27-5	5989275	743	(R)-p-mentha-1,8-diene	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
5989-54-8	5989548	744	(S)-p-mentha-1,8-diene	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
599-04-2	599042	3296	2,4-dihydroxy-3,3-dimethylbutyric a	130.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
599-61-1	599611	3298	3,3'-sulphonyldianiline	248.31	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
599-64-4	599644	3299	P-Cumylphenol	212.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
60-00-4	60004	71	edetic acid	292.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
60-09-3	60093	746	4-aminoazobenzene	197.24	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
60111-54-8	60111548	3304	3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5	432.89	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
60-12-8	60128	3306	2-phenylethanol	122.17	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
603-35-0	603350	751	triphenylphosphine	262.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6041-94-7	6041947	3310	4-[(2,5-dichlorophenyl)azo]-3-hydro	436.3	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
60658-04-0	60658040	4438	Ethyl 2-(3-benzoylphenyl)propanoa	282.34	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
608-25-3	608253	3317	2-methylresorcinol	124.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
611-06-3	611063	755	1,3-dichloro-4-nitrobenzene	192	3_REACH	8	8	0	1	0.00025	3	0.15	0	0.00025	8	0	28000	486956.5
611-19-8	611198	3326	2-Chlorobenzyl chloride	161.03	3_REACH	2	2	0	1	0.00025	3	0.15	0	0.00025	2	0	7000	121739.1
611-70-1	611701	3328	isobutyrophenone	148.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
61260-55-7	61260557	3330	N,N'-bis(2,2,6,6-tetramethylpiperidi	394.7	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
613-62-7	613627	4310	2-(phenylmethoxy)naphthalene	234.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
614-45-9	614459	3334	tert-butyl perbenzoate	194.23	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
615-20-3	615203	3338	2-chlorobenzothiazole	169.63	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
615-60-1	615601	3339	4-chloro-o-xylene	140.61	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
61597-98-6	61597986	3340	L-Menthyl lactate	228.33	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
616-45-5	616455	757	2-pyrrolidone	85.107	3_REACH	207	207	0	0	0	3	0.15	0	0.15	207	0	724500	12600000.0
616-47-7	616477	3346	1-methylimidazole	82.108	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6166-86-5	6166865	3347	2,4,6,8,10-pentamethylcyclopentas	295.6	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
61826-76-4	61826764	4625	(S)-2-Hydroxy-2-(3-phenoxyphenyl)	225.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
61847-48-1	61847481	3356	methyl 4-[[(2,5-dichlorophenyl)amin	643.49	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
618-62-2	618622	759	3,5-dichloronitrobenzene	192	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
618-88-2	618882	3358	5-nitroisophthalic acid	211.13	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6197-30-4	6197304	3360	octocrilene	361.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
621-29-4	621294	3362	m-tolyl isocyanate	133.15	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
62-23-7	62237	761	4-nitrobenzoic acid	167.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
622-40-2	622402	762	2-morpholinoethanol	131.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
622-58-2	622582	3365	p-tolyl isocyanate	133.15	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
623-03-0	623030	763	4-chlorobenzonitrile	137.57	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
623-40-5	623405	4785	2-Pentanone oxime	101.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
624-54-4	624544	3370	pentyl propionate	144.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
62-53-3	62533	765	aniline	93.13	3_REACH	1.333333333	1.333333333	0	1	0.00025	1	3	0	0.00025	1.33333333	0	4666.666667	81159.4
62-56-6	62566	767	thiourea	76.123	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6259-76-3	6259763	3375	hexyl salicylate	222.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
626-43-7	626437	768	3,5-dichloroaniline	162.02	3_REACH	1	1	0	1	0.00025	3	0.15	0	0.00025	1	0	3500	60869.6
6284-40-8	6284408	770	meglumine	195.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
62889-66-1	62889661	3379	613-099-6	315.54	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
628-89-7	628897	3380	2-(2-chloroethoxy)ethanol	124.57	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
628-96-6	628966	3382	ethylene dinitrate	152.06	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
629-11-8	629118	3385	hexane-1,6-diol	118.18	3_REACH	400	400	0	0	0	1	3	0	3	400	0	1400000	24347826.1
6291-95-8	6291958	4276	1,3,5-tris(2-methyl-2-propenyl)-1,3,!	291.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
629-40-3	629403	771	suberonitrile	136.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
629-50-5	629505	3389	tridecane	184.37	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
629-59-4	629594	3390	tetradecane	198.39	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
629-62-9	629629	772	pentadecane	212.42	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
629-73-2	629732	3391	hexadec-1-ene	224.43	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
629-82-3	629823	3392	dioctyl ether	242.45	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
63-05-8	63058	75	androst-4-ene-3,17-dione	286.42	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6309-51-9	6309519	3394	isopentyl laurate	270.46	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
6331-96-0	6331960	3399	2-amino-4,5-dichlorobenzenesulfon	242.08	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
63562-34-5	63562345	3405	bis(2-hydroxyethyl) (6H-dibenz[c,e][	434.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6358-30-1	6358301	3406	8,18-dichloro-5,15-diethyl-5,15-dihy	589.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6358-37-8	6358378	3408	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	657.56	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6358-64-1	6358641	3409	4-chloro-2,5-dimethoxyaniline	187.63	3_REACH	20	20	0	1	0.00025	3	0.15	0	0.00025	20	0	70000	1217391.3
6358-85-6	6358856	3410	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4	629.51	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
636-30-6	636306	774	2,4,5-trichloroaniline	196.47	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6386-38-5	6386385	3420	methyl 3-(3,5-di-tert-butyl-4-hydroxy	292.42	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
6410-32-8	6410328	3424	3-hydroxy-4-[(2-methyl-4-nitropheny	440.46	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6410-41-9	6410419	3425	N-(5-chloro-2,4-dimethoxyphenyl)-4	627.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6419-19-8	6419198	3429	nitrilotrimethylenetris(phosphonic ac	299.05	3_REACH	150	150	0	0	0	3	0.15	0	0.15	150	0	525000	9130434.8
6422-86-2	6422862	3430	bis(2-ethylhexyl) terephthalate	390.56	3_REACH	79	79	0	0	0	1	3	0	3	79	0	276500	4808695.7
6425-39-4	6425394	3432	2,2'-dimorpholinyldiethyl ether	244.34	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
64354-92-3	64354923	3434	3-(isodecyloxy)propiononitrile	211.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6440-58-0	6440580	779	1,3-bis(hydroxymethyl)-5,5-dimethy	188.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6448-95-9	6448959	3436	3-hydroxy-4-[(2-methyl-5-nitropheny	426.44	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
645-62-5	645625	3438	2-ethylhex-2-enal	126.2	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
646-24-2	646242	3439	nonamethylenediamine	158.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6485-40-1	6485401	781	l-p-mentha-1(6),8-dien-2-one	150.22	3_REACH			1	1	0.00025	2	0.91	0	0.00025	0.00025	1	0.875	15.2
6485-55-8	6485558	3445	cis-2,6-dimethylmorpholine	115.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6485-67-2	6485672	4453	(2R)-2-amino-2-phenylacetamide	150.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
6486-23-3	6486233	3446	2-[(4-chloro-2-nitrophenyl)azo]-N-(2	395.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6528-34-3	6528343	3450	2-[(4-methoxy-2-nitrophenyl)azo]-N	386.37	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
65405-77-8	65405778	3452	(Z)-3-hexenyl salicylate	220.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
65-45-2	65452	784	salicylamide	137.14	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
65520-46-9	65520469	3455	bis[2-[2-(2-butoxyethoxy)ethoxy]eth	522.68	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
65-85-0	65850	785	benzoic acid	122.12	3_REACH	500	500	0	0	0	1	3	0	3	500	0	1750000	30434782.6
65855-02-9	65855029	4291	1-benzyl-5-ethoxyimidazolidine-2,4-	234.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6600-31-3	6600313	3458	3,9-dicyclohex-3-enyl-2,4,8,10-tetra	320.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
66063-15-8	66063158	3459	4-chloro-N-cyclopentylbenzylamine	209.72	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
66068-84-6	66068846	3460	4-(5,5,6-trimethylbicyclo[2.2.1]hept-	236.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6610-29-3	6610293	3462	4-methylthiosemicarbazide	105.17	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
66423-13-0	66423130	3473	octyl (R)-2-(4-chloro-2-methylpheno	326.86	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
66492-51-1	66492511	3475	(5-ethyl-1,3-dioxan-5-yl)methyl acry	200.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6674-22-2	6674222	3481	1,8-diazabicyclo[5.4.0]undec-7-ene	152.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
67075-37-0	67075370	3484	2,9-bis(2-phenylethyl)anthra[2,1,9-c	598.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
6711-48-4	6711484	3485	N'-[3-(dimethylamino)propyl]-N,N-di	187.33	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6712-98-7	6712987	3486	1-(N,N-bis(2-hydroxyethyl)amino)pr	163.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
67151-63-7	67151637	3487	1-[bis[3-(dimethylamino)propyl]amir	245.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6731-36-8	6731368	3488	di-tert-butyl 3,3,5-trimethylcyclohex	302.45	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
67-43-6	67436	82	N-carboxymethyliminobis(ethylener	393.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
674-82-8	674828	3493	but-3-en-3-olide	84.074	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
67801-15-4	67801154	3500	3-methyl-5-(2,2,3-trimethyl-3-cyclop	206.33	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
6786-83-0	6786830	3502	alpha,alpha-Bis[4-(dimethylamino)p	487.65	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
67990-05-0	67990050	3504	N-(5-chloro-2-methoxyphenyl)-3-hy	581.03	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
68-11-1	68111	798	mercaptoacetic acid	92.116	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
68134-22-5	68134225	3507	N-(2,3-dihydro-2-oxo-1H-benzimida	405.34	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
682-01-9	682019	3509	tetrapropyl orthosilicate	264.44	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
682-09-7	682097	3510	2,2-bis(allyloxymethyl)butan-1-ol	214.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
682-11-1	682111	3511	2-allyloxymethyl-2-ethylpropanediol	174.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
68227-78-1	68227781	3512	N-(5-chloro-2-methylphenyl)-3-hydr	565.03	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
68-26-8	68268	3514	retinol	286.46	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
6842-62-2	6842622	3515	614-477-3	239.1	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6843-66-9	6843669	3516	dimethoxydiphenylsilane	244.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6850-63-1	6850631	801	2,6-dimethylcyclohexylamine	127.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
68516-73-4	68516734	3518	tetramethyl 2,2'-[1,4-phenylenebis[i	716.67	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
68610-86-6	68610866	3522	Butanamide, 2,2'-[(3,3'-dichloro[1,1'	687.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
687-47-8	687478	3526	ethyl (S)-2-hydroxypropionate	118.13	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
68855-18-5	68855185	3527	(3-Hydroxy-2,2-dimethylpropyl) hep	216.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
688-84-6	688846	3529	2-ethylhexyl methacrylate	198.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
69045-84-7	69045847	4322	2,3-dichloro-5-trifluoromethylpyridin	215.99	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6925-69-5	6925695	3537	12H-phthaloperin-12-one	270.29	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
693-21-0	693210	804	oxydiethylene dinitrate	196.12	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
693-23-2	693232	3538	dodecanedioic acid	230.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
693-36-7	693367	3539	dioctadecyl 3,3'-thiodipropionate	683.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
693-57-2	693572	3540	12-aminododecanoic acid	215.34	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6938-94-9	6938949	3541	diisopropyl adipate	230.3	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
693-98-1	693981	806	2-methylimidazole	82.108	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
6940-53-0	6940530	3543	1-chloro-2,5-dimethoxy-4-nitrobenz	217.61	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
694-83-7	694837	807	cyclohex-1,2-ylenediamine	114.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
700-13-0	700130	3554	2,3,5-trimethylhydroquinone	152.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
70356-09-1	70356091	3560	1-[4-(1,1-dimethylethyl)phenyl]-3-(4	310.39	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
70445-33-9	70445339	4370	3-(2-ethylhexyloxy)propane-1,2-dio	204.31	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
70516-41-5	70516415	3563	2'-anilino-6'-[ethyl(3-methylbutyl)am	518.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
70-55-3	70553	85	toluene-4-sulphonamide	171.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
706-14-9	706149	813	decan-4-olide	170.25	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
7069-42-3	7069423	3567	retinyl propionate	342.52	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
70969-58-3	70969583	815	diisobutyl hexahydrophthalate	284.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
71048-82-3	71048823	3577	(2E)-1-[(1R,2S)-2,6,6-Trimethylcycl	192.3	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
712-50-5	712505	818	cyclohexyl phenyl ketone	188.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
713-95-1	713951	3581	dodecan-5-olide	198.31	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
71604-74-5	71604745	3586	m-(2,3-epoxypropoxy)-N,N-bis(2,3-	277.32	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
71617-10-2	71617102	3587	isopentyl p-methoxycinnamate	248.32	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
71735-74-5	71735745	3588	ethyl 3-[[bis(1-methylethoxy)phosph	314.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7173-62-8	7173628	3589	(Z)-N-9-octadecenylpropane-1,3-dia	324.6	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
71902-23-3	71902233	3594	6-[(1-oxomethyloctyl)amino]hexano	271.4	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
7195-44-0	7195440	3595	bis(2,3-epoxypropyl) terephthalate	278.26	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
72361-35-4	72361354	3603	triisotridecyl benzene-1,2,4-tricarbo	757.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
7300-34-7	7300347	3612	3,3'-[butane-1,4-diylbis(oxy)]bisprop	204.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7305-71-7	7305717	4342	2-amino-5-methylthiazole	114.17	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
732-26-3	732263	829	2,4,6-tri-tert-butylphenol	262.44	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
7328-22-5	7328225	3618	2-(2-butoxyethoxy)ethyl methacryla	230.3	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
7381-13-7	7381137	3627	1,1'-(1,3-Phenylenedicarbonyl)diaz	356.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7396-58-9	7396589	3629	N-methyldidecylamine	311.6	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7397-62-8	7397628	3630	butyl glycollate	132.16	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
74338-72-0	74338720	4323	2,4,4,7-tetramethyl-6-octen-3-one	182.31	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
74441-05-7	74441057	3635	N-[4-(aminocarbonyl)phenyl]-4-[[1-[	499.49	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7473-98-5	7473985	3642	2-hydroxy-2-methylpropiophenone	164.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
75-12-7	75127	851	formamide	45.042	3_REACH	40	40	0	0	0	3	0.15	0	0.15	40	0	140000	2434782.6
7526-26-3	7526263	3659	diphenyl methylphosphonate	248.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7534-94-3	7534943	3668	exo-1,7,7-trimethylbicyclo[2.2.1]hep	222.33	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
75490-39-0	75490390	4313	2,2,4-trimethyl-4-phenyl-butane-nitr	187.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
756-80-9	756809	864	O,O-dimethyl hydrogen dithiophosp	158.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
75-75-2	75752	3683	methanesulphonic acid	96.104	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
7575-23-7	7575237	3684	pentaerythritol tetrakis(3-mercaptop	488.66	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
75980-60-8	75980608	3692	diphenyl(2,4,6-trimethylbenzoyl)pho	348.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
75-98-9	75989	868	pivalic acid	102.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
76-03-9	76039	90	trichloroacetic acid	163.39	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7605-52-9	7605529	3696	methyl cis-3-methylcyclohexanecar	156.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7

760-67-8	760678	3697	2-ethylhexanoyl chloride	162.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
76114-73-3	76114733	3699	2-Propynyl butylcarbamate	155.2	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
76201-56-4	76201564	3704	3-[dimethyl(3-{[(3,3,4,4,5,5,6,6,7,7,8	650.47	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
762-04-9	762049	3705	diethyl phosphonate	138.1	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
76-22-2	76222	872	bornan-2-one	152.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
763-69-9	763699	3710	ethyl 3-ethoxypropionate	146.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
764-99-8	764998	3714	1,1'-[oxybis(ethyleneoxy)]diethylene	158.2	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
76524-94-2	76524942	3715	N-[3-(Triethoxysilyl)propyl]formamic	249.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7659-86-1	7659861	3721	2-ethylhexyl mercaptoacetate	204.33	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
76855-69-1	76855691	4234	Azetidon	287.43	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
768-94-5	768945	878	amantadine	151.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7695-91-2	7695912	3727	3,4-dihydro-2,5,7,8-tetramethyl-2-(4	472.75	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
770-35-4	770354	3730	1-phenoxypropan-2-ol	152.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
77-09-8	77098	879	phenolphthalein	318.33	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7747-35-5	7747355	880	7a-ethyldihydro-1H,3H,5H-oxazolo[	143.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
77501-63-4	77501634	882	Lactofen	461.78	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
77-71-4	77714	883	5,5-dimethylhydantoin	128.13	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
77-73-6	77736	884	3a,4,7,7a-tetrahydro-4,7-methanoin	132.21	3_REACH	4	4	0	0	0	3	0.15	0	0.15	4	0	14000	243478.3
77-78-1	77781	886	dimethyl sulphate	126.13	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
77804-81-0	77804810	3736	2,2'-[ethylenebis(oxyphenyl-2,1-ene	732.72	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
77-83-8	77838	3738	ethyl 2,3-epoxy-3-phenylbutyrate	206.24	3_REACH	35	35	0	1	0.00025	3	0.15	0	0.00025	35	0	122500	2130434.8
7785-26-4	7785264	887	(-)-pin-2(3)-ene	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
7785-70-8	7785708	888	(+)-pin-2(3)-ene	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
77-86-1	77861	3739	trometamol	121.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
7787-93-1	7787931	3741	dichloro(3-chloropropyl)methylsilan	191.56	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
778-94-9	778949	3743	2-nitro-4-(trifluoromethyl)benzonitril	216.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
77-90-7	77907	3744	tributyl O-acetylcitrate	402.48	3_REACH	100	100	0	0	0	1	3	0	3	100	0	350000	6086956.5
77-92-9	77929	889	citric acid	192.12	3_REACH	666.6666667	666.6666667	0	0	0	3	0.15	0	0.15	666.666667	0	2333333.333	40579710.1
77-93-0	77930	92	triethyl citrate	276.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
77-94-1	77941	3745	tributyl citrate	360.45	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
77-99-6	77996	890	propylidynetrimethanol	134.18	3_REACH	67	67	0	0	0	1	3	0	3	67	0	234500	4078260.9
780-69-8	780698	891	triethoxy(phenyl)silane	240.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-08-0	78080	3746	triethoxy(vinyl)silane	190.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-11-5	78115	892	pentaerithrityl tetranitrate	316.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-27-3	78273	893	1-ethynylcyclohexanol	124.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-40-0	78400	894	triethyl phosphate	182.16	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
78-42-2	78422	895	tris(2-ethylhexyl) phosphate	434.64	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-51-3	78513	93	tris(2-butoxyethyl) phosphate	398.48	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78521-39-8	78521398	3751	6-[[(4-methylphenyl)sulphonyl]amin	285.36	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78531-61-0	78531610	4400	4-(trans-4-propylcyclohexyl)acetopl	244.38	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
78-59-1	78591	897	3,5,5-trimethylcyclohex-2-enone	138.21	3_REACH	500	500	0	1	0.00025	2	0.91	0	0.00025	500	0	1750000	30434782.6
78605-96-6	78605966	3752	alpha-Amylcinnamaldehyde	202.3	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
78-63-7	78637	3753	di-tert-butyl 1,1,4,4-tetramethyltetra	290.44	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-67-1	78671	3754	2,2'-dimethyl-2,2'-azodipropiononitr	164.22	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
78-69-3	78693	3755	3,7-dimethyloctan-3-ol	158.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-70-6	78706	899	linalool	154.25	3_REACH	117	117	0	0	0	3	0.15	0	0.15	117	0	409500	7121739.1
78850-37-0	78850370	5023	methyl (3aR,4R,7aR)-2-methyl-4-(1	413.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
78-97-7	78977	3762	lactonitrile	71.08	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
79-06-1	79061	911	acrylamide	71.08	3_REACH	0.17	0.17	0	1	0.00025	3	0.15	0	0.00025	0.17	0	595	10347.8
79-07-2	79072	3765	2-chloroacetamide	93.514	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
79-08-3	79083	912	bromoacetic acid	138.95	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
79-11-8	79118	915	chloroacetic acid	94.497	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
791-28-6	791286	95	triphenylphosphine oxide	278.29	3_REACH	2	2	0	0	0	3	0.15	0	0.15	2	0	7000	121739.1
79-14-1	79141	3766	glycollic acid	76.051	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
79-16-3	79163	3767	N-methylacetamide	73.096	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
793-24-8	793248	3771	N-1,3-dimethylbutyl-N'-phenyl-p-ph	268.41	3_REACH	4	4	0	0	0	3	0.15	0	0.15	4	0	14000	243478.3
79-33-4	79334	920	l-(+)-lactic acid	90.078	3_REACH	570	570	0	0	0	3	0.15	0	0.15	570	0	1995000	34695652.2
79-41-4	79414	3776	methacrylic acid	86.09	3_REACH	50	50	0	0	0	3	0.15	0	0.15	50	0	175000	3043478.3
79456-26-1	79456261	4391	3-chloro-5-trifluoromethyl-2-pyridyla	196.56	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
79-74-3	79743	3781	2,5-di-tert-pentylhydroquinone	250.38	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
79-77-6	79776	926	(E)-4-(2,6,6-trimethyl-1-cyclohexen-	192.3	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
79815-20-6	79815206	4252	(S)-2,3-dihydro-1H-indole-2-carbox	163.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
79-94-7	79947	929	2,2',6,6'-tetrabromo-4,4'-isopropylid	543.9	3_REACH	16	16	0	0	0	3	0.15	0	0.15	16	0	56000	973913.0
80-04-6	80046	931	4,4'-isopropylidenedicyclohexanol	240.39	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
80-05-7	80057	96	4,4'-isopropylidenediphenol	228.29	3_REACH	5	5	0	0	0	3	0.15	0	0.15	5	0	17500	304347.8
80-07-9	80079	3786	bis(4-chlorophenyl) sulphone	287.16	3_REACH	1.5	1.5	0	0	0	3	0.15	0	0.15	1.5	0	5250	91304.3
80-10-4	80104	3788	dichloro(diphenyl)silane	253.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
80-15-9	80159	932	Cumene hydroperoxide	152.19	3_REACH	15	15	0	0	0	1	3	0	3	15	0	52500	913043.5
80-26-2	80262	934	p-menth-1-en-8-yl acetate	196.29	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
80-43-3	80433	3791	Dicumyl peroxide	270.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
80-46-6	80466	936	p-(1,1-dimethylpropyl)phenol	164.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
80-51-3	80513	3792	4,4'-oxydi(benzenesulphonohydrazi	358.4	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
80-54-6	80546	3794	2-(4-tert-butylbenzyl)propionaldehy	204.31	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
80-56-8	80568	937	pin-2(3)-ene	136.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
80-73-9	80739	3797	1,3-dimethylimidazolidin-2-one	114.15	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
81-07-2	81072	98	1,2-benzisothiazol-3(2H)-one 1,1-di	183.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
81-19-6	81196	939	1,3-Dichloro-2-(dichloromethyl)benz	229.92	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
81-25-4	81254	100	cholic acid	408.58	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
81-33-4	81334	3804	perylene-3,4:9,10-tetracarboxydiimi	390.36	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
81782-77-6	81782776	3814	4-methyl-3-decen-5-ol	170.3	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
818-61-1	818611	943	2-hydroxyethyl acrylate	116.12	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
82199-12-0	82199120	3820	N-(2,3-dihydro-2-oxo-1H-benzimida	367.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
822-06-0	822060	3822	hexamethylene diisocyanate	168.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
826-36-8	826368	3834	2,2,6,6-tetramethyl-4-piperidone	155.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
82985-35-1	82985351	3839	bis(trimethoxysilylpropyl)amine	341.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
830-13-7	830137	3840	cyclododecanone	182.31	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
83066-88-0	83066880	950	(2R)-2-[4-[[5-(trifluoromethyl)-2-pyri	327.26	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
83261-15-8	83261158	3844	isobutyl (S)-2-chloropropionate	164.63	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
83-32-9	83329	952	acenaphthene	154.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
83-42-1	83421	954	2-chloro-6-nitrotoluene	171.58	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
83524-75-8	83524758	3848	2,9-bis(p-methoxybenzyl)anthra[2,1	630.66	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
83-73-8	83738	3850	diiodohydroxyquinoline	396.95	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
83926-73-2	83926732	4796	4-cyclohexyl-2-methyl-2-butanol	170.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
84170-74-1	84170741	3857	(2,2-Dimethyl-1,3-propanediyl)bis(o	328.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
84281-74-3	84281743	3859	1,3-Benzenediamine, coupled with	346.41	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
84418-63-3	84418633	3863	Isononanoic acid, mixed esters with	328.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
84434-11-7	84434117	3864	ethyl phenyl(2,4,6-trimethylbenzoyl)	316.34	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
84583-68-6	84583686	3868	2-Butenoic acid, 4-oxo-4-(tridecylar	297.44	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
84-65-1	84651	960	anthraquinone	208.22	3_REACH	31	31	0	1	0.00025	3	0.15	0	0.00025	31	0	108500	1886956.5
84-66-2	84662	961	diethyl phthalate	222.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
84-69-5	84695	962	diisobutyl phthalate	278.35	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
84713-17-7	84713177	3874	2,2,4(or 2,4,4)-trimethylhexanedinit	150.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
84-74-2	84742	963	dibutyl phthalate	278.35	3_REACH	0.666666667	0.666666667	0	0	0	1	3	0	3	0.66666667	0	2333.333333	40579.7
84852-15-3	84852153	964	Phenol, 4-nonyl-, branched	220.36	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
84852-53-9	84852539	3878	1,1'-(ethane-1,2-diyl)bis[pentabrom	971.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
85-41-6	85416	965	phthalimide	147.13	3_REACH	250	250	0	0	0	3	0.15	0	0.15	250	0	875000	15217391.3
85-42-7	85427	3889	cyclohexane-1,2-dicarboxylic anhyc	154.16	3_REACH	100	100	0	0	0	3	0.15	0	0.15	100	0	350000	6086956.5
85-68-7	85687	968	benzyl butyl phthalate	312.37	3_REACH	50	50	0	0	0	1	3	0	3	50	0	175000	3043478.3
85702-79-0	85702790	3896	6-(isononanoylamino)hexanoic acid	271.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
85-73-4	85734	3897	phthalylsulfathiazole	403.44	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
86261-90-7	86261907	3902	2-(2-oxoimidazolidin-1-yl)ethyl meth	198.22	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
867-13-0	867130	3910	triethyl phosphonoacetate	224.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
86-73-7	86737	973	fluorene	166.22	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
86-74-8	86748	974	carbazole	167.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
868-77-9	868779	975	2-hydroxyethyl methacrylate	130.14	3_REACH	100	100	0	0	0	1	3	0	3	100	0	350000	6086956.5
86960-46-5	86960465	3914	4-(decanoyloxy)benzoic acid	292.38	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
872-05-9	872059	3921	dec-1-ene	140.27	3_REACH	1000	1000	0	0	0	1	3	0	3	1000	0	3500000	60869565.2
872-36-6	872366	3923	vinylene carbonate	86.046	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
872-50-4	872504	977	1-methyl-2-pyrrolidone	99.134	3_REACH	160	160	0	0	0	3	0.15	0	0.15	160	0	560000	9739130.4
87305-03-1	87305031	3924	(1R,4R,5S)-6,6-Dimethyl-4-(tribrom	376.89	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
873-32-5	873325	3927	2-chlorobenzonitrile	137.57	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
87333-22-0	87333220	4632	methyl 2-(acetylamino)-3-chloropro	195.599	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
87-59-2	87592	978	2,3-xylidine	121.18	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
87-61-6	87616	979	1,2,3-trichlorobenzene	181.45	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
87-62-7	87627	980	2,6-xylidine	121.18	3_REACH	150	150	0	0	0	1	3	0	3	150	0	525000	9130434.8
87-99-0	87990	3944	xylitol	152.15	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
88-12-0	88120	3948	1-vinyl-2-pyrrolidone	111.15	3_REACH	1	1	0	0	0	3	0.15	0	0.15	1	0	3500	60869.6
88150-62-3	88150623	4393	3-ethyl 5-methyl 4-(2-chlorophenyl)-	538.99	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
88-18-6	88186	983	2-tert-butylphenol	150.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
88-27-7	88277	3954	2,6-DI-Tert-butyl-4-(dimethylamino)	263.43	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
88374-05-4	88374054	3955	2-(2-Fluorophenyl)-2-(4-fluoropheny	232.23	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
88-44-8	88448	3956	4-aminotoluene-3-sulphonic acid	187.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
88-45-9	88459	3957	2,5-diaminobenzenesulphonic acid	188.21	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
88-51-7	88517	3959	4-amino-6-chlorotoluene-3-sulphon	221.66	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
88-60-8	88608	3961	6-tert-butyl-m-cresol	164.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
88-72-2	88722	985	2-nitrotoluene	137.14	3_REACH	50	50	0	1	0.00025	3	0.15	0	0.00025	50	0	175000	3043478.3
88-73-3	88733	986	1-chloro-2-nitrobenzene	157.56	3_REACH	0.25	0.25	0	1	0.00025	3	0.15	0	0.00025	0.25	0	875	15217.4
88-74-4	88744	987	2-nitroaniline	138.13	3_REACH	50	50	0	1	0.00025	3	0.15	0	0.00025	50	0	175000	3043478.3
88-75-5	88755	988	2-nitrophenol	139.11	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
88-85-7	88857	989	dinoseb	240.22	3_REACH	0.333333333	0.333333333	0	1	0.00025	3	0.15	0	0.00025	0.33333333	0	1166.666667	20289.9
88-99-3	88993	990	phthalic acid	166.13	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
89182-60-5	89182605	3969	D-Glucitol, 1-deoxy-1-(formylamino	209.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
89-48-5	89485	3976	menthyl acetate	198.31	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
89604-91-1	89604911	4680	3-[2-(1,3-benzothiazol-2-ylsulfanyl)-	351.43	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
89-62-3	89623	991	2-nitro-p-toluidine	152.16	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
89-63-4	89634	992	4-chloro-2-nitroaniline	172.57	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
89-72-5	89725	993	2-sec-butylphenol	150.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
89-83-8	89838	996	thymol	150.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
89-98-5	89985	997	2-chlorobenzaldehyde	140.57	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
90-02-8	90028	998	salicylaldehyde	122.12	3_REACH	10	10	0	1	0.00025	1	3	0	0.00025	10	0	35000	608695.7
90-04-0	90040	999	o-anisidine	123.16	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
90-05-1	90051	3990	guaiacol	124.14	3_REACH	67	67	0	0	0	1	3	0	3	67	0	234500	4078260.9
90-12-0	90120	1000	1-methylnaphthalene	142.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
901-44-0	901440	3991	2,2'-isopropylidenebis(p-phenylene	316.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
9016-45-9	9016459	1001	Nonylphenol, ethoxylated	308.462	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
90-17-5	90175	3992	2,2,2-trichloro-1-phenylethyl acetate	267.54	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
90268-23-8	90268238	3995	Butanamide, 2,2'-[(3,3'-dichloro[1,1'	659.54	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
90268-24-9	90268249	3996	Butanamide, 2,2'-[(3,3'-dichloro[1,1'	752.06	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
90-30-2	90302	1002	N-1-naphthylaniline	219.29	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
90-43-7	90437	106	biphenyl-2-ol	170.21	3_REACH	39	39	0	0	0	3	0.15	0	0.15	39	0	136500	2373913.0
90474-13-8	90474138	4000	diethyl 1,2-cyclopentanedicarboxyla	214.26	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
90498-90-1	90498901	4387	3,9-bis(2-(3-(3-tert-butyl-4-hydroxy-	740.98	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
90-51-7	90517	4001	6-amino-4-hydroxynaphthalene-2-s	239.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
90-72-2	90722	4003	2,4,6-tris(dimethylaminomethyl)phe	265.4	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
90-80-2	90802	4006	D-glucono-1,5-lactone	178.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
91-15-6	91156	1004	phthalonitrile	128.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
91-17-8	91178	1005	decahydronaphthalene	138.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
91-20-3	91203	107	naphthalene	128.17	3_REACH	71	71	0	0	0	3	0.15	0	0.15	71	0	248500	4321739.1
91-22-5	91225	1006	quinoline	129.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
91273-04-0	91273040	4271	1-(N,N-bis(2-ethylhexyl)aminometh	322.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
91-57-6	91576	1007	2-methylnaphthalene	142.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
91-64-5	91645	1008	coumarin	146.15	3_REACH	10	10	0	1	0.00025	3	0.15	0	0.00025	10	0	35000	608695.7
91-66-7	91667	1009	N,N-diethylaniline	149.24	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
91-68-9	91689	4019	3-diethylaminophenol	165.24	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
91-76-9	91769	4021	6-phenyl-1,3,5-triazine-2,4-diyldiam	187.21	3_REACH	19	19	0	1	0.00025	3	0.15	0	0.00025	19	0	66500	1156521.7
919-30-2	919302	4023	3-aminopropyltriethoxysilane	221.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
91-97-4	91974	4025	3,3'-dimethylbiphenyl-4,4'-diyl diiso	264.29	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
923-02-4	923024	4030	N-(hydroxymethyl)methacrylamide	115.13	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
925-21-3	925213	4038	butyl hydrogen maleate	172.18	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
92-52-4	92524	1012	biphenyl	154.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
92-69-3	92693	1013	biphenyl-4-ol	170.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
92-70-6	92706	4045	3-hydroxy-2-naphthoic acid	188.18	3_REACH	12	12	0	0	0	3	0.15	0	0.15	12	0	42000	730434.8
927-07-1	927071	4046	tert-butyl peroxypivalate	174.24	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
92-84-2	92842	4051	phenothiazine	199.28	3_REACH	6	6	0	0	0	3	0.15	0	0.15	6	0	21000	365217.4
92-88-6	92886	1015	biphenyl-4,4'-diol	186.21	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
928-96-1	928961	1016	cis-hex-3-en-1-ol	100.16	3_REACH	127	127	0	0	0	1	3	0	3	127	0	444500	7730434.8
929-06-6	929066	4053	2-(2-aminoethoxy)ethanol	105.14	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
92952-81-3	92952813	4412	4-[(3-hydroxypropyl)amino]-3-nitrop	212.21	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
93-04-9	93049	1017	methyl 2-naphthyl ether	158.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
931-36-2	931362	4059	2-ethyl-4-methylimidazole	110.16	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4

93-17-4	93174	4063	3,4-dimethoxyphenylacetonitrile	177.2	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
93-20-9	93209	4065	2-(2-naphthyloxy)ethanol	188.23	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
932-64-9	932649	4066	1,2-dihydro-5-nitro-3H-1,2,4-triazol-	130.07	3_REACH			1	1	0.00025	1	0.15	0	0.00025	0.00025	1	0.875	15.2
93413-62-8	93413628	4069	4-[2-(Dimethylamino)-1-(1-hydroxyc	263.38	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
93-58-3	93583	4073	methyl benzoate	136.15	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
936-49-2	936492	4076	2-phenyl-2-imidazoline	146.19	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
93-69-6	93696	4079	1-o-tolylbiguanide	191.24	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
93-70-9	93709	4080	2'-chloroacetoacetanilide	211.65	3_REACH			1	0	0	1	0.15	0	0.15	0.15	1	525	9130.4
93-92-5	93925	4093	1-phenylethyl acetate	164.2	3_REACH	50	50	0	0	0	1	3	0	3	50	0	175000	3043478.3
93957-50-7	93957507	4490	3-(3-(4-fluorophenyl)-1-(1-methylet	307.37	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
939-87-9	939979	4095	4-tert-butylbenzaldehyde	162.23	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
94-04-2	94042	4096	vinyl 2-ethylhexanoate	170.25	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
94050-90-5	94050905	4248	(R)-2-(4-hydroxyphenoxy)propanoic	182.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
94-13-3	94133	109	propyl 4-hydroxybenzoate	180.2	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
941-69-5	941695	4098	N-phenylmaleimide	173.17	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
947-04-6	947046	4110	dodecane-12-lactam	197.32	3_REACH	25	25	0	0	0	3	0.15	0	0.15	25	0	87500	1521739.1
947-19-3	947193	4112	hydroxycyclohexyl phenyl ketone	204.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
94723-86-1	94723861	4485	2-butanoyl-3-hydroxy-5-(thiazn-3-yl)	282.4	3_REACH			1	1	0.00025	1	0.15	0	0.00025	0.00025	1	0.875	15.2
947753-66-4	947753664	4115	2-Ethylhexyl-2-cyano-3-(4-methoxy	391.51	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
94-91-7	94917	4116	N,N'-Bis(salicylidene)-1,2-propanec	282.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
94-96-2	94962	1024	2-ethylhexane-1,3-diol	146.23	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
95-14-7	95147	112	benzotriazole	119.13	3_REACH	98.33333333	98.33333333	0	0	0	3	0.15	0	0.15	98.3333333	0	344166.6667	5985507.2
95-16-9	95169	113	benzothiazole	135.19	3_REACH	1.7	1.7	0	0	0	3	0.15	0	0.15	1.7	0	5950	103478.3
95235-30-6	95235306	4398	4-(4-isopropoxyphenylsulfonyl)pher	292.35	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
95-31-8	95318	4124	N-tert-butylbenzothiazole-2-sulpher	238.38	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
95-33-0	95330	4125	N-cyclohexylbenzothiazole-2-sulfer	264.42	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
95-38-5	95385	4126	2-(2-heptadec-8-enyl-2-imidazolin-1	350.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
95-48-7	95487	1029	o-cresol	108.14	3_REACH	67	67	0	0	0	1	3	0	3	67	0	234500	4078260.9
95-49-8	95498	1030	2-chlorotoluene	126.59	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
95-51-2	95512	1031	2-chloroaniline	127.58	3_REACH	3.333333333	3.333333333	0	1	0.00025	3	0.15	0	0.00025	3.33333333	0	11666.66667	202898.6
95-53-4	95534	1032	o-toluidine	107.16	3_REACH	7.833333333	7.833333333	0	1	0.00025	1	3	0	0.00025	7.83333333	0	27416.66667	476811.6
95-54-5	95545	1033	o-phenylenediamine	108.15	3_REACH	20	20	0	1	0.00025	1	3	0	0.00025	20	0	70000	1217391.3
95-63-6	95636	1035	1,2,4-trimethylbenzene	120.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
95-68-1	95681	1036	2,4-xylidine	121.18	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
95-74-9	95749	1037	3-chloro-p-toluidine	141.6	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
95-80-7	95807	1039	4-methyl-m-phenylenediamine	122.17	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
95-82-9	95829	1040	2,5-dichloroaniline	162.02	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
95962-14-4	95962144	4305	2-(2-(4-methyl-3-cyclohexen-1-yl)pr	220.36	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
95-96-5	95965	4140	dilactide	144.13	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
96-09-3	96093	1044	(epoxyethyl)benzene	120.15	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-12-8	96128	1045	1,2-dibromo-3-chloropropane	236.35	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-18-4	96184	1047	1,2,3-trichloropropane	147.43	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-23-1	96231	1049	1,3-dichloropropan-2-ol	128.99	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-24-2	96242	1050	3-chloropropane-1,2-diol	110.54	3_REACH	0.08	0.08	0	1	0.00025	3	0.15	0	0.00025	0.08	0	280	4869.6
96-29-7	96297	1051	butanone oxime	87.123	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
96-31-1	96311	1052	1,3-dimethylurea	88.112	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
96-45-7	96457	1054	imidazolidine-2-thione	102.16	3_REACH	5	5	0	0	0	1	0.15	0	0.15	5	0	17500	304347.8
96-48-0	96480	4148	Butyrolactone	86.09	3_REACH	112	112	0	0	0	1	3	0	3	112	0	392000	6817391.3
96-49-1	96491	4149	ethylene carbonate	88.062	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
96-67-3	96673	4151	3-amino-2-hydroxy-5-nitrobenzenes	234.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-69-5	96695	4152	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	358.54	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
96-76-4	96764	4153	2,4-di-tert-butylphenol	206.33	3_REACH	150	150	0	0	0	1	3	0	3	150	0	525000	9130434.8
96-93-5	96935	4156	3-amino-4-hydroxy-5-nitrobenzenes	234.19	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-96-8	96968	4157	2-nitro-p-anisidine	168.15	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
96-97-9	96979	4158	5-nitrosalicylic acid	183.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
97-00-7	97007	1056	1-chloro-2,4-dinitrobenzene	202.56	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
97-39-2	97392	4164	1,3-di-o-tolylguanidine	239.32	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
97-52-9	97529	4165	4-nitro-o-anisidine	168.15	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
97-53-0	97530	1057	eugenol	164.2	3_REACH	67	67	0	1	0.00025	1	3	0	0.00025	67	0	234500	4078260.9
97-65-4	97654	4168	itaconic acid	130.1	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
976-71-6	976716	4170	camrenone	340.46	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
97-74-5	97745	1059	tetramethylthiuram monosulphide	208.37	3_REACH			1	0	0	1	0.15	0	0.15	0.15	1	525	9130.4
97-78-9	97789	4172	N-lauroylsarcosine	271.4	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
97-88-1	97881	1061	butyl methacrylate	142.2	3_REACH	120	120	0	0	0	1	3	0	3	120	0	420000	7304347.8
97-90-5	97905	4175	ethylene dimethacrylate	198.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98-00-0	98000	1063	furfuryl alcohol	98.101	3_REACH	53	53	0	0	0	3	0.15	0	0.15	53	0	185500	3226087.0
980-26-7	980267	4177	5,12-dihydro-2,9-dimethylquino[2,3	340.38	3_REACH	1000	1000	0	1	0.00025	3	0.15	0	0.00025	1000	0	3500000	60869565.2
98-07-7	98077	1065	Benzotrichloride	195.48	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
98-09-9	98099	1066	benzenesulphonyl chloride	176.62	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
98-13-5	98135	1067	trichloro(phenyl)silane	211.55	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
98-16-8	98168	1068	3-Trifluoromethylaniline	161.13	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
98-17-9	98179	1069	3-(Trifluoromethyl)phenol	162.11	3_REACH			1	0	0	1	0.15	0	0.15	0.15	1	525	9130.4
98-29-3	98293	4181	4-tert-butylpyrocatechol	166.22	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98-37-3	98373	4183	3-amino-4-hydroxybenzenesulphon	189.19	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98377-35-6	98377356	4501	1-(2-chlorophenyl)-1,2-dihydro-5H-i	198.6	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
98-44-2	98442	4185	2-aminobenzene-1,4-disulphonic ac	253.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98-51-1	98511	1071	4-tert-butyltoluene	148.25	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98-52-2	98522	1072	4-tert-butylcyclohexanol	156.27	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98-53-3	98533	4186	4-tert-butylcyclohexanone	154.25	3_REACH			1	0	0	2	0.91	0	0.91	0.91	1	3185	55391.3
98-54-4	98544	1073	4-tert-butylphenol	150.22	3_REACH	60	60	0	0	0	1	3	0	3	60	0	210000	3652173.9
98-55-5	98555	1074	p-menth-1-en-8-ol	154.25	3_REACH	250	250	0	0	0	3	0.15	0	0.15	250	0	875000	15217391.3
98-59-9	98599	4188	tosyl chloride	190.65	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
98730-04-2	98730042	4191	2,2-Dichloro-1-(3-methyl-2,3-dihydr	260.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
98-73-7	98737	1075	4-tert-butylbenzoic acid	178.23	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98-82-8	98828	1076	cumene	120.19	3_REACH	154	154	0	0	0	1	3	0	3	154	0	539000	9373913.0
98-83-9	98839	4193	2-phenylpropene	118.18	3_REACH	40	40	0	0	0	1	3	0	3	40	0	140000	2434782.6
98-85-1	98851	4194	1-phenylethanol	122.17	3_REACH	31	31	0	0	0	1	3	0	3	31	0	108500	1886956.5
98-86-2	98862	1077	acetophenone	120.15	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
98967-40-9	98967409	1081	N-(2,6-difluorophenyl)-5-methyl[1,2	325.3	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
99-08-1	99081	1082	3-nitrotoluene	137.14	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
99189-60-3	99189603	4198	2-[1-(2-Amino-2-oxoethyl)cyclohex	199.25	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
993-13-5	993135	4203	methylphosphonic acid	96.022	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
99-34-3	99343	4204	3,5-dinitrobenzoic acid	212.12	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
99-54-7	99547	1087	1,2-dichloro-4-nitrobenzene	192	3_REACH	4	4	0	1	0.00025	3	0.15	0	0.00025	4	0	14000	243478.3
99-55-8	99558	1088	5-nitro-o-toluidine	152.16	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
99-57-0	99570	4206	2-amino-4-nitrophenol	154.13	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
99591-74-9	99591749	4207	1,5,2,4-dioxadithiane 2,2,4,4-tetrac	188.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
99607-70-2	99607702	1089	Heptan-2-yl [(5-chloroquinolin-8-yl)o	335.83	3_REACH			1	0	0	3	0.15	0	0.15	0.15	1	525	9130.4
99-62-7	99627	4210	1,3-diisopropylbenzene	162.28	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
99-63-8	99638	4214	isophthaloyl dichloride	203.02	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
99-75-2	99752	4215	methyl p-toluate	150.18	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
99-76-3	99763	4216	methyl 4-hydroxybenzoate	152.15	3_REACH	1030	1030	0	0	0	1	3	0	3	1030	0	3605000	62699652.2
99817-36-4	99817364	4328	2-chloro-3-ethyl-6-nitrophenol	236.06	3_REACH			1	1	0.00025	3	0.15	0	0.00025	0.00025	1	0.875	15.2
99-87-6	99876	1092	p-cymene	134.22	3_REACH	154	154	0	0	0	1	3	0	3	154	0	539000	9373913.0
99-88-7	99887	4221	4-isopropylaniline	135.21	3_REACH	6	6	0	1	0.00025	1	3	0	0.00025	6	0	21000	365217.4
99-93-4	99934	4222	4'-hydroxyacetophenone	136.15	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
99-96-7	99967	1093	4-hydroxybenzoic acid	138.12	3_REACH			1	0	0	1	3	0	3	3	1	10500	182608.7
99-97-8	99978	1094	N,N-dimethyl-p-toluidine	135.21	3_REACH			1	1	0.00025	1	3	0	0.00025	0.00025	1	0.875	15.2
99-99-0	99990	1095	4-nitrotoluene	137.14	3_REACH	125	125	0	1	0.00025	3	0.15	0	0.00025	125	0	437500	7608695.7

						Daphnids, acute						Daphnids, chronic						Daphnids, chronic & reproduction					
CAS	CAS_NR	ID	Compound	MW	Emissions	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value [1=YES]	Final Tox conc (ug/l)	Final Tox conc (mol/m3)	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value [1=YES]	Final Tox conc (ug/l)	Final Tox conc (mol/m3)	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value [1=YES]	Final Tox conc (ug/l)	Final Tox conc (mol/m3)
100986-85-4	100986854	139	Levofloxacin	361.38	1_Pharma				1	0.3	8.3015E-07				1	0.03	8.3015E-08				1	0.03	8.30151E-08
10238-21-8	10238218	152	Glibenklamid	494.01	1_Pharma				1	0.3	6.0728E-07				1	0.03	6.0728E-08				1	0.03	6.07275E-08
103-90-2	103902	165	paracetamol	151.17	1_Pharma	10.66666667		10.66666667	0	10.6666667	7.0561E-05				1	0.03	1.9845E-07				1	0.03	1.98452E-07
114-07-8	114078	336	erythromycin	733.94	1_Pharma	7483.333333		7483.333333	0	7483.33333	0.01019611	11100		11100	0	11100	0.01512385	11100		11100	0	11100	0.015123852
114798-26-4	114798264	1626	Losartan	422.93	1_Pharma				1	0.3	7.0934E-07				1	0.03	7.0934E-08				1	0.03	7.09337E-08
120-51-4	120514	359	benzyl benzoate	212.25	1_Pharma				1	0.3	1.4134E-06				1	0.03	1.4134E-07				1	0.03	1.41343E-07
121-75-5	121755	374	Malathion	330.36	1_Pharma	0.032666667		0.032666667	0	0.03266667	9.8882E-08	0.06		0.06	0	0.06	1.8162E-07	0.06		0.06	0	0.06	1.8162E-07
123-99-9	123999	1782	azelaic acid	188.22	1_Pharma				1	0.3	1.5939E-06				1	0.03	1.5939E-07				1	0.03	1.59388E-07
126-07-8	126078	1144	Griseofulvin	352.77	1_Pharma	333333.3333		333333.3333	0	333333.333	0.94490272				1	0.03	8.5041E-08				1	0.03	8.50412E-08
127-07-1	127071	411	Hydroxikarbamid	76.057	1_Pharma				1	0.3	3.9444E-06				1	0.03	3.9444E-07				1	0.03	3.94441E-07
128-13-2	128132	1816	Ursodiol	392.58	1_Pharma				1	0.3	7.6418E-07				1	0.03	7.6418E-08				1	0.03	7.64175E-08
130-26-7	130267	1834	Clioquinol	305.5	1_Pharma				1	0.3	9.82E-07				1	0.03	9.82E-08				1	0.03	9.81997E-08
13311-84-7	13311847	427	Flutamid	276.22	1_Pharma				1	0.3	1.0861E-06				1	0.03	1.0861E-07				1	0.03	1.08609E-07
134523-00-5	134523005	431	Atorvastatin	558.65	1_Pharma	1		1	0	1	1.79E-06				1	0.03	5.3701E-08				1	0.03	5.37009E-08
137862-53-4	137862534	442	Valsartan	435.53	1_Pharma	193333.3333		193333.3333	0	193333.333	0.4439036	5600		5600	0	5600	0.0128579	5600		5600	0	5600	0.012857897
138402-11-6	138402116	444	Irbesartan	428.55	1_Pharma	86400		86400	0	86400	0.20161008	10400		10400	0	10400	0.02426788				1	0.03	7.00035E-08
139481-59-7	139481597	447	Candesartan	440.47	1_Pharma	40000		40000	0	40000	0.09081209	10000		10000	0	10000	0.02270302				1	0.03	6.81091E-08
15307-86-5	15307865	31	diclofenac	296.15	1_Pharma	15200		15200	0	15200	0.05132534	0.36		0.36	0	0.36	1.2156E-06	0.36		0.36	0	0.36	1.2156E-06
15687-27-1	15687271	493	ibuprofen	206.29	1_Pharma	10.66666667		10.66666667	0	10.6666667	5.1707E-05	1230		1230	0	1230	0.00596248	1230		1230	0	1230	0.00596248
20830-75-5	20830755	529	Digoxin	780.95	1_Pharma				1	0.3	3.8415E-07				1	0.03	3.8415E-08				1	0.03	3.84148E-08
22204-53-1	22204531	539	Naproxen	230.26	1_Pharma	10.66666667		10.66666667	0	10.6666667	4.6324E-05				1	0.03	1.3029E-07				1	0.03	1.30288E-07
23593-75-1	23593751	553	Klotrimazol	344.85	1_Pharma				1	0.3	8.6994E-07				1	0.03	8.6994E-08				1	0.03	8.69943E-08
25812-30-0	25812300	570	Gemfibrozil	250.34	1_Pharma	3466.666667		3466.666667	0	3466.66667	0.01384783	32000		32000	0	32000	0.12782616				1	0.03	1.19837E-07
26787-78-0	26787780	574	amoxicillin	365.41	1_Pharma	333333.3333		333333.3333	0	333333.333	0.91221733				1	0.03	8.21E-08				1	0.03	8.20996E-08
29122-68-7	29122687	44	Atenolol	266.34	1_Pharma	104333.3333		104333.3333	0	104333.333	0.39172987				1	0.03	1.1264E-07				1	0.03	1.12638E-07
298-46-4	298464	45	Carbamazepine	236.28	1_Pharma	12000		12000	0	12000	0.0507872	0.5		0.5	0	0.5	2.1161E-06	0.5		0.5	0	0.5	2.11613E-06
3380-34-5	3380345	48	triclosan	289.55	1_Pharma	100		100	0	100	0.00034536				1	0.03	1.0361E-07				1	0.03	1.03609E-07
37350-58-6	37350586	50	Metoprolol	267.37	1_Pharma	21300		21300	0	21300	0.07966488	3200		3200	0	3200	0.01196843				1	0.03	1.12204E-07
3930-20-9	3930209	51	Sotalol	272.37	1_Pharma	333333.3333		333333.3333	0	333333.333	1.22382543				1	0.03	1.1014E-07				1	0.03	1.10144E-07
41859-67-0	41859670	53	Bezafibrat	361.83	1_Pharma	10100		10100	0	10100	0.02791366				1	0.03	8.2912E-08				1	0.03	8.29119E-08
42200-33-9	42200339	1154	Nadolol	309.41	1_Pharma	33333.33333		33333.33333	0	33333.3333	0.10773192				1	0.03	9.6959E-08				1	0.03	9.69587E-08
439-14-5	439145	640	Diazepam	284.75	1_Pharma				1	0.3	1.0536E-06				1	0.03	1.0536E-07				1	0.03	1.05356E-07
443-48-1	443481	642	Metronidazol	171.16	1_Pharma	70333.33333		70333.33333	0	70333.3333	0.41092155				1	0.03	1.7527E-07				1	0.03	1.75275E-07
49562-28-9	49562289	649	fenofibrate	360.84	1_Pharma	16706.66667		16706.66667	0	16706.6667	0.04629938				1	0.03	8.3139E-08				1	0.03	8.31393E-08
50-02-2	50022	652	Dexametason	392.47	1_Pharma	16100		16100	0	16100	0.04102224				1	0.03	7.6439E-08				1	0.03	7.6439E-08
50-06-6	50066	4945	phenobarbital	232.24	1_Pharma				1	0.3	1.2918E-06				1	0.03	1.2918E-07				1	0.03	1.29177E-07
50-18-0	50180	1131	Cyclophosphamid	261.09	1_Pharma				1	0.3	1.149E-06				1	0.03	1.149E-07				1	0.03	1.14903E-07
50-24-8	50248	656	prednisolone	360.45	1_Pharma				1	0.3	8.3229E-07				1	0.03	8.3229E-08				1	0.03	8.32293E-08
50-28-2	50282	55	estradiol	272.39	1_Pharma				1	0.3	1.1014E-06				1	0.03	1.1014E-07				1	0.03	1.10136E-07
50-78-2	50782	666	O-acetylsalicylic acid	180.16	1_Pharma	38100		38100	0	38100	0.21147869	1000		1000	0	1000	0.00555062	1000		1000	0	1000	0.005550622
51-21-8	51218	668	fluorouracil	130.08	1_Pharma				1	0.3	2.3063E-06				1	0.03	2.3063E-07				1	0.03	2.30627E-07
51481-61-9	51481619	1129	Cimetidin	252.35	1_Pharma	90433.33333		90433.33333	0	90433.3333	0.35836471				1	0.03	1.1888E-07				1	0.03	1.18883E-07
51-52-5	51525	5108	propylthiouracil	170.24	1_Pharma				1	0.3	1.7622E-06				1	0.03	1.7622E-07				1	0.03	1.76222E-07
525-66-6	525666	59	Propranolol	259.35	1_Pharma	800		800	0	800	0.00308463	55		55	0	55	0.00021207	55		55	0	55	0.000212069
52645-53-1	52645531	676	Permethrin	391.29	1_Pharma	0.032		0.032	0	0.032	8.1781E-08	0.039		0.039	0	0.039	9.967E-08				1	0.03	7.66695E-08
53-86-1	53861	1101	Indometacin	357.79	1_Pharma				1	0.3	8.3848E-07				1	0.03	8.3848E-08				1	0.03	8.38481E-08
54-11-5	54115	5067	nicotine	162.24	1_Pharma	80.66666667		80.66666667	0	80.6666667	0.00049721	70		70	0	70	0.00043146				1	0.03	1.84911E-07
54-31-9	54319	62	Furosemid	330.75	1_Pharma				1	0.3	9.0703E-07				1	0.03	9.0703E-08				1	0.03	9.07029E-08
54739-18-3	54739183	689	Fluvoxamin	318.34	1_Pharma				1	0.3	9.4239E-07				1	0.03	9.4239E-08				1	0.03	9.42389E-08
54-85-3	54853	691	Isoniazid	137.15	1_Pharma				1	0.3	2.1874E-06				1	0.03	2.1874E-07				1	0.03	2.18739E-07
54910-89-3	54910893	692	Fluoxetin	309.33	1_Pharma	0.1		0.1	0	0.1	3.2328E-07	48.3333333		48.33333333	0	48.3333333	0.00015625				1	0.03	9.69838E-08
55-56-1	55561	3175	chlorhexidine	505.47	1_Pharma				1	0.3	5.9351E-07				1	0.03	5.9351E-08				1	0.03	5.93507E-08
55-63-0	55630	702	glycerol trinitrate	227.09	1_Pharma	10666.66667		10666.66667	0	10666.6667	0.0469711				1	0.03	1.3211E-07				1	0.03	1.32106E-07
56-75-7	56757	64	Chloramphenicol	323.13	1_Pharma	75666.66667		75666.66667	0	75666.6667	0.23416788				1	0.03	9.2842E-08				1	0.03	9.28419E-08
56-81-5	56815	716	glycerol	92.094	1_Pharma	3333333.333		3333333.333	0	3333333.33	36.1949023				1	0.03	3.2575E-07				1	0.03	3.25754E-07
56-86-0	56860	3214	glutamic acid	147.13	1_Pharma				1	0.3	2.039E-06				1	0.03	2.039E-07				1	0.03	2.03901E-07
57-13-6	57136	719	urea	60.058	1_Pharma	1303333.333		1303333.333	0	1303333.33	21.7012444				1	0.03	4.9952E-07				1	0.03	4.99517E-07
57-63-6	57636	724	Etinylestradiol	296.41	1_Pharma	863.4666667		863.4666667	0	863.466667	0.00291308	0.0001		0.0001	0	0.0001	3.3737E-10	0.0001		0.0001	0	0.0001	3.37371E-10
58-08-2	58082	66	caffeine	194.2	1_Pharma				1	0.3	1.5448E-06				1	0.03	1.5448E-07				1	0.03	1.5448E-07
58-22-0	58220	67	testosterone	288.43	1_Pharma	2000		2000	0	2000	0.00693409	10		10	0	10	3.467E-05	10		10	0	10	3.46705E-05
58-55-9	58559	730	theophylline	180.17	1_Pharma				1	0.3	1.6651E-06				1	0.03	1.6651E-07				1	0.03	1.66509E-07
59-05-2	59052	732	Metotrexat	454.45	1_Pharma				1	0.3	6.6014E-07				1	0.03	6.6014E-08				1	0.03	6.60139E-08
59277-89-3	59277893	735	Aciklovir	225.21	1_Pharma				1	0.3	1.3321E-06				1	0.03	1.3321E-07				1	0.03	1.33209E-07
59467-70-8	59467708	736	Midazolam	325.78	1_Pharma				1	0.3	9.2087E-07				1	0.03	9.2087E-08				1	0.03	9.20867E-08
59-67-6	59676	739	Niacin	123.11	1_Pharma				1	0.3	2.4368E-06				1	0.03	2.4368E-07				1	0.03	2.43685E-07
59-92-7	59927	745	Levodopa	197.19	1_Pharma	17400		17400	0	17400	0.08823977				1	0.03	1.5214E-07				1	0.03	1.52138E-07
60-54-8	60548	754	Tetracycline	444.44	1_Pharma				1	0.3	6.7501E-07	100		100	0	100	0.000225	100		100	0	100	0.000225002
61-68-7	61687	1150	Mefenamic acid	241.29	1_Pharma				1	0.3	1.2433E-06				1	0.03	1.2433E-07				1	0.03	1.24332E-07
61869-08-7	61869087	760	Paroxetin	329.37	1_Pharma				1	0.3	9.1083E-07				1	0.03	9.1083E-08				1	0.03	9.1083E-08
62571-86-2	62571862	1103	Captopril	217.29	1_Pharma	33333.33333		33333.33333	0	33333.3333	0.15340482				1	0.03	1.3806E-07				1	0.03	1.38064E-07
657-24-9	657249	79	Metformin	129.17	1_Pharma	21333.33333		21333.33333	0	21333.3333	0.16515703				1	0.03	2.3225E-07				1	0.03	2.32252E-07
66357-35-5	66357355	789	ranitidine	314.41	1_Pharma				1	0.3	9.5417E-07				1	0.03	9.5417E-08				1	0.03	9.54168E-08
67-20-9	67209	791	Nitrofurantoin	238.16	1_Pharma				1	0.3	1.2597E-06				1	0.03	1.2597E-07				1	0.03	1.25966E-07
68-35-9	68359	1165	Sulfadiazin	250.28	1_Pharma	19000		19000	0	19000	0.07591498				1	0.03	1.1987E-07				1	0.03	1.19866E-07
69-53-4	69534	808	ampicillin	349.41	1_Pharma	333333.3333		333333.3333	0	333333.333	0.95398911				1	0.03	8.5859E-08				1	0.03	8.5859E-08
69-72-7	69727	84	salicylic acid	138.12	1_Pharma	10.66666667		10.66666667	0	10.6666667	7.7228E-05	1000		1000	0	1000	0.00724008	1000		1000	0	1000	0.007240081
70458-96-7	70458967	812	Norfloxacin	319.34	1_Pharma				1	0.3	9.3944E-07				1	0.03	9.3944E-08				1	0.03	9.39438E-08
723-46-6	723466	86	Sulfametoxazol	253.28	1_Pharma	8400		8400	0	8400	0.03316488				1	0.03	1.1845E-07				1	0.03	1.18446E-07
72956-09-3	72956093	826	Carvedilol	406.48	1_Pharma				1	0.3	7.3804E-07				1	0.03	7.3804E-08				1	0.03	7.38044E-08
73334-07-3	73334073	4988	Iopromide	791.11	1_Pharma				1	0.3	3.7921E-07				1	0.03	3.7921E-08				1	0.03	3.79214E-08
738-70-5	738705	89	Trimetoprim	290.33	1_Pharma	30666.66667		30666.66667	0	30666.6667	0.10562693	6000		6000	0	6000	0.02066614	6000		6000	0	6000	0.020666139
76824-35-6	76824356	1100	Famotidine	337.45	1_Pharma				1	0.3	8.8902E-07				1	0.03	8.8902E-08				1	0.03	8.89021E-08
78439-06-2	78439062	896	Ceftazidim	546.59	1_Pharma				1	0.3	5.4886E-07				1	0.03	5.4886E-08				1	0.03	5.48857E-08
79-57-2	79572	923	Oxitetracyklin	460.44	1_Pharma	7546.666667		7546.666667	0	7546.66667	0.01639012				1	0.03	6.5155E-08				1	0.03	6.51551E-08
79617-96-2	79617962	924	Sertraline	306.24	1_Pharma	1		1	0	1	3.2654E-06	32		32	0	32	0.00010449	32		32	0	32	0.000104493
80-08-0	80080	3787	dapsone	248.31	1_Pharma				1	0.3	1.2082E-06				1	0.03	1.2082E-07				1	0.03	1.20817E-07
81103-11-9	81103119	99	Claritromycin	747.97	1_Pharma	8573.333333		8573.333333	0	8573.33333	0.01146214				1	0.03	4.0109E-08				1	0.03	4.01086E-08
81-13-0	81130	3802	dexpanthenol	205.26	1_Pharma				1	0.3	1.4616E-06				1	0.03	1.4616E-07				1	0.03	1.46156E-07
81-81-2	81812	942	warfarin	308.33	1_Pharma	5666.666667		5666.666667	0	5666.66667	0.01837858				1	0.03	9.7298E-08				1	0.03	9.72983E-08
82419-36-1	82419361	945	Ofloxacin	361.38	1_Pharma	10583.33333		10583.33333	0	10583.3333	0.02928589				1	0.03	8.3015E-08				1	0.03	8.30151E-08
83799-24-0	83799240	956	Fexofenadine	501.67	1_Pharma	260000		260000	0	260000	0.51826898				1	0.03	5.98E-08				1	0.03	5.98003E-08
83905-01-5	83905015	957	Azithromycin	749	1_Pharma	40000		40000	0	40000	0.05340454				1	0.03	4.0053E-08				1	0.03	4.00534E-08
84057-84-1	84057841	102	Lamotrigin	256.1	1_Pharma	18666.66667		18666.66667	0	18666.6667	0.07288819				1	0.03	1.1714E-07				1	0.03	1.17142E-07
85721-33-1	85721331	969	Ciprofloxacin	331.35	1_Pharma	333.3333333		333.3333333	0	333.333333	0.00100599				1	0.03	9.0539E-08				1	0.03	9.05387E-08
86386-73-4	86386734	970	Fluconazole	306.28	1_Pharma	20000		20000	0	20000	0.06529973				1	0.03	9.795E-08				1	0.03	9.79496E-08
88150-42-9	88150429	982	Amlodipine	408.88	1_Pharma				1	0.3	7.3371E-07				1	0.03	7.3371E-08				1	0.03	7.33712E-08
89-57-6	89576	3980	Mesalamine	153.14	1_Pharma				1	0.3	1.959E-06				1	0.03	1.959E-07				1	0.03	1.95899E-07
89-78-1	89781	994	menthol	156.27	1_Pharma				1	0.3	1.9198E-06				1	0.03	1.9198E-07				1	0.03	1.91975E-07
90-82-4	90824	4008	pseudoephedrine	165.24	1_Pharma				1	0.3	1.8155E-06				1	0.03	1.8155E-07				1	0.03	1.81554E-07
93413-69-5	93413695	1019	Venlafaxine	277.41	1_Pharma				1	0.3	1.0814E-06				1	0.03	1.0814E-07				1	0.03	1.08143E-07
94-09-7	94097	1020	Bensokain	165.19	1_Pharma				1	0.3	1.8161E-06				1	0.03	1.8161E-07				1	0.03	1.81609E-07
94-36-0	94360	4103	dibenzoyl peroxide	242.23	1_Pharma				1	0.3	1.2385E-06				1	0.03	1.2385E-07				1	0.03	1.23849E-07
97-77-8	97778	1060	disulfiram	296.54	1_Pharma	40		40	0	40	0.00013489				1	0.03	1.0117E-07				1	0.03	1.01167E-07
98-92-0	98920	1079	nicotinamide	122.13	1_Pharma				1	0.3	2.4564E-06				1	0.03	2.4564E-07				1	0.03	2.4564E-07
99-66-1	99661	1091	Valproic acid	144.21	1_Pharma				1	0.3	2.0803E-06				1	0.03	2.0803E-07				1	0.03	2.0803E-07
2164-08-1	2164081	114	Lenacil	234.3	2_Pest	11000		11000	0	11000	0.04694836				1	0.03	1.2804E-07				1	0.03	1.28041E-07
2439-01-2	2439012	5114	Quinomethionate	234.3	2_Pest	40		40	0	40	0.00017072	2.45		2.45	0	2.45	1.0457E-05	22		22	0	22	9.38967E-05
3813-05-6	3813056	116	Benazolin	243.67	2_Pest	77800		77800	0	77800	0.31928428				1	0.03	1.2312E-07				1	0.03	1.23117E-07
10004-44-1	10004441	121	Hymexazol	99.09	2_Pest	9890		9890	0	9890	0.09980826				1	0.03	3.0276E-07				1	0.03	3.02755E-07
100646-51-3	100646513	5117	Quizalofop-P-ethyl	372.81	2_Pest	160		160	0	160	0.00042917	23		23	0	23	6.1694E-05	74000		74000	0	74000	0.19849253
101-05-3	101053	141	Anilazine	275.53	2_Pest	320		320	0	320	0.0011614	58		58	0	58	0.0002105				1	0.03	1.08881E-07
101200-48-0	101200480	142	Tribenuron-methyl	395.4	2_Pest	240000		240000	0	240000	0.60698027	28000		28000	0	28000	0.07081437	54000		54000	0	54000	0.136570561
101205-02-1	101205021	144	Cycloxydim	325.47	2_Pest	44333.33333		44333.33333	0	44333.3333	0.13621327				1	0.03	9.2174E-08				1	0.03	9.21744E-08
101-21-3	101213	145	Chlorpropham	213.66	2_Pest	770		770	0	770	0.00360386				1	0.03	1.4041E-07				1	0.03	1.4041E-07
101-42-8	101428	147	Fenuron	164.21	2_Pest				1	0.3	1.8269E-06				1	0.03	1.8269E-07				1	0.03	1.82693E-07
101463-69-8	101463698	148	Flufenoxuron	488.77	2_Pest	0.014333333		0.014333333	0	0.01433333	2.9325E-08	0.0032		0.0032	0	0.0032	6.547E-09				1	0.03	6.13786E-08
1014-69-3	1014693	149	Desmetryn	213.31	2_Pest	8666.666667		8666.666667	0	8666.66667	0.04062944				1	0.03	1.4064E-07				1	0.03	1.4064E-07
10265-92-6	10265926	153	Methamidophos	141.13	2_Pest	8.666666667		8.666666667	0	8.66666667	6.1409E-05	4.49		4.49	0	4.49	3.1815E-05	11.9		11.9	0	11.9	8.43194E-05
102851-06-9	102851069	157	Tau-fluvalinate	502.92	2_Pest	0.22		0.22	0	0.22	4.3745E-07	0.1		0.1	0	0.1	1.9884E-07				1	0.03	5.96516E-08
103055-07-8	103055078	158	Lufenuron	511.15	2_Pest				1	0.3	5.8691E-07				1	0.03	5.8691E-08				1	0.03	5.86912E-08
10311-84-9	10311849	4894	Dialifos	393.85	2_Pest				1	0.3	7.6171E-07				1	0.03	7.6171E-08				1	0.03	7.61711E-08
104040-78-0	104040780	166	Flazasulfuron	407.33	2_Pest	106000		106000	0	106000	0.26023126	6390		6390	0	6390	0.01568753				1	0.03	7.36504E-08
104206-82-8	104206828	167	Mesotrione	339.32	2_Pest	622000		622000	0	622000	1.83307792	180000		180000	0	180000	0.53047271	300000		300000	0	300000	0.884121184
10453-86-8	10453868	1114	Resmethrin	338.45	2_Pest	0.11		0.11	0	0.11	3.2501E-07	0.06		0.06	0	0.06	1.7728E-07				1	0.03	8.86394E-08
10552-74-6	10552746	176	Nitrothal-isopropyl	295.29	2_Pest	946.6666667		946.6666667	0	946.666667	0.00320589				1	0.03	1.016E-07				1	0.03	1.01595E-07
10605-21-7	10605217	3	Carbendazim	191.19	2_Pest	6.666666667		6.666666667	0	6.66666667	3.4869E-05	3.1		3.1	0	3.1	1.6214E-05	3.1		3.1	0	3.1	1.62142E-05
1071-83-6	1071836	212	Glyphosate	169.07	2_Pest	1700		1700	0	1700	0.01005501				1	0.03	1.7744E-07				1	0.03	1.77441E-07
107534-96-3	107534963	221	Tebuconazole	307.83	2_Pest	6.2		6.2	0	6.2	2.0141E-05	120		120	0	120	0.00038983	120		120	0	120	0.000389826
1085-98-9	1085989	241	Dichlofluanid	333.23	2_Pest	620		620	0	620	0.00186058				1	0.03	9.0028E-08				1	0.03	9.00279E-08
110488-70-5	110488705	4906	Dimethomorph	387.86	2_Pest	10600		10600	0	10600	0.02732945	100		100	0	100	0.00025782	310		310	0	310	0.000799257
1113-02-6	1113026	295	Omethoate	213.19	2_Pest	7		7	0	7	3.2835E-05				1	0.03	1.4072E-07				1	0.03	1.4072E-07
111479-05-1	111479051	303	Propaquizafop	443.89	2_Pest	666.6666667		666.6666667	0	666.666667	0.00150187				1	0.03	6.7584E-08				1	0.03	6.75843E-08
111988-49-9	111988499	6	Thiacloprid	252.73	2_Pest	9100		9100	0	9100	0.03600681	560		560	0	560	0.0022158	560		560	0	560	0.002215803
111991-09-4	111991094	319	Nicosulfuron	410.42	2_Pest	1000000		1000000	0	1000000	2.43652843	43000		43000	0	43000	0.10477072	48000		48000	0	48000	0.116953365
112281-77-3	112281773	323	Tetraconazole	372.15	2_Pest	250		250	0	250	0.00067177	190		190	0	190	0.00051055	190		190	0	190	0.000510547
112410-23-8	112410238	328	Tebufenozide	352.48	2_Pest	600		600	0	600	0.00170222	29		29	0	29	8.2274E-05	32		32	0	32	9.07853E-05
113136-77-9	113136779	334	Cyclanilide	274.1	2_Pest	3200		3200	0	3200	0.01167457	12000		12000	0	12000	0.04377964				1	0.03	1.09449E-07
113158-40-0	113158400	335	Fenoxaprop-P	333.73	2_Pest	417		417	0	417	0.00124951	340		340	0	340	0.00101879				1	0.03	8.9893E-08
1134-23-2	1134232	4878	Cycloate	215.36	2_Pest	1866.666667		1866.666667	0	1866.66667	0.00866766				1	0.03	1.393E-07				1	0.03	1.39302E-07
114-26-1	114261	337	Propoxur	209.25	2_Pest	0.333333333		0.333333333	0	0.33333333	1.593E-06	16		16	0	16	7.6464E-05	23		23	0	23	0.000109916
114369-43-6	114369436	338	Fenbuconazole	336.83	2_Pest	750		750	0	750	0.00222664	12		12	0	12	3.5626E-05	37		37	0	37	0.000109848
115-29-7	115297	4921	Endosulfan	406.93	2_Pest	0.1		0.1	0	0.1	2.4574E-07	2.7		2.7	0	2.7	6.635E-06	170		170	0	170	0.000417762
115-32-2	115322	340	Dicofol	370.49	2_Pest	26.66666667		26.66666667	0	26.6666667	7.1977E-05				1	0.03	8.0974E-08				1	0.03	8.09738E-08
116-06-3	116063	342	Aldicarb	190.27	2_Pest	17		17	0	17	8.9347E-05	20		20	0	20	0.00010511	20		20	0	20	0.000105114
116255-48-2	116255482	343	Bromuconazole	377.08	2_Pest	20		20	0	20	5.3039E-05	6		6	0	6	1.5912E-05	17		17	0	17	4.50833E-05
116-29-0	116290	344	Tetradifon	356.05	2_Pest	2966.666667		2966.666667	0	2966.66667	0.00833216				1	0.03	8.4258E-08				1	0.03	8.42578E-08
118134-30-8	118134308	347	Spiroxamine	297.48	2_Pest	440		440	0	440	0.00147909	34		34	0	34	0.00011429				1	0.03	1.00847E-07
119168-77-3	119168773	350	Tebufenpyrad	333.87	2_Pest	26		26	0	26	7.7875E-05				1	0.03	8.9855E-08				1	0.03	8.98553E-08
119446-68-3	119446683	351	Difenoconazole	406.27	2_Pest	520		520	0	520	0.00127994	5		5	0	5	1.2307E-05	5		5	0	5	1.23071E-05
1194-65-6	1194656	352	dichlobenil	172.01	2_Pest	1233.333333		1233.333333	0	1233.33333	0.00717013	560		560	0	560	0.00325562	560		560	0	560	0.003255625
120068-37-3	120068373	11	Fipronil	437.15	2_Pest	22		22	0	22	5.0326E-05	9.6		9.6	0	9.6	2.196E-05				1	0.03	6.86263E-08
120-36-5	120365	4895	Dichlorprop	235.07	2_Pest	1300		1300	0	1300	0.00553027	400		400	0	400	0.00170162	400		400	0	400	0.001701621
120928-09-8	120928098	366	Fenazaquin	306.41	2_Pest	0.8		0.8	0	0.8	2.6109E-06	0.2		0.2	0	0.2	6.5272E-07	0.52		0.52	0	0.52	1.69707E-06
121552-61-2	121552612	371	Cyprodinil	225.3	2_Pest	22.3		22.3	0	22.3	9.8979E-05	2.3		2.3	0	2.3	1.0209E-05	7.3		7.3	0	7.3	3.24012E-05
122-14-5	122145	378	Fenitrothion	277.24	2_Pest	0.066666667		0.066666667	0	0.06666667	2.4047E-07	0.087		0.087	0	0.087	3.1381E-07				1	0.03	1.08209E-07
122-34-9	122349	15	Simazine	201.67	2_Pest	333.3333333		333.3333333	0	333.333333	0.00165287	2500		2500	0	2500	0.01239649				1	0.03	1.48758E-07
122-42-9	122429	5107	Propham	179.22	2_Pest	2666.666667		2666.666667	0	2666.66667	0.01487929				1	0.03	1.6739E-07				1	0.03	1.67392E-07
122453-73-0	122453730	380	Chlorfenapyr	407.63	2_Pest	2.7		2.7	0	2.7	6.6237E-06	3.57		3.57	0	3.57	8.7579E-06				1	0.03	7.35962E-08
122931-48-0	122931480	383	Rimsulfuron	431.45	2_Pest	120000		120000	0	120000	0.27813188				1	0.03	6.9533E-08				1	0.03	6.9533E-08
123312-89-0	123312890	387	Pymetrozine	217.24	2_Pest	19200		19200	0	19200	0.08838151	25.1		25.1	0	25.1	0.00011554				1	0.03	1.38096E-07
123-33-1	123331	389	Maleic hydrazide	112.09	2_Pest	18000		18000	0	18000	0.16058524				1	0.03	2.6764E-07				1	0.03	2.67642E-07
125116-23-6	125116236	405	Metconazole	319.84	2_Pest				1	0.3	9.3797E-07				1	0.03	9.3797E-08				1	0.03	9.37969E-08
126833-17-8	126833178	409	Fenhexamid	302.2	2_Pest	10100		10100	0	10100	0.03342158	1000		1000	0	1000	0.00330907	9700		9700	0	9700	0.032097948
13071-79-9	13071799	416	Terbufos	288.43	2_Pest	0.18		0.18	0	0.18	6.2407E-07	0.03		0.03	0	0.03	1.0401E-07				1	0.03	1.04011E-07
13121-70-5	13121705	419	Cyhexatin	385.16	2_Pest	0.056666667		0.056666667	0	0.05666667	1.4713E-07				1	0.03	7.789E-08				1	0.03	7.78897E-08
131341-86-1	131341861	420	Fludioxonil	248.19	2_Pest	500		500	0	500	0.00201459	19		19	0	19	7.6554E-05				1	0.03	1.20875E-07
13171-21-6	13171216	5093	Phosphamidon	299.69	2_Pest	2.933333333		2.933333333	0	2.93333333	9.7879E-06	1.5		1.5	0	1.5	5.0052E-06				1	0.03	1.00103E-07
131807-57-3	131807573	421	Famoxadone	374.4	2_Pest	3.5		3.5	0	3.5	9.3483E-06	0.085		0.085	0	0.085	2.2703E-07	0.085		0.085	0	0.085	2.2703E-07
13181-17-4	13181174	422	Bromofenoxim	461.04	2_Pest	400		400	0	400	0.0008676				1	0.03	6.507E-08				1	0.03	6.50703E-08
131860-33-8	131860338	423	Azoxystrobin	403.4	2_Pest	31.66666667		31.66666667	0	31.6666667	7.8499E-05	44		44	0	44	0.00010907	44		44	0	44	0.000109073
13194-48-4	13194484	4930	Ethoprophos	242.34	2_Pest	32		32	0	32	0.00013205	0.8		0.8	0	0.8	3.3011E-06	2.4		2.4	0	2.4	9.90344E-06
131983-72-7	131983727	424	Triticonazole	317.82	2_Pest	1800		1800	0	1800	0.00566358	190		190	0	190	0.00059782				1	0.03	9.43931E-08
132-66-1	132661	5059	Naptalam	291.31	2_Pest	39500		39500	0	39500	0.13559438				1	0.03	1.0298E-07				1	0.03	1.02983E-07
133-06-2	133062	425	Captan	300.59	2_Pest	100		100	0	100	0.00033268	560		560	0	560	0.001863	1000		1000	0	1000	0.003326791
133-07-3	133073	426	Folpet	296.56	2_Pest	8.5		8.5	0	8.5	2.8662E-05	1.88		1.88	0	1.88	6.3394E-06				1	0.03	1.0116E-07
13360-45-7	13360457	428	Chlorbromuron	293.56	2_Pest	1933.333333		1933.333333	0	1933.33333	0.00658582				1	0.03	1.0219E-07				1	0.03	1.02194E-07
134098-61-6	134098616	429	Fenpyroximate	421.5	2_Pest	0.78		0.78	0	0.78	1.8505E-06	0.68		0.68	0	0.68	1.6133E-06				1	0.03	7.11744E-08
13457-18-6	13457186	432	Pyrazophos	373.37	2_Pest	0.06		0.06	0	0.06	1.607E-07				1	0.03	8.0349E-08				1	0.03	8.03493E-08
13593-03-8	13593038	437	Quinalphos	298.3	2_Pest				1	0.3	1.0057E-06				1	0.03	1.0057E-07				1	0.03	1.0057E-07
136426-54-5	136426545	438	Fluquinconazole	376.18	2_Pest				1	0.3	7.9749E-07	650		650	0	650	0.0017279				1	0.03	7.97491E-08
13684-56-5	13684565	439	Desmedipham	300.32	2_Pest	560		560	0	560	0.00186468				1	0.03	9.9893E-08				1	0.03	9.98934E-08
13684-63-4	13684634	440	Phenmedipham	300.32	2_Pest	166.6666667		166.6666667	0	166.666667	0.00055496				1	0.03	9.9893E-08				1	0.03	9.98934E-08
137-26-8	137268	441	thiram	240.43	2_Pest	3.333333333		3.333333333	0	3.33333333	1.3864E-05				1	0.03	1.2478E-07				1	0.03	1.24776E-07
138261-41-3	138261413	443	Imidacloprid	255.67	2_Pest	1233.333333		1233.333333	0	1233.33333	0.00482393	1250		1250	0	1250	0.00488911	7300		7300	0	7300	0.028552431
139-40-2	139402	446	propazine	229.72	2_Pest	5320		5320	0	5320	0.02315863	47		47	0	47	0.0002046				1	0.03	1.30594E-07
139528-85-1	139528851	1922	Metosulam	419.27	2_Pest				1	0.3	7.1553E-07				1	0.03	7.1553E-08				1	0.03	7.15529E-08
140923-17-7	140923177	453	Iprovalicarb	320.44	2_Pest				1	0.3	9.3621E-07	1890		1890	0	1890	0.00589814	1890		1890	0	1890	0.00589814
141517-21-7	141517217	5178	Trifloxystrobine	408.38	2_Pest	18		18	0	18	4.4077E-05	2.76		2.76	0	2.76	6.7584E-06	12		12	0	12	2.93844E-05
141776-32-1	141776321	457	Sulfosulfuron	470.49	2_Pest	96000		96000	0	96000	0.20404259	102000		102000	0	102000	0.21679526				1	0.03	6.37633E-08
1420-07-1	1420071	4911	Dinoterb	240.22	2_Pest	156.6666667		156.6666667	0	156.666667	0.00065218				1	0.03	1.2489E-07				1	0.03	1.24886E-07
14214-32-5	14214325	4902	Difenoxuron	286.33	2_Pest	26333.33333		26333.33333	0	26333.3333	0.09196847				1	0.03	1.0477E-07				1	0.03	1.04774E-07
142459-58-3	142459583	461	Flufenacet	363.34	2_Pest				1	0.3	8.2567E-07	6300		6300	0	6300	0.01733913	6300		6300	0	6300	0.017339131
143390-89-0	143390890	470	Kresoxim-Methyl	313.35	2_Pest	160		160	0	160	0.00051061				1	0.03	9.574E-08				1	0.03	9.57396E-08
145701-23-1	145701231	473	Florasulam	359.283	2_Pest	5500		5500	0	5500	0.01530827	38900		38900	0	38900	0.1082712				1	0.03	8.34996E-08
14816-18-3	14816183	475	Phoxim	298.3	2_Pest	0.27		0.27	0	0.27	9.0513E-07				1	0.03	1.0057E-07				1	0.03	1.0057E-07
148-79-8	148798	476	Thiabendazole	201.25	2_Pest	100		100	0	100	0.00049689	42		42	0	42	0.0002087				1	0.03	1.49068E-07

149961-52-4	149961524	481	Dimoxystrobin	326.4	2 Pest	13.13333333	13.13333333	0	13.1333333	4.0237E-05	12.5	12.5	0	12.5	3.8297E-05			1	0.03	9.19118E-08
149979-41-9	149979419	5148	Tepraloxydim	341.84	2 Pest	2900	2900	0	2900	0.0084835			1	0.03	8.776E-08			1	0.03	8.77604E-08
150-68-5	150685	482	Monuron	198.66	2 Pest	19000	19000	0	19000	0.09564079			1	0.03	1.5101E-07			1	0.03	1.51012E-07
15165-67-0	15165670	4896	Dichlorprop-P	235.07	2 Pest	64000	64000	0	64000	0.27225933			1	0.03	1.2762E-07			1	0.03	1.27622E-07
15299-99-7	15299997	5058	Napropamide	271.36	2 Pest	5600	5600	0	5600	0.02063679	8.4	8.4	0	8.4	3.0955E-05			1	0.03	1.10554E-07
153719-23-4	153719234	487	Thiamethoxam	291.72	2 Pest	36000	36000	0	36000	0.12340601	50000	50000	0	50000	0.17139723			1	0.03	1.02838E-07
15457-05-3	15457053	4958	Fluorodifen	328.2	2 Pest			1	0.3	9.1408E-07			1	0.03	9.1408E-08			1	0.03	9.14077E-08
15545-48-9	15545489	32	Chlorotoluron	212.68	2 Pest	22333.33333	22333.33333	0	22333.3333	0.10500909			1	0.03	1.4106E-07			1	0.03	1.41057E-07
156052-68-5	156052685	490	Zoxamide	336.65	2 Pest	780	780	0	780	0.00231695	39	39	0	39	0.00011585	160	160	0	160	0.000475271
1563-66-2	1563662	491	Carbofuran	221.26	2 Pest	1.8	1.8	0	1.8	8.1352E-06	9.8	9.8	0	9.8	4.4292E-05			1	0.03	1.35587E-07
1582-09-8	1582098	496	Trifluralin	335.29	2 Pest	64.33333333	64.33333333	0	64.3333333	0.00019187	2.4	2.4	0	2.4	7.158E-06	14	14	0	14	4.17549E-05
15972-60-8	15972608	497	Alachlor	269.77	2 Pest	5600	5600	0	5600	0.02075842	110	110	0	110	0.00040775			1	0.03	1.11206E-07
161050-58-4	161050584	5021	Methoxyfenozide	368.48	2 Pest	1700	1700	0	1700	0.00461355	200	200	0	200	0.00054277	710	710	0	710	0.001926835
161326-34-7	161326347	499	Fenamidone	311.41	2 Pest	29.3	29.3	0	29.3	9.4088E-05	12.5	12.5	0	12.5	4.014E-05			1	0.03	9.6336E-08
163515-14-8	163515148	502	Dimethenamid-P	275.8	2 Pest	3400	3400	0	3400	0.01232777			1	0.03	1.0877E-07			1	0.03	1.08774E-07
16672-87-0	16672870	505	Ethephon	144.49	2 Pest	10566.66667	10566.66667	0	10566.6667	0.07313078	17000	17000	0	17000	0.1176552			1	0.03	2.07627E-07
16752-77-5	16752775	506	Methomyl	162.21	2 Pest	2.133333333	2.133333333	0	2.13333333	1.3152E-05	0.4	0.4	0	0.4	2.4659E-06	1.6	1.6	0	1.6	9.86376E-06
1689-83-4	1689834	507	Ioxynil	370.91	2 Pest	1300	1300	0	1300	0.00350489			1	0.03	8.0882E-08			1	0.03	8.08822E-08
1689-84-5	1689845	34	Bromoxynil	276.93	2 Pest	13.66666667	13.66666667	0	13.6666667	4.9351E-05	20	20	0	20	7.222E-05			1	0.03	1.08331E-07
1698-60-8	1698608	35	Chloridazon	221.65	2 Pest	60	60	0	60	0.0002707			1	0.03	1.3535E-07			1	0.03	1.35349E-07
1702-17-6	1702176	509	Clopyralid	192	2 Pest	75000	75000	0	75000	0.390625			1	0.03	1.5625E-07			1	0.03	1.5625E-07
173159-57-4	173159574	510	Foramsulfuron	452.45	2 Pest	33333.33333	33333.33333	0	33333.3333	0.07367297	100000	100000	0	100000	0.2210189			1	0.03	6.63057E-08
1746-81-2	1746812	511	Monolinuron	214.65	2 Pest	3.333333333	3.333333333	0	3.33333333	1.5529E-05			1	0.03	1.3976E-07			1	0.03	1.39762E-07
175013-18-0	175013180	512	Pyraclostrobin	387.83	2 Pest	0.71	0.71	0	0.71	1.8307E-06	4	4	0	4	1.0314E-05	4	4	0	4	1.03138E-05
17804-35-2	17804352	513	Benomyl	290.33	2 Pest	5	5	0	5	1.7222E-05	3.1	3.1	0	3.1	1.0678E-05	3.1	3.1	0	3.1	1.06775E-05
18181-80-1	18181801	4865	Bromopropylate	428.13	2 Pest	56.66666667	56.66666667	0	56.6666667	0.00013236			1	0.03	7.0072E-08			1	0.03	7.00722E-08
1861-40-1	1861401	514	Benfluralin	335.29	2 Pest	728.6666667	728.6666667	0	728.666667	0.00217324	15.5	15.5	0	15.5	4.6229E-05	30.7	30.7	0	30.7	9.15625E-05
18691-97-9	18691979	515	Methabenzthiazuron	221.29	2 Pest	10200	10200	0	10200	0.04609336			1	0.03	1.3557E-07			1	0.03	1.35569E-07
188425-85-6	188425856	36	Boscalid	343.21	2 Pest	1590	1590	0	1590	0.00463273	1310	1310	0	1310	0.00381691	1310	1310	0	1310	0.003816905
1897-45-6	1897456	516	Chlorothalonil	265.92	2 Pest	6.8	6.8	0	6.8	2.5572E-05	0.28	0.28	0	0.28	1.0529E-06			1	0.03	1.12816E-07
19044-88-3	19044883	517	Oryzalin	346.37	2 Pest	700	700	0	700	0.00202096	358	358	0	358	0.00103358	1000	1000	0	1000	0.002887086
1912-24-9	1912249	37	atrazine	215.69	2 Pest	80	80	0	80	0.0003709	140	140	0	140	0.00064908	500	500	0	500	0.002318142
1918-00-9	1918009	519	Dicamba	221.04	2 Pest	18000	18000	0	18000	0.08143322			1	0.03	1.3572E-07			1	0.03	1.35722E-07
1918-16-7	1918167	520	Propachlor	211.69	2 Pest	800	800	0	800	0.00377911	97	97	0	97	0.00045822	612	612	0	612	0.00289102
1929-77-7	1929777	521	Vernolate	203.35	2 Pest	900	900	0	900	0.00442587			1	0.03	1.4753E-07			1	0.03	1.47529E-07
19666-30-9	19666309	526	Oxadiazon	345.23	2 Pest	130	130	0	130	0.00037656	30	30	0	30	8.6899E-05			1	0.03	8.68986E-08
1967-16-4	1967164	4870	Chlorbufam	223.66	2 Pest			1	0.3	1.3413E-06			1	0.03	1.3413E-07			1	0.03	1.34132E-07
19937-59-8	19937598	527	Metoxuron	228.68	2 Pest	53333.33333	53333.33333	0	53333.3333	0.23322255			1	0.03	1.3119E-07			1	0.03	1.31188E-07
2032-65-7	2032657	528	Methiocarb	225.31	2 Pest	2	2	0	2	8.8767E-06	0.1	0.1	0	0.1	4.4383E-07			1	0.03	1.3315E-07
208465-21-8	208465218	5020	Mesosulfuron-methyl	503.51	2 Pest	90200	90200	0	90200	0.17914242	2000	2000	0	2000	0.00397212	50100	50100	0	50100	0.099501499
21087-64-9	21087649	531	Metribuzin	214.29	2 Pest	1000	1000	0	1000	0.00466657	320	320	0	320	0.0014933	320	320	0	320	0.001493303
2164-17-2	2164172	534	Fluometuron	232.21	2 Pest	1800	1800	0	1800	0.0077516	1730	1730	0	1730	0.00745015			1	0.03	1.29193E-07
21725-46-2	21725462	535	Cyanazine	240.7	2 Pest	10000	10000	0	10000	0.04154549			1	0.03	1.2464E-07			1	0.03	1.24636E-07
2212-67-1	2212671	537	Molinate	187.31	2 Pest	233.3333333	233.3333333	0	233.333333	0.00124571	380	380	0	380	0.00202872			1	0.03	1.60162E-07
22224-92-6	22224926	540	Fenamiphos	303.36	2 Pest	0.76	0.76	0	0.76	2.5053E-06	0.12	0.12	0	0.12	3.9557E-07			1	0.03	9.88924E-08
2275-23-2	2275232	543	Vamidothion	287.34	2 Pest	63.33333333	63.33333333	0	63.3333333	0.00022041			1	0.03	1.0441E-07			1	0.03	1.04406E-07
22781-23-3	22781233	544	Bendiocarb	223.23	2 Pest	10	10	0	10	4.4797E-05	0.74	0.74	0	0.74	3.315E-06	1.4	1.4	0	1.4	6.27156E-06
2303-17-5	2303175	545	Tri-allate	304.67	2 Pest	43	43	0	43	0.00014114	13	13	0	13	4.2669E-05			1	0.03	9.84672E-08
2310-17-0	2310170	546	Phosalone	367.81	2 Pest	0.133333333	0.133333333	0	0.13333333	3.6251E-07			1	0.03	8.1564E-08			1	0.03	8.15639E-08
23103-98-2	23103982	547	Pirimicarb	238.29	2 Pest	2.6	2.6	0	2.6	1.0911E-05	0.9	0.9	0	0.9	3.7769E-06			1	0.03	1.25897E-07
23135-22-0	23135220	549	Oxamyl	219.27	2 Pest	140	140	0	140	0.00063848	26.8	26.8	0	26.8	0.00012222			1	0.03	1.36818E-07
23560-59-0	23560590	551	Heptenophos	250.62	2 Pest	0.666666667	0.666666667	0	0.66666667	2.6601E-06			1	0.03	1.197E-07			1	0.03	1.19703E-07
23564-05-8	23564058	552	Thiophanate-methyl	342.4	2 Pest	866.6666667	866.6666667	0	866.666667	0.00253115	666.666667	666.6666667	0	666.666667	0.00194704			1	0.03	8.76168E-08
23947-60-6	23947606	555	Ethirimol	209.3	2 Pest	17666.66667	17666.66667	0	17666.6667	0.08440835			1	0.03	1.4333E-07			1	0.03	1.43335E-07
23950-58-5	23950585	556	Propyzamide	256.13	2 Pest	5600	5600	0	5600	0.0218639	600	600	0	600	0.00234256			1	0.03	1.17128E-07
24017-47-8	24017478	557	Triazophos	313.32	2 Pest	1	1	0	1	3.1916E-06	0.025	0.025	0	0.025	7.9791E-08	0.05	0.05	0	0.05	1.59581E-07
24579-73-5	24579735	5105	Propamocarb	188.27	2 Pest	106000	106000	0	106000	0.56302119	8900	8900	0	8900	0.04727253			1	0.03	1.59346E-07
24934-91-6	24934916	564	Chlormephos	234.7	2 Pest			1	0.3	1.2782E-06			1	0.03	1.2782E-07			1	0.03	1.27823E-07
25057-89-0	25057890	39	Bentazone	240.28	2 Pest	21333.33333	21333.33333	0	21333.3333	0.08878531			1	0.03	1.2485E-07			1	0.03	1.24854E-07
25311-71-1	25311711	567	Isofenphos	345.4	2 Pest	1	1	0	1	2.8952E-06	0.21	0.21	0	0.21	6.0799E-07			1	0.03	8.68558E-08
2540-82-1	2540821	569	Formothion	257.27	2 Pest	5366.666667	5366.666667	0	5366.66667	0.02086006			1	0.03	1.1661E-07			1	0.03	1.16609E-07
2593-15-9	2593159	571	Etridiazole	247.53	2 Pest	2000	2000	0	2000	0.00807983	370	370	0	370	0.00149477	970	970	0	970	0.003918717
26225-79-6	26225796	573	Ethofumesate	286.35	2 Pest	21333.33333	21333.33333	0	21333.3333	0.0745009	250	250	0	250	0.00087306			1	0.03	1.04767E-07
2642-71-9	2642719	40	Azinphos-ethyl	345.38	2 Pest	1.066666667	1.066666667	0	1.06666667	3.0884E-06			1	0.03	8.6861E-08			1	0.03	8.68608E-08
26644-46-2	26644462	5180	Triforine	434.97	2 Pest	7200	7200	0	7200	0.01655287			1	0.03	6.897E-08			1	0.03	6.89703E-08
27314-13-2	27314132	5073	Norflurazon	303.67	2 Pest	15000	15000	0	15000	0.04939573	1000	1000	0	1000	0.00329305			1	0.03	9.87915E-08
2764-72-9	2764729	4912	Diquat	184.24	2 Pest	400	400	0	400	0.00217108			1	0.03	1.6283E-07			1	0.03	1.62831E-07
2797-51-5	2797515	5113	Quinoclamine	207.62	2 Pest			1	0.3	1.4449E-06			1	0.03	1.4449E-07			1	0.03	1.44495E-07
28249-77-6	28249776	580	Thiobencarb	257.78	2 Pest	72	72	0	72	0.00027931	1	1	0	1	3.8793E-06			1	0.03	1.16378E-07
28434-01-7	28434017	581	Bioresmethrin	338.45	2 Pest	0.521	0.521	0	0.521	1.5394E-06			1	0.03	8.8639E-08			1	0.03	8.86394E-08
29091-05-2	29091052	4910	Dinitramine	322.25	2 Pest	320	320	0	320	0.00099302			1	0.03	9.3095E-08			1	0.03	9.30954E-08
29104-30-1	29104301	4847	Benzoximate	363.8	2 Pest			1	0.3	8.2463E-07			1	0.03	8.2463E-08			1	0.03	8.24629E-08
2921-88-2	2921882	585	Chlorpyrifos	350.59	2 Pest	0.001	0.001	0	0.001	2.8523E-09	0.0075	0.0075	0	0.0075	2.1393E-08	0.03	0.03	0	0.03	8.557E-08
29232-93-7	29232937	586	Pirimiphos-Methyl	305.34	2 Pest	0.01	0.01	0	0.01	3.275E-08			1	0.03	9.8251E-08			1	0.03	9.82511E-08
298-00-0	298000	5086	Parathion-Methyl	263.21	2 Pest	0.046666667	0.046666667	0	0.04666667	1.773E-07	0.13266499	0.132664992	0	0.13266499	5.0403E-07	0.178	0.178	0	0.178	6.76266E-07
298-02-2	298022	589	Phorate	260.38	2 Pest	12	12	0	12	4.6086E-05	0.21	0.21	0	0.21	8.0651E-07	0.8	0.8	0	0.8	3.07243E-06
298-04-4	298044	590	Disulfoton	274.4	2 Pest	0.766666667	0.766666667	0	0.76666667	2.794E-06	0.037	0.037	0	0.037	1.3484E-07	0.037	0.037	0	0.037	1.3484E-07
29973-13-5	29973135	593	Ethiofencarb	225.31	2 Pest	73.33333333	73.33333333	0	73.3333333	0.00032548			1	0.03	1.3315E-07			1	0.03	1.3315E-07
300-76-5	300765	594	Naled	380.8	2 Pest	0.1	0.1	0	0.1	2.6261E-07	0.098	0.098	0	0.098	2.5735E-07	0.098	0.098	0	0.098	2.57353E-07
301-12-2	301122	595	Oxydemeton-methyl	246.28	2 Pest	1.1	1.1	0	1.1	4.4665E-06	27	27	0	27	0.00010963			1	0.03	1.21813E-07
30560-19-1	30560191	596	Acephate	183.17	2 Pest	200	200	0	200	0.00109188	150	150	0	150	0.00081891			1	0.03	1.63782E-07
3060-89-7	3060897	598	Metobromuron	259.11	2 Pest	14666.66667	14666.66667	0	14666.6667	0.05660402			1	0.03	1.1578E-07			1	0.03	1.15781E-07
314-40-9	314409	4864	Bromacil	261.13	2 Pest	83000	83000	0	83000	0.31784935	8200	8200	0	8200	0.03140198			1	0.03	1.14885E-07
330-54-1	330541	46	diuron	233.1	2 Pest	133.3333333	133.3333333	0	133.333333	0.000572	6	6	0	6	2.574E-05			1	0.03	1.287E-07
330-55-2	330552	602	Linuron	249.1	2 Pest	100	100	0	100	0.00040145	130	130	0	130	0.00052188	240	240	0	240	0.000963468
33089-61-1	33089611	603	Amitraz	293.42	2 Pest	10	10	0	10	3.4081E-05	1.1	1.1	0	1.1	3.7489E-06			1	0.03	1.02243E-07
333-41-5	333415	47	Diazinon	304.35	2 Pest	0.156666667	0.156666667	0	0.15666667	5.1476E-07	0.1	0.1	0	0.1	3.2857E-07	0.2	0.2	0	0.2	6.57138E-07
3347-22-6	3347226	604	Dithianon	296.33	2 Pest			1	0.3	1.0124E-06			1	0.03	1.0124E-07			1	0.03	1.01238E-07
33629-47-9	33629479	605	Butralin	295.34	2 Pest	40	40	0	40	0.00013544			1	0.03	1.0158E-07			1	0.03	1.01578E-07
33693-04-8	33693048	606	Terbumeton	225.3	2 Pest	14666.66667	14666.66667	0	14666.6667	0.06509839			1	0.03	1.3316E-07			1	0.03	1.33156E-07
33820-53-0	33820530	4982	Isopropalin	309.37	2 Pest	10	10	0	10	3.2324E-05			1	0.03	9.6971E-08			1	0.03	9.69713E-08
34014-18-1	34014181	607	Tebuthiuron	228.32	2 Pest	99000	99000	0	99000	0.43360196	21800	21800	0	21800	0.09548003			1	0.03	1.31395E-07
34123-59-6	34123596	49	Isoproturon	206.29	2 Pest	169000	169000	0	169000	0.81923506			1	0.03	1.4543E-07			1	0.03	1.45426E-07
34256-82-1	34256821	608	Acetochlor	269.77	2 Pest	5500	5500	0	5500	0.02038774	22.1	22.1	0	22.1	8.1922E-05			1	0.03	1.11206E-07
34681-10-2	34681102	610	Butocarboxim	190.27	2 Pest	1066.666667	1066.666667	0	1066.66667	0.00560607			1	0.03	1.5767E-07			1	0.03	1.57671E-07
35367-38-5	35367385	612	Diflubenzuron	310.69	2 Pest	0.32	0.32	0	0.32	1.03E-06	0.06	0.06	0	0.06	1.9312E-07	0.06	0.06	0	0.06	1.93119E-07
35554-44-0	35554440	614	Imazalil	297.19	2 Pest	1800	1800	0	1800	0.00605673			1	0.03	1.0095E-07			1	0.03	1.00946E-07
36734-19-7	36734197	616	Iprodione	330.17	2 Pest	130	130	0	130	0.00039374	170	170	0	170	0.00051489			1	0.03	9.08623E-08
3689-24-5	3689245	5137	Sulfotep	322.32	2 Pest	1	1	0	1	3.1025E-06			1	0.03	9.3075E-08			1	0.03	9.30752E-08
3878-19-1	3878191	622	Fuberidazole	184.2	2 Pest	1866.666667	1866.666667	0	1866.66667	0.01013391			1	0.03	1.6287E-07			1	0.03	1.62866E-07
39515-41-8	39515418	624	Fenpropathrin	349.43	2 Pest	0.176666667	0.176666667	0	0.17666667	5.0559E-07	0.2	0.2	0	0.2	5.7236E-07			1	0.03	8.58541E-08
39807-15-3	39807153	626	Oxadiargyl	341.2	2 Pest			1	0.3	8.7925E-07			1	0.03	8.7925E-08			1	0.03	8.7925E-08
40487-42-1	40487421	628	Pendimethalin	281.32	2 Pest	26.66666667	26.66666667	0	26.6666667	9.4791E-05	14	14	0	14	4.9765E-05			1	0.03	1.0664E-07
41083-11-8	41083118	630	Azocyclotin	436.21	2 Pest	13.33333333	13.33333333	0	13.3333333	3.0566E-05			1	0.03	6.8774E-08			1	0.03	6.87742E-08
41394-05-2	41394052	632	Metamitron	202.22	2_Pest	33333.33333	33333.33333	0	33333.3333	0.16483698			1	0.03	1.4835E-07			1	0.03	1.48353E-07
41483-43-6	41483436	633	Bupirimate	316.43	2_Pest	2433.333333	2433.333333	0	2433.33333	0.00768996			1	0.03	9.4808E-08			1	0.03	9.48077E-08
42576-02-3	42576023	4851	Bifenox	342.13	2 Pest	350	350	0	350	0.001023			1	0.03	8.7686E-08			1	0.03	8.7686E-08
42874-03-3	42874033	638	Oxyfluorfen	361.7	2_Pest	20	20	0	20	5.5294E-05	13	13	0	13	3.5941E-05	13	13	0	13	3.59414E-05
43121-43-3	43121433	639	Triadimefon	293.76	2 Pest	600	600	0	600	0.00204248	52	52	0	52	0.00017702	283	283	0	283	0.000963371
4685-14-7	4685147	5085	Paraquat	186.26	2 Pest	600	600	0	600	0.0032213			1	0.03	1.6107E-07			1	0.03	1.61065E-07
470-90-6	470906	1098	Chlorfenvinphos	359.57	2 Pest	0.033333333	0.033333333	0	0.03333333	9.2703E-08			1	0.03	8.3433E-08			1	0.03	8.3433E-08
49866-87-7	49866877	4903	Difenzoquat	249.34	2 Pest	876.6666667	876.6666667	0	876.666667	0.00351595			1	0.03	1.2032E-07			1	0.03	1.20318E-07
50471-44-8	50471448	661	Vinclozolin	286.12	2 Pest	1000	1000	0	1000	0.00349504	790	790	0	790	0.00276108	2400	2400	0	2400	0.008388089
50563-36-5	50563365	663	Dimethachlor	255.75	2 Pest	4733.333333	4733.333333	0	4733.33333	0.01850766			1	0.03	1.173E-07			1	0.03	1.17302E-07
50594-66-6	50594666	4828	Acifluorfen	361.66	2 Pest			1	0.3	8.2951E-07			1	0.03	8.2951E-08			1	0.03	8.29508E-08
51218-45-2	51218452	56	Metolachlor	283.8	2 Pest	5200	5200	0	5200	0.01832276	354	354	0	354	0.00124736	3200	3200	0	3200	0.011275546
51276-47-2	51276472	4969	Glufosinate	181.13	2 Pest			1	0.3	1.6563E-06			1	0.03	1.6563E-07			1	0.03	1.65627E-07
51630-58-1	51630581	1111	Fenvalerate	419.91	2 Pest	0.03	0.03	0	0.03	7.1444E-08	0.032	0.032	0	0.032	7.6207E-08			1	0.03	7.14439E-08
51707-55-2	51707552	5158	Thidiazuron	220.26	2 Pest	1200	1200	0	1200	0.00544811	100	100	0	100	0.00045401			1	0.03	1.36203E-07
52315-07-8	52315078	1099	Cypermethrin	416.31	2 Pest	0.085	0.085	0	0.085	2.0417E-07	0.0009	0.0009	0	0.0009	2.1619E-09	0.015	0.015	0	0.015	3.60308E-08
5234-68-4	5234684	673	Carboxin	235.31	2 Pest	11000	11000	0	11000	0.04674684			1	0.03	1.2749E-07			1	0.03	1.27491E-07
52-68-6	52686	677	Trichlorfon	257.44	2 Pest	0.026666667	0.026666667	0	0.02666667	1.0358E-07	0.0056	0.0056	0	0.0056	2.1753E-08			1	0.03	1.16532E-07
52888-80-9	52888809	60	Prosulfocarb	251.39	2 Pest	170	170	0	170	0.00067624	45	45	0	45	0.000179			1	0.03	1.19336E-07
52918-63-5	52918635	679	Deltamethrin	505.22	2 Pest	0.001	0.001	0	0.001	1.9793E-09	0.0041	0.0041	0	0.0041	8.1153E-09			1	0.03	5.93801E-08
53112-28-0	53112280	681	Pyrimethanil	199.26	2 Pest	1400	1400	0	1400	0.007026	8.9	8.9	0	8.9	4.4665E-05	8.9	8.9	0	8.9	4.46653E-05
55179-31-2	55179312	693	Bitertanol	337.43	2 Pest	933.3333333	933.3333333	0	933.333333	0.00276601	3.7	3.7	0	3.7	1.0965E-05	11	11	0	11	3.25994E-05
55219-65-3	55219653	694	Triadimenol	295.77	2 Pest	1000	1000	0	1000	0.00338101	100	100	0	100	0.0003381	432	432	0	432	0.001460594
55283-68-6	55283686	695	Ethalfluralin	333.27	2_Pest	6.033333333	6.033333333	0	6.03333333	1.8103E-05	23.7	23.7	0	23.7	7.1114E-05	37.4	37.4	0	37.4	0.000112221
55285-14-8	55285148	696	Carbosulfan	380.55	2 Pest	0.5	0.5	0	0.5	1.3139E-06	3.2	3.2	0	3.2	8.4089E-06			1	0.03	7.88333E-08
55335-06-3	55335063	698	Triclopyr	256.47	2_Pest	400	400	0	400	0.00155964			1	0.03	1.1697E-07			1	0.03	1.16973E-07
55-38-9	55389	699	Fenthion	278.33	2_Pest	0.18	0.18	0	0.18	6.4671E-07	0.013	0.013	0	0.013	4.6707E-08	0.08	0.08	0	0.08	2.87429E-07
55512-33-9	55512339	701	Pyridate	378.92	2_Pest	276.6666667	276.6666667	0	276.666667	0.00073015			1	0.03	7.9172E-08			1	0.03	7.91724E-08
555-37-3	555373	5063	Neburon	275.18	2 Pest			1	0.3	1.0902E-06			1	0.03	1.0902E-07			1	0.03	1.0902E-07
5598-13-0	5598130	709	Chlorpyrifos-Methyl	322.54	2 Pest	0.37	0.37	0	0.37	1.1471E-06			1	0.03	9.3012E-08			1	0.03	9.30117E-08
563-12-2	563122	711	Ethion	384.48	2 Pest	0.018666667	0.018666667	0	0.01866667	4.855E-08	0.025	0.025	0	0.025	6.5023E-08			1	0.03	7.80275E-08
56-38-2	56382	713	Parathion	291.26	2 Pest	0.009333333	0.009333333	0	0.00933333	3.2045E-08	0.002	0.002	0	0.002	6.8667E-09	0.002	0.002	0	0.002	6.86672E-09
57018-04-9	57018049	718	Tolclofos-methyl	301.13	2 Pest			1	0.3	9.9625E-07			1	0.03	9.9625E-08			1	0.03	9.96247E-08
57646-30-7	57646307	725	Furalaxyl	301.34	2 Pest	13000	13000	0	13000	0.04314064			1	0.03	9.9555E-08			1	0.03	9.95553E-08
57837-19-1	57837191	726	Metalaxyl	279.34	2 Pest	6000	6000	0	6000	0.0214792	1200	1200	0	1200	0.00429584	1200	1200	0	1200	0.00429584
57966-95-7	57966957	727	Cymoxanil	198.19	2 Pest	560	560	0	560	0.00282557	67	67	0	67	0.00033806	67	67	0	67	0.000338059
58138-08-2	58138082	5176	Tridiphane	320.43	2 Pest	83.33333333	83.33333333	0	83.3333333	0.00026007			1	0.03	9.3624E-08			1	0.03	9.36242E-08
58-89-9	58899	68	Lindane	290.83	2 Pest	33.33333333	33.33333333	0	33.3333333	0.00011461	14.4568323	14.45683229	0	14.4568323	4.9709E-05	14.45683229	14.45683229	0	14.45683229	4.97089E-05
5902-51-2	5902512	5149	Terbacil	216.67	2 Pest	21666.66667	21666.66667	0	21666.6667	0.09999846	50	50	0	50	0.00023077			1	0.03	1.38459E-07
5915-41-3	5915413	70	Terbuthylazine	229.72	2 Pest	9800	9800	0	9800	0.04266063			1	0.03	1.3059E-07			1	0.03	1.30594E-07
60168-88-9	60168889	747	Fenarimol	331.2	2 Pest	2266.666667	2266.666667	0	2266.66667	0.0068438	113	113	0	113	0.00034118	113	113	0	113	0.000341184
60207-90-1	60207901	748	Propiconazole	342.23	2 Pest	2.7	2.7	0	2.7	7.8894E-06	310	310	0	310	0.00090582			1	0.03	8.76603E-08
60-51-5	60515	753	Dimethoate	229.26	2 Pest	0.866666667	0.866666667	0	0.86666667	3.7803E-06	29	29	0	29	0.00012649	33	33	0	33	0.000143941
61213-25-0	61213250	4960	Flurochloridone	312.12	2 Pest	1700	1700	0	1700	0.00544662			1	0.03	9.6117E-08			1	0.03	9.61169E-08
62-73-7	62737	4897	Dichlorvos	220.98	2 Pest	0.02	0.02	0	0.02	9.0506E-08	0.17027625	0.170276246	0	0.17027625	7.7055E-07			1	0.03	1.35759E-07
62850-32-2	62850322	4946	Fenothiocarb	253.37	2 Pest	2233.333333	2233.333333	0	2233.33333	0.00881451			1	0.03	1.184E-07			1	0.03	1.18404E-07
63-25-2	63252	76	Carbaryl	201.23	2 Pest	0.22	0.22	0	0.22	1.0933E-06	1	1	0	1	4.9694E-06	1.5	1.5	0	1.5	7.45416E-06
63284-71-9	63284719	773	Nuarimol	314.75	2 Pest	2666.666667	2666.666667	0	2666.66667	0.00847233			1	0.03	9.5314E-08			1	0.03	9.53137E-08
640-15-3	640153	775	Thiometon	246.35	2 Pest	1830	1830	0	1830	0.00742846			1	0.03	1.2178E-07			1	0.03	1.21778E-07
64902-72-3	64902723	783	Chlorsulfuron	357.78	2 Pest	10.54092553	10.54092553	0	10.5409255	2.9462E-05	12000	12000	0	12000	0.03354016	20000	20000	0	20000	0.055900274
66215-27-8	66215278	4881	Cyromazine	166.19	2 Pest	1070	1070	0	1070	0.00643841	310	310	0	310	0.00186533			1	0.03	1.80516E-07
66230-04-4	66230044	786	Esfenvalerate	419.91	2 Pest	0.006666667	0.006666667	0	0.00666667	1.5876E-08	0.005	0.005	0	0.005	1.1907E-08	0.203333333	0.203333333	0	0.203333333	4.84231E-07
66246-88-6	66246886	787	Penconazole	284.19	2 Pest	2250	2250	0	2250	0.00791724			1	0.03	1.0556E-07			1	0.03	1.05563E-07
66332-96-5	66332965	4961	Flutolanil	323.32	2 Pest	2200	2200	0	2200	0.0068044	530	530	0	530	0.00163924	530	530	0	530	0.001639243
668-34-8	668348	790	Fentin	350.01	2 Pest	4.666666667	4.666666667	0	4.66666667	1.3333E-05	0.1	0.1	0	0.1	2.8571E-07			1	0.03	8.57118E-08
66841-25-6	66841256	5167	Tralomethrin	665.04	2 Pest	0.013	0.013	0	0.013	1.9548E-08	0.0044	0.0044	0	0.0044	6.6161E-09			1	0.03	4.51101E-08
67129-08-2	67129082	81	Metazachlor	277.76	2 Pest	7333.333333	7333.333333	0	7333.33333	0.02640169			1	0.03	1.0801E-07			1	0.03	1.08007E-07
67306-00-7	67306007	792	Fenpropidin	273.46	2_Pest	180	180	0	180	0.00065823	320	320	0	320	0.00117019			1	0.03	1.09705E-07
67375-30-8	67375308	1108	alpha-Cypermethrin	416.31	2 Pest	0.033333333	0.033333333	0	0.03333333	8.0069E-08			1	0.03	7.2062E-08			1	0.03	7.20617E-08
67564-91-4	67564914	4949	Fenpropimorph	303.49	2 Pest	1000	1000	0	1000	0.003295	71	71	0	71	0.00023395			1	0.03	9.885E-08
67747-09-5	67747095	797	Prochloraz	376.67	2 Pest	866.6666667	866.6666667	0	866.666667	0.00230086	139.3679	139.3679	0	139.3679	0.00037	139.3679	139.3679	0	139.3679	0.00037
68694-11-1	68694111	802	Triflumizole	345.76	2 Pest	320	320	0	320	0.0009255	140	140	0	140	0.00040491	140	140	0	140	0.000404905
6923-22-4	6923224	803	Monocrotophos	223.17	2 Pest			1	0.3	1.3443E-06			1	0.03	1.3443E-07			1	0.03	1.34427E-07
69377-81-7	69377817	805	Fluroxypyr	255.03	2 Pest	33333.33333	33333.33333	0	33333.3333	0.13070358			1	0.03	1.1763E-07			1	0.03	1.17633E-07
69806-34-4	69806344	810	Haloxyfop	361.7	2 Pest			1	0.3	8.2942E-07			1	0.03	8.2942E-08			1	0.03	8.29417E-08
7003-89-6	7003896	4871	Chlormequat	122.62	2 Pest	5633.333333	5633.333333	0	5633.33333	0.04594139			1	0.03	2.4466E-07			1	0.03	2.44658E-07
70124-77-5	70124775	811	Flucythrinate	451.47	2 Pest	2.766666667	2.766666667	0	2.76666667	6.1281E-06			1	0.03	6.645E-08			1	0.03	6.64496E-08
70630-17-0	70630170	1113	Metalaxyl-M	279.34	2 Pest	39000	39000	0	39000	0.13961481	100	100	0	100	0.00035799	1000	1000	0	1000	0.003579867
709-98-8	709988	816	Propanil	218.08	2 Pest	590	590	0	590	0.00270543	75	75	0	75	0.00034391	75	75	0	75	0.00034391
71626-11-4	71626114	823	Benalaxyl	325.41	2 Pest			1	0.3	9.2191E-07			1	0.03	9.2191E-08			1	0.03	9.21914E-08
71751-41-2	71751412	1097	Abamectin	873.09	2 Pest	0.31	0.31	0	0.31	3.5506E-07	0.03	0.03	0	0.03	3.4361E-08			1	0.03	3.43607E-08
72178-02-0	72178020	824	Fomesafen	438.77	2 Pest	98000	98000	0	98000	0.22335164	50000	50000	0	50000	0.11395492			1	0.03	6.8373E-08
72490-01-8	72490018	825	Fenoxycarb	301.34	2 Pest	50	50	0	50	0.00016593	0.0016	0.0016	0	0.0016	5.3096E-09	0.0016	0.0016	0	0.0016	5.30962E-09
7287-19-6	7287196	87	Prometryn	241.37	2 Pest	3233.333333	3233.333333	0	3233.33333	0.01339575	1000	1000	0	1000	0.00414302			1	0.03	1.24291E-07
731-27-1	731271	827	Tolylfluanid	347.26	2 Pest	33	33	0	33	9.503E-05	100	100	0	100	0.00028797	320	320	0	320	0.0009215
732-11-6	732116	828	Phosmet	317.32	2 Pest	0.014	0.014	0	0.014	4.412E-08	0.78	0.78	0	0.78	2.4581E-06			1	0.03	9.45418E-08
74051-80-2	74051802	834	Sethoxydim	327.49	2 Pest	1100	1100	0	1100	0.00335888			1	0.03	9.1606E-08			1	0.03	9.16059E-08
74070-46-5	74070465	835	Aclonifen	264.67	2 Pest	400	400	0	400	0.00151132	16	16	0	16	6.0453E-05	16	16	0	16	6.04526E-05
74223-64-6	74223646	836	Metsulfuron-methyl	381.37	2 Pest	50000	50000	0	50000	0.13110627	5100	5100	0	5100	0.01337284			1	0.03	7.86638E-08
74738-17-3	74738173	4948	Fenpiclonil	237.09	2 Pest	433.3333333	433.3333333	0	433.333333	0.00182772			1	0.03	1.2653E-07			1	0.03	1.26534E-07
75-99-0	75990	4884	Dalapon	142.97	2 Pest	3666.666667	3666.666667	0	3666.66667	0.02564641			1	0.03	2.0983E-07			1	0.03	2.09834E-07
759-94-4	759944	869	EPTC	189.32	2 Pest	1700	1700	0	1700	0.00897951	810	810	0	810	0.00427847			1	0.03	1.58462E-07
76578-12-6	76578126	5116	Quizalofop	344.76	2 Pest			1	0.3	8.7017E-07			1	0.03	8.7017E-08			1	0.03	8.70171E-08
76674-21-0	76674210	875	Flutriafol	301.3	2 Pest	5600	5600	0	5600	0.01858613	100	100	0	100	0.0003319	100	100	0	100	0.000331895
76738-62-0	76738620	5082	Paclobutrazol	293.8	2 Pest	12400	12400	0	12400	0.04220558			1	0.03	1.0211E-07			1	0.03	1.0211E-07
76-87-9	76879	1110	Fentin hydroxide	367.01	2 Pest	3.333333333	3.333333333	0	3.33333333	9.0824E-06	0.77	0.77	0	0.77	2.098E-06			1	0.03	8.17416E-08
77732-09-3	77732093	5080	Oxadixyl	278.31	2 Pest	220000	220000	0	220000	0.79048543			1	0.03	1.0779E-07			1	0.03	1.07793E-07
7786-34-7	7786347	5035	Mevinphos	224.15	2 Pest	0.053333333	0.053333333	0	0.05333333	2.3794E-07			1	0.03	1.3384E-07			1	0.03	1.33839E-07
78587-05-0	78587050	4974	Hexythiazox	352.89	2 Pest	300	300	0	300	0.00085012	6.1	6.1	0	6.1	1.7286E-05			1	0.03	8.50123E-08
786-19-6	786196	898	carbophenothion	342.87	2 Pest	26.66666667	26.66666667	0	26.6666667	7.7775E-05			1	0.03	8.7497E-08			1	0.03	8.74967E-08
79241-46-6	79241466	4954	Fluazifop-P-butyl	383.37	2 Pest	333.3333333	333.3333333	0	333.333333	0.00086948			1	0.03	7.8253E-08			1	0.03	7.82534E-08
79277-27-3	79277273	918	Thifensulfuron-methyl	387.4	2 Pest	333333.3333	333333.3333	0	333333.333	0.8604371			1	0.03	7.7439E-08			1	0.03	7.74393E-08
79538-32-2	79538322	922	Tefluthrin	418.74	2 Pest	0.023333333	0.023333333	0	0.02333333	5.5723E-08	0.0079	0.0079	0	0.0079	1.8866E-08	0.025	0.025	0	0.025	5.97029E-08
79622-59-6	79622596	925	Fluazinam	465.1	2 Pest	26.5	26.5	0	26.5	5.6977E-05	68	68	0	68	0.00014621	68	68	0	68	0.000146205
79983-71-4	79983714	930	Hexaconazole	314.22	2 Pest	620	620	0	620	0.00197314	226	226	0	226	0.00071924			1	0.03	9.54745E-08
80-33-1	80331	935	Chlorfenson	303.16	2 Pest			1	0.3	9.8958E-07			1	0.03	9.8958E-08			1	0.03	9.89576E-08
81335-37-7	81335377	4977	Imazaquin	311.34	2 Pest	93333.33333	93333.33333	0	93333.3333	0.29977945			1	0.03	9.6358E-08			1	0.03	9.63577E-08
81777-89-1	81777891	941	Clomazone	239.7	2 Pest	400	400	0	400	0.00166875	2200	2200	0	2200	0.00917814			1	0.03	1.25156E-07
82097-50-5	82097505	944	Triasulfuron	401.83	2 Pest	33333.33333	33333.33333	0	33333.3333	0.08295382	104750	104750	0	104750	0.26068238			1	0.03	7.46584E-08
82558-50-7	82558507	946	Isoxaben	332.4	2 Pest	1300	1300	0	1300	0.00391095	690	690	0	690	0.00207581			1	0.03	9.02527E-08
82560-54-1	82560541	947	Benfuracarb	410.54	2 Pest	6.666666667	6.666666667	0	6.66666667	1.6239E-05			1	0.03	7.3074E-08			1	0.03	7.30745E-08

82657-04-3	82657043	948	Bifenthrin	422.87	2_Pest	0.036666667	0.036666667	0	0.03666667	8.6709E-08	0.0013	0.0013	0	0.0013	3.0742E-09	0.003	0.003	0	0.003	7.09438E-09
82-68-8	82688	5115	Quintozene	295.34	2_Pest	130	130	0	130	0.00044017	18	18	0	18	6.0947E-05			1	0.03	1.01578E-07
83055-99-6	83055996	949	Bensulfuron-methyl	410.41	2_Pest	33000	33000	0	33000	0.0804074	17000	17000	0	17000	0.04142199			1	0.03	7.30976E-08
83121-18-0	83121180	5144	Teflubenzuron	381.11	2_Pest			1	0.3	7.8717E-07			1	0.03	7.8717E-08			1	0.03	7.87174E-08
83164-33-4	83164334	951	Diflufenican	394.3	2_Pest	3333.333333	3333.333333	0	3333.33333	0.0084538	52	52	0	52	0.00013188			1	0.03	7.60842E-08
834-12-8	834128	953	ametryn	227.34	2_Pest	12000	12000	0	12000	0.05278438	240	240	0	240	0.00105569	240	240	0	240	0.001055688
83657-24-3	83657243	955	Diniconazole	326.23	2_Pest	2466.666667	2466.666667	0	2466.66667	0.00756113			1	0.03	9.196E-08			1	0.03	9.19597E-08
84087-01-4	84087014	958	Quinclorac	242.06	2_Pest	8500	8500	0	8500	0.03511526	110000	110000	0	110000	0.45443279			1	0.03	1.23936E-07
841-06-5	841065	959	Methoprotryne	271.39	2_Pest	14000	14000	0	14000	0.05158628			1	0.03	1.1054E-07			1	0.03	1.10542E-07
85509-19-9	85509199	967	Flusilazole	315.4	2_Pest			1	0.3	9.5117E-07	270	270	0	270	0.00085606	270	270	0	270	0.000856056
86479-06-3	86479063	971	Hexaflumuron	461.15	2_Pest	0.04	0.04	0	0.04	8.674E-08	0.001	0.001	0	0.001	2.1685E-09			1	0.03	6.50548E-08
86-50-0	86500	972	Azinphos-methyl	317.33	2_Pest	0.7	0.7	0	0.7	2.2059E-06	0.1	0.1	0	0.1	3.1513E-07	0.2	0.2	0	0.2	6.30259E-07
87392-12-9	87392129	1115	S-Metolachlor	283.8	2_Pest	4800	4800	0	4800	0.01691332	5170	5170	0	5170	0.01821705			1	0.03	1.05708E-07
87674-68-8	87674688	1109	Dimethenamid	275.8	2_Pest	12000	12000	0	12000	0.04350979	680	680	0	680	0.00246555			1	0.03	1.08774E-07
87820-88-0	87820880	981	Tralkoxydim	329.44	2_Pest	1250	1250	0	1250	0.00379432	2100	2100	0	2100	0.00637445	2100	2100	0	2100	0.006374454
886-50-0	886500	104	Terbutryn	241.37	2_Pest	560	560	0	560	0.00232009			1	0.03	1.2429E-07			1	0.03	1.24291E-07
88671-89-0	88671890	984	Myclobutanil	288.79	2_Pest	3200	3200	0	3200	0.01108072			1	0.03	1.0388E-07			1	0.03	1.03882E-07
90717-03-6	90717036	1003	Quinmerac	221.64	2_Pest	49566.66667	49566.66667	0	49566.6667	0.22363593			1	0.03	1.3535E-07			1	0.03	1.35355E-07
91465-08-6	91465086	5001	Lambda-Cyhalothrin	449.86	2_Pest	0.02	0.02	0	0.02	4.4458E-08	0.0019	0.0019	0	0.0019	4.2235E-09			1	0.03	6.66874E-08
919-86-8	919868	1010	Demeton-S-methyl	230.29	2_Pest			1	0.3	1.3027E-06			1	0.03	1.3027E-07			1	0.03	1.30271E-07
93-65-2	93652	108	Mecoprop	214.65	2_Pest			1	0.3	1.3976E-06	3333.33333	3333.333333	0	3333.33333	0.01552916			1	0.03	1.39762E-07
94125-34-5	94125345	1021	Prosulfuron	419.39	2_Pest	120000	120000	0	120000	0.28612986	148000	148000	0	148000	0.35289349			1	0.03	7.15325E-08
94361-06-5	94361065	1022	Cyproconazole	291.79	2_Pest	4600	4600	0	4600	0.01576476	19	19	0	19	6.5115E-05	19	19	0	19	6.51153E-05
944-22-9	944229	1023	Fonofos	246.33	2_Pest	0.9	0.9	0	0.9	3.6536E-06	0.08	0.08	0	0.08	3.2477E-07			1	0.03	1.21788E-07
94-74-6	94746	110	MCPA	200.62	2_Pest	3666.666667	3666.666667	0	3666.66667	0.01827668	100000	100000	0	100000	0.49845479	100000	100000	0	100000	0.49845479
94-75-7	94757	111	2,4-D	221.04	2_Pest	1066.666667	1066.666667	0	1066.66667	0.00482567	3333.33333	3333.333333	0	3333.33333	0.01508023	151000	151000	0	151000	0.683134274
94-81-5	94815	5015	MCPB	228.68	2_Pest			1	0.3	1.3119E-06			1	0.03	1.3119E-07			1	0.03	1.31188E-07
94-82-6	94826	4327	2,4-DB	249.09	2_Pest	8400	8400	0	8400	0.03372275			1	0.03	1.2044E-07			1	0.03	1.20438E-07
950-37-8	950378	1025	Methidathion	302.33	2_Pest	1.8	1.8	0	1.8	5.9538E-06	0.5	0.5	0	0.5	1.6538E-06			1	0.03	9.92293E-08
95266-40-3	95266403	1026	Trinexapac-Ethyl	252.27	2_Pest	47500	47500	0	47500	0.18829032	2400	2400	0	2400	0.00951362	21000	21000	0	21000	0.083244143
95465-99-9	95465999	1027	Cadusafos	270.39	2_Pest	0.31	0.31	0	0.31	1.1465E-06	0.23	0.23	0	0.23	8.5062E-07			1	0.03	1.10951E-07
95617-09-7	95617097	4947	Fenoxaprop	333.73	2_Pest			1	0.3	8.9893E-07			1	0.03	8.9893E-08			1	0.03	8.9893E-08
96489-71-3	96489713	1055	Pyridaben	364.94	2_Pest	0.15	0.15	0	0.15	4.1103E-07	0.013	0.013	0	0.013	3.5622E-08			1	0.03	8.22053E-08
99105-77-8	99105778	1083	Sulcotrione	328.77	2_Pest			1	0.3	9.1249E-07	75000	75000	0	75000	0.228123	75000	75000	0	75000	0.228123004
99129-21-2	99129212	1084	Clethodim	359.92	2_Pest	5500	5500	0	5500	0.01528117	940	940	0	940	0.00261169	3000	3000	0	3000	0.008335186
99-30-9	99309	1085	Dicloran	207.02	2_Pest	1000	1000	0	1000	0.00483045			1	0.03	1.4491E-07			1	0.03	1.44914E-07
2458-08-4	2458084	1246	12-Ketochenodeoxycholic acid	406.56	3_REACH			1	0.3	7.379E-07			1	0.03	7.379E-08			1	0.03	7.37898E-08
2478-10-6	2478106	1247	4-hydroxybutyl acrylate	144.17	3_REACH			1	0.3	2.0809E-06			1	0.03	2.0809E-07			1	0.03	2.08088E-07
2536-05-2	2536052	1249	2,2'-methylenediphenyl diisocyanate	250.26	3_REACH			1	0.3	1.1988E-06			1	0.03	1.1988E-07			1	0.03	1.19875E-07
2550-02-9	2550029	1250	triethoxypropylsilane	206.36	3_REACH			1	0.3	1.4538E-06			1	0.03	1.4538E-07			1	0.03	1.45377E-07
2550-06-3	2550063	1251	trichloro(3-chloropropyl)silane	211.98	3_REACH			1	0.3	1.4152E-06			1	0.03	1.4152E-07			1	0.03	1.41523E-07
2554-06-5	2554065	1252	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	344.66	3_REACH			1	0.3	8.7042E-07			1	0.03	8.7042E-08			1	0.03	8.70423E-08
2643-07-4	2643074	1253	p-[(2-chloroethyl)ethylamino]benzaldehyde	211.69	3_REACH			1	0.3	1.4172E-06			1	0.03	1.4172E-07			1	0.03	1.41717E-07
2680-03-7	2680037	1254	N,N-dimethylacrylamide	99.134	3_REACH			1	0.3	3.0262E-06			1	0.03	3.0262E-07			1	0.03	3.02621E-07
3081-01-4	3081014	1257	N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	282.43	3_REACH			1	0.3	1.0622E-06			1	0.03	1.0622E-07			1	0.03	1.06221E-07
3302-10-1	3302101	1259	3,5,5-trimethylhexanoic acid	158.24	3_REACH			1	0.3	1.8959E-06			1	0.03	1.8959E-07			1	0.03	1.89585E-07
3452-07-1	3452071	1261	icos-1-ene	280.54	3_REACH			1	0.3	1.0694E-06			1	0.03	1.0694E-07			1	0.03	1.06937E-07
3913-02-8	3913028	1263	2-butyloctan-1-ol	186.34	3_REACH			1	0.3	1.61E-06			1	0.03	1.61E-07			1	0.03	1.60996E-07
4130-08-9	4130089	1265	triacetoxyvinylsilane	232.26	3_REACH			1	0.3	1.2917E-06			1	0.03	1.2917E-07			1	0.03	1.29166E-07
4223-03-4	4223034	1266	N-(1,1,3,3-tetramethylbutyl)acrylamide	183.3	3_REACH			1	0.3	1.6367E-06			1	0.03	1.6367E-07			1	0.03	1.63666E-07
4292-10-8	4292108	1267	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	342.53	3_REACH			1	0.3	8.7584E-07			1	0.03	8.7584E-08			1	0.03	8.75836E-08
4719-04-4	4719044	117	2,2',2''-(hexahydro-1,3,5-triazine-1,3,5-triyl)triethanol	219.29	3_REACH	7500	7500	0	7500	0.03420129			1	0.03	1.3681E-07			1	0.03	1.36805E-07
5117-12-4	5117124	4397	4-(1-oxo-2-propenyl)-morpholine	141.17	3_REACH			1	0.3	2.1251E-06			1	0.03	2.1251E-07			1	0.03	2.1251E-07
6318-09-8	6318098	1282	2,4,6-Tri(propan-2-yl)benzene-1,3-diamine	234.39	3_REACH			1	0.3	1.2799E-06			1	0.03	1.2799E-07			1	0.03	1.27992E-07
6992-11-6	6992116	1287	4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxynaphthalene-2-carboxamide	492.33	3_REACH			1	0.3	6.0935E-07			1	0.03	6.0935E-08			1	0.03	6.09347E-08
7027-11-4	7027114	4392	3-cyano-3,5,5-trimethylcyclohexanone	165.24	3_REACH			1	0.3	1.8155E-06			1	0.03	1.8155E-07			1	0.03	1.81554E-07
7651-02-7	7651027	1289	N-[3-(dimethylamino)propyl]stearamide	368.65	3_REACH			1	0.3	8.1378E-07			1	0.03	8.1378E-08			1	0.03	8.1378E-08
100-00-5	100005	119	1-chloro-4-nitrobenzene	157.56	3_REACH	900	900	0	900	0.00571211	190	190	0	190	0.00120589	190	190	0	190	0.00120589
100-01-6	100016	120	4-nitroaniline	138.13	3_REACH	8000	8000	0	8000	0.05791646			1	0.03	2.1719E-07			1	0.03	2.17187E-07
100-02-7	100027	1	4-nitrophenol	139.11	3_REACH	2500	2500	0	2500	0.01797139	1300	1300	0	1300	0.00934512	1300	1300	0	1300	0.009345123
1001354-72-8	1001354728	4779	3-Aminooctan-4-ol	145.25	3_REACH			1	0.3	2.0654E-06			1	0.03	2.0654E-07			1	0.03	2.0654E-07
10016-20-3	10016203	1295	cyclohexapentylose	972.85	3_REACH			1	0.3	3.0837E-07			1	0.03	3.0837E-08			1	0.03	3.08372E-08
100-18-5	100185	1296	1,4-diisopropylbenzene	162.28	3_REACH			1	0.3	1.8487E-06			1	0.03	1.8487E-07			1	0.03	1.84866E-07
100-20-9	100209	1297	terephthaloyl dichloride	203.02	3_REACH			1	0.3	1.4777E-06			1	0.03	1.4777E-07			1	0.03	1.47769E-07
100-21-0	100210	122	terephthalic acid	166.13	3_REACH	0.085	0.085	0	0.085	5.1165E-07			1	0.03	1.8058E-07			1	0.03	1.80581E-07
1003-52-7	1003527	1302	4-methyloxazole-5-carbonitrile	108.1	3_REACH			1	0.3	2.7752E-06			1	0.03	2.7752E-07			1	0.03	2.77521E-07
100-37-8	100378	123	2-diethylaminoethanol	117.19	3_REACH			1	0.3	2.5599E-06			1	0.03	2.5599E-07			1	0.03	2.55995E-07
10042-59-8	10042598	1306	2-propylheptan-1-ol	158.29	3_REACH			1	0.3	1.8953E-06			1	0.03	1.8953E-07			1	0.03	1.89526E-07
100-46-9	100469	127	benzylamine	107.16	3_REACH			1	0.3	2.7996E-06			1	0.03	2.7996E-07			1	0.03	2.79955E-07
100-47-0	100470	128	benzonitrile	103.13	3_REACH	10310	10310	0	10310	0.09997091			1	0.03	2.9089E-07			1	0.03	2.90895E-07
100-51-6	100516	129	benzyl alcohol	108.14	3_REACH	18333.33333	18333.33333	0	18333.3333	0.16953332			1	0.03	2.7742E-07			1	0.03	2.77418E-07
100-52-7	100527	130	benzaldehyde	106.12	3_REACH	16666.66667	16666.66667	0	16666.6667	0.15705491			1	0.03	2.827E-07			1	0.03	2.82699E-07
100-54-9	100549	131	nicotinonitrile	104.11	3_REACH			1	0.3	2.8816E-06			1	0.03	2.8816E-07			1	0.03	2.88157E-07
100-61-8	100618	133	N-methylaniline	107.16	3_REACH	50	50	0	50	0.00046659			1	0.03	2.7996E-07			1	0.03	2.79955E-07
100-63-0	100630	134	phenylhydrazine	108.15	3_REACH	400	400	0	400	0.00369857			1	0.03	2.7739E-07			1	0.03	2.77393E-07
100-64-1	100641	135	cyclohexanone oxime	113.16	3_REACH			1	0.3	2.6511E-06			1	0.03	2.6511E-07			1	0.03	2.65111E-07
100-69-6	100696	1309	2-vinylpyridine	105.14	3_REACH			1	0.3	2.8533E-06			1	0.03	2.8533E-07			1	0.03	2.85334E-07
10081-67-1	10081671	1310	4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline	405.59	3_REACH			1	0.3	7.3966E-07			1	0.03	7.3966E-08			1	0.03	7.39663E-08
100-83-4	100834	138	3-hydroxybenzaldehyde	122.12	3_REACH			1	0.3	2.4566E-06			1	0.03	2.4566E-07			1	0.03	2.4566E-07
100-97-0	100970	2	methenamine	140.19	3_REACH			1	0.3	2.14E-06			1	0.03	2.14E-07			1	0.03	2.13995E-07
10097-02-6	10097026	4315	2,2-bis(hydroxymethyl)butanoic acid	148.16	3_REACH			1	0.3	2.0248E-06			1	0.03	2.0248E-07			1	0.03	2.02484E-07
101-02-0	101020	140	triphenyl phosphite	310.29	3_REACH			1	0.3	9.6684E-07			1	0.03	9.6684E-08			1	0.03	9.66837E-08
101-14-4	101144	1315	4,4'-methylenebis[2-chloroaniline]	267.16	3_REACH			1	0.3	1.1229E-06			1	0.03	1.1229E-07			1	0.03	1.12292E-07
101-20-2	101202	143	triclocarban	315.59	3_REACH			1	0.3	9.506E-07			1	0.03	9.506E-08			1	0.03	9.506E-08
101238-01-1	101238011	1317	2,2,6,6-Tetramethylpiperidin-4-yl dodecanoate	339.57	3_REACH			1	0.3	8.8347E-07			1	0.03	8.8347E-08			1	0.03	8.8347E-08
101-37-1	101371	1318	2,4,6-triallyloxy-1,3,5-triazine	249.27	3_REACH			1	0.3	1.2035E-06			1	0.03	1.2035E-07			1	0.03	1.20351E-07
1013-88-3	1013883	4621	diphenylmethanimine	181.24	3_REACH			1	0.3	1.6553E-06			1	0.03	1.6553E-07			1	0.03	1.65526E-07
101-39-3	101393	1320	alpha-Methylcinnamaldehyde	146.19	3_REACH			1	0.3	2.0521E-06			1	0.03	2.0521E-07			1	0.03	2.05212E-07
101-41-7	101417	1321	methyl phenylacetate	150.18	3_REACH			1	0.3	1.9976E-06			1	0.03	1.9976E-07			1	0.03	1.9976E-07
101-43-9	101439	1322	cyclohexyl methacrylate	168.24	3_REACH			1	0.3	1.7832E-06			1	0.03	1.7832E-07			1	0.03	1.78317E-07
101-54-2	101542	1323	N-(4-aminophenyl)aniline	184.24	3_REACH			1	0.3	1.6283E-06			1	0.03	1.6283E-07			1	0.03	1.62831E-07
101-68-8	101688	1325	4,4'-methylenediphenyl diisocyanate	250.26	3_REACH			1	0.3	1.1988E-06			1	0.03	1.1988E-07			1	0.03	1.19875E-07
1017183-70-8	1017183708	4503	3-(4-fluorophenyl)-2-methylpropionylchloride	200.64	3_REACH			1	0.3	1.4952E-06			1	0.03	1.4952E-07			1	0.03	1.49522E-07
101-72-4	101724	1326	N-isopropyl-N'-phenyl-p-phenylenediamine	226.32	3_REACH			1	0.3	1.3256E-06			1	0.03	1.3256E-07			1	0.03	1.32556E-07
101-77-9	101779	1328	4,4'-methylenedianiline	198.27	3_REACH			1	0.3	1.5131E-06			1	0.03	1.5131E-07			1	0.03	1.51309E-07
101-80-4	101804	1329	4,4'-oxydianiline	200.24	3_REACH			1	0.3	1.4982E-06			1	0.03	1.4982E-07			1	0.03	1.4982E-07
101-84-8	101848	150	diphenyl ether	170.21	3_REACH	223.3333333	223.3333333	0	223.333333	0.0013121			1	0.03	1.7625E-07			1	0.03	1.76253E-07
101-96-2	101962	1331	N,N'-di-sec-butyl-p-phenylenediamine	220.36	3_REACH			1	0.3	1.3614E-06			1	0.03	1.3614E-07			1	0.03	1.36141E-07
102-01-2	102012	1334	acetoacetanilide	177.2	3_REACH			1	0.3	1.693E-06			1	0.03	1.693E-07			1	0.03	1.693E-07
102-06-7	102067	1335	1,3-diphenylguanidine	211.27	3_REACH			1	0.3	1.42E-06			1	0.03	1.42E-07			1	0.03	1.41998E-07
102-08-9	102089	151	1,3-diphenyl-2-thiourea	228.32	3_REACH	22333.33333	22333.33333	0	22333.3333	0.09781593			1	0.03	1.3139E-07			1	0.03	1.31395E-07
102-09-0	102090	1336	diphenyl carbonate	214.22	3_REACH			1	0.3	1.4004E-06			1	0.03	1.4004E-07			1	0.03	1.40043E-07
10233-13-3	10233133	1339	isopropyl laurate	242.4	3_REACH			1	0.3	1.2376E-06			1	0.03	1.2376E-07			1	0.03	1.23762E-07
102-36-3	102363	1341	3,4-dichlorophenyl isocyanate	188.01	3_REACH			1	0.3	1.5957E-06			1	0.03	1.5957E-07			1	0.03	1.59566E-07
10254-57-6	10254576	1344	4,4'-methylene bis(dibutyldithiocarbamate)	422.79	3_REACH			1	0.3	7.0957E-07			1	0.03	7.0957E-08			1	0.03	7.09572E-08
102-60-3	102603	1347	1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol	292.42	3_REACH			1	0.3	1.0259E-06			1	0.03	1.0259E-07			1	0.03	1.02592E-07
102-69-2	102692	154	tripropylamine	143.28	3_REACH			1	0.3	2.0938E-06			1	0.03	2.0938E-07			1	0.03	2.0938E-07
102-71-6	102716	155	2,2',2''-nitrilotriethanol	149.19	3_REACH	463333.3333	463333.3333	0	463333.333	3.10565945	16000	16000	0	16000	0.10724579	16000	16000	0	16000	0.107245794
102-76-1	102761	1352	triacetin	218.21	3_REACH			1	0.3	1.3748E-06			1	0.03	1.3748E-07			1	0.03	1.37482E-07
102-77-2	102772	1353	2-(morpholinothio)benzothiazole	252.36	3_REACH			1	0.3	1.1888E-06			1	0.03	1.1888E-07			1	0.03	1.18878E-07
102-81-8	102818	1354	2-dibutylaminoethanol	173.3	3_REACH			1	0.3	1.7311E-06			1	0.03	1.7311E-07			1	0.03	1.7311E-07
102-82-9	102829	156	tributylamine	185.36	3_REACH			1	0.3	1.6185E-06			1	0.03	1.6185E-07			1	0.03	1.61847E-07
102985-93-3	102985933	4723	2,2-dimethyl-3-oxopropyl dodecanoate	284.44	3_REACH			1	0.3	1.0547E-06			1	0.03	1.0547E-07			1	0.03	1.0547E-07
103-09-3	103093	1359	2-ethylhexyl acetate	172.27	3_REACH			1	0.3	1.7415E-06			1	0.03	1.7415E-07			1	0.03	1.74145E-07
103-11-7	103117	159	2-ethylhexyl acrylate	184.28	3_REACH	3333.333333	3333.333333	0	3333.33333	0.01808842			1	0.03	1.628E-07			1	0.03	1.62796E-07
103-23-1	103231	160	bis(2-ethylhexyl) adipate	370.57	3_REACH	220	220	0	220	0.00059368	35.3270435	35.32704347	0	35.3270435	9.5332E-05	35.32704347	35.32704347	0	35.32704347	9.53316E-05
103-26-4	103264	1362	methyl cinnamate	162.19	3_REACH			1	0.3	1.8497E-06			1	0.03	1.8497E-07			1	0.03	1.84968E-07
10326-41-7	10326417	161	(R)-lactic acid	90.078	3_REACH			1	0.3	3.3304E-06			1	0.03	3.3304E-07			1	0.03	3.33045E-07
103-45-7	103457	1367	phenethyl acetate	164.2	3_REACH			1	0.3	1.827E-06			1	0.03	1.827E-07			1	0.03	1.82704E-07
103-49-1	103491	1368	dibenzylamine	197.28	3_REACH			1	0.3	1.5207E-06			1	0.03	1.5207E-07			1	0.03	1.52068E-07
103-50-4	103504	1369	dibenzyl ether	198.26	3_REACH			1	0.3	1.5132E-06			1	0.03	1.5132E-07			1	0.03	1.51316E-07
103-60-6	103606	1374	2-phenoxyethyl isobutyrate	208.26	3_REACH			1	0.3	1.4405E-06			1	0.03	1.4405E-07			1	0.03	1.44051E-07
103694-68-4	103694684	4367	Trimethylbenzenepropanol	178.28	3_REACH			1	0.3	1.6827E-06			1	0.03	1.6827E-07			1	0.03	1.68275E-07
103-69-5	103695	162	N-ethylaniline	121.18	3_REACH	140	140	0	140	0.00115531			1	0.03	2.4757E-07			1	0.03	2.47566E-07
103-71-9	103719	1378	phenyl isocyanate	119.12	3_REACH			1	0.3	2.5185E-06			1	0.03	2.5185E-07			1	0.03	2.51847E-07
103-74-2	103742	163	2-(2-pyridyl)ethanol	123.16	3_REACH	4606.666667	4606.666667	0	4606.66667	0.03740392			1	0.03	2.4359E-07			1	0.03	2.43586E-07
103-83-3	103833	164	benzyldimethylamine	135.21	3_REACH			1	0.3	2.2188E-06			1	0.03	2.2188E-07			1	0.03	2.21877E-07
103-95-7	103957	1382	3-p-cumenyl-2-methylpropionaldehyde	190.29	3_REACH			1	0.3	1.5765E-06			1	0.03	1.5765E-07			1	0.03	1.57654E-07
10411-92-4	10411924	1383	cis-4-tert-butylcyclohexyl acetate	198.31	3_REACH			1	0.3	1.5128E-06			1	0.03	1.5128E-07			1	0.03	1.51278E-07
10420-33-4	10420334	1387	dimethyl acetylsuccinate	188.18	3_REACH			1	0.3	1.5942E-06			1	0.03	1.5942E-07			1	0.03	1.59422E-07
104-23-4	104234	1388	4'-aminoazobenzene-4-sulphonic acid	277.31	3_REACH			1	0.3	1.0818E-06			1	0.03	1.0818E-07			1	0.03	1.08182E-07
104-38-1	104381	1393	2,2'-p-phenylenedioxydiethanol	198.22	3_REACH			1	0.3	1.5135E-06			1	0.03	1.5135E-07			1	0.03	1.51347E-07
104468-21-5	104468215	4316	2,2-dimethyl 3-methyl-3-butenyl propanoate	170.25	3_REACH			1	0.3	1.7621E-06			1	0.03	1.7621E-07			1	0.03	1.76211E-07
104-55-2	104552	168	cinnamaldehyde	132.16	3_REACH	320	320	0	320	0.00242131			1	0.03	2.27E-07			1	0.03	2.26998E-07
104-61-0	104610	1395	nonan-4-olide	156.22	3_REACH			1	0.3	1.9204E-06			1	0.03	1.9204E-07			1	0.03	1.92037E-07
104-66-5	104665	1397	1,2-diphenoxyethane	214.26	3_REACH			1	0.3	1.4002E-06			1	0.03	1.4002E-07			1	0.03	1.40017E-07
104-67-6	104676	1398	undecan-4-olide	184.28	3_REACH			1	0.3	1.628E-06			1	0.03	1.628E-07			1	0.03	1.62796E-07
104-68-7	104687	1399	2-(2-phenoxyethoxy)ethanol	182.22	3_REACH			1	0.3	1.6464E-06			1	0.03	1.6464E-07			1	0.03	1.64636E-07
1047-16-1	1047161	1400	5,12-dihydroquino[2,3-b]acridine-7,14-dione	312.33	3_REACH			1	0.3	9.6052E-07			1	0.03	9.6052E-08			1	0.03	9.60523E-08
104-75-6	104756	169	2-ethylhexylamine	129.25	3_REACH	733.3333333	733.3333333	0	733.333333	0.00567376			1	0.03	2.3211E-07			1	0.03	2.32108E-07
104-76-7	104767	170	2-ethylhexan-1-ol	144.26	3_REACH			1	0.3	2.0796E-06			1	0.03	2.0796E-07			1	0.03	2.07958E-07
104-88-1	104881	171	4-chlorobenzaldehyde	140.57	3_REACH			1	0.3	2.1342E-06			1	0.03	2.1342E-07			1	0.03	2.13417E-07
104-90-5	104905	172	5-ethyl-2-methylpyridine	121.18	3_REACH			1	0.3	2.4757E-06			1	0.03	2.4757E-07			1	0.03	2.47566E-07
104-93-8	104938	1403	4-methylanisole	122.17	3_REACH			1	0.3	2.4556E-06			1	0.03	2.4556E-07			1	0.03	2.45559E-07
105-05-5	105055	1405	1,4-diethylbenzene	134.22	3_REACH			1	0.3	2.2351E-06			1	0.03	2.2351E-07			1	0.03	2.23514E-07
10543-57-4	10543574	175	N,N'-ethylenebis[N-acetylacetamide]	228.25	3_REACH	1000000	1000000	0	1000000	4.38116101			1	0.03	1.3143E-07			1	0.03	1.31435E-07
105-53-3	105533	177	diethyl malonate	160.17	3_REACH			1	0.3	1.873E-06			1	0.03	1.873E-07			1	0.03	1.87301E-07
105-55-5	105555	178	1,3-diethyl-2-thiourea	132.23	3_REACH	64333.33333	64333.33333	0	64333.3333	0.486526			1	0.03	2.2688E-07			1	0.03	2.26877E-07
105-56-6	105566	1415	ethyl cyanoacetate	113.12	3_REACH			1	0.3	2.6521E-06			1	0.03	2.6521E-07			1	0.03	2.65205E-07
105-59-9	105599	1416	2,2'-methyliminodiethanol	119.17	3_REACH			1	0.3	2.5174E-06			1	0.03	2.5174E-07			1	0.03	2.51741E-07

105-60-2	105602	180	Caprolactam	113.16	3_REACH	2333333.333	2333333.333	0	2333333.33	20.6197714			1	0.03	2.6511E-07			1	0.03	2.65111E-07
10563-26-5	10563265	1417	N,N'-bis(3-aminopropyl)ethylenediamine	174.3	3_REACH			1	0.3	1.7212E-06			1	0.03	1.7212E-07			1	0.03	1.72117E-07
10563-29-8	10563298	1418	N'-(3-aminopropyl)-N,N-dimethylpropane-1,3-diamine	159.28	3_REACH			1	0.3	1.8835E-06			1	0.03	1.8835E-07			1	0.03	1.88348E-07
105-67-9	105679	181	2,4-xylenol	122.17	3_REACH	700	700	0	700	0.00572972			1	0.03	2.4556E-07			1	0.03	2.45559E-07
105-75-9	105759	182	dibutyl fumarate	228.29	3_REACH			1	0.3	1.3141E-06			1	0.03	1.3141E-07			1	0.03	1.31412E-07
105-76-0	105760	183	dibutyl maleate	228.29	3_REACH			1	0.3	1.3141E-06			1	0.03	1.3141E-07			1	0.03	1.31412E-07
105812-81-5	105812815	4223	(-)-trans-4-(4'-fluorophenyl)-3-hydroxymethyl-N-methylpiperidine	223.29	3_REACH			1	0.3	1.3435E-06			1	0.03	1.3435E-07			1	0.03	1.34354E-07
105827-91-6	105827916	4348	2-chloro-5-chloromethylthiazole	168.05	3_REACH			1	0.3	1.7852E-06			1	0.03	1.7852E-07			1	0.03	1.78518E-07
105-83-9	105839	1420	N,N-bis(3-aminopropyl)methylamine	145.25	3_REACH			1	0.3	2.0654E-06			1	0.03	2.0654E-07			1	0.03	2.0654E-07
105-95-3	105953	1422	1,4-dioxacycloheptadecane-5,17-dione	270.37	3_REACH			1	0.3	1.1096E-06			1	0.03	1.1096E-07			1	0.03	1.10959E-07
105-99-7	105997	184	dibutyl adipate	258.36	3_REACH			1	0.3	1.1612E-06			1	0.03	1.1612E-07			1	0.03	1.16117E-07
106-02-5	106025	1425	pentadecan-15-olide	240.39	3_REACH			1	0.3	1.248E-06			1	0.03	1.248E-07			1	0.03	1.24797E-07
106-20-7	106207	1430	bis(2-ethylhexyl)amine	241.46	3_REACH			1	0.3	1.2424E-06			1	0.03	1.2424E-07			1	0.03	1.24244E-07
106-21-8	106218	1431	3,7-dimethyloctan-1-ol	158.29	3_REACH			1	0.3	1.8953E-06			1	0.03	1.8953E-07			1	0.03	1.89526E-07
106-22-9	106229	185	citronellol	156.27	3_REACH			1	0.3	1.9198E-06			1	0.03	1.9198E-07			1	0.03	1.91975E-07
106-23-0	106230	1432	citronellal	154.25	3_REACH			1	0.3	1.9449E-06			1	0.03	1.9449E-07			1	0.03	1.94489E-07
106-24-1	106241	186	geraniol	154.25	3_REACH			1	0.3	1.9449E-06			1	0.03	1.9449E-07			1	0.03	1.94489E-07
106-25-2	106252	187	nerol	154.25	3_REACH			1	0.3	1.9449E-06			1	0.03	1.9449E-07			1	0.03	1.94489E-07
106-26-3	106263	1433	(Z)-3,7-dimethylocta-2,6-dienal	152.24	3_REACH			1	0.3	1.9706E-06			1	0.03	1.9706E-07			1	0.03	1.97057E-07
106-43-4	106434	190	4-chlorotoluene	126.59	3_REACH			1	0.3	2.3699E-06			1	0.03	2.3699E-07			1	0.03	2.36986E-07
106-44-5	106445	191	p-cresol	108.14	3_REACH	466.6666667	466.6666667	0	466.666667	0.00431539	1000	1000	0	1000	0.00924727	1000	1000	0	1000	0.009247272
106461-41-0	106461410	4581	2,4-dihydro-4-(4-(4-(4-hydroxyphenyl)-1-piperazinyl)phenyl)-2-(1-methylpropyl)-3H-1,2,4-triazol-3-one	393.5	3_REACH			1	0.3	7.6239E-07			1	0.03	7.6239E-08			1	0.03	7.62389E-08
106-46-7	106467	192	1,4-dichlorobenzene	147	3_REACH	0.233333333	0.233333333	0	0.23333333	1.5873E-06	300	300	0	300	0.00204082	300	300	0	300	0.002040816
106-47-8	106478	193	4-chloroaniline	127.58	3_REACH	16.66666667	16.66666667	0	16.6666667	0.00013064	10	10	0	10	7.8382E-05	10	10	0	10	7.83822E-05
106-48-9	106489	194	4-chlorophenol	128.56	3_REACH	833.3333333	833.3333333	0	833.333333	0.00648206	630	630	0	630	0.00490044	630	630	0	630	0.004900436
106-49-0	106490	195	p-toluidine	107.16	3_REACH			1	0.3	2.7996E-06			1	0.03	2.7996E-07			1	0.03	2.79955E-07
106-50-3	106503	196	p-phenylenediamine	108.15	3_REACH			1	0.3	2.7739E-06			1	0.03	2.7739E-07			1	0.03	2.77393E-07
106-51-4	106514	197	p-benzoquinone	108.1	3_REACH			1	0.3	2.7752E-06			1	0.03	2.7752E-07			1	0.03	2.77521E-07
1067-33-0	1067330	199	dibutyltin di(acetate)	351.01	3_REACH			1	0.3	8.5468E-07			1	0.03	8.5468E-08			1	0.03	8.54677E-08
106-79-6	106796	1446	dimethyl sebacate	230.3	3_REACH			1	0.3	1.3026E-06			1	0.03	1.3026E-07			1	0.03	1.30265E-07
106797-53-9	106797539	4354	2-hydroxy-4'-hydroxyethoxy-2-methylpropiophenone	224.26	3_REACH			1	0.3	1.3377E-06			1	0.03	1.3377E-07			1	0.03	1.33773E-07
106-91-2	106912	1449	2,3-epoxypropyl methacrylate	142.15	3_REACH			1	0.3	2.1104E-06			1	0.03	2.1104E-07			1	0.03	2.11045E-07
1071-22-3	1071223	1455	3-(trichlorosilyl)propiononitrile	188.52	3_REACH			1	0.3	1.5913E-06			1	0.03	1.5913E-07			1	0.03	1.59134E-07
1072-63-5	1072635	1457	1-vinylimidazole	94.119	3_REACH			1	0.3	3.1875E-06			1	0.03	3.1875E-07			1	0.03	3.18745E-07
1073-69-4	1073694	1461	(4-chlorophenyl)hydrazine	142.59	3_REACH			1	0.3	2.1039E-06			1	0.03	2.1039E-07			1	0.03	2.10393E-07
107-41-5	107415	219	2-methylpentane-2,4-diol	118.18	3_REACH	1066666.667	1066666.667	0	1066666.67	9.02577988			1	0.03	2.5385E-07			1	0.03	2.5385E-07
107-56-2	107562	1465	O,O-diisopropyl hydrogen dithiophosphate	214.29	3_REACH			1	0.3	1.4E-06			1	0.03	1.4E-07			1	0.03	1.39997E-07
107-58-4	107584	1466	N-tert-butylacrylamide	127.19	3_REACH			1	0.3	2.3587E-06			1	0.03	2.3587E-07			1	0.03	2.35868E-07
107-66-4	107664	1467	dibutyl hydrogen phosphate	210.21	3_REACH			1	0.3	1.4271E-06			1	0.03	1.4271E-07			1	0.03	1.42714E-07
107737-97-3	107737973	4619	2,2-Dimethyl-3-(3-methylphenyl)propanal	176.26	3_REACH			1	0.3	1.702E-06			1	0.03	1.702E-07			1	0.03	1.70203E-07
107-75-5	107755	1468	7-hydroxycitronellal	172.27	3_REACH			1	0.3	1.7415E-06			1	0.03	1.7415E-07			1	0.03	1.74145E-07
107-88-0	107880	1470	butane-1,3-diol	90.122	3_REACH			1	0.3	3.3288E-06			1	0.03	3.3288E-07			1	0.03	3.32882E-07
107898-54-4	107898544	4225	Supersantol	222.37	3_REACH			1	0.3	1.3491E-06			1	0.03	1.3491E-07			1	0.03	1.3491E-07
107-92-6	107926	224	butyric acid	88.106	3_REACH	650000	650000	0	650000	7.37747713			1	0.03	3.405E-07			1	0.03	3.40499E-07
107-93-7	107937	225	trans-crotonic acid	86.09	3_REACH			1	0.3	3.4847E-06			1	0.03	3.4847E-07			1	0.03	3.48473E-07
107-96-0	107960	1473	3-mercaptopropionic acid	106.14	3_REACH			1	0.3	2.8265E-06			1	0.03	2.8265E-07			1	0.03	2.82646E-07
108-39-4	108394	237	m-cresol	108.14	3_REACH	2966.666667	2966.666667	0	2966.66667	0.02743357			1	0.03	2.7742E-07			1	0.03	2.77418E-07
108-42-9	108429	238	3-chloroaniline	127.58	3_REACH	33.33333333	33.33333333	0	33.3333333	0.00026127	13	13	0	13	0.0001019	13	13	0	13	0.000101897
108-44-1	108441	239	m-toluidine	107.16	3_REACH	243.3333333	243.3333333	0	243.333333	0.00227075	12	12	0	12	0.00011198			1	0.03	2.79955E-07
108-45-2	108452	1484	m-phenylenediamine	108.15	3_REACH			1	0.3	2.7739E-06			1	0.03	2.7739E-07			1	0.03	2.77393E-07
108-46-3	108463	240	resorcinol	110.11	3_REACH	83.33333333	83.33333333	0	83.3333333	0.00075682			1	0.03	2.7245E-07			1	0.03	2.72455E-07
108-67-8	108678	242	mesitylene	120.19	3_REACH	16666.66667	16666.66667	0	16666.6667	0.13866933	400	400	0	400	0.00332806	400	400	0	400	0.003328064
108-68-9	108689	243	3,5-xylenol	122.17	3_REACH			1	0.3	2.4556E-06			1	0.03	2.4556E-07			1	0.03	2.45559E-07
108-69-0	108690	244	3,5-xylidine	121.18	3_REACH			1	0.3	2.4757E-06			1	0.03	2.4757E-07			1	0.03	2.47566E-07
108-78-1	108781	4	melamine	126.13	3_REACH			1	0.3	2.3785E-06			1	0.03	2.3785E-07			1	0.03	2.3785E-07
108-80-5	108805	245	cyanuric acid	129.08	3_REACH	56.66666667	56.66666667	0	56.6666667	0.000439			1	0.03	2.3241E-07			1	0.03	2.32414E-07
108-83-8	108838	1490	2,6-dimethylheptan-4-one	142.24	3_REACH			1	0.3	2.1091E-06			1	0.03	2.1091E-07			1	0.03	2.10911E-07
108-93-0	108930	250	cyclohexanol	100.16	3_REACH			1	0.3	2.9952E-06			1	0.03	2.9952E-07			1	0.03	2.99521E-07
108-95-2	108952	252	phenol	94.113	3_REACH	1250	1250	0	1250	0.01328191	160	160	0	160	0.00170008	2380	2380	0	2380	0.025288749
108-98-5	108985	1491	benzenethiol	110.18	3_REACH			1	0.3	2.7228E-06			1	0.03	2.7228E-07			1	0.03	2.72282E-07
109-13-7	109137	1494	tert-butyl peroxyisobutyrate	160.21	3_REACH			1	0.3	1.8725E-06			1	0.03	1.8725E-07			1	0.03	1.87254E-07
109-16-0	109160	1495	2,2'-ethylenedioxydiethyl dimethacrylate	286.32	3_REACH			1	0.3	1.0478E-06			1	0.03	1.0478E-07			1	0.03	1.04778E-07
109-52-4	109524	256	valeric acid	102.13	3_REACH			1	0.3	2.9374E-06			1	0.03	2.9374E-07			1	0.03	2.93743E-07
109-77-3	109773	266	malononitrile	66.065	3_REACH			1	0.3	4.541E-06			1	0.03	4.541E-07			1	0.03	4.54098E-07
110-15-6	110156	274	succinic acid	118.09	3_REACH	124733.3333	124733.3333	0	124733.333	1.05625653			1	0.03	2.5404E-07			1	0.03	2.54044E-07
110-16-7	110167	275	maleic acid	116.07	3_REACH	53333.33333	53333.33333	0	53333.3333	0.45949283			1	0.03	2.5846E-07			1	0.03	2.58465E-07
110-25-8	110258	1515	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	353.55	3_REACH			1	0.3	8.4854E-07			1	0.03	8.4854E-08			1	0.03	8.48536E-08
110-41-8	110418	1519	2-methylundecanal	184.32	3_REACH			1	0.3	1.6276E-06			1	0.03	1.6276E-07			1	0.03	1.6276E-07
110-42-9	110429	1520	methyl decanoate	186.29	3_REACH			1	0.3	1.6104E-06			1	0.03	1.6104E-07			1	0.03	1.61039E-07
110-44-1	110441	1521	hexa-2,4-dienoic acid	112.13	3_REACH			1	0.3	2.6755E-06			1	0.03	2.6755E-07			1	0.03	2.67547E-07
110-63-4	110634	1526	butane-1,4-diol	90.122	3_REACH			1	0.3	3.3288E-06			1	0.03	3.3288E-07			1	0.03	3.32882E-07
110-64-5	110645	1527	but-2-ene-1,4-diol	88.106	3_REACH			1	0.3	3.405E-06			1	0.03	3.405E-07			1	0.03	3.40499E-07
110-65-6	110656	281	but-2-yne-1,4-diol	86.09	3_REACH			1	0.3	3.4847E-06			1	0.03	3.4847E-07			1	0.03	3.48473E-07
110-77-0	110770	283	2-(ethylthio)ethanol	106.19	3_REACH	9866.666667	9866.666667	0	9866.66667	0.09291521			1	0.03	2.8251E-07			1	0.03	2.82512E-07
110-93-0	110930	291	6-methylhept-5-en-2-one	126.2	3_REACH			1	0.3	2.3772E-06			1	0.03	2.3772E-07			1	0.03	2.37718E-07
110964-79-9	110964799	1534	4-(methylsulfonyl)-2-nitrobenzoic acid	245.21	3_REACH			1	0.3	1.2234E-06			1	0.03	1.2234E-07			1	0.03	1.22344E-07
110-97-4	110974	292	1,1'-iminodipropan-2-ol	133.19	3_REACH			1	0.3	2.2524E-06			1	0.03	2.2524E-07			1	0.03	2.25242E-07
111-11-5	111115	1538	methyl octanoate	158.24	3_REACH			1	0.3	1.8959E-06			1	0.03	1.8959E-07			1	0.03	1.89585E-07
111-14-8	111148	293	heptanoic acid	130.19	3_REACH			1	0.3	2.3043E-06			1	0.03	2.3043E-07			1	0.03	2.30432E-07
111-18-2	111182	1540	N,N,N',N'-tetramethylhexamethylenediamine	172.32	3_REACH			1	0.3	1.7409E-06			1	0.03	1.7409E-07			1	0.03	1.74095E-07
111-21-7	111217	1542	2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate	234.25	3_REACH			1	0.3	1.2807E-06			1	0.03	1.2807E-07			1	0.03	1.28068E-07
111-27-3	111273	294	hexan-1-ol	102.18	3_REACH	67000	67000	0	67000	0.65570562			1	0.03	2.936E-07			1	0.03	2.936E-07
111-30-8	111308	296	glutaral	100.12	3_REACH	600	600	0	600	0.00599281	4200	4200	0	4200	0.04194966			1	0.03	2.9964E-07
111-40-0	111400	299	2,2'-iminodi(ethylamine)	103.17	3_REACH	17833.33333	17833.33333	0	17833.3333	0.17285387			1	0.03	2.9078E-07			1	0.03	2.90782E-07
111-41-1	111411	1547	2-(2-aminoethylamino)ethanol	104.16	3_REACH			1	0.3	2.8802E-06			1	0.03	2.8802E-07			1	0.03	2.88018E-07
111-42-2	111422	300	2,2'-iminodiethanol	105.14	3_REACH	716.6666667	716.6666667	0	716.666667	0.00681631	3200	3200	0	3200	0.03043561	3200	3200	0	3200	0.03043561
111-44-4	111444	301	bis(2-chloroethyl) ether	143.01	3_REACH	80000	80000	0	80000	0.55940144			1	0.03	2.0978E-07			1	0.03	2.09776E-07
111-46-6	111466	302	2,2'-oxydiethanol	106.12	3_REACH	3333333.333	3333333.333	0	3333333.33	31.4109813			1	0.03	2.827E-07			1	0.03	2.82699E-07
111-64-8	111648	1551	octanoyl chloride	162.66	3_REACH			1	0.3	1.8443E-06			1	0.03	1.8443E-07			1	0.03	1.84434E-07
111-69-3	111693	307	adiponitrile	108.15	3_REACH	148333.3333	148333.3333	0	148333.333	1.37155186			1	0.03	2.7739E-07			1	0.03	2.77393E-07
111-70-6	111706	308	heptan-1-ol	116.2	3_REACH	16333.33333	16333.33333	0	16333.3333	0.14056225			1	0.03	2.5818E-07			1	0.03	2.58176E-07
1117-31-3	1117313	1555	1,3-butylene diacetate	174.2	3_REACH			1	0.3	1.7222E-06			1	0.03	1.7222E-07			1	0.03	1.72216E-07
111-75-1	111751	1556	2-butylaminoethanol	117.19	3_REACH			1	0.3	2.5599E-06			1	0.03	2.5599E-07			1	0.03	2.55995E-07
111-76-2	111762	309	2-butoxyethanol	118.18	3_REACH	573333.3333	573333.3333	0	573333.333	4.85135669			1	0.03	2.5385E-07			1	0.03	2.5385E-07
111-77-3	111773	310	2-(2-methoxyethoxy)ethanol	120.15	3_REACH	930000	930000	0	930000	7.74032459			1	0.03	2.4969E-07			1	0.03	2.49688E-07
1117-86-8	1117868	1557	octane-1,2-diol	146.23	3_REACH			1	0.3	2.0516E-06			1	0.03	2.0516E-07			1	0.03	2.05156E-07
111-81-9	111819	1558	methyl undec-10-enoate	198.31	3_REACH			1	0.3	1.5128E-06			1	0.03	1.5128E-07			1	0.03	1.51278E-07
111-82-0	111820	1559	methyl laurate	214.35	3_REACH			1	0.3	1.3996E-06			1	0.03	1.3996E-07			1	0.03	1.39958E-07
111-85-3	111853	1561	1-chlorooctane	148.68	3_REACH			1	0.3	2.0178E-06			1	0.03	2.0178E-07			1	0.03	2.01776E-07
111-86-4	111864	313	octylamine	129.25	3_REACH			1	0.3	2.3211E-06			1	0.03	2.3211E-07			1	0.03	2.32108E-07
111-87-5	111875	314	octan-1-ol	130.23	3_REACH	6666.666667	6666.666667	0	6666.66667	0.05119148	1000	1000	0	1000	0.00767872	1000	1000	0	1000	0.007678722
111-88-6	111886	1563	octane-1-thiol	146.3	3_REACH			1	0.3	2.0506E-06			1	0.03	2.0506E-07			1	0.03	2.05058E-07
111-90-0	111900	315	2-(2-ethoxyethoxy)ethanol	134.18	3_REACH	1113333.333	1113333.333	0	1113333.33	8.29731207			1	0.03	2.2358E-07			1	0.03	2.2358E-07
111-91-1	111911	316	bis(2-chloroethoxy)methane	173.04	3_REACH	67000	67000	0	67000	0.38719371			1	0.03	1.7337E-07			1	0.03	1.7337E-07
111-92-2	111922	317	dibutylamine	129.25	3_REACH	53333.33333	53333.33333	0	53333.3333	0.41263701			1	0.03	2.3211E-07			1	0.03	2.32108E-07
1120-21-4	1120214	1567	undecane	156.31	3_REACH			1	0.3	1.9193E-06			1	0.03	1.9193E-07			1	0.03	1.91926E-07
1120-24-7	1120247	1568	decyldimethylamine	185.36	3_REACH			1	0.3	1.6185E-06			1	0.03	1.6185E-07			1	0.03	1.61847E-07
112-02-7	112027	7	cetrimonium chloride	320.01	3_REACH	3.333333333	3.333333333	0	3.33333333	1.0416E-05			1	0.03	9.3747E-08			1	0.03	9.37471E-08
1120-36-1	1120361	1569	tetradec-1-ene	196.38	3_REACH			1	0.3	1.5277E-06			1	0.03	1.5277E-07			1	0.03	1.52765E-07
112-05-0	112050	320	nonanoic acid	158.24	3_REACH	39000	39000	0	39000	0.24646107			1	0.03	1.8959E-07			1	0.03	1.89585E-07
1120-71-4	1120714	1572	1,3-propanesultone	122.14	3_REACH			1	0.3	2.4562E-06			1	0.03	2.4562E-07			1	0.03	2.4562E-07
112-07-2	112072	1573	2-butoxyethyl acetate	160.21	3_REACH			1	0.3	1.8725E-06			1	0.03	1.8725E-07			1	0.03	1.87254E-07
112-15-2	112152	1577	2-(2-ethoxyethoxy)ethyl acetate	176.21	3_REACH			1	0.3	1.7025E-06			1	0.03	1.7025E-07			1	0.03	1.70251E-07
112-16-3	112163	1578	lauroyl chloride	218.77	3_REACH			1	0.3	1.3713E-06			1	0.03	1.3713E-07			1	0.03	1.3713E-07
112-18-5	112185	321	dodecyldimethylamine	213.41	3_REACH			1	0.3	1.4057E-06			1	0.03	1.4057E-07			1	0.03	1.40574E-07
112-25-4	112254	1580	2-hexyloxyethanol	146.23	3_REACH			1	0.3	2.0516E-06			1	0.03	2.0516E-07			1	0.03	2.05156E-07
112-27-6	112276	322	2,2'-(ethylenedioxy)diethanol	150.17	3_REACH	17466.66667	17466.66667	0	17466.6667	0.11631262			1	0.03	1.9977E-07			1	0.03	1.99774E-07
112-29-8	112298	324	1-bromodecane	221.19	3_REACH	24.66666667	24.66666667	0	24.6666667	0.00011152			1	0.03	1.3563E-07			1	0.03	1.3563E-07
112-30-1	112301	325	decan-1-ol	158.29	3_REACH	2800	2800	0	2800	0.01768905	110	110	0	110	0.00069493	210	210	0	210	0.001326679
112-31-2	112312	1581	decanal	156.27	3_REACH			1	0.3	1.9198E-06			1	0.03	1.9198E-07			1	0.03	1.91975E-07
112-33-4	112334	1583	2-[2-(3-aminopropoxy)ethoxy]ethanol	163.22	3_REACH			1	0.3	1.838E-06			1	0.03	1.838E-07			1	0.03	1.83801E-07
112-34-5	112345	326	2-(2-butoxyethoxy)ethanol	162.23	3_REACH	950000	950000	0	950000	5.85588362			1	0.03	1.8492E-07			1	0.03	1.84923E-07
112-35-6	112356	1584	2-(2-(2-methoxyethoxy)ethoxy)ethanol	164.2	3_REACH			1	0.3	1.827E-06			1	0.03	1.827E-07			1	0.03	1.82704E-07
112-36-7	112367	327	bis(2-ethoxyethyl) ether	162.23	3_REACH			1	0.3	1.8492E-06			1	0.03	1.8492E-07			1	0.03	1.84923E-07
112-38-9	112389	1585	undec-10-enoic acid	184.28	3_REACH			1	0.3	1.628E-06			1	0.03	1.628E-07			1	0.03	1.62796E-07
112-40-3	112403	1587	dodecane	170.34	3_REACH			1	0.3	1.7612E-06			1	0.03	1.7612E-07			1	0.03	1.76118E-07
112-41-4	112414	1588	dodec-1-ene	168.32	3_REACH			1	0.3	1.7823E-06			1	0.03	1.7823E-07			1	0.03	1.78232E-07
112-42-5	112425	329	undecan-1-ol	172.31	3_REACH			1	0.3	1.741E-06			1	0.03	1.741E-07			1	0.03	1.74105E-07
112-44-7	112447	1589	undecanal	170.3	3_REACH			1	0.3	1.7616E-06			1	0.03	1.7616E-07			1	0.03	1.7616E-07
112-45-8	112458	1590	undec-10-enal	168.28	3_REACH			1	0.3	1.7827E-06			1	0.03	1.7827E-07			1	0.03	1.78274E-07
112-49-2	112492	330	1,2-bis(2-methoxyethoxy)ethane	178.23	3_REACH			1	0.3	1.6832E-06			1	0.03	1.6832E-07			1	0.03	1.68322E-07
112-50-5	112505	331	2-(2-(2-ethoxyethoxy)ethoxy)ethanol	178.23	3_REACH			1	0.3	1.6832E-06			1	0.03	1.6832E-07			1	0.03	1.68322E-07
112-53-8	112538	332	dodecan-1-ol	186.34	3_REACH			1	0.3	1.61E-06			1	0.03	1.61E-07			1	0.03	1.60996E-07
112-54-9	112549	333	dodecanal	184.32	3_REACH			1	0.3	1.6276E-06			1	0.03	1.6276E-07			1	0.03	1.6276E-07
112-55-0	112550	1592	dodecane-1-thiol	202.4	3_REACH			1	0.3	1.4822E-06			1	0.03	1.4822E-07			1	0.03	1.48221E-07
112-59-4	112594	1593	2-(2-hexyloxyethoxy)ethanol	190.28	3_REACH			1	0.3	1.5766E-06			1	0.03	1.5766E-07			1	0.03	1.57662E-07
112-67-4	112674	1597	palmitoyl chloride	274.88	3_REACH			1	0.3	1.0914E-06			1	0.03	1.0914E-07			1	0.03	1.09139E-07
112-69-6	112696	1598	hexadecyldimethylamine	269.52	3_REACH			1	0.3	1.1131E-06			1	0.03	1.1131E-07			1	0.03	1.11309E-07
112-72-1	112721	1599	tetradecanol	214.39	3_REACH			1	0.3	1.3993E-06			1	0.03	1.3993E-07			1	0.03	1.39932E-07
112-73-2	112732	1600	bis(2-butoxyethyl) ether	218.34	3_REACH			1	0.3	1.374E-06			1	0.03	1.374E-07			1	0.03	1.374E-07
112-75-4	112754	1601	dimethyl(tetradecyl)amine	241.46	3_REACH			1	0.3	1.2424E-06			1	0.03	1.2424E-07			1	0.03	1.24244E-07
112-76-5	112765	1602	stearoyl chloride	302.93	3_REACH			1	0.3	9.9033E-07			1	0.03	9.9033E-08			1	0.03	9.90328E-08
112-85-6	112856	1608	docosanoic acid	340.59	3_REACH			1	0.3	8.8082E-07			1	0.03	8.8082E-08			1	0.03	8.80824E-08
112-88-9	112889	1609	octadec-1-ene	252.49	3_REACH			1	0.3	1.1882E-06			1	0.03	1.1882E-07			1	0.03	1.18817E-07
112-92-5	112925	1611	octadecan-1-ol	270.5	3_REACH			1	0.3	1.1091E-06			1	0.03	1.1091E-07			1	0.03	1.10906E-07
1134-94-7	1134947	4363	2-Phenylsulfanylaniline	201.29	3_REACH			1	0.3	1.4904E-06			1	0.03	1.4904E-07			1	0.03	1.49039E-07
114772-54-2	114772542	1625	4'-(Bromomethyl)-2-cyanobiphenyl	272.15	3_REACH			1	0.3	1.1023E-06			1	0.03	1.1023E-07			1	0.03	1.10233E-07
115-27-5	115275	1635	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	370.83	3_REACH			1	0.3	8.09E-07			1	0.03	8.09E-08			1	0.03	8.08996E-08
1154308-86-7	1154308867	1636	N-(2-Hydroxyethyl)-3,5,5-trimethylhexanamide	201.31	3_REACH			1	0.3	1.4902E-06			1	0.03	1.4902E-07			1	0.03	1.49024E-07
115-70-8	115708	1638	2-amino-2-ethylpropanediol	119.17	3_REACH			1	0.3	2.5174E-06			1	0.03	2.5174E-07			1	0.03	2.51741E-07
115-77-5	115775	341	pentaerythritol	136.15	3_REACH	12966666.67	12966666.67	0	12966666.7	95.2380952			1	0.03	2.2035E-07			1	0.03	2.20345E-07
115-86-6	115866	9	triphenyl phosphate	326.29	3_REACH	333.3333333	333.3333333	0	333.333333	0.00102159			1	0.03	9.1943E-08			1	0.03	9.19428E-08
115-95-7	115957	1640	linalyl acetate	196.29	3_REACH			1	0.3	1.5284E-06			1	0.03	1.5284E-07			1	0.03	1.52835E-07
115-96-8	115968	10	tris(2-chloroethyl) phosphate	285.49	3_REACH	100000	100000	0	100000	0.35027497	10	10	0	10	3.5027E-05	10	10	0	10	3.50275E-05
116-37-0	116370	1648	1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol	344.45	3_REACH			1	0.3	8.7095E-07			1	0.03	8.7095E-08			1	0.03	8.70954E-08

116539-55-0	116539550	1651	(1S)-3-(methylamino)-1-(2-thienyl)propan-1-ol	171.26	3_REACH			1	0.3	1.7517E-06			1	0.03	1.7517E-07			1	0.03	1.75172E-07
116-75-6	116756	1653	1,4-bis(mesitylamino)anthraquinone	474.61	3_REACH			1	0.3	6.321E-07			1	0.03	6.321E-08			1	0.03	6.32098E-08
117-08-8	117088	1655	tetrachlorophthalic anhydride	285.9	3_REACH			1	0.3	1.0493E-06			1	0.03	1.0493E-07			1	0.03	1.04932E-07
117-21-5	117215	1657	3-chlorophthalic anhydride	182.56	3_REACH			1	0.3	1.6433E-06			1	0.03	1.6433E-07			1	0.03	1.6433E-07
117-61-3	117613	1661	benzidine-2,2'-disulphonic acid	344.37	3_REACH			1	0.3	8.7116E-07			1	0.03	8.7116E-08			1	0.03	8.71156E-08
117-81-7	117817	346	bis(2-ethylhexyl) phthalate	390.56	3_REACH	44.33333333	44.33333333	0	44.3333333	0.00011351	77	77	0	77	0.00019715			1	0.03	7.68128E-08
118135-28-7	118135287	1666	8-tert-Butyl-2-(chloromethyl)-1,4-dioxaspiro[4.5]decane	246.78	3_REACH			1	0.3	1.2157E-06			1	0.03	1.2157E-07			1	0.03	1.21566E-07
118-45-6	118456	1670	4-chlorophthalic anhydride	182.56	3_REACH			1	0.3	1.6433E-06			1	0.03	1.6433E-07			1	0.03	1.6433E-07
118-48-9	118489	1671	4H-3,1-benzoxazine-2,4(1H)-dione	163.13	3_REACH			1	0.3	1.839E-06			1	0.03	1.839E-07			1	0.03	1.83902E-07
118-58-1	118581	1674	benzyl salicylate	228.25	3_REACH			1	0.3	1.3143E-06			1	0.03	1.3143E-07			1	0.03	1.31435E-07
118-60-5	118605	1675	2-ethylhexyl salicylate	250.34	3_REACH			1	0.3	1.1984E-06			1	0.03	1.1984E-07			1	0.03	1.19837E-07
118-69-4	118694	1676	2,6-dichlorotoluene	161.03	3_REACH			1	0.3	1.863E-06			1	0.03	1.863E-07			1	0.03	1.86301E-07
118-75-2	118752	1677	tetrachloro-p-benzoquinone	245.88	3_REACH			1	0.3	1.2201E-06			1	0.03	1.2201E-07			1	0.03	1.22011E-07
118-79-6	118796	348	2,4,6-tribromophenol	330.82	3_REACH			1	0.3	9.0684E-07			1	0.03	9.0684E-08			1	0.03	9.06838E-08
118-82-1	118821	1679	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	424.67	3_REACH			1	0.3	7.0643E-07			1	0.03	7.0643E-08			1	0.03	7.06431E-08
1189-08-8	1189088	1682	1-methyltrimethylene dimethacrylate	226.27	3_REACH			1	0.3	1.3258E-06			1	0.03	1.3258E-07			1	0.03	1.32585E-07
118-92-3	118923	1683	anthranilic acid	137.14	3_REACH			1	0.3	2.1875E-06			1	0.03	2.1875E-07			1	0.03	2.18755E-07
118-96-7	118967	349	2,4,6-trinitrotoluene	227.13	3_REACH	326.6666667	326.6666667	0	326.666667	0.00143824	480	480	0	480	0.00211333	480	480	0	480	0.002113327
119-17-5	119175	1686	m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphonic acid	254.27	3_REACH			1	0.3	1.1798E-06			1	0.03	1.1798E-07			1	0.03	1.17985E-07
119313-12-1	119313121	4343	2-benzyl-2-dimethylamino-4-morpholinobutyrophenone	366.51	3_REACH			1	0.3	8.1853E-07			1	0.03	8.1853E-08			1	0.03	8.18532E-08
119462-56-5	119462565	4277	1,3-bis(3-methyl-2,5-dioxo-1H-pyrrolinylmethyl)benzene	324.34	3_REACH			1	0.3	9.2496E-07			1	0.03	9.2496E-08			1	0.03	9.24955E-08
119-53-9	119539	1694	benzoin	212.25	3_REACH			1	0.3	1.4134E-06			1	0.03	1.4134E-07			1	0.03	1.41343E-07
119-61-9	119619	354	benzophenone	182.22	3_REACH	93.33333333	93.33333333	0	93.3333333	0.0005122			1	0.03	1.6464E-07			1	0.03	1.64636E-07
119-64-2	119642	355	1,2,3,4-tetrahydronaphthalene	132.21	3_REACH	804	804	0	804	0.00608123			1	0.03	2.2691E-07			1	0.03	2.26912E-07
119-65-3	119653	356	isoquinoline	129.16	3_REACH	8366.666667	8366.666667	0	8366.66667	0.06477754			1	0.03	2.3227E-07			1	0.03	2.3227E-07
119-80-2	119802	357	2,2'-dithiodi(benzoic acid)	306.36	3_REACH			1	0.3	9.7924E-07			1	0.03	9.7924E-08			1	0.03	9.7924E-08
119851-28-4	119851284	1700	1-[2-Chloro-4-(4-chlorophenoxy)phenyl]ethanone	281.14	3_REACH			1	0.3	1.0671E-06			1	0.03	1.0671E-07			1	0.03	1.06708E-07
120068-79-3	120068793	4457	PYRAZOLE MB 45897	321.09	3_REACH			1	0.3	9.3432E-07			1	0.03	9.3432E-08			1	0.03	9.34317E-08
120100-77-8	120100778	1704	2-Chloro-4-(methylsulfonyl)-3-[(2,2,2-trifluoroethoxy)methyl]benzoic acid	346.71	3_REACH			1	0.3	8.6528E-07			1	0.03	8.6528E-08			1	0.03	8.65276E-08
120-12-7	120127	358	anthracene	178.23	3_REACH	31.66666667	31.66666667	0	31.6666667	0.00017767			1	0.03	1.6832E-07			1	0.03	1.68322E-07
120-18-3	120183	12	naphthalene-2-sulphonic acid	208.24	3_REACH			1	0.3	1.4406E-06			1	0.03	1.4406E-07			1	0.03	1.44065E-07
120298-38-6	120298386	4257	(S,S)-trans-4-(acetylamino)-5,6-dihydro-6-methyl-7,7-dioxo-4H-thieno[2,3-b]thiopyran-2-sulfonamide	338.43	3_REACH			1	0.3	8.8645E-07			1	0.03	8.8645E-08			1	0.03	8.86446E-08
120-40-1	120401	13	N,N-bis(2-hydroxyethyl)dodecanamide	287.44	3_REACH			1	0.3	1.0437E-06			1	0.03	1.0437E-07			1	0.03	1.0437E-07
120-46-7	120467	1712	1,3-diphenylpropane-1,3-dione	224.26	3_REACH			1	0.3	1.3377E-06			1	0.03	1.3377E-07			1	0.03	1.33773E-07
120-47-8	120478	14	ethyl 4-hydroxybenzoate	166.18	3_REACH			1	0.3	1.8053E-06			1	0.03	1.8053E-07			1	0.03	1.80527E-07
120-55-8	120558	1714	oxydiethylene dibenzoate	314.34	3_REACH			1	0.3	9.5438E-07			1	0.03	9.5438E-08			1	0.03	9.54381E-08
120-57-0	120570	1715	piperonal	150.13	3_REACH			1	0.3	1.9983E-06			1	0.03	1.9983E-07			1	0.03	1.99827E-07
120570-77-6	120570776	1716	2-(2-Formyloxyethoxy)ethyl formate	162.14	3_REACH			1	0.3	1.8503E-06			1	0.03	1.8503E-07			1	0.03	1.85025E-07
120578-03-2	120578032	4461	3-(2-(7-Chloroquinolin-2-yl)vinyl)benzaldehyde	293.75	3_REACH			1	0.3	1.0213E-06			1	0.03	1.0213E-07			1	0.03	1.02128E-07
120-61-6	120616	1717	dimethyl terephthalate	194.19	3_REACH			1	0.3	1.5449E-06			1	0.03	1.5449E-07			1	0.03	1.54488E-07
120-78-5	120785	360	di(benzothiazol-2-yl) disulphide	332.49	3_REACH			1	0.3	9.0228E-07			1	0.03	9.0228E-08			1	0.03	9.02283E-08
120-80-9	120809	361	pyrocatechol	110.11	3_REACH			1	0.3	2.7245E-06			1	0.03	2.7245E-07			1	0.03	2.72455E-07
120-82-1	120821	362	1,2,4-trichlorobenzene	181.45	3_REACH	400	400	0	400	0.00220446	60	60	0	60	0.00033067			1	0.03	1.65335E-07
120-83-2	120832	363	2,4-dichlorophenol	163	3_REACH	0.87	0.87	0	0.87	5.3374E-06	210	210	0	210	0.00128834	210	210	0	210	0.001288344
120-93-4	120934	367	2-imidazolidone	86.096	3_REACH	1866666.667	1866666.667	0	1866666.67	21.6812241			1	0.03	3.4845E-07			1	0.03	3.48448E-07
121219-07-6	121219076	4298	1-Ethoxy-2,3-Difluorobenzene	158.15	3_REACH			1	0.3	1.8969E-06			1	0.03	1.8969E-07			1	0.03	1.89693E-07
121-32-4	121324	368	3-ethoxy-4-hydroxybenzaldehyde	166.18	3_REACH			1	0.3	1.8053E-06			1	0.03	1.8053E-07			1	0.03	1.80527E-07
121-33-5	121335	369	vanillin	152.15	3_REACH			1	0.3	1.9717E-06			1	0.03	1.9717E-07			1	0.03	1.97174E-07
121-57-3	121573	372	sulphanilic acid	173.19	3_REACH			1	0.3	1.7322E-06			1	0.03	1.7322E-07			1	0.03	1.7322E-07
121-60-8	121608	1730	N-acetylsulphanilyl chloride	233.67	3_REACH			1	0.3	1.2839E-06			1	0.03	1.2839E-07			1	0.03	1.28386E-07
121-69-7	121697	373	N,N-dimethylaniline	121.18	3_REACH	5500	5500	0	5500	0.04538703			1	0.03	2.4757E-07			1	0.03	2.47566E-07
121-82-4	121824	375	perhydro-1,3,5-trinitro-1,3,5-triazine	222.12	3_REACH	5000	5000	0	5000	0.02251035			1	0.03	1.3506E-07			1	0.03	1.35062E-07
121-86-8	121868	376	2-chloro-4-nitrotoluene	171.58	3_REACH	1333.333333	1333.333333	0	1333.33333	0.00777091			1	0.03	1.7485E-07			1	0.03	1.74846E-07
121-91-5	121915	1739	isophthalic acid	166.13	3_REACH			1	0.3	1.8058E-06			1	0.03	1.8058E-07			1	0.03	1.80581E-07
122-00-9	122009	1740	4'-methylacetophenone	134.18	3_REACH			1	0.3	2.2358E-06			1	0.03	2.2358E-07			1	0.03	2.2358E-07
122-01-0	122010	1741	4-chlorobenzoyl chloride	175.01	3_REACH			1	0.3	1.7142E-06			1	0.03	1.7142E-07			1	0.03	1.71419E-07
122-03-2	122032	377	4-isopropylbenzaldehyde	148.21	3_REACH			1	0.3	2.0242E-06			1	0.03	2.0242E-07			1	0.03	2.02415E-07
122-20-3	122203	1743	1,1',1''-nitrilotripropan-2-ol	191.27	3_REACH			1	0.3	1.5685E-06			1	0.03	1.5685E-07			1	0.03	1.56846E-07
12225-08-0	12225080	1744	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2,5-dimethoxy-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide	576.59	3_REACH			1	0.3	5.203E-07			1	0.03	5.203E-08			1	0.03	5.203E-08
12225-18-2	12225182	1745	N-(4-chloro-2,5-dimethoxyphenyl)-2-[[2,5-dimethoxy-4-[(phenylamino)sulphonyl]phenyl]azo]-3-oxobutyramide	591.04	3_REACH			1	0.3	5.0758E-07			1	0.03	5.0758E-08			1	0.03	5.0758E-08
12236-62-3	12236623	1747	2-[(4-chloro-2-nitrophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide	416.79	3_REACH			1	0.3	7.1979E-07			1	0.03	7.1979E-08			1	0.03	7.19787E-08
12236-64-5	12236645	1748	N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxynaphthalene-2-carboxamide	501.94	3_REACH			1	0.3	5.9768E-07			1	0.03	5.9768E-08			1	0.03	5.97681E-08
122-39-4	122394	379	diphenylamine	169.23	3_REACH	46.66666667	46.66666667	0	46.6666667	0.00027576	160	160	0	160	0.00094546			1	0.03	1.77274E-07
122-52-1	122521	1751	triethyl phosphite	166.16	3_REACH			1	0.3	1.8055E-06			1	0.03	1.8055E-07			1	0.03	1.80549E-07
122-57-6	122576	1752	4-phenylbutenone	146.19	3_REACH			1	0.3	2.0521E-06			1	0.03	2.0521E-07			1	0.03	2.05212E-07
122-62-3	122623	1755	bis(2-ethylhexyl) sebacate	426.68	3_REACH			1	0.3	7.031E-07			1	0.03	7.031E-08			1	0.03	7.03103E-08
122-99-6	122996	384	2-phenoxyethanol	138.17	3_REACH			1	0.3	2.1712E-06			1	0.03	2.1712E-07			1	0.03	2.17124E-07
123-04-6	123046	1760	3-(chloromethyl)heptane	148.68	3_REACH			1	0.3	2.0178E-06			1	0.03	2.0178E-07			1	0.03	2.01776E-07
123-05-7	123057	1761	2-ethylhexanal	128.22	3_REACH			1	0.3	2.3397E-06			1	0.03	2.3397E-07			1	0.03	2.33973E-07
123-11-5	123115	1763	anisaldehyde	136.15	3_REACH			1	0.3	2.2035E-06			1	0.03	2.2035E-07			1	0.03	2.20345E-07
123-17-1	123171	1764	2,6,8-trimethylnonan-4-ol	186.34	3_REACH			1	0.3	1.61E-06			1	0.03	1.61E-07			1	0.03	1.60996E-07
123-30-8	123308	386	4-aminophenol	109.13	3_REACH	80	80	0	80	0.00073307			1	0.03	2.749E-07			1	0.03	2.74901E-07
123-31-9	123319	388	hydroquinone	110.11	3_REACH	30	30	0	30	0.00027245			1	0.03	2.7245E-07			1	0.03	2.72455E-07
123-39-7	123397	392	N-methylformamide	59.069	3_REACH			1	0.3	5.0788E-06			1	0.03	5.0788E-07			1	0.03	5.07881E-07
123-42-2	123422	393	4-hydroxy-4-methylpentan-2-one	116.16	3_REACH	2916666.667	2916666.667	0	2916666.67	25.109045			1	0.03	2.5826E-07			1	0.03	2.58264E-07
123-68-2	123682	1773	allyl hexanoate	156.22	3_REACH			1	0.3	1.9204E-06			1	0.03	1.9204E-07			1	0.03	1.92037E-07
123-77-3	123773	1775	C,C'-azodi(formamide)	116.08	3_REACH			1	0.3	2.5844E-06			1	0.03	2.5844E-07			1	0.03	2.58442E-07
1238449-42-7	1238449427	1776	bis(2-propylheptyl) carbonate	342.56	3_REACH			1	0.3	8.7576E-07			1	0.03	8.7576E-08			1	0.03	8.75759E-08
123-96-6	123966	399	octan-2-ol	130.23	3_REACH			1	0.3	2.3036E-06			1	0.03	2.3036E-07			1	0.03	2.30362E-07
124-04-9	124049	400	adipic acid	146.14	3_REACH			1	0.3	2.0528E-06			1	0.03	2.0528E-07			1	0.03	2.05283E-07
124-07-2	124072	401	octanoic acid	144.21	3_REACH			1	0.3	2.0803E-06			1	0.03	2.0803E-07			1	0.03	2.0803E-07
124-09-4	124094	1783	hexamethylenediamine	116.21	3_REACH			1	0.3	2.5815E-06			1	0.03	2.5815E-07			1	0.03	2.58153E-07
124-13-0	124130	1786	octanal	128.22	3_REACH			1	0.3	2.3397E-06			1	0.03	2.3397E-07			1	0.03	2.33973E-07
124-17-4	124174	1787	2-(2-butoxyethoxy)ethyl acetate	204.27	3_REACH			1	0.3	1.4686E-06			1	0.03	1.4686E-07			1	0.03	1.46864E-07
124-18-5	124185	402	decane	142.29	3_REACH	6000	6000	0	6000	0.0421674			1	0.03	2.1084E-07			1	0.03	2.10837E-07
1241-94-7	1241947	403	2-ethylhexyl diphenyl phosphate	362.41	3_REACH	50	50	0	50	0.00013797			1	0.03	8.2779E-08			1	0.03	8.27792E-08
124-19-6	124196	1788	nonanal	142.24	3_REACH			1	0.3	2.1091E-06			1	0.03	2.1091E-07			1	0.03	2.10911E-07
124-26-5	124265	1789	stearamide	283.5	3_REACH			1	0.3	1.0582E-06			1	0.03	1.0582E-07			1	0.03	1.0582E-07
124-28-7	124287	1790	dimantine	297.57	3_REACH			1	0.3	1.0082E-06			1	0.03	1.0082E-07			1	0.03	1.00817E-07
124-30-1	124301	1791	octadecylamine	269.52	3_REACH			1	0.3	1.1131E-06			1	0.03	1.1131E-07			1	0.03	1.11309E-07
124655-09-0	124655090	4568	tert-butyl2-[(4R,6S)-6-(hydroxymethyl)-2,2-dimethyl-1,3-dioxan-4-yl]acetate	260.33	3_REACH			1	0.3	1.1524E-06			1	0.03	1.1524E-07			1	0.03	1.15238E-07
125-12-2	125122	1796	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	196.29	3_REACH			1	0.3	1.5284E-06			1	0.03	1.5284E-07			1	0.03	1.52835E-07
12542-30-2	12542302	1797	hexahydro-4,7-methano-1H-indenyl acrylate	204.27	3_REACH			1	0.3	1.4686E-06			1	0.03	1.4686E-07			1	0.03	1.46864E-07
125971-57-5	125971575	1800	(2Z)-2-Benzylidene-4-methyl-3-oxo-N-phenylpentanamide	293.37	3_REACH			1	0.3	1.0226E-06			1	0.03	1.0226E-07			1	0.03	1.0226E-07
125971-96-2	125971962	4497	4-(4-F-PHENYL)-4-OXO-3-PHENYL-2-ISOBUTYRYL-N-PHENYLBUTANAMID	417.48	3_REACH			1	0.3	7.186E-07			1	0.03	7.186E-08			1	0.03	7.18597E-08
126-33-0	126330	406	tetrahydrothiophene 1,1-dioxide	120.17	3_REACH			1	0.3	2.4965E-06			1	0.03	2.4965E-07			1	0.03	2.49646E-07
126586-91-2	126586912	4597	N2-[1-(S)-ethoxycarbonyl-3-phenylpropyl]-N6-trifluoroacetyl-L-lysyl-N2-carboxy anhydride	414.43	3_REACH			1	0.3	7.2389E-07			1	0.03	7.2389E-08			1	0.03	7.23886E-08
126-71-6	126716	18	triisobutyl phosphate	266.32	3_REACH	5800	5800	0	5800	0.02177831			1	0.03	1.1265E-07			1	0.03	1.12646E-07
126-73-8	126738	19	tributyl phosphate	266.32	3_REACH	700	700	0	700	0.00262842	730	730	0	730	0.00274106	730	730	0	730	0.002741063
127-47-9	127479	1812	retinyl acetate	328.5	3_REACH			1	0.3	9.1324E-07			1	0.03	9.1324E-08			1	0.03	9.13242E-08
128-37-0	128370	413	2,6-di-tert-butyl-p-cresol	220.36	3_REACH	480	480	0	480	0.00217825			1	0.03	1.3614E-07			1	0.03	1.36141E-07
128-39-2	128392	1820	2,6-di-tert-butylphenol	206.33	3_REACH			1	0.3	1.454E-06			1	0.03	1.454E-07			1	0.03	1.45398E-07
128-69-8	128698	1822	perylene-3,4:9,10-tetracarboxylic dianhydride	392.32	3_REACH			1	0.3	7.6468E-07			1	0.03	7.6468E-08			1	0.03	7.64682E-08
129-00-0	129000	21	pyrene	202.26	3_REACH	341.3333333	341.3333333	0	341.333333	0.0016876			1	0.03	1.4832E-07			1	0.03	1.48324E-07
129909-90-6	129909906	415	Amicarbazone	241.3	3_REACH	25200	25200	0	25200	0.10443431	252	252	0	252	0.00104434	470	470	0	470	0.001947783
13048-33-4	13048334	1837	hexamethylene diacrylate	226.27	3_REACH			1	0.3	1.3258E-06			1	0.03	1.3258E-07			1	0.03	1.32585E-07
130755-46-3	130755463	1842	4,4'-dithiobis[5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1H-pyrazole]	704.3	3_REACH			1	0.3	4.2595E-07			1	0.03	4.2595E-08			1	0.03	4.25955E-08
13076-17-0	13076170	1843	Lactide, D-	144.13	3_REACH			1	0.3	2.0815E-06			1	0.03	2.0815E-07			1	0.03	2.08145E-07
130841-23-5	130841235	1844	Benzene,1,4-dichloro-2-(1,1,2,3,3,3-hexafluoropropoxy)-5-nitro-	358.02	3_REACH			1	0.3	8.3794E-07			1	0.03	8.3794E-08			1	0.03	8.37942E-08
131-11-3	131113	417	dimethyl phthalate	194.19	3_REACH	11000	11000	0	11000	0.05664555	9600	9600	0	9600	0.04943612			1	0.03	1.54488E-07
131-17-9	131179	418	diallyl phthalate	246.26	3_REACH	6666.666667	6666.666667	0	6666.66667	0.02707166	3200	3200	0	3200	0.0129944	3200	3200	0	3200	0.012994396
13122-18-4	13122184	1847	tert-butyl 3,5,5-trimethylperoxyhexanoate	230.35	3_REACH			1	0.3	1.3024E-06			1	0.03	1.3024E-07			1	0.03	1.30237E-07
13127-18-9	13127189	1848	Erythromycin oxime	748.95	3_REACH			1	0.3	4.0056E-07			1	0.03	4.0056E-08			1	0.03	4.00561E-08
1315251-11-6	1315251116	1849	7,7,8,9,9-pentamethyl-6,7,8,9-tetrahydro-5H-cyclopenta[h]quinazoline	242.37	3_REACH			1	0.3	1.2378E-06			1	0.03	1.2378E-07			1	0.03	1.23778E-07
131538-00-6	131538006	4321	2,3-bis((2-mercaptoethyl)thio)-1-propanethiol	260.52	3_REACH			1	0.3	1.1515E-06			1	0.03	1.1515E-07			1	0.03	1.15154E-07
131-56-6	131566	1850	2,4-dihydroxybenzophenone	214.22	3_REACH			1	0.3	1.4004E-06			1	0.03	1.4004E-07			1	0.03	1.40043E-07
131-57-7	131577	22	oxybenzone	228.25	3_REACH			1	0.3	1.3143E-06			1	0.03	1.3143E-07			1	0.03	1.31435E-07

13170-23-5	13170235	1851	diacetoxydi-tert-butoxysilane	292.4	3_REACH			1	0.3	1.026E-06			1	0.03	1.026E-07			1	0.03	1.02599E-07
132694-65-6	132694656	4685	4-[4-[(1-Oxo-2-propenyl)oxy]butoxy]benzoic acid 1,4-phenylene ester	602.64	3_REACH			1	0.3	4.9781E-07			1	0.03	4.9781E-08			1	0.03	4.9781E-08
1333-07-9	1333079	1866	toluenesulphonamide	171.22	3_REACH			1	0.3	1.7521E-06			1	0.03	1.7521E-07			1	0.03	1.75213E-07
133467-41-1	133467411	4415	4-[4-(2-ethylhexyloxy)phenyl](1,4	339.5	3_REACH			1	0.3	8.8365E-07			1	0.03	8.8365E-08			1	0.03	8.83652E-08
13361-34-7	13361347	1870	2-ethylhexyl cyanoacetate	197.28	3_REACH			1	0.3	1.5207E-06			1	0.03	1.5207E-07			1	0.03	1.52068E-07
133636-82-5	133636825	4540	Spiro[bicyclo[3.1.1]heptane-3,1'-[2]cyclohexen]-4'-one, 2,6,6-trimethyl-, (1S,1'S,2S,5R)-	218.34	3_REACH			1	0.3	1.374E-06			1	0.03	1.374E-07			1	0.03	1.374E-07
133-91-5	133915	1872	3,5-diiodosalicylic acid	389.91	3_REACH			1	0.3	7.6941E-07			1	0.03	7.6941E-08			1	0.03	7.69408E-08
13393-93-6	13393936	1873	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	292.51	3_REACH			1	0.3	1.0256E-06			1	0.03	1.0256E-07			1	0.03	1.02561E-07
13402-02-3	13402023	1875	hexadecyl acrylate	296.5	3_REACH			1	0.3	1.0118E-06			1	0.03	1.0118E-07			1	0.03	1.0118E-07
134605-64-4	134605644	433	1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl]benzoate	474.82	3_REACH	8600	8600	0	8600	0.01811213	9	9	0	9	1.8955E-05	36	36	0	36	7.58182E-05
134701-20-5	134701205	4329	2,4-dimethyl-6-(1-methylpentadecyl)phenol	346.6	3_REACH			1	0.3	8.6555E-07			1	0.03	8.6555E-08			1	0.03	8.65551E-08
13472-08-7	13472087	1882	2,2'-azobis[2-methylbutyronitrile]	192.27	3_REACH			1	0.3	1.5603E-06			1	0.03	1.5603E-07			1	0.03	1.56031E-07
13501-76-3	13501763	1885	(3-chloropropyl)diethoxymethylsilane	209.77	3_REACH			1	0.3	1.4301E-06			1	0.03	1.4301E-07			1	0.03	1.43014E-07
13515-40-7	13515407	1887	2-[(4-chloro-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide	390.79	3_REACH			1	0.3	7.6768E-07			1	0.03	7.6768E-08			1	0.03	7.67676E-08
135-19-3	135193	435	2-naphthol	144.17	3_REACH	1180	1180	0	1180	0.00818478			1	0.03	2.0809E-07			1	0.03	2.08088E-07
135590-91-9	135590919	436	1-(2,4-Dichlorophenyl)-4,5-dihydro-5-methyl-1H-pyrazole-3,5-dicarboxylic acid 3,5-diethyl ester	373.24	3_REACH	3970	3970	0	3970	0.01063659			1	0.03	8.0377E-08			1	0.03	8.03772E-08
136210-30-5	136210305	4527	1,4-diethyl 2-{[4-({4-[(1,4-diethoxy-1,4-dioxobutan-2-yl)amino]cyclohexyl}methyl)cyclohexyl]amino}butanedioate	554.73	3_REACH			1	0.3	5.408E-07			1	0.03	5.408E-08			1	0.03	5.40804E-08
136239-66-2	136239662	4294	1-butoxy-2,3-difluorobenzene	186.2	3_REACH			1	0.3	1.6112E-06			1	0.03	1.6112E-07			1	0.03	1.61117E-07
136465-81-1	136465811	4454	PHIO	238.38	3_REACH			1	0.3	1.2585E-06			1	0.03	1.2585E-07			1	0.03	1.25849E-07
1364731-90-7	1364731907	1900	2,6-dimethylphenyl 4-hydroxybenzenesulfonate	278.33	3_REACH			1	0.3	1.0779E-06			1	0.03	1.0779E-07			1	0.03	1.07786E-07
13674-84-5	13674845	24	tris(2-chloro-1-methylethyl) phosphate	327.57	3_REACH	33500	33500	0	33500	0.10226822	32000	32000	0	32000	0.09768904	32000	32000	0	32000	0.097689044
13674-87-8	13674878	25	tris[2-chloro-1-(chloromethyl)ethyl] phosphate	430.91	3_REACH	1600	1600	0	1600	0.00371307			1	0.03	6.962E-08			1	0.03	6.96201E-08
13749-61-6	13749616	1909	N-isopropylmethacrylamide	127.19	3_REACH			1	0.3	2.3587E-06			1	0.03	2.3587E-07			1	0.03	2.35868E-07
13752-51-7	13752517	1911	4-[(morpholinothio)thioxomethyl]morpholine	248.37	3_REACH			1	0.3	1.2079E-06			1	0.03	1.2079E-07			1	0.03	1.20788E-07
137863-20-8	137863208	1913	Valsartan benzyl ester	525.66	3_REACH			1	0.3	5.7071E-07			1	0.03	5.7071E-08			1	0.03	5.70711E-08
138564-59-7	138564597	4458	5-methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile	259.283	3_REACH			1	0.3	1.157E-06			1	0.03	1.157E-07			1	0.03	1.15704E-07
138-59-0	138590	445	(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid	174.15	3_REACH			1	0.3	1.7227E-06			1	0.03	1.7227E-07			1	0.03	1.72265E-07
139007-06-0	139007060	1915	(E)-2-Ethoxy-N-(2-methyl-1-phenylpropylidene)ethylamine	219.33	3_REACH			1	0.3	1.3678E-06			1	0.03	1.3678E-07			1	0.03	1.3678E-07
139122-17-1	139122171	4737	2-(3-chloro-2-oxo-2,3-dihydro-1H-indol-4-yl) ethyl benzoate	315.76	3_REACH			1	0.3	9.5009E-07			1	0.03	9.5009E-08			1	0.03	9.50089E-08
139-13-9	139139	27	nitrilotriacetic acid	191.14	3_REACH	26333.33333	26333.33333	0	26333.3333	0.13776987			1	0.03	1.5695E-07			1	0.03	1.56953E-07
139189-30-3	139189303	4566	Phosphoric acid, P,P'-1,3-phenylene P,P,P',P'-tetrakis(2,6-dimethylphenyl) ester	686.68	3_REACH			1	0.3	4.3688E-07			1	0.03	4.3688E-08			1	0.03	4.36885E-08
139504-68-0	139504680	4286	1-[(2-tert-butylcyclohexyl)oxy]butan-2-ol	228.38	3_REACH			1	0.3	1.3136E-06			1	0.03	1.3136E-07			1	0.03	1.3136E-07
140-11-4	140114	448	benzyl acetate	150.18	3_REACH			1	0.3	1.9976E-06			1	0.03	1.9976E-07			1	0.03	1.9976E-07
140-29-4	140294	1926	phenylacetonitrile	117.15	3_REACH			1	0.3	2.5608E-06			1	0.03	2.5608E-07			1	0.03	2.56082E-07
140-31-8	140318	449	2-piperazin-1-ylethylamine	129.21	3_REACH			1	0.3	2.3218E-06			1	0.03	2.3218E-07			1	0.03	2.3218E-07
14064-10-9	14064109	450	diethyl chloromalonate	194.61	3_REACH			1	0.3	1.5415E-06			1	0.03	1.5415E-07			1	0.03	1.54154E-07
140-66-9	140669	451	4-(1,1,3,3-tetramethylbutyl)phenol	206.33	3_REACH	3.666666667	3.666666667	0	3.66666667	1.7771E-05			1	0.03	1.454E-07			1	0.03	1.45398E-07
14073-97-3	14073973	1929	L-menthan-3-one	154.25	3_REACH			1	0.3	1.9449E-06			1	0.03	1.9449E-07			1	0.03	1.94489E-07
14078-41-2	14078412	1930	3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diol	358.48	3_REACH			1	0.3	8.3687E-07			1	0.03	8.3687E-08			1	0.03	8.36867E-08
141-05-9	141059	454	diethyl maleate	172.18	3_REACH			1	0.3	1.7424E-06			1	0.03	1.7424E-07			1	0.03	1.74236E-07
141-10-6	141106	1932	6,10-dimethylundeca-3,5,9-trien-2-one	192.3	3_REACH			1	0.3	1.5601E-06			1	0.03	1.5601E-07			1	0.03	1.56006E-07
141-17-3	141173	1933	bis(2-(2-butoxyethoxy)ethyl) adipate	434.57	3_REACH			1	0.3	6.9034E-07			1	0.03	6.9034E-08			1	0.03	6.90338E-08
141-18-4	141184	1934	bis(2-butoxyethyl) adipate	346.46	3_REACH			1	0.3	8.659E-07			1	0.03	8.659E-08			1	0.03	8.65901E-08
141-27-5	141275	1935	(E)-3,7-dimethylocta-2,6-dienal	152.24	3_REACH			1	0.3	1.9706E-06			1	0.03	1.9706E-07			1	0.03	1.97057E-07
141-62-8	141628	1939	decamethyltetrasiloxane	310.69	3_REACH			1	0.3	9.6559E-07			1	0.03	9.6559E-08			1	0.03	9.65593E-08
141-63-9	141639	1940	dodecamethylpentasiloxane	384.85	3_REACH			1	0.3	7.7952E-07			1	0.03	7.7952E-08			1	0.03	7.79524E-08
141-97-9	141979	459	ethyl acetoacetate	130.14	3_REACH	263333.3333	263333.3333	0	263333.333	2.02346191			1	0.03	2.3052E-07			1	0.03	2.30521E-07
141-98-0	141980	460	O-isopropyl ethylthiocarbamate	147.24	3_REACH			1	0.3	2.0375E-06			1	0.03	2.0375E-07			1	0.03	2.03749E-07
142-16-5	142165	1948	bis(2-ethylhexyl) maleate	340.5	3_REACH			1	0.3	8.8106E-07			1	0.03	8.8106E-08			1	0.03	8.81057E-08
142-19-8	142198	1950	allyl heptanoate	170.25	3_REACH			1	0.3	1.7621E-06			1	0.03	1.7621E-07			1	0.03	1.76211E-07
14246-53-8	14246538	1956	N-(1-oxooctyl)glycine	201.27	3_REACH			1	0.3	1.4905E-06			1	0.03	1.4905E-07			1	0.03	1.49054E-07
142-62-1	142621	462	hexanoic acid	116.16	3_REACH			1	0.3	2.5826E-06			1	0.03	2.5826E-07			1	0.03	2.58264E-07
142-90-5	142905	465	dodecyl methacrylate	254.41	3_REACH			1	0.3	1.1792E-06			1	0.03	1.1792E-07			1	0.03	1.1792E-07
142-91-6	142916	1957	isopropyl palmitate	298.51	3_REACH			1	0.3	1.005E-06			1	0.03	1.005E-07			1	0.03	1.00499E-07
142-92-7	142927	466	hexyl acetate	144.21	3_REACH			1	0.3	2.0803E-06			1	0.03	2.0803E-07			1	0.03	2.0803E-07
143-07-7	143077	468	lauric acid	200.32	3_REACH	11666.66667	11666.66667	0	11666.6667	0.05824015			1	0.03	1.4976E-07			1	0.03	1.4976E-07
143-08-8	143088	469	nonan-1-ol	144.26	3_REACH			1	0.3	2.0796E-06			1	0.03	2.0796E-07			1	0.03	2.07958E-07
143-22-6	143226	1959	2-(2-(2-butoxyethoxy)ethoxy)ethanol	206.28	3_REACH			1	0.3	1.4543E-06			1	0.03	1.4543E-07			1	0.03	1.45433E-07
143-24-8	143248	28	bis(2-(2-methoxyethoxy)ethyl) ether	222.28	3_REACH			1	0.3	1.3496E-06			1	0.03	1.3496E-07			1	0.03	1.34965E-07
143-28-2	143282	1962	(Z)-octadec-9-enol	268.49	3_REACH			1	0.3	1.1174E-06			1	0.03	1.1174E-07			1	0.03	1.11736E-07
14338-82-0	14338820	1965	dibutyl methylenedithiodi(acetate)	308.46	3_REACH			1	0.3	9.7257E-07			1	0.03	9.7257E-08			1	0.03	9.72573E-08
144-19-4	144194	1974	2,2,4-trimethylpentane-1,3-diol	146.23	3_REACH			1	0.3	2.0516E-06			1	0.03	2.0516E-07			1	0.03	2.05156E-07
14433-76-2	14433762	471	N,N-dimethyldecan-1-amide	199.34	3_REACH			1	0.3	1.505E-06			1	0.03	1.505E-07			1	0.03	1.50497E-07
144-62-7	144627	472	oxalic acid	90.034	3_REACH	45633.33333	45633.33333	0	45633.3333	0.50684556			1	0.03	3.3321E-07			1	0.03	3.33207E-07
144-83-2	144832	29	sulfapyridine	249.29	3_REACH			1	0.3	1.2034E-06			1	0.03	1.2034E-07			1	0.03	1.20342E-07
1453-58-3	1453583	1985	3-methylpyrazole	82.108	3_REACH			1	0.3	3.6537E-06			1	0.03	3.6537E-07			1	0.03	3.65372E-07
145783-14-8	145783148	1988	4,6-dichloro-5-nitro-2-(propylthio)pyrimidine	268.13	3_REACH			1	0.3	1.1189E-06			1	0.03	1.1189E-07			1	0.03	1.11886E-07
1459-93-4	1459934	1990	dimethyl isophthalate	194.19	3_REACH			1	0.3	1.5449E-06			1	0.03	1.5449E-07			1	0.03	1.54488E-07
146421-65-0	146421650	4455	URACROSS P 3307	400.52	3_REACH			1	0.3	7.4903E-07			1	0.03	7.4903E-08			1	0.03	7.49026E-08
14657-64-8	14657648	4379	3-(hydroxyphenylphosphinyl)propanoic acid	214.16	3_REACH			1	0.3	1.4008E-06			1	0.03	1.4008E-07			1	0.03	1.40082E-07
147315-50-2	147315502	4308	2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-((hexyl)oxy)phenol	425.54	3_REACH			1	0.3	7.0499E-07			1	0.03	7.0499E-08			1	0.03	7.04987E-08
147504-92-5	147504925	4409	4,6-bis[2-(4-hydroxyphenyl)isopropylidene]resorcinol	378.47	3_REACH			1	0.3	7.9267E-07			1	0.03	7.9267E-08			1	0.03	7.92665E-08
1477-55-0	1477550	1997	m-phenylenebis(methylamine)	136.2	3_REACH			1	0.3	2.2026E-06			1	0.03	2.2026E-07			1	0.03	2.20264E-07
147-85-3	147853	1999	L-proline	115.13	3_REACH			1	0.3	2.6058E-06			1	0.03	2.6058E-07			1	0.03	2.60575E-07
14814-09-6	14814096	2001	3-(triethoxysilyl)propanethiol	238.42	3_REACH			1	0.3	1.2583E-06			1	0.03	1.2583E-07			1	0.03	1.25828E-07
148528-05-6	148528056	2002	2-Methyloctane-1,8-diamine	158.29	3_REACH			1	0.3	1.8953E-06			1	0.03	1.8953E-07			1	0.03	1.89526E-07
14858-73-2	14858732	2004	bis(2-ethylhexyl) carbonate	286.46	3_REACH			1	0.3	1.0473E-06			1	0.03	1.0473E-07			1	0.03	1.04727E-07
14901-07-6	14901076	477	4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one	192.3	3_REACH			1	0.3	1.5601E-06			1	0.03	1.5601E-07			1	0.03	1.56006E-07
149-30-4	149304	478	benzothiazole-2-thiol	167.25	3_REACH			1	0.3	1.7937E-06			1	0.03	1.7937E-07			1	0.03	1.79372E-07
1493-13-6	1493136	2005	trifluoromethanesulphonic acid	150.07	3_REACH			1	0.3	1.9991E-06			1	0.03	1.9991E-07			1	0.03	1.99907E-07
149-57-5	149575	479	2-ethylhexanoic acid	144.21	3_REACH			1	0.3	2.0803E-06			1	0.03	2.0803E-07			1	0.03	2.0803E-07
149-74-6	149746	2006	dichloro(methyl)(phenyl)silane	191.13	3_REACH			1	0.3	1.5696E-06			1	0.03	1.5696E-07			1	0.03	1.56961E-07
149850-30-6	149850306	5029	methyl N-[3-acetylamino)-4-(2-cyano-4-nitrophenylazo)phenyl]-N-[(1-methoxy)acetyl]glycinate	468.43	3_REACH			1	0.3	6.4044E-07			1	0.03	6.4044E-08			1	0.03	6.40437E-08
150-76-5	150765	483	mequinol	124.14	3_REACH	2400	2400	0	2400	0.01933301			1	0.03	2.4166E-07			1	0.03	2.41663E-07
150-78-7	150787	484	1,4-dimethoxybenzene	138.17	3_REACH			1	0.3	2.1712E-06			1	0.03	2.1712E-07			1	0.03	2.17124E-07
150-84-5	150845	2012	citronellyl acetate	198.31	3_REACH			1	0.3	1.5128E-06			1	0.03	1.5128E-07			1	0.03	1.51278E-07
15214-89-8	15214898	2021	2-acrylamido-2-methylpropanesulphonic acid	207.25	3_REACH			1	0.3	1.4475E-06			1	0.03	1.4475E-07			1	0.03	1.44753E-07
152402-98-7	152402987	2023	2-[[(3-Methyl-4-nitro-pyridin-2-yl)methyl]sulfanyl]-1H-benzoimidazole	300.34	3_REACH			1	0.3	9.9887E-07			1	0.03	9.9887E-08			1	0.03	9.98868E-08
15267-95-5	15267955	2025	(chloromethyl)triethoxysilane	212.75	3_REACH			1	0.3	1.4101E-06			1	0.03	1.4101E-07			1	0.03	1.41011E-07
1530-32-1	1530321	2028	ethyltriphenylfosfonium bromide	371.26	3_REACH			1	0.3	8.0806E-07			1	0.03	8.0806E-08			1	0.03	8.08059E-08
15307-79-6	15307796	30	sodium [2-[(2,6-dichlorophenyl)amino]phenyl]acetate	318.14	3_REACH	10000	10000	0	10000	0.0314327	8300	8300	0	8300	0.02608914	8300	8300	0	8300	0.026089143
15356-60-2	15356602	486	(+)-menthol	156.27	3_REACH			1	0.3	1.9198E-06			1	0.03	1.9198E-07			1	0.03	1.91975E-07
153719-38-1	153719381	4548	N-nitro-N-(3-methyl-3,6-dihydro-2H-1,3,5-oxadiazin-4-yl)amine	160.14	3_REACH			1	0.3	1.8734E-06			1	0.03	1.8734E-07			1	0.03	1.87336E-07
15396-00-6	15396006	2033	3-(trimethoxysilyl)propyl isocyanate	205.29	3_REACH			1	0.3	1.4613E-06			1	0.03	1.4613E-07			1	0.03	1.46135E-07
154279-60-4	154279604	2034	4,4'-methylenebis(N-sec-butylcyclohexanamine)	322.58	3_REACH			1	0.3	9.3E-07			1	0.03	9.3E-08			1	0.03	9.30002E-08
15471-17-7	15471177	2039	1-(3-sulphonatopropyl)pyridinium	201.25	3_REACH			1	0.3	1.4907E-06			1	0.03	1.4907E-07			1	0.03	1.49068E-07
15520-10-2	15520102	2040	2-methylpentane-1,5-diamine	116.21	3_REACH			1	0.3	2.5815E-06			1	0.03	2.5815E-07			1	0.03	2.58153E-07
15625-89-5	15625895	2046	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	296.32	3_REACH			1	0.3	1.0124E-06			1	0.03	1.0124E-07			1	0.03	1.01242E-07
156-43-4	156434	2048	p-phenetidine	137.18	3_REACH			1	0.3	2.1869E-06			1	0.03	2.1869E-07			1	0.03	2.18691E-07
1570-64-5	1570645	495	4-chloro-o-cresol	142.59	3_REACH	96.66666667	96.66666667	0	96.6666667	0.00067793			1	0.03	2.1039E-07			1	0.03	2.10393E-07
15721-78-5	15721785	2055	bis(4-(1,1,3,3-tetramethylbutyl)phenyl)amine	393.66	3_REACH			1	0.3	7.6208E-07			1	0.03	7.6208E-08			1	0.03	7.62079E-08
15827-60-8	15827608	2059	[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid	573.2	3_REACH			1	0.3	5.2338E-07			1	0.03	5.2338E-08			1	0.03	5.23378E-08

15834-04-5	15834045	2060	2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate	472.62	3_REACH			1	0.3	6.3476E-07			1	0.03	6.3476E-08			1	0.03	6.34759E-08
15848-49-4	15848494	2062	Ethyl 2-(cyclopent-2-EN-1-YL)acetate	154.21	3_REACH			1	0.3	1.9454E-06			1	0.03	1.9454E-07			1	0.03	1.9454E-07
15894-70-9	15894709	2065	N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]	250.32	3_REACH			1	0.3	1.1985E-06			1	0.03	1.1985E-07			1	0.03	1.19847E-07
15993-42-7	15993427	2069	N-(5-chloro-2-methoxyphenyl)-2-[(2-methoxy-4-nitrophenyl)azo]-3-oxobutyramide	420.81	3_REACH			1	0.3	7.1291E-07			1	0.03	7.1291E-08			1	0.03	7.12911E-08
16111-62-9	16111629	2079	bis(2-ethylhexyl) peroxydicarbonate	346.46	3_REACH			1	0.3	8.659E-07			1	0.03	8.659E-08			1	0.03	8.65901E-08
161462-35-7	161462357	4456	1-cyclopropyl-3-(2-methylthio-4-trifluoromethylphenyl)-1,3-propanedione	302.31	3_REACH			1	0.3	9.9236E-07			1	0.03	9.9236E-08			1	0.03	9.92359E-08
16219-75-3	16219753	2083	5-ethylidene-8,9,10-trinorborn-2-ene	120.19	3_REACH			1	0.3	2.496E-06			1	0.03	2.496E-07			1	0.03	2.49605E-07
162208-27-7	162208277	4901	Diethyl thiophosphoril-(z)-(2 aminothiazol-4-yl)-(methoxyimino)acetate	353.36	3_REACH			1	0.3	8.4899E-07			1	0.03	8.4899E-08			1	0.03	8.48993E-08
16298-38-7	16298387	4407	4,4'-methylenebis(2-isopropyl-6-methylaniline)	310.49	3_REACH			1	0.3	9.6621E-07			1	0.03	9.6621E-08			1	0.03	9.66215E-08
16415-12-6	16415126	2092	hexadecyltrimethoxysilane	346.63	3_REACH			1	0.3	8.6548E-07			1	0.03	8.6548E-08			1	0.03	8.65476E-08
164578-11-4	164578114	4335	2,9-bis[N-[3-	696.9	3_REACH			1	0.3	4.3048E-07			1	0.03	4.3048E-08			1	0.03	4.30478E-08
165184-98-5	165184985	2096	alpha-Hexylcinnamaldehyde	216.32	3_REACH			1	0.3	1.3868E-06			1	0.03	1.3868E-07			1	0.03	1.38683E-07
16634-82-5	16634825	4584	2-Chloro-N-(4-methylphenyl)acetamide	183.64	3_REACH			1	0.3	1.6336E-06			1	0.03	1.6336E-07			1	0.03	1.63363E-07
166524-65-8	166524658	2105	2-ethoxy-4,6-	160.13	3_REACH			1	0.3	1.8735E-06			1	0.03	1.8735E-07			1	0.03	1.87348E-07
167004-78-6	167004786	2110	3-	261.26	3_REACH			1	0.3	1.1483E-06			1	0.03	1.1483E-07			1	0.03	1.14828E-07
16712-64-4	16712644	2111	6-hydroxy-2-naphthoic acid	188.18	3_REACH			1	0.3	1.5942E-06			1	0.03	1.5942E-07			1	0.03	1.59422E-07
1696-20-4	1696204	2118	4-acetylmorpholine	129.16	3_REACH			1	0.3	2.3227E-06			1	0.03	2.3227E-07			1	0.03	2.3227E-07
1704-62-7	1704627	2119	2-[2-(dimethylamino)ethoxy]ethanol	133.19	3_REACH			1	0.3	2.2524E-06			1	0.03	2.2524E-07			1	0.03	2.25242E-07
1709-70-2	1709702	2121	Tris-bht mesitylene	775.22	3_REACH			1	0.3	3.8699E-07			1	0.03	3.8699E-08			1	0.03	3.86987E-08
1724-39-6	1724396	2126	cyclododecanol	184.32	3_REACH			1	0.3	1.6276E-06			1	0.03	1.6276E-07			1	0.03	1.6276E-07
172529-93-0	172529930	2128	1,3-dimethyl 2-[2-(2-amino-6-chloro-9H-purin-9-yl)ethyl]propanedioate	327.73	3_REACH			1	0.3	9.1539E-07			1	0.03	9.1539E-08			1	0.03	9.15388E-08
1738-25-6	1738256	2132	3-dimethylaminopropiononitrile	98.151	3_REACH			1	0.3	3.0565E-06			1	0.03	3.0565E-07			1	0.03	3.05651E-07
173904-11-5	173904115	2133	N,N'-[cyclohexane-1,3-diylbis(methylene)]bis(2-methylpropan-1-imine)	250.43	3_REACH			1	0.3	1.1979E-06			1	0.03	1.1979E-07			1	0.03	1.19794E-07
1739-84-0	1739840	2135	1,2-dimethylimidazole	96.135	3_REACH			1	0.3	3.1206E-06			1	0.03	3.1206E-07			1	0.03	3.12061E-07
174489-43-1	174489431	2137	1-(allyloxy)-2-methyl-1-oxopropan-2-yl 5-amino-2-chlorobenzoate	297.74	3_REACH			1	0.3	1.0076E-06			1	0.03	1.0076E-07			1	0.03	1.00759E-07
174489-76-0	174489760	2138	1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-nitrobenzoate	327.72	3_REACH			1	0.3	9.1542E-07			1	0.03	9.1542E-08			1	0.03	9.15416E-08
1746-23-2	1746232	2139	p-tert-butylstyrene	160.26	3_REACH			1	0.3	1.872E-06			1	0.03	1.872E-07			1	0.03	1.87196E-07
1760-24-3	1760243	2145	N-(3-(trimethoxysilyl)propyl)ethylenediamine	222.36	3_REACH			1	0.3	1.3492E-06			1	0.03	1.3492E-07			1	0.03	1.34916E-07
17689-77-9	17689779	2148	triacetoxyethylsilane	234.28	3_REACH			1	0.3	1.2805E-06			1	0.03	1.2805E-07			1	0.03	1.28052E-07
176969-34-9	176969349	2150	3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid	176.12	3_REACH			1	0.3	1.7034E-06			1	0.03	1.7034E-07			1	0.03	1.70338E-07
17796-82-6	17796826	2153	N-(cyclohexylthio)phthalimide	261.34	3_REACH			1	0.3	1.1479E-06			1	0.03	1.1479E-07			1	0.03	1.14793E-07
17832-28-9	17832289	2154	4-(vinyloxy)butan-1-ol	116.16	3_REACH			1	0.3	2.5826E-06			1	0.03	2.5826E-07			1	0.03	2.58264E-07
17865-07-5	17865075	2155	propyltriacetoxysilane	248.31	3_REACH			1	0.3	1.2082E-06			1	0.03	1.2082E-07			1	0.03	1.20817E-07
17928-28-8	17928288	2158	1,1,1,3,5,5,5-heptamethyl-3[(trimethylsilyl)oxy]trisiloxane	310.69	3_REACH			1	0.3	9.6559E-07			1	0.03	9.6559E-08			1	0.03	9.65593E-08
18063-03-1	18063031	2163	2,6-difluorobenzamide	157.12	3_REACH			1	0.3	1.9094E-06			1	0.03	1.9094E-07			1	0.03	1.90937E-07
1809-19-4	1809194	2164	dibutyl phosphonate	194.21	3_REACH			1	0.3	1.5447E-06			1	0.03	1.5447E-07			1	0.03	1.54472E-07
18127-01-0	18127010	2166	3-(4-tert-butylphenyl)propionaldehyde	190.29	3_REACH			1	0.3	1.5765E-06			1	0.03	1.5765E-07			1	0.03	1.57654E-07
181587-01-9	181587019	4655	Ethiprole	397.21	3_REACH			1	0.3	7.5527E-07			1	0.03	7.5527E-08			1	0.03	7.55268E-08
18171-19-2	18171192	2172	(3-chloropropyl)dimethoxymethylsilane	182.72	3_REACH			1	0.3	1.6419E-06			1	0.03	1.6419E-07			1	0.03	1.64186E-07
18379-25-4	18379254	2187	trichloro(2,4,4-trimethylpentyl)silane	247.67	3_REACH			1	0.3	1.2113E-06			1	0.03	1.2113E-07			1	0.03	1.21129E-07
1843-03-4	1843034	2190	4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol]	544.82	3_REACH			1	0.3	5.5064E-07			1	0.03	5.5064E-08			1	0.03	5.50641E-08
18479-58-8	18479588	2192	2,6-dimethyloct-7-en-2-ol	156.27	3_REACH			1	0.3	1.9198E-06			1	0.03	1.9198E-07			1	0.03	1.91975E-07
1852-17-1	1852171	2196	perhydropyrimidin-2-one	100.12	3_REACH			1	0.3	2.9964E-06			1	0.03	2.9964E-07			1	0.03	2.9964E-07
18600-59-4	18600594	4312	2,2-(1,4-phenylene)bis((4H-3,1-benzoxazine-4-one)	368.35	3_REACH			1	0.3	8.1444E-07			1	0.03	8.1444E-08			1	0.03	8.14443E-08
1860-26-0	1860260	2200	2-ethyl-N,N-bis(2-ethylhexyl)hexylamine	353.68	3_REACH			1	0.3	8.4822E-07			1	0.03	8.4822E-08			1	0.03	8.48224E-08
186817-80-1	186817801	2203	Propanoic acid, 2-hydroxy-, 2-ethylhexyl ester, (2S)	202.29	3_REACH			1	0.3	1.483E-06			1	0.03	1.483E-07			1	0.03	1.48302E-07
1879-09-0	1879090	2209	6-tert-butyl-2,4-xylenol	178.28	3_REACH			1	0.3	1.6827E-06			1	0.03	1.6827E-07			1	0.03	1.68275E-07
18835-33-1	18835331	2210	hexacos-1-ene	364.7	3_REACH			1	0.3	8.2259E-07			1	0.03	8.2259E-08			1	0.03	8.22594E-08
18835-34-2	18835342	2211	octacos-1-ene	392.76	3_REACH			1	0.3	7.6383E-07			1	0.03	7.6383E-08			1	0.03	7.63825E-08
1889-67-4	1889674	2214	1,1'-(1,1,2,2-tetramethylethylene)dibenzene	238.37	3_REACH			1	0.3	1.2585E-06			1	0.03	1.2585E-07			1	0.03	1.25855E-07
19234-20-9	19234209	2228	2-(1-methylethoxy)ethyl acetate	146.19	3_REACH			1	0.3	2.0521E-06			1	0.03	2.0521E-07			1	0.03	2.05212E-07
19444-21-4	19444214	2233	allyl 2-hydroxy-2-methylpropanoate	144.17	3_REACH			1	0.3	2.0809E-06			1	0.03	2.0809E-07			1	0.03	2.08088E-07
1948-33-0	1948330	523	2-tert-butylhydroquinone	166.22	3_REACH			1	0.3	1.8048E-06			1	0.03	1.8048E-07			1	0.03	1.80484E-07
1955-46-0	1955460	2235	methyl 5-nitrohydrogen isophthalate	225.16	3_REACH			1	0.3	1.3324E-06			1	0.03	1.3324E-07			1	0.03	1.33239E-07
1962-75-0	1962750	525	dibutyl terephthalate	278.35	3_REACH			1	0.3	1.0778E-06			1	0.03	1.0778E-07			1	0.03	1.07778E-07
1975-78-6	1975786	2239	decanenitrile	153.27	3_REACH			1	0.3	1.9573E-06			1	0.03	1.9573E-07			1	0.03	1.95733E-07
1999-85-5	1999855	2247	alpha,alpha'-Dihydroxy-1,3-diisopropylbenzene	194.27	3_REACH			1	0.3	1.5442E-06			1	0.03	1.5442E-07			1	0.03	1.54424E-07
20030-30-2	20030302	2248	2,5,6-trimethylcyclohex-2-en-1-one	138.21	3_REACH			1	0.3	2.1706E-06			1	0.03	2.1706E-07			1	0.03	2.17061E-07
20120-33-6	20120336	2250	dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate	211.16	3_REACH			1	0.3	1.4207E-06			1	0.03	1.4207E-07			1	0.03	1.42072E-07
20292-08-4	20292084	2257	2-ethylhexyl laurate	312.54	3_REACH			1	0.3	9.5988E-07			1	0.03	9.5988E-08			1	0.03	9.59877E-08
20298-69-5	20298695	2258	cis-2-tert-butylcyclohexyl acetate	198.31	3_REACH			1	0.3	1.5128E-06			1	0.03	1.5128E-07			1	0.03	1.51278E-07
2031-67-6	2031676	2259	triethoxy(methyl)silane	178.3	3_REACH			1	0.3	1.6826E-06			1	0.03	1.6826E-07			1	0.03	1.68256E-07
2040-90-6	2040906	4576	2-chloro-6-fluoro-phenol	146.55	3_REACH			1	0.3	2.0471E-06			1	0.03	2.0471E-07			1	0.03	2.04708E-07
2044-64-6	2044646	2265	N,N-dimethyl-3-oxobutyramide	129.16	3_REACH			1	0.3	2.3227E-06			1	0.03	2.3227E-07			1	0.03	2.3227E-07
204918-22-9	204918229	2267	1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-isocyanatobenzoate	323.73	3_REACH			1	0.3	9.267E-07			1	0.03	9.267E-08			1	0.03	9.26698E-08
20592-85-2	20592852	2271	[nitrilotris(methylene)]trisphosphonic acid, sodium salt	299.05	3_REACH			1	0.3	1.0032E-06			1	0.03	1.0032E-07			1	0.03	1.00318E-07
20749-68-2	20749682	2272	8,9,10,11-tetrachloro-12H-phthaloperin-12-one	408.07	3_REACH			1	0.3	7.3517E-07			1	0.03	7.3517E-08			1	0.03	7.35168E-08
2082-81-7	2082817	2277	tetramethylene dimethacrylate	226.27	3_REACH			1	0.3	1.3258E-06			1	0.03	1.3258E-07			1	0.03	1.32585E-07
21282-97-3	21282973	2288	2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate	214.22	3_REACH			1	0.3	1.4004E-06			1	0.03	1.4004E-07			1	0.03	1.40043E-07
2135-17-3	2135173	532	flumetasone	410.46	3_REACH			1	0.3	7.3089E-07			1	0.03	7.3089E-08			1	0.03	7.30887E-08
2146-71-6	2146716	2295	vinyl laurate	226.36	3_REACH			1	0.3	1.3253E-06			1	0.03	1.3253E-07			1	0.03	1.32532E-07
21542-96-1	21542961	2298	N,N-dimethyldocosylamine	353.68	3_REACH			1	0.3	8.4822E-07			1	0.03	8.4822E-08			1	0.03	8.48224E-08
2156-97-0	2156970	533	dodecyl acrylate	240.39	3_REACH			1	0.3	1.248E-06			1	0.03	1.248E-07			1	0.03	1.24797E-07
2162-73-4	2162734	2299	2,4,6-triisopropyl-m-phenylene diisocyanate	286.38	3_REACH			1	0.3	1.0476E-06			1	0.03	1.0476E-07			1	0.03	1.04756E-07
2162-74-5	2162745	2300	bis(2,6-diisopropylphenyl)carbodiimide	362.56	3_REACH			1	0.3	8.2745E-07			1	0.03	8.2745E-08			1	0.03	8.27449E-08
2163-00-0	2163000	2301	1,6-dichlorohexane	155.07	3_REACH			1	0.3	1.9346E-06			1	0.03	1.9346E-07			1	0.03	1.93461E-07
2163-42-0	2163420	4357	2-methyl-1,3-propanediol	90.122	3_REACH			1	0.3	3.3288E-06			1	0.03	3.3288E-07			1	0.03	3.32882E-07
21643-42-5	21643425	2302	tetradecyl acrylate	268.44	3_REACH			1	0.3	1.1176E-06			1	0.03	1.1176E-07			1	0.03	1.11757E-07
21743-27-1	21743271	4770	4-((Triethoxysilyl)methyl)morpholine	263.41	3_REACH			1	0.3	1.1389E-06			1	0.03	1.1389E-07			1	0.03	1.13891E-07
2186-92-7	2186927	2308	p-(dimethoxymethyl)anisole	182.22	3_REACH			1	0.3	1.6464E-06			1	0.03	1.6464E-07			1	0.03	1.64636E-07
22047-49-0	22047490	2316	2-ethylhexyl stearate	396.7	3_REACH			1	0.3	7.5624E-07			1	0.03	7.5624E-08			1	0.03	7.56239E-08
220727-26-4	220727264	4596	S-(3-(triethoxysilyl)propyl)octanethioate	364.616	3_REACH			1	0.3	8.2278E-07			1	0.03	8.2278E-08			1	0.03	8.22783E-08
22094-93-5	22094935	2317	2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	754.51	3_REACH			1	0.3	3.9761E-07			1	0.03	3.9761E-08			1	0.03	3.97609E-08
2210-79-9	2210799	2319	2,3-epoxypropyl o-tolyl ether	164.2	3_REACH			1	0.3	1.827E-06			1	0.03	1.827E-07			1	0.03	1.82704E-07
2216-51-5	2216515	538	L-menthol	156.27	3_REACH			1	0.3	1.9198E-06			1	0.03	1.9198E-07			1	0.03	1.91975E-07
2224-33-1	2224331	2325	butan-2-one O,O',O''-(vinylsilylidyne)trioxime	313.48	3_REACH			1	0.3	9.57E-07			1	0.03	9.57E-08			1	0.03	9.56999E-08
2226-96-2	2226962	2327	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	173.26	3_REACH			1	0.3	1.7315E-06			1	0.03	1.7315E-07			1	0.03	1.7315E-07
2235-00-9	2235009	2331	1-vinylhexahydro-2H-azepin-2-one	139.2	3_REACH			1	0.3	2.1552E-06			1	0.03	2.1552E-07			1	0.03	2.15517E-07
224049-04-1	224049041	2333	Isotianil	298.15	3_REACH			1	0.3	1.0062E-06			1	0.03	1.0062E-07			1	0.03	1.0062E-07
2243-62-1	2243621	542	1,5-naphthylenediamine	158.21	3_REACH			1	0.3	1.8962E-06			1	0.03	1.8962E-07			1	0.03	1.89621E-07
2280-49-1	2280491	2338	N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide	382.72	3_REACH			1	0.3	7.8386E-07			1	0.03	7.8386E-08			1	0.03	7.83863E-08
22871-58-5	22871585	2340	3-Amino-5-((2-hydroxyethyl)carbamoyl)-2,4,6-triiodobenzoic acid	601.89	3_REACH			1	0.3	4.9843E-07			1	0.03	4.9843E-08			1	0.03	4.9843E-08
22984-54-9	22984549	2341	butan-2-one O,O',O''-(methylsilylidyne)trioxime	301.47	3_REACH			1	0.3	9.9512E-07			1	0.03	9.9512E-08			1	0.03	9.95124E-08
2312-35-8	2312358	548	propargite	350.48	3_REACH	23.2	23.2	0	23.2	6.6195E-05	9	9	0	9	2.5679E-05			1	0.03	8.55969E-08
232938-43-1	232938431	4564	3-(3-Tosylureido)phenyl p-toluenesulfonate	460.53	3_REACH			1	0.3	6.5142E-07			1	0.03	6.5142E-08			1	0.03	6.51423E-08
23410-40-4	23410404	2351	N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine	220.39	3_REACH			1	0.3	1.3612E-06			1	0.03	1.3612E-07			1	0.03	1.36122E-07
2362-14-3	2362143	2353	4,4'-cyclohexylidenedi-o-cresol	296.41	3_REACH			1	0.3	1.0121E-06			1	0.03	1.0121E-07			1	0.03	1.01211E-07
2370-88-9	2370889	2355	2,4,6,8-	236.48	3_REACH			1	0.3	1.2686E-06			1	0.03	1.2686E-07			1	0.03	1.26861E-07
2372-82-9	2372829	554	N-(3-aminopropyl)-N-dodecylpropane-1,3-diamine	299.55	3_REACH	25	25	0	25	8.3459E-05			1	0.03	1.0015E-07			1	0.03	1.0015E-07
23779-32-0	23779320	2358	[3-(triethoxysilyl)propyl]urea	264.4	3_REACH			1	0.3	1.1346E-06			1	0.03	1.1346E-07			1	0.03	1.13464E-07
23783-42-8	23783428	2359	3,6,9,12-tetraoxotridecanol	208.25	3_REACH			1	0.3	1.4406E-06			1	0.03	1.4406E-07			1	0.03	1.44058E-07
2380-86-1	2380861	4816	6-hydroxyindole	133.15	3_REACH			1	0.3	2.2531E-06			1	0.03	2.2531E-07			1	0.03	2.2531E-07
23847-08-7	23847087	2360	1,1'-dithiobis[hexahydro-2H-azepin-2-one]	288.43	3_REACH			1	0.3	1.0401E-06			1	0.03	1.0401E-07			1	0.03	1.04011E-07
2385-77-5	2385775	2361	(R)-3,7-dimethyloct-6-enal	154.25	3_REACH			1	0.3	1.9449E-06			1	0.03	1.9449E-07			1	0.03	1.94489E-07
2386-87-0	2386870	2362	7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate	252.31	3_REACH			1	0.3	1.189E-06			1	0.03	1.189E-07			1	0.03	1.18901E-07
2402-79-1	2402791	2367	2,3,5,6-tetrachloropyridine	216.88	3_REACH			1	0.3	1.3833E-06			1	0.03	1.3833E-07			1	0.03	1.38325E-07

2403-88-5	2403885	2368	2,2,6,6-tetramethylpiperidin-4-ol	157.26	3_REACH			1	0.3	1.9077E-06			1	0.03	1.9077E-07			1	0.03	1.90767E-07
2403-89-6	2403896	2369	1,2,2,6,6-pentamethylpiperidin-4-ol	171.29	3_REACH			1	0.3	1.7514E-06			1	0.03	1.7514E-07			1	0.03	1.75142E-07
24085-06-1	24085061	2372	(5-Acetyl-2-acetyloxyphenyl)methyl acetate	250.25	3_REACH			1	0.3	1.1988E-06			1	0.03	1.1988E-07			1	0.03	1.1988E-07
2409-55-4	2409554	2373	2-tert-butyl-o-cresol	164.25	3_REACH			1	0.3	1.8265E-06			1	0.03	1.8265E-07			1	0.03	1.82648E-07
2416-94-6	2416946	558	2,3,6-trimethylphenol	136.19	3_REACH			1	0.3	2.2028E-06			1	0.03	2.2028E-07			1	0.03	2.2028E-07
24199-460	24199460	2376	6-methyloct-5-en-2-one	140.23	3_REACH			1	0.3	2.1393E-06			1	0.03	2.1393E-07			1	0.03	2.13934E-07
2421-28-5	2421285	2378	benzophenone-3,3',4,4'-tetracarboxylic dianhydride	322.23	3_REACH			1	0.3	9.3101E-07			1	0.03	9.3101E-08			1	0.03	9.31012E-08
2425-77-6	2425776	2381	2-hexyldecan-1-ol	242.45	3_REACH			1	0.3	1.2374E-06			1	0.03	1.2374E-07			1	0.03	1.23737E-07
24279-39-8	24279398	4333	2,6-dichloro-4-trifluoromethylaniline	230.02	3_REACH			1	0.3	1.3042E-06			1	0.03	1.3042E-07			1	0.03	1.30423E-07
24293-43-4	24293434	2384	bis(2-ethylhexyl) 2,2'-thiobisacetate	374.58	3_REACH			1	0.3	8.009E-07			1	0.03	8.009E-08			1	0.03	8.00897E-08
2439-35-2	2439352	2391	2-(dimethylamino)ethyl acrylate	143.19	3_REACH			1	0.3	2.0951E-06			1	0.03	2.0951E-07			1	0.03	2.09512E-07
24424-99-5	24424995	2393	diitert-butyl carbonate	218.25	3_REACH			1	0.3	1.3746E-06			1	0.03	1.3746E-07			1	0.03	1.37457E-07
24468-13-1	24468131	2395	2-ethylhexyl chloroformate	192.69	3_REACH			1	0.3	1.5595E-06			1	0.03	1.5595E-07			1	0.03	1.55955E-07
24549-06-2	24549062	2397	6-ethyl-2-toluidine	135.21	3_REACH			1	0.3	2.2188E-06			1	0.03	2.2188E-07			1	0.03	2.21877E-07
2461-15-6	2461156	561	[[(2-ethylhexyl)oxy]methyl]oxirane	186.29	3_REACH			1	0.3	1.6104E-06			1	0.03	1.6104E-07			1	0.03	1.61039E-07
24650-42-8	24650428	2400	2,2-dimethoxy-1,2-diphenylethan-1-one	256.3	3_REACH			1	0.3	1.1705E-06			1	0.03	1.1705E-07			1	0.03	1.1705E-07
24800-44-0	24800440	2404	[(methylethylene)bis(oxy)]dipropanol	192.26	3_REACH			1	0.3	1.5604E-06			1	0.03	1.5604E-07			1	0.03	1.56039E-07
24863-70-5	24863705	2405	1-Cyclopentene-1-acetic acid, 3-oxo-2-pentyl-, methyl ester	224.3	3_REACH			1	0.3	1.3376E-06			1	0.03	1.3376E-07			1	0.03	1.33749E-07
2495-37-6	2495376	565	benzyl methacrylate	176.22	3_REACH			1	0.3	1.7024E-06			1	0.03	1.7024E-07			1	0.03	1.70242E-07
2500-88-1	2500881	2411	dioctadecyl disulfide	571.12	3_REACH			1	0.3	5.2528E-07			1	0.03	5.2528E-08			1	0.03	5.25284E-08
25013-15-4	25013154	2412	vinyltoluene	118.18	3_REACH			1	0.3	2.5365E-06			1	0.03	2.5365E-07			1	0.03	2.5365E-07
2512-29-0	2512290	2416	2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-phenylbutyramide	340.34	3_REACH			1	0.3	8.8147E-07			1	0.03	8.8147E-08			1	0.03	8.814715E-08
25265-71-8	25265718	566	dipropylene glycol	134.18	3_REACH			1	0.3	2.2368E-06			1	0.03	2.2368E-07			1	0.03	2.2368E-07
25265-77-4	25265774	2426	isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	216.32	3_REACH			1	0.3	1.3868E-06			1	0.03	1.3868E-07			1	0.03	1.38683E-07
2526-62-7	2526627	2427	3-(trimethoxysilyl)propiononitrile	175.26	3_REACH			1	0.3	1.7117E-06			1	0.03	1.7117E-07			1	0.03	1.711745-07
2528-61-2	2528612	2428	benzoyl chloride	140.57	3_REACH			1	0.3	2.0184E-06			1	0.03	2.0184E-07			1	0.03	2.01844E-07
25307-17-9	25307179	2429	2,2'-(octadec-9-enylimino)bisethanol	355.61	3_REACH			1	0.3	8.4362E-07			1	0.03	8.4362E-08			1	0.03	8.43621E-08
2530-87-2	2530872	2430	3-chloropropyltrimethoxysilane	198.72	3_REACH			1	0.3	1.5097E-06			1	0.03	1.5097E-07			1	0.03	1.50966E-07
25322-69-4	25322694	568	Propane-1,2-diol, propoxylated	134.175	3_REACH			1	0.3	2.2369E-06			1	0.03	2.2369E-07			1	0.03	2.23669E-07
25498-49-1	25498491	2436	[2-(2-methoxymethylethoxy)methylethoxy]propanol	206.28	3_REACH			1	0.3	1.4543E-06			1	0.03	1.4543E-07			1	0.03	1.45433E-07
2550-26-7	2550267	2437	4-phenylbutan-2-one	148.21	3_REACH			1	0.3	2.0242E-06			1	0.03	2.0242E-07			1	0.03	2.02415E-07
25601-41-6	25601416	2440	Methyl 5-decanone	184.28	3_REACH			1	0.3	1.6288E-06			1	0.03	1.6288E-07			1	0.03	1.62799E-07
256473-04-8	256473048	2441	2-Chloro-3-(2,2,2-trifluoroethoxy)quinoline	211.57	3_REACH			1	0.3	1.418E-06			1	0.03	1.418E-07			1	0.03	1.41797E-07
256473-05-9	256473059	2442	2-(isopropylthio)-3-(2,2,2-trifluoroethoxy)quinoline	251.27	3_REACH			1	0.3	1.1939E-06			1	0.03	1.1939E-07			1	0.03	1.19393E-07
2568-90-3	2568903	2443	1,1'-[methylenebis(oxy)]dibutane	160.26	3_REACH			1	0.3	1.872E-06			1	0.03	1.872E-07			1	0.03	1.87196E-07
2602-34-8	2602348	2449	[3-(2,3-epoxypropoxy)propyl]triethoxysilane	278.42	3_REACH			1	0.3	1.0776E-06			1	0.03	1.0776E-07			1	0.03	1.07761E-07
2605-79-0	2605790	2452	N,N-dimethyldecylamine N-oxide	201.35	3_REACH			1	0.3	1.4899E-06			1	0.03	1.4899E-07			1	0.03	1.48994E-07
2612-57-9	2612579	2455	2,4-dichlorophenyl isocyanate	188.01	3_REACH			1	0.3	1.5967E-06			1	0.03	1.5967E-07			1	0.03	1.59666E-07
26159-31-9	26159319	572	(±)-2-(6-methoxy-2-naphthyl)propionic acid	230.26	3_REACH			1	0.3	1.3029E-06			1	0.03	1.3029E-07			1	0.03	1.30288E-07
26218-04-2	26218042	4353	2-ethylhexyl 4-aminobenzoate	249.35	3_REACH			1	0.3	1.2031E-06			1	0.03	1.2031E-07			1	0.03	1.20313E-07
26272-90-2	26272902	2460	hexadecyl chloroformate	304.9	3_REACH			1	0.3	9.8393E-07			1	0.03	9.8393E-08			1	0.03	9.83929E-08
2627-86-3	2627863	2461	L-1-Phenylethylamine	121.18	3_REACH			1	0.3	2.4757E-06			1	0.03	2.4757E-07			1	0.03	2.47666E-07
26364-65-8	26364658	4511	2-thiazolidinylidenecyanamide	127.17	3_REACH			1	0.3	2.359E-06			1	0.03	2.359E-07			1	0.03	2.35905E-07
26399-02-0	26399020	2468	2-ethylhexyl oleate	394.68	3_REACH			1	0.3	7.6011E-07			1	0.03	7.6011E-08			1	0.03	7.60109E-08
26523-78-4	26523784	2474	tris(nonylphenyl) phosphite	689.02	3_REACH			1	0.3	4.354E-07			1	0.03	4.354E-08			1	0.03	4.35401E-08
26586-02-7	26586027	2480	(E)-3-formylbut-2-enyl acetate	142.15	3_REACH			1	0.3	2.1104E-06			1	0.03	2.1104E-07			1	0.03	2.11045E-07
26741-53-7	26741537	2485	3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane	604.71	3_REACH			1	0.3	4.9611E-07			1	0.03	4.9611E-08			1	0.03	4.96105E-08
26761-45-5	26761455	2487	2,3-epoxypropyl neodecanoate	228.33	3_REACH			1	0.3	1.3139E-06			1	0.03	1.3139E-07			1	0.03	1.31389E-07
2687-91-4	2687914	2489	1-ethylpyrrolidin-2-one	113.16	3_REACH			1	0.3	2.6511E-06			1	0.03	2.6511E-07			1	0.03	2.65111E-07
26896-20-8	26896208	2491	neodecanoic acid	172.27	3_REACH			1	0.3	1.7418E-06			1	0.03	1.7418E-07			1	0.03	1.74185E-07
2691-41-0	2691410	575	octanoyl chloride	296.16	3_REACH	15000	15000	0	15000	0.0005483			1	0.03	1.0135E-07			1	0.03	1.01297E-07
2705-87-5	2705876	2493	allyl 3-cyclohexylpropionate	196.29	3_REACH			1	0.3	1.5284E-06			1	0.03	1.5284E-07			1	0.03	1.52835E-07
27458-94-2	27458942	2507	isononyl alcohol	144.26	3_REACH			1	0.3	2.0796E-06			1	0.03	2.0796E-07			1	0.03	2.07968E-07
2752-17-2	2752172	2511	2,2'-oxydi(ethylamine)	104.16	3_REACH			1	0.3	2.8802E-06			1	0.03	2.8802E-07			1	0.03	2.88018E-07
2778-42-9	2778429	2517	1,3-bis(1-isocyanato-1-methylethyl)benzene	244.3	3_REACH			1	0.3	1.228E-06			1	0.03	1.228E-07			1	0.03	1.2285-07
2786-76-7	2786767	2520	4-[[4-(aminocarbonyl)phenyl]azo]-N-(2-ethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide	454.49	3_REACH			1	0.3	6.6006E-07			1	0.03	6.6006E-08			1	0.03	6.60061E-08
27955-94-8	27955948	4403	4,4',4''-(ethan-1,1,1-triyl)trisphenol	306.36	3_REACH			1	0.3	9.7924E-07			1	0.03	9.7924E-08			1	0.03	9.79245-08
2809-21-4	2809214	578	etidronic acid	206.03	3_REACH	33333.33333	33333.33333	0	33333.3333	0.16178874	100	100	0	100	0.00048537			1	0.03	1.45615E-07
281-23-2	281232	579	tricyclo[3.3.1.13,7]decane	136.24	3_REACH			1	0.3	2.202E-06			1	0.03	2.202E-07			1	0.03	2.202E-07
28219-61-6	28219616	2525	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol	208.35	3_REACH			1	0.3	1.4399E-06			1	0.03	1.4399E-07			1	0.03	1.43988E-07
28479-22-3	28479223	2533	3-chloroundecyl isocyanate	167.6	3_REACH			1	0.3	1.79E-06			1	0.03	1.79E-07			1	0.03	1.78998E-07
28535-81-1	28535811	2535	Methyl 3alpha,7alpha-diacetoxy-12-oxo-5beta-cholanoate	504.66	3_REACH			1	0.3	5.9446E-07			1	0.03	5.9446E-08			1	0.03	5.94465-08
2855-13-2	2855132	2536	3-aminomethyl-3,5,5-trimethylcyclohexylamine	170.3	3_REACH			1	0.3	1.7616E-06			1	0.03	1.7616E-07			1	0.03	1.76165-07
28553-12-0	28553120	582	di-"isononyl" phthalate	418.62	3_REACH			1	0.3	7.1684E-07	34	34	0	34	8.1219E-05			1	0.03	7.16845-08
2867-47-2	2867472	583	2-dimethylaminoethyl methacrylate	157.21	3_REACH			1	0.3	1.9083E-06			1	0.03	1.9083E-07			1	0.03	1.90825E-07
28768-32-3	28768323	2543	4,4'-methylenebis[N,N-bis(2,3-epoxypropyl)aniline]	422.53	3_REACH			1	0.3	7.1001E-07			1	0.03	7.1001E-08			1	0.03	7.10009E-08
288-13-1	288131	43	pyrazole	68.081	3_REACH			1	0.3	4.4065E-06			1	0.03	4.4065E-07			1	0.03	4.40652E-07
288-88-0	288880	584	1,2,4-triazole	69.07	3_REACH	98100	98100	0	98100	1.42029825			1	0.03	4.3434E-07			1	0.03	4.34342E-07
2896-70-0	2896700	2550	2,2,6,6-tetramethyl-4-oxopiperidinooxy	171.24	3_REACH			1	0.3	1.7619E-06			1	0.03	1.7619E-07			1	0.03	1.76193E-07
2915-57-3	2915573	2559	bis(2-ethylhexyl) succinate	342.52	3_REACH			1	0.3	8.7686E-07			1	0.03	8.7686E-08			1	0.03	8.76861E-08
29171-20-8	29171208	2560	3,7-dimethyloct-6-en-1-yn-3-ol	152.24	3_REACH			1	0.3	1.9706E-06			1	0.03	1.9706E-07			1	0.03	1.97067E-07
2920-38-9	2920389	2561	p-phenylbenzonitrile	179.22	3_REACH			1	0.3	1.6739E-06			1	0.03	1.6739E-07			1	0.03	1.67392E-07
2935-90-2	2935902	2563	methyl 3-mercaptoproiionate	120.17	3_REACH			1	0.3	2.4965E-06			1	0.03	2.4965E-07			1	0.03	2.49656E-07
2942-59-8	2942598	2566	2-chloronicotinic acid	157.56	3_REACH			1	0.3	1.2045E-06			1	0.03	1.2045E-07			1	0.03	1.20445E-07
2943-75-1	2943751	2567	triethoxyoctylsilane	276.49	3_REACH			1	0.3	1.0865E-06			1	0.03	1.0865E-07			1	0.03	1.08603E-07
294-62-2	294622	587	cyclododecane	168.32	3_REACH	7000	7000	0	7000	0.04158745			1	0.03	1.7623E-07			1	0.03	1.76232E-07
294-90-6	294906	4493	1,4,7,10-tetraazacyclododecane	172.28	3_REACH			1	0.3	1.7414E-06			1	0.03	1.7414E-07			1	0.03	1.74135E-07
29761-21-5	29761215	588	isodecyl diphenyl phosphate	390.46	3_REACH			1	0.3	7.6832E-06			1	0.03	7.6832E-08			1	0.03	7.68325E-08
298-06-6	298066	591	O,O-diethyl hydrogen phosphorodithioate	186.23	3_REACH	180	180	0	180	0.00096665			1	0.03	1.6109E-07			1	0.03	1.61091E-07
29806-73-3	29806733	2572	2-ethylhexyl palmitate	368.65	3_REACH			1	0.3	8.1378E-07			1	0.03	8.1378E-08			1	0.03	8.13785-08
298-07-7	298077	592	bis(2-ethylhexyl) hydrogen phosphate	322.43	3_REACH	9066.666667	9066.666667	0	9066.66667	0.0281198			1	0.03	9.3043E-06			1	0.03	9.30435E-08
298-12-4	298124	2573	glyoxylic acid	74.035	3_REACH			1	0.3	4.0521E-06			1	0.03	4.0521E-07			1	0.03	4.05214E-07
29911-28-2	29911282	2578	1-(2-butoxy-1-methylethoxy)propan-2-ol	190.28	3_REACH			1	0.3	1.5766E-06			1	0.03	1.5766E-07			1	0.03	1.57662E-07
29920-31-8	29920318	2579	dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]terephthalate	453.42	3_REACH			1	0.3	6.6164E-07			1	0.03	6.6164E-08			1	0.03	6.61638E-08
29964-84-9	29964849	2581	isodecyl methacrylate	226.36	3_REACH			1	0.3	1.3283E-06			1	0.03	1.3283E-07			1	0.03	1.32832E-07
2996-92-1	2996921	2582	trimethoxyphenylsilane	198.29	3_REACH			1	0.3	1.5129E-06			1	0.03	1.5129E-07			1	0.03	1.51294E-07
3030-47-5	3030476	2590	bis(2-dimethylaminoethyl)(methyl)amine	173.31	3_REACH			1	0.3	1.731E-06			1	0.03	1.731E-07			1	0.03	1.7315-07
3031-66-1	3031661	2591	hex-3-yne-2,5-diol	114.14	3_REACH			1	0.3	2.6284E-06			1	0.03	2.6284E-07			1	0.03	2.62835E-07
3033-62-3	3033623	2592	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	160.26	3_REACH			1	0.3	1.872E-06			1	0.03	1.872E-07			1	0.03	1.87196E-07
3047-32-3	3047323	2598	3-ethyloxetane-3-methanol	116.16	3_REACH			1	0.3	2.5826E-06			1	0.03	2.5826E-07			1	0.03	2.58264E-07
3049-71-6	3049716	2600	2,9-bis[4-(phenylazo)phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone	750.78	3_REACH			1	0.3	3.9958E-07			1	0.03	3.9958E-08			1	0.03	3.99584E-08
3061-75-4	3061754	2604	diproxpenamide	338.61	3_REACH			1	0.3	8.8337E-07			1	0.03	8.8337E-08			1	0.03	8.83368E-08
30674-80-7	30674807	2606	2-isocyanatoethyl methacrylate	155.15	3_REACH			1	0.3	1.9336E-06			1	0.03	1.9336E-07			1	0.03	1.93361E-07
3069-29-2	3069292	2608	N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine	206.36	3_REACH			1	0.3	1.4538E-06			1	0.03	1.4538E-07			1	0.03	1.45377E-07
3069-40-7	3069407	2609	trimethoxyoctylsilane	234.41	3_REACH			1	0.3	1.2796E-06			1	0.03	1.2796E-07			1	0.03	1.27961E-07
3081-14-9	3081149	2612	N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine	304.52	3_REACH			1	0.3	9.8516E-07			1	0.03	9.8516E-08			1	0.03	9.85167E-08
3089-16-5	3089165	2614	4,11-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	381.22	3_REACH			1	0.3	7.8695E-07			1	0.03	7.8695E-08			1	0.03	7.86947E-08
3089-17-6	3089176	2615	2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	381.22	3_REACH			1	0.3	7.8695E-07			1	0.03	7.8695E-08			1	0.03	7.86947E-08
31024-56-3	31024563	2617	N-[3-(trimethoxysilyl)propyl]butylamine	235.4	3_REACH			1	0.3	1.2744E-06			1	0.03	1.2744E-07			1	0.03	1.27443E-07
31027-31-3	31027313	2618	p-isopropylphenyl isocyanate	161.21	3_REACH			1	0.3	1.8609E-06			1	0.03	1.8609E-07			1	0.03	1.86093E-07
3115-49-9	3115499	2619	(4-nonylphenoxy)acetic acid	278.39	3_REACH			1	0.3	1.0776E-06			1	0.03	1.0776E-07			1	0.03	1.07762E-07
31335-74-7	31335747	2625	2,2-dimethyl-1,3-propanediyl dioctanoate	356.55	3_REACH			1	0.3	8.414E-07			1	0.03	8.414E-08			1	0.03	8.41397E-08
3148-73-0	3148730	2627	N,N'-diacetylhydrazine	116.12	3_REACH			1	0.3	2.5836E-06			1	0.03	2.5836E-07			1	0.03	2.58353E-07
3173-72-6	3173726	2631	1,5-naphthylene diisocyanate	210.19	3_REACH			1	0.3	1.4273E-06			1	0.03	1.4273E-07			1	0.03	1.42728E-07
31775-20-9	31775209	2632	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-ethoxyphenyl)-3-oxobutyramide]	717.62	3_REACH			1	0.3	4.1805E-06			1	0.03	4.1805E-08			1	0.03	4.18049E-08
31775-89-0	31775890	2633	3-[(3-sulfanylbutanoyl)oxy]-2,2-bis[[(3-sulfanylbutanoyl)oxy]methyl]propyl 3-sulfanylbutanoate	544.77	3_REACH			1	0.3	5.5069E-07			1	0.03	5.5069E-08			1	0.03	5.50691E-08

31778-10-6	31778106	2634	butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthyl]azo]benzoate	523.55	3_REACH			1	0.3	5.7301E-07			1	0.03	5.7301E-08	1	0.03	5.73011E-08
3179-47-3	3179473	2635	decyl methacrylate	226.36	3_REACH			1	0.3	1.3253E-06			1	0.03	1.3253E-07	1	0.03	1.32532E-07
3179-63-3	3179633	2636	3-dimethylaminopropan-1-ol	103.17	3_REACH			1	0.3	2.9078E-06			1	0.03	2.9078E-07	1	0.03	2.90782E-07
3179-76-8	3179768	2637	3-(diethoxymethylsilyl)propylamine	191.35	3_REACH			1	0.3	1.5678E-06			1	0.03	1.5678E-07	1	0.03	1.56781E-07
31837-42-0	31837420	2639	2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzoic acid	381.35	3_REACH			1	0.3	7.8668E-07			1	0.03	7.8668E-08	1	0.03	7.86679E-08
319002-92-1	319002921	4599	Propyl (2S)-2-(2-methylbutan-2	202.29	3_REACH			1	0.3	1.483E-06			1	0.03	1.483E-07	1	0.03	1.48302E-07
3209-22-1	3209221	600	1,2-dichloro-3-nitrobenzene	192	3_REACH	533.3333333	533.3333333	0	533.333333	0.00277778			1	0.03	1.5625E-07	1	0.03	1.5625E-07
3234-85-3	3234853	2648	tetradecyl myristate	424.75	3_REACH			1	0.3	7.063E-07			1	0.03	7.063E-08	1	0.03	7.06298E-08
32388-55-9	32388559	2651	Acetyl cedrene	246.39	3_REACH			1	0.3	1.2176E-06			1	0.03	1.2176E-07	1	0.03	1.21758E-07
329-01-1	329011	2668	3-(Trifluoromethyl)phenyl isocyanate	187.12	3_REACH			1	0.3	1.6032E-06			1	0.03	1.6032E-07	1	0.03	1.60325E-07
3290-92-4	3290924	2669	propylidynetrimethyl trimethacrylate	338.4	3_REACH			1	0.3	8.8652E-07			1	0.03	8.8652E-08	1	0.03	8.86525E-08
3296-90-0	3296900	2671	2,2-bis(bromomethyl)propane-1,3-diol	261.95	3_REACH			1	0.3	1.1453E-06			1	0.03	1.1453E-07	1	0.03	1.14526E-07
3320-83-0	3320830	2677	2-chlorophenyl isocyanate	153.57	3_REACH			1	0.3	1.9535E-06			1	0.03	1.9535E-07	1	0.03	1.95351E-07
3332-27-2	3332272	2679	N,N-dimethyltetradecylamine N-oxide	257.46	3_REACH			1	0.3	1.1652E-06			1	0.03	1.1652E-07	1	0.03	1.16523E-07
33329-35-0	33329350	2680	N,N-bis[3-(dimethylamino)propyl]-N',N'-dimethylpropane-1,3-diamine	272.49	3_REACH			1	0.3	1.101E-06			1	0.03	1.101E-07	1	0.03	1.10096E-07
33704-61-9	33704619	2684	1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one	206.33	3_REACH			1	0.3	1.454E-06			1	0.03	1.454E-07	1	0.03	1.45398E-07
337906-36-2	337906362	2686	2-(methoxymethyl)benzene-1,4-diamine	152.2	3_REACH			1	0.3	1.9711E-06			1	0.03	1.9711E-07	1	0.03	1.97109E-07
3407-42-9	3407429	2689	3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	236.4	3_REACH			1	0.3	1.269E-06			1	0.03	1.269E-07	1	0.03	1.26904E-07
34090-76-1	34090761	2690	tetrahydro-4-methylphthalic anhydride	166.18	3_REACH			1	0.3	1.8053E-06			1	0.03	1.8053E-07	1	0.03	1.80527E-07
34206-40-1	34206401	2694	butan-2-one O,O',O'',O'''-silanetetrayltetraoxime	372.55	3_REACH			1	0.3	8.0526E-07			1	0.03	8.0526E-08	1	0.03	8.05261E-08
342-25-6	342256	2695	2,4'-difluorobenzophenone	218.2	3_REACH			1	0.3	1.3749E-06			1	0.03	1.3749E-07	1	0.03	1.37489E-07
34316-64-8	34316648	2700	hexyl laurate	284.48	3_REACH			1	0.3	1.0546E-06			1	0.03	1.0546E-07	1	0.03	1.05456E-07
3437-84-1	3437841	2701	bisisobutyryl peroxide	174.2	3_REACH			1	0.3	1.7222E-06			1	0.03	1.7222E-07	1	0.03	1.72216E-07
34396-03-7	34396037	2702	trimethoxy(2,4,4-trimethylpentyl)silane	234.41	3_REACH			1	0.3	1.2798E-06			1	0.03	1.2798E-07	1	0.03	1.27981E-07
3452-97-9	3452979	609	3,5,5-trimethylhexan-1-ol	144.26	3_REACH			1	0.3	2.0796E-06			1	0.03	2.0796E-07	1	0.03	2.07958E-07
345-92-6	345926	2710	bis(4-fluorophenyl) ketone	218.2	3_REACH			1	0.3	1.3749E-06			1	0.03	1.3749E-07	1	0.03	1.37489E-07
34690-00-1	34690001	2714	[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid	685.42	3_REACH			1	0.3	4.3769E-07			1	0.03	4.3769E-08	1	0.03	4.37688E-08
34893-92-0	34893920	2717	1,3-dichloro-5-isocyanatobenzene	188.01	3_REACH			1	0.3	1.5957E-06			1	0.03	1.5957E-07	1	0.03	1.59566E-07
350-46-9	350469	611	1-fluoro-4-nitrobenzene	141.1	3_REACH			1	0.3	2.1262E-06			1	0.03	2.1262E-07	1	0.03	2.12615E-07
3508-98-3	3508983	4362	2-phenylhexanenitrile	173.26	3_REACH			1	0.3	1.7315E-06			1	0.03	1.7315E-07	1	0.03	1.7315E-07
35265-04-4	35265044	2726	2-[(1-methylpropyl)amino]ethanol	117.19	3_REACH			1	0.3	2.5599E-06			1	0.03	2.5599E-07	1	0.03	2.55995E-07
35435-21-3	35435213	2734	triethoxy(2,4,4-trimethylpentyl)silane	276.49	3_REACH			1	0.3	1.085E-06			1	0.03	1.085E-07	1	0.03	1.08503E-07
3547-33-9	3547339	613	2-(octylthio)ethanol	190.35	3_REACH	60	60	0	60	0.00031521			1	0.03	1.576E-07	1	0.03	1.57604E-07
35636-63-6	35636636	2742	dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]terephthalate	453.42	3_REACH			1	0.3	6.6164E-07			1	0.03	6.6164E-08	1	0.03	6.61638E-08
3576-88-3	3576883	2746	2,2'-iminobis[4,6-diamino-1,3,5-triazine]	235.23	3_REACH			1	0.3	1.2753E-06			1	0.03	1.2753E-07	1	0.03	1.27535E-07
35836-72-7	35836727	2750	2-Pinene-10-methyl acetate	208.3	3_REACH			1	0.3	1.4402E-06			1	0.03	1.4402E-07	1	0.03	1.44023E-07
35948-25-5	35948255	2754	6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide	216.18	3_REACH			1	0.3	1.3877E-06			1	0.03	1.3877E-07	1	0.03	1.38773E-07
36177-92-1	36177921	2761	N-butyl-2,2,6,6-tetramethylpiperidin-4-	212.38	3_REACH			1	0.3	1.4126E-06			1	0.03	1.4126E-07	1	0.03	1.41256E-07
3622-84-2	3622842	2763	N-butylbenzenesulphonamide	213.3	3_REACH			1	0.3	1.4065E-06			1	0.03	1.4065E-07	1	0.03	1.40647E-07
3634-83-1	3634831	2766	1,3-bis(isocyanatomethyl)benzene	188.19	3_REACH			1	0.3	1.5941E-06			1	0.03	1.5941E-07	1	0.03	1.59413E-07
36443-68-2	36443682	2767	ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)propionate]	586.77	3_REACH			1	0.3	5.1127E-07			1	0.03	5.1127E-08	1	0.03	5.11274E-08
36483-57-5	36483575	2768	2,2-dimethylpropan-1-ol, tribromo derivative	324.86	3_REACH			1	0.3	9.2347E-07			1	0.03	9.2347E-08	1	0.03	9.23475E-08
36635-56-0	36635560	2772	N-[[(4-methylphenyl)sulfonyl]methyl]formamide	213.26	3_REACH			1	0.3	1.4067E-06			1	0.03	1.4067E-07	1	0.03	1.40673E-07
36727-29-4	36727294	2775	3,5,5-trimethylhexanoyl chloride	176.69	3_REACH			1	0.3	1.6979E-06			1	0.03	1.6979E-07	1	0.03	1.69789E-07
36768-62-4	36768624	2776	2,2,6,6-tetramethyl-4-piperidylamine	156.28	3_REACH			1	0.3	1.9196E-06			1	0.03	1.9196E-07	1	0.03	1.91963E-07
3681-71-8	3681718	2779	(Z)-hex-3-enyl acetate	142.2	3_REACH			1	0.3	2.1097E-06			1	0.03	2.1097E-07	1	0.03	2.1097E-07
3687-22-7	3687227	4777	2,4-Dinitro-6-(1-methylheptyl)phenol	296.32	3_REACH			1	0.3	1.0124E-06			1	0.03	1.0124E-07	1	0.03	1.01242E-07
369634-22-0	369634220	4583	Octalynol	140.18	3_REACH			1	0.3	2.1401E-06			1	0.03	2.1401E-07	1	0.03	2.14011E-07
3699-54-5	3699545	2788	1-(2-hydroxyethyl)imidazolidin-2-one	130.15	3_REACH			1	0.3	2.305E-06			1	0.03	2.305E-07	1	0.03	2.30503E-07
37052-78-1	37052781	2789	1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione	180.23	3_REACH			1	0.3	1.6645E-06			1	0.03	1.6645E-07	1	0.03	1.66454E-07
3710-84-7	3710847	2791	N,N-diethylhydroxylamine	89.139	3_REACH			1	0.3	3.3655E-06			1	0.03	3.3655E-07	1	0.03	3.36553E-07
3717-40-6	3717406	2792	N,N-Dimethyladamantan-1-amine	179.31	3_REACH			1	0.3	1.6731E-06			1	0.03	1.6731E-07	1	0.03	1.67308E-07
372-09-8	372098	2794	cyanoacetic acid	85.063	3_REACH			1	0.3	3.5268E-06			1	0.03	3.5268E-07	1	0.03	3.5268E-07
373-44-4	373444	2796	octamethylenediamine	144.26	3_REACH			1	0.3	2.0796E-06			1	0.03	2.0796E-07	1	0.03	2.07958E-07
3741-80-8	3741808	5041	N-(1,1-dimethylethyl)bis(2-benzothiazolesulfen)amide	403.61	3_REACH			1	0.3	7.4329E-07			1	0.03	7.4329E-08	1	0.03	7.43292E-08
3748-13-8	3748138	2798	m-bis(1-methylvinyl)benzene	158.24	3_REACH			1	0.3	1.8959E-06			1	0.03	1.8959E-07	1	0.03	1.89585E-07
3749-87-9	3749879	2800	Methyl 3,7-di-O-acetylcholate	506.68	3_REACH			1	0.3	5.9209E-07			1	0.03	5.9209E-08	1	0.03	5.9209E-08
3779-63-3	3779633	2809	(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene) isocyanate	504.59	3_REACH			1	0.3	5.9454E-07			1	0.03	5.9454E-08	1	0.03	5.94542E-08
37971-36-1	37971361	2811	2-phosphonobutane-1,2,4-tricarboxylic acid	270.13	3_REACH			1	0.3	1.1106E-06			1	0.03	1.1106E-07	1	0.03	1.11058E-07
38051-10-4	38051104	2812	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	582.99	3_REACH			1	0.3	5.1459E-07			1	0.03	5.1459E-08	1	0.03	5.14589E-08
38083-17-9	38083179	620	climbazole	292.77	3_REACH	5330	5330	0	5330	0.01820542			1	0.03	1.0247E-07	1	0.03	1.0247E-07
3845-76-9	3845769	2822	N-[3-(dimethylamino)propyl]acrylamide	156.23	3_REACH			1	0.3	1.9202E-06			1	0.03	1.9202E-07	1	0.03	1.92025E-07
3851-87-4	3851874	2823	bis(3,5,5-trimethylhexanoyl) peroxide	314.47	3_REACH			1	0.3	9.5399E-07			1	0.03	9.5399E-08	1	0.03	9.53986E-08
3855-32-1	3855321	2824	N-[3-(dimethylamino)propyl]-N,N',N'-trimethylpropane-1,3-diamine	201.36	3_REACH			1	0.3	1.4899E-06			1	0.03	1.4899E-07	1	0.03	1.48987E-07
38668-48-3	38668483	2825	1,1'-(p-tolylimino)dipropan-2-ol	223.32	3_REACH			1	0.3	1.3434E-06			1	0.03	1.3434E-07	1	0.03	1.34336E-07
3886-69-9	3886699	2827	D-alpha-Methylbenzylamine	121.18	3_REACH			1	0.3	2.4757E-06			1	0.03	2.4757E-07	1	0.03	2.47566E-07
38888-98-1	38888981	2828	(phenylethyl)benzene	182.27	3_REACH			1	0.3	1.6459E-06			1	0.03	1.6459E-07	1	0.03	1.64591E-07
393509-79-0	393509790	4634	methyl 2-chlorosulfonyl-4-(methanesulfonylaminomethyl) benzoate	341.79	3_REACH			1	0.3	8.7773E-07			1	0.03	8.7773E-08	1	0.03	8.77732E-08
39515-51-0	39515510	625	m-phenoxybenzaldehyde	198.22	3_REACH	16.66666667	16.66666667	0	16.6666667	8.4082E-05			1	0.03	1.5135E-07	1	0.03	1.51347E-07
39670-09-2	39670092	2846	2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate	246.3	3_REACH			1	0.3	1.218E-06			1	0.03	1.218E-07	1	0.03	1.21803E-07
40306-75-0	40306750	2857	3-acetamido-5-amino-4-hydroxybenzenesulphonic acid	246.24	3_REACH			1	0.3	1.2183E-06			1	0.03	1.2183E-07	1	0.03	1.21832E-07
40601-76-1	40601761	2859	1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6-xylyl]methyl]-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	699.94	3_REACH			1	0.3	4.2861E-07			1	0.03	4.2861E-08	1	0.03	4.28608E-08
4065-45-6	4065456	52	sulisobenzone	308.31	3_REACH			1	0.3	9.7305E-07			1	0.03	9.7305E-08	1	0.03	9.73047E-08
4073-98-7	4073987	2864	4,4'-methylenebis(2,6-xylidine)	254.38	3_REACH			1	0.3	1.1793E-06			1	0.03	1.1793E-07	1	0.03	1.17934E-07
40758-65-4	40758654	2865	4,6-Dichloro-2-ethoxypyrimidine	193.04	3_REACH			1	0.3	1.5541E-06			1	0.03	1.5541E-07	1	0.03	1.55408E-07
4083-64-1	4083641	629	p-toluenesulphonyl isocyanate	197.21	3_REACH			1	0.3	1.5212E-06			1	0.03	1.5212E-07	1	0.03	1.52122E-07
4098-71-9	4098719	2867	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	222.29	3_REACH			1	0.3	1.3496E-06			1	0.03	1.3496E-07	1	0.03	1.34959E-07
41198-08-7	41198087	631	Profenofos	373.64	3_REACH	0.32	0.32	0	0.32	8.5644E-07	0.2	0.2	0	0.2	5.3527E-07	1	0.03	8.02912E-08
41340-36-7	41340367	4309	2-(7-ethyl-1H-indol-3-yl)ethanol	189.26	3_REACH			1	0.3	1.5851E-06			1	0.03	1.5851E-07	1	0.03	1.58512E-07
41620-33-1	41620331	4337	2-[[2-(acetyloxy)-3-(1,1-dimethylethyl)-5-methylphenyl]methyl]-6-(1,1-dimethylethyl)-4-methylphenol	382.54	3_REACH			1	0.3	7.8423E-07			1	0.03	7.8423E-08	1	0.03	7.84232E-08
4180-23-8	4180238	635	(E)-anethole	148.21	3_REACH	5600	5600	0	5600	0.03778423			1	0.03	2.0242E-07	1	0.03	2.02415E-07
42019-78-3	42019783	2886	4-chloro-4'-hydroxybenzophenone	232.67	3_REACH			1	0.3	1.2894E-06			1	0.03	1.2894E-07	1	0.03	1.28938E-07
42125-46-2	42125462	2889	4-tert-butylcyclohexyl chloroformate	218.72	3_REACH			1	0.3	1.3716E-06			1	0.03	1.3716E-07	1	0.03	1.37162E-07
4245-76-5	4245765	2892	610-029-6	118.1	3_REACH			1	0.3	2.5402E-06			1	0.03	2.5402E-07	1	0.03	2.54022E-07
4246-51-9	4246519	2893	3,3'-oxybis(ethyleneoxy)bis(propylamine)	220.32	3_REACH			1	0.3	1.3617E-06			1	0.03	1.3617E-07	1	0.03	1.36166E-07
4253-34-3	4253343	2896	methylsilanetriyl triacetate	220.25	3_REACH			1	0.3	1.3621E-06			1	0.03	1.3621E-07	1	0.03	1.36209E-07
43057-68-7	43057687	4478	2-Ethyl-2-methyl-1,3-dihydroperimidine	212.3	3_REACH			1	0.3	1.4131E-06			1	0.03	1.4131E-07	1	0.03	1.41309E-07
4378-61-4	4378614	2916	4,10-dibromodibenzo[def,mno]chrysene-6,12-dione	464.12	3_REACH			1	0.3	6.4638E-07			1	0.03	6.4638E-08	1	0.03	6.46385E-08
4394-85-8	4394858	2918	4-morpholinecarbaldehyde	115.13	3_REACH			1	0.3	2.6058E-06			1	0.03	2.6058E-07	1	0.03	2.60575E-07
4402-30-6	4402306	2919	1,1'-(methylimino)dipropan-2-ol	147.22	3_REACH			1	0.3	2.0378E-06			1	0.03	2.0378E-07	1	0.03	2.03777E-07

4404-43-7	**4404437**	641	4,4'-bis[4-[bis(2-hydroxyethyl)amino]-6-anilino-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonic acid	917.01	3_REACH			**1**	**0.3**	**3.2715E-07**			**1**	**0.03**	**3.2715E-08**			**1**	**0.03**	**3.2715E-08**
4431-83-8	**4431838**	2921	2,5,7,10-tetraoxaundecane	164.2	3_REACH			**1**	**0.3**	**1.827E-06**			**1**	**0.03**	**1.827E-07**			**1**	**0.03**	**1.82704E-07**
4443-26-9	**4443269**	2925	1,3-dihydro-1,3-dioxo-2H-isoindole-2-hexanoic acid	261.28	3_REACH			**1**	**0.3**	**1.1482E-06**			**1**	**0.03**	**1.1482E-07**			**1**	**0.03**	**1.14819E-07**
4457-71-0	**4457710**	2927	3-methylpentane-1,5-diol	118.18	3_REACH			**1**	**0.3**	**2.5385E-06**			**1**	**0.03**	**2.5385E-07**			**1**	**0.03**	**2.5385E-07**
4488-57-7	**4488577**	2933	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	134.22	3_REACH			**1**	**0.3**	**2.2351E-06**			**1**	**0.03**	**2.2351E-07**			**1**	**0.03**	**2.23514E-07**
4500-29-2	**4500292**	2936	2,2'-(cyclohexylimino)bisethanol	187.28	3_REACH			**1**	**0.3**	**1.6019E-06**			**1**	**0.03**	**1.6019E-07**			**1**	**0.03**	**1.60188E-07**
4511-42-6	**4511426**	2938	(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione	144.13	3_REACH			**1**	**0.3**	**2.0815E-06**			**1**	**0.03**	**2.0815E-07**			**1**	**0.03**	**2.08145E-07**
4531-49-1	**4531491**	2939	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methoxyphenyl)-3-oxobutyramide]	689.56	3_REACH			**1**	**0.3**	**4.3506E-07**			**1**	**0.03**	**4.3506E-08**			**1**	**0.03**	**4.3506E-08**
4559-86-8	**4559868**	2943	tetrabutylurea	284.49	3_REACH			**1**	**0.3**	**1.0545E-06**			**1**	**0.03**	**1.0545E-07**			**1**	**0.03**	**1.05452E-07**
461-58-5	**461585**	2948	cyanoguanidine	84.086	3_REACH			**1**	**0.3**	**3.5678E-06**			**1**	**0.03**	**3.5678E-07**			**1**	**0.03**	**3.56778E-07**
462-94-2	**462942**	2950	pentamethylenediamine	102.18	3_REACH			**1**	**0.3**	**2.936E-06**			**1**	**0.03**	**2.936E-07**			**1**	**0.03**	**2.936E-07**
4635-59-0	**4635590**	2951	4-chlorobutyryl chloride	141	3_REACH			**1**	**0.3**	**2.1277E-06**			**1**	**0.03**	**2.1277E-07**			**1**	**0.03**	**2.12766E-07**
4651-67-6	**4651676**	2954	Nutriacholic acid	390.56	3_REACH			**1**	**0.3**	**7.6813E-07**			**1**	**0.03**	**7.6813E-08**			**1**	**0.03**	**7.68128E-08**
4672-38-2	**4672382**	2957	propylphosphonic acid	124.08	3_REACH			**1**	**0.3**	**2.4178E-06**			**1**	**0.03**	**2.4178E-07**			**1**	**0.03**	**2.41779E-07**
470-82-6	**470826**	645	cineole	154.25	3_REACH			**1**	**0.3**	**1.9449E-06**			**1**	**0.03**	**1.9449E-07**			**1**	**0.03**	**1.94489E-07**
4724-48-5	**4724485**	2964	octylphosphonic acid	194.21	3_REACH			**1**	**0.3**	**1.5447E-06**			**1**	**0.03**	**1.5447E-07**			**1**	**0.03**	**1.54472E-07**
474-25-9	**474259**	2966	chenodeoxycholic acid	392.58	3_REACH			**1**	**0.3**	**7.6418E-07**			**1**	**0.03**	**7.6418E-08**			**1**	**0.03**	**7.64175E-08**
479-27-6	**479276**	646	1,8-naphthylenediamine	158.21	3_REACH			**1**	**0.3**	**1.8962E-06**			**1**	**0.03**	**1.8962E-07**			**1**	**0.03**	**1.89621E-07**
4813-57-4	**4813574**	2971	octadecyl acrylate	324.55	3_REACH			**1**	**0.3**	**9.2436E-07**			**1**	**0.03**	**9.2436E-08**			**1**	**0.03**	**9.24357E-08**
48145-04-6	**48145046**	2972	2-phenoxyethyl acrylate	192.21	3_REACH			**1**	**0.3**	**1.5608E-06**			**1**	**0.03**	**1.5608E-07**			**1**	**0.03**	**1.56079E-07**
482-89-3	**482893**	647	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	262.27	3_REACH			**1**	**0.3**	**1.1439E-06**			**1**	**0.03**	**1.1439E-07**			**1**	**0.03**	**1.14386E-07**
4904-61-4	**4904614**	648	cyclododeca-1,5,9-triene	162.28	3_REACH			**1**	**0.3**	**1.8487E-06**			**1**	**0.03**	**1.8487E-07**			**1**	**0.03**	**1.84866E-07**
4948-15-6	**4948156**	2983	2,9-bis(3,5-dimethylphenyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone	598.66	3_REACH			**1**	**0.3**	**5.0112E-07**			**1**	**0.03**	**5.0112E-08**			**1**	**0.03**	**5.01119E-08**
497-18-7	**497187**	2989	carbonohydrazide	90.09	3_REACH			**1**	**0.3**	**3.33E-06**			**1**	**0.03**	**3.33E-07**			**1**	**0.03**	**3.33E-07**
4979-32-2	**4979322**	2990	N,N-dicyclohexylbenzothiazole-2-sulphenamide	346.56	3_REACH			**1**	**0.3**	**8.6565E-07**			**1**	**0.03**	**8.6565E-08**			**1**	**0.03**	**8.65651E-08**
50-21-5	**50215**	654	lactic acid	90.078	3_REACH	250000	250000	**0**	**250000**	**2.77537245**			**1**	**0.03**	**3.3304E-07**			**1**	**0.03**	**3.33045E-07**
502-44-3	**502443**	2999	hexan-6-olide	114.14	3_REACH			**1**	**0.3**	**2.6284E-06**			**1**	**0.03**	**2.6284E-07**			**1**	**0.03**	**2.62835E-07**
5026-74-4	**5026744**	3000	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	277.32	3_REACH			**1**	**0.3**	**1.0818E-06**			**1**	**0.03**	**1.0818E-07**			**1**	**0.03**	**1.08178E-07**
5036-48-6	**5036486**	3003	1H-imidazole-1-propylamine	125.18	3_REACH			**1**	**0.3**	**2.3965E-06**			**1**	**0.03**	**2.3965E-07**			**1**	**0.03**	**2.39655E-07**
503-74-2	**503742**	657	isovaleric acid	102.13	3_REACH			**1**	**0.3**	**2.9374E-06**			**1**	**0.03**	**2.9374E-07**			**1**	**0.03**	**2.93743E-07**
504-29-0	**504290**	658	2-pyridylamine	94.119	3_REACH			**1**	**0.3**	**3.1875E-06**			**1**	**0.03**	**3.1875E-07**			**1**	**0.03**	**3.18745E-07**
504-63-2	**504632**	660	propane-1,3-diol	76.095	3_REACH	2472333.333	2472333.333	**0**	**2472333.33**	**32.4900891**			**1**	**0.03**	**3.9424E-07**			**1**	**0.03**	**3.94244E-07**
506-30-9	**506309**	3012	icosanoic acid	312.54	3_REACH			**1**	**0.3**	**9.5988E-07**			**1**	**0.03**	**9.5988E-08**			**1**	**0.03**	**9.59877E-08**
507448-65-9	**507448659**	3018	ethyl (2Z)-4,4,4-trifluoro-3-(methylamino)but-2-enoate	197.16	3_REACH			**1**	**0.3**	**1.5216E-06**			**1**	**0.03**	**1.5216E-07**			**1**	**0.03**	**1.52161E-07**
5089-70-3	**5089703**	3022	(3-chloropropyl)triethoxysilane	240.8	3_REACH			**1**	**0.3**	**1.2458E-06**			**1**	**0.03**	**1.2458E-07**			**1**	**0.03**	**1.24585E-07**
5102-83-0	**5102830**	3025	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	685.62	3_REACH			**1**	**0.3**	**4.3756E-07**			**1**	**0.03**	**4.3756E-08**			**1**	**0.03**	**4.3756E-08**
51-03-6	**51036**	667	2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether	338.44	3_REACH	150	150	**0**	**150**	**0.00044321**	30	30	**0**	**30**	**8.8642E-05**	250	250	**0**	**250**	**0.000738683**
51167-18-1	**51167181**	3028	2'-[2,4-dichloro-5-(1-methylethoxy)phenyl]-2,2-dimethylpropionohydrazide	319.23	3_REACH			**1**	**0.3**	**9.3976E-07**			**1**	**0.03**	**9.3976E-08**			**1**	**0.03**	**9.39761E-08**
5124-30-1	**5124301**	3030	4,4'-methylenedicyclohexyl diisocyanate	262.36	3_REACH			**1**	**0.3**	**1.1435E-06**			**1**	**0.03**	**1.1435E-07**			**1**	**0.03**	**1.14347E-07**
51-28-5	**51285**	57	2,4-dinitrophenol	184.11	3_REACH	1000	1000	**0**	**1000**	**0.00543154**	2000	2000	**0**	**2000**	**0.01086307**	2000	2000	**0**	**2000**	**0.010863071**
5131-66-8	**5131668**	3032	1-butoxypropan-2-ol	132.2	3_REACH			**1**	**0.3**	**2.2693E-06**			**1**	**0.03**	**2.2693E-07**			**1**	**0.03**	**2.26929E-07**
51920-12-8	**51920128**	3049	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-methyl-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide	560.6	3_REACH			**1**	**0.3**	**5.3514E-07**			**1**	**0.03**	**5.3514E-08**			**1**	**0.03**	**5.35141E-08**
5208-93-5	**5208935**	3052	3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol	220.36	3_REACH			**1**	**0.3**	**1.3614E-06**			**1**	**0.03**	**1.3614E-07**			**1**	**0.03**	**1.36141E-07**
521-18-6	**521186**	672	androstanolone	290.45	3_REACH			**1**	**0.3**	**1.0329E-06**			**1**	**0.03**	**1.0329E-07**			**1**	**0.03**	**1.03288E-07**
52449-76-0	**52449760**	3059	Methyl 4-cyano-2-nitrobenzoate	206.16	3_REACH			**1**	**0.3**	**1.4552E-06**			**1**	**0.03**	**1.4552E-07**			**1**	**0.03**	**1.45518E-07**
52-51-7	**52517**	674	bronopol	200	3_REACH	560	560	**0**	**560**	**0.0028**			**1**	**0.03**	**0.00000015**			**1**	**0.03**	**0.00000015**
52722-86-8	**52722868**	3072	4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	201.31	3_REACH			**1**	**0.3**	**1.4902E-06**			**1**	**0.03**	**1.4902E-07**			**1**	**0.03**	**1.49024E-07**
5280-68-2	**5280682**	3074	N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide	611.06	3_REACH			**1**	**0.3**	**4.9095E-07**			**1**	**0.03**	**4.9095E-08**			**1**	**0.03**	**4.9095E-08**
5280-80-8	**5280808**	3076	3,3'-[(2,5-dimethyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]	916.66	3_REACH			**1**	**0.3**	**3.2728E-07**			**1**	**0.03**	**3.2728E-08**			**1**	**0.03**	**3.27275E-08**
52829-07-9	**52829079**	3077	bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	480.74	3_REACH			**1**	**0.3**	**6.2404E-07**			**1**	**0.03**	**6.2404E-08**			**1**	**0.03**	**6.24038E-08**
5283-66-9	**5283669**	678	octyltrichlorosilane	247.67	3_REACH	100000	100000	**0**	**100000**	**0.40376307**			**1**	**0.03**	**1.2113E-07**			**1**	**0.03**	**1.21129E-07**
52846-56-7	**52846567**	3078	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(4-nitrophenyl)azo]-3-oxobutyramide	382.34	3_REACH			**1**	**0.3**	**7.8464E-07**			**1**	**0.03**	**7.8464E-08**			**1**	**0.03**	**7.84642E-08**
5292-45-5	**5292455**	680	dimethyl 2-nitroterephthalate	239.18	3_REACH			**1**	**0.3**	**1.2543E-06**			**1**	**0.03**	**1.2543E-07**			**1**	**0.03**	**1.25429E-07**
5308-25-8	**5308258**	3087	1-ethylpiperazine	114.19	3_REACH			**1**	**0.3**	**2.6272E-06**			**1**	**0.03**	**2.6272E-07**			**1**	**0.03**	**2.6272E-07**
53-16-7	**53167**	61	estrone	270.37	3_REACH			**1**	**0.3**	**1.1096E-06**			**1**	**0.03**	**1.1096E-07**			**1**	**0.03**	**1.10959E-07**
53306-54-0	**53306540**	3094	bis(2-propylheptyl) phthalate	446.67	3_REACH			**1**	**0.3**	**6.7164E-07**			**1**	**0.03**	**6.7164E-08**			**1**	**0.03**	**6.71637E-08**
5333-42-6	**5333426**	3096	2-octyldodecan-1-ol	298.56	3_REACH			**1**	**0.3**	**1.0048E-06**			**1**	**0.03**	**1.0048E-07**			**1**	**0.03**	**1.00482E-07**
5333-84-6	**5333846**	3097	1,2,3,6-tetrahydro-3-methylphthalic anhydride	166.18	3_REACH			**1**	**0.3**	**1.8053E-06**			**1**	**0.03**	**1.8053E-07**			**1**	**0.03**	**1.80527E-07**
534-03-2	**534032**	3100	2-aminopropane-1,3-diol	91.111	3_REACH			**1**	**0.3**	**3.2927E-06**			**1**	**0.03**	**3.2927E-07**			**1**	**0.03**	**3.29269E-07**
5343-92-0	**5343920**	3102	pentane-1,2-diol	104.15	3_REACH			**1**	**0.3**	**2.8805E-06**			**1**	**0.03**	**2.8805E-07**			**1**	**0.03**	**2.88046E-07**
53445-37-7	**53445377**	3103	2,2,4(or 2,4,4)-trimethyladipic acid	188.22	3_REACH			**1**	**0.3**	**1.5939E-06**			**1**	**0.03**	**1.5939E-07**			**1**	**0.03**	**1.59388E-07**
534-52-1	**534521**	682	2-methyl-4,6-dinitro-phenol DNOC	198.14	3_REACH	48.33333333	48.33333333	**0**	**48.3333333**	**0.00024394**	210	210	**0**	**210**	**0.00105986**	600	600	**0**	**600**	**0.003028162**
53651-69-7	**53651697**	3107	Propanoic acid	132.16	3_REACH			**1**	**0.3**	**2.27E-06**			**1**	**0.03**	**2.27E-07**			**1**	**0.03**	**2.26998E-07**
5372-81-6	**5372816**	683	dimethyl 2-aminoterephthalate	209.2	3_REACH			**1**	**0.3**	**1.434E-06**			**1**	**0.03**	**1.434E-07**			**1**	**0.03**	**1.43403E-07**
540-97-6	**540976**	3124	dodecamethylcyclohexasiloxane	444.93	3_REACH			**1**	**0.3**	**6.7426E-07**			**1**	**0.03**	**6.7426E-08**			**1**	**0.03**	**6.74263E-08**
541-02-6	**541026**	3125	decamethylcyclopentasiloxane	370.77	3_REACH			**1**	**0.3**	**8.0913E-07**			**1**	**0.03**	**8.0913E-08**			**1**	**0.03**	**8.09127E-08**
5413-60-5	**5413605**	3128	3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate	192.26	3_REACH			**1**	**0.3**	**1.5604E-06**			**1**	**0.03**	**1.5604E-07**			**1**	**0.03**	**1.56039E-07**
541-73-1	**541731**	685	1,3-dichlorobenzene	147	3_REACH	400	400	**0**	**400**	**0.00272109**	300	300	**0**	**300**	**0.00204082**	500	500	**0**	**500**	**0.003401361**
542-05-2	**542052**	3134	3-oxoglutaric acid	146.1	3_REACH			**1**	**0.3**	**2.0534E-06**			**1**	**0.03**	**2.0534E-07**			**1**	**0.03**	**2.05339E-07**
5435-64-3	**5435643**	3140	3,5,5-trimethylhexanal	142.24	3_REACH			**1**	**0.3**	**2.1091E-06**			**1**	**0.03**	**2.1091E-07**			**1**	**0.03**	**2.10911E-07**
544-01-4	**544014**	3141	diisopentyl ether	158.29	3_REACH			**1**	**0.3**	**1.8953E-06**			**1**	**0.03**	**1.8953E-07**			**1**	**0.03**	**1.89526E-07**
54423-67-5	**54423675**	3143	vinyl neononanoate	184.28	3_REACH			**1**	**0.3**	**1.628E-06**			**1**	**0.03**	**1.628E-07**			**1**	**0.03**	**1.62796E-07**
5466-77-3	**5466773**	3151	2-ethylhexyl 4-methoxycinnamate	290.4	3_REACH			**1**	**0.3**	**1.0331E-06**			**1**	**0.03**	**1.0331E-07**			**1**	**0.03**	**1.03306E-07**
5468-75-7	**5468757**	3152	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide]	657.56	3_REACH			**1**	**0.3**	**4.5623E-07**			**1**	**0.03**	**4.5623E-08**			**1**	**0.03**	**4.56232E-08**
54839-24-6	**54839246**	3154	2-ethoxy-1-methylethyl acetate	146.19	3_REACH			**1**	**0.3**	**2.0521E-06**			**1**	**0.03**	**2.0521E-07**			**1**	**0.03**	**2.05212E-07**
54914-37-3	**54914373**	3156	1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]cyclohexanemethylamine	278.49	3_REACH			**1**	**0.3**	**1.0772E-06**			**1**	**0.03**	**1.0772E-07**			**1**	**0.03**	**1.07724E-07**
5521-31-3	**5521313**	3163	2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone	418.41	3_REACH			**1**	**0.3**	**7.17E-07**			**1**	**0.03**	**7.17E-08**			**1**	**0.03**	**7.17E-08**
55314-16-4	**55314164**	3166	611-255-8	176.22	3_REACH			**1**	**0.3**	**1.7024E-06**			**1**	**0.03**	**1.7024E-07**			**1**	**0.03**	**1.70242E-07**
553-86-6	**553866**	3169	(3H)-benzofuran-2-one	134.13	3_REACH			**1**	**0.3**	**2.2366E-06**			**1**	**0.03**	**2.2366E-07**			**1**	**0.03**	**2.23664E-07**
554-00-7	**554007**	700	2,4-dichloroaniline	162.02	3_REACH	166.6666667	166.6666667	**0**	**166.666667**	**0.00102868**	15	15	**0**	**15**	**9.2581E-05**			**1**	**0.03**	**1.85162E-07**
556-67-2	**556672**	705	octamethylcyclotetrasiloxane	296.62	3_REACH			**1**	**0.3**	**1.0114E-06**	5.04975247	5.049752469	**0**	**5.04975247**	**1.7024E-05**	5.049752469	5.049752469	**0**	**5.049752469**	**1.70243E-05**
5567-15-7	**5567157**	706	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]	818.5	3_REACH			**1**	**0.3**	**3.6652E-07**			**1**	**0.03**	**3.6652E-08**			**1**	**0.03**	**3.66524E-08**
556-88-7	**556887**	707	1-nitroguanidine	104.07	3_REACH	341333.3333	341333.3333	**0**	**341333.333**	**3.27984369**			**1**	**0.03**	**2.8827E-07**			**1**	**0.03**	**2.88268E-07**
5578-42-7	**5578427**	3177	dichlorocyclohexylmethylsilane	197.18	3_REACH			**1**	**0.3**	**1.5215E-06**			**1**	**0.03**	**1.5215E-07**			**1**	**0.03**	**1.52145E-07**
5580-57-4	**5580574**	3178	3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(3-chloro-o-tolyl)benzamide]	937.08	3_REACH			**1**	**0.3**	**3.2014E-07**			**1**	**0.03**	**3.2014E-08**			**1**	**0.03**	**3.20143E-08**
5580-58-5	**5580585**	3179	3,3'-[(2,5-dichloro-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]	957.49	3_REACH			**1**	**0.3**	**3.1332E-07**			**1**	**0.03**	**3.1332E-08**			**1**	**0.03**	**3.13319E-08**
55934-93-5	**55934935**	3182	[(butoxymethylethoxy)methylethoxy]propan-1-ol	248.36	3_REACH			**1**	**0.3**	**1.2079E-06**			**1**	**0.03**	**1.2079E-07**			**1**	**0.03**	**1.20792E-07**
561-41-1	**561411**	3187	4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol	375.52	3_REACH			**1**	**0.3**	**7.9889E-07**			**1**	**0.03**	**7.9889E-08**			**1**	**0.03**	**7.98892E-08**
56-18-8	**56188**	3188	3,3'-iminodi(propylamine)	131.23	3_REACH			**1**	**0.3**	**2.2861E-06**			**1**	**0.03**	**2.2861E-07**			**1**	**0.03**	**2.28606E-07**
56309-94-5	**56309945**	4472	4-(1,4-dioxa-spiro[4.5]dec-8-yl)-cyclohexanone	238.33	3_REACH			**1**	**0.3**	**1.2588E-06**			**1**	**0.03**	**1.2588E-07**			**1**	**0.03**	**1.25876E-07**
56358-17-9	**56358179**	3192	N-(2-ethylhexyl)naphthalen-2-amine	255.41	3_REACH			**1**	**0.3**	**1.1746E-06**			**1**	**0.03**	**1.1746E-07**			**1**	**0.03**	**1.17458E-07**
56-41-7	**56417**	3198	L-alanine	89.095	3_REACH			**1**	**0.3**	**3.3672E-06**			**1**	**0.03**	**3.3672E-07**			**1**	**0.03**	**3.36719E-07**
56519-71-2	**56519712**	3200	Propane-1,3-diyl dioctanoate	328.49	3_REACH			**1**	**0.3**	**9.1327E-07**			**1**	**0.03**	**9.1327E-08**			**1**	**0.03**	**9.1327E-08**
56539-66-3	**56539663**	3201	3-methoxy-3-methylbutan-1-ol	118.18	3_REACH			**1**	**0.3**	**2.5385E-06**			**1**	**0.03**	**2.5385E-07**			**1**	**0.03**	**2.5385E-07**
56677-60-2	**56677602**	3208	tetradecyl chloroformate	276.85	3_REACH			**1**	**0.3**	**1.0836E-06**			**1**	**0.03**	**1.0836E-07**			**1**	**0.03**	**1.08362E-07**
56706-10-6	**56706106**	3209	4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecane	474.83	3_REACH			**1**	**0.3**	**6.3181E-07**			**1**	**0.03**	**6.3181E-08**			**1**	**0.03**	**6.31805E-08**

56718-71-9	56718710	3211	p-(2-methoxyethyl)phenol	152.19	3_REACH			1	0.3	1.9712E-06			1	0.03	1.9712E-07			1	0.03	1.97122E-07
56-84-8	56848	3212	aspartic acid	133.1	3_REACH			1	0.3	2.2538E-06			1	0.03	2.2538E-07			1	0.03	2.25384E-07
56962-04-0	56962040	3217	3-Bromo-5-chlorophenol	207.46	3_REACH			1	0.3	1.4461E-06			1	0.03	1.4461E-07			1	0.03	1.44605E-07
56973-87-6	56973876	4267	1-(3,3-dimethylcyclohexyl)pent-4-en-1-one	194.32	3_REACH			1	0.3	1.5438E-06			1	0.03	1.5438E-07			1	0.03	1.54385E-07
57090-45-6	57090456	4249	(R)-3-chloropropane-1,2-diol	110.54	3_REACH			1	0.3	2.7139E-06			1	0.03	2.7139E-07			1	0.03	2.71395E-07
5726-19-2	5726192	3228	2-methylcyclohexyl acetate	156.22	3_REACH			1	0.3	1.9204E-06			1	0.03	1.9204E-07			1	0.03	1.92037E-07
57374-49-9	57374499	4553	methyl 3-acetoxy-2-pentyl-2-cyclopentene-1-acetate	268.35	3_REACH			1	0.3	1.1176E-06			1	0.03	1.1176E-07			1	0.03	1.11764E-07
576-26-1	576261	723	2,6-xylenol	122.17	3_REACH			1	0.3	2.4556E-06			1	0.03	2.4556E-07			1	0.03	2.45559E-07
5766-67-6	5766676	3236	ethylenediaminetetraacetonitrile	216.25	3_REACH			1	0.3	1.3873E-06			1	0.03	1.3873E-07			1	0.03	1.38728E-07
57843-53-5	57843536	3238	N,N,N',N'-tetakis(2-hydroxypropyl)adipamide	376.5	3_REACH			1	0.3	7.9681E-07			1	0.03	7.9681E-08			1	0.03	7.96813E-08
58190-57-1	58190571	3242	2-Propanone, 2,2',2"-(O,O',O"-(ethylsilylidyne)trioxime)	273.41	3_REACH			1	0.3	1.0973E-06			1	0.03	1.0973E-07			1	0.03	1.09725E-07
583-39-1	583391	3244	benzimidazole-2-thiol	150.21	3_REACH			1	0.3	1.9972E-06			1	0.03	1.9972E-07			1	0.03	1.99725E-07
583-78-8	583788	728	2,4,6-trichlorophenol	197	3_REACH			1	0.3	1.8405E-06			1	0.03	1.8405E-07			1	0.03	1.84046E-07
58430-94-7	58430947	3247	3,5,5-trimethylhexyl acetate	186.29	3_REACH			1	0.3	1.6104E-06			1	0.03	1.6104E-07			1	0.03	1.61039E-07
584-84-9	584849	729	4-methyl-m-phenylene diisocyanate	174.16	3_REACH			1	0.3	1.7226E-06			1	0.03	1.7226E-07			1	0.03	1.72265E-07
58567-11-6	58567116	3249	(ethoxymethoxy)cyclododecane	242.4	3_REACH			1	0.3	1.2376E-06			1	0.03	1.2376E-07			1	0.03	1.23762E-07
586-62-9	586629	731	α-mentha-1,4(8)-diene	136.24	3_REACH	1950	1950	0	1950	0.01431269			1	0.03	2.202E-07			1	0.03	2.2025E-07
58670-89-6	58670896	3252	2-decyltetradecanol	354.66	3_REACH			1	0.3	8.4598E-07			1	0.03	8.4598E-08			1	0.03	8.45981E-08
5888-33-5	5888335	3257	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate	208.3	3_REACH			1	0.3	1.4402E-06			1	0.03	1.4402E-07			1	0.03	1.44023E-07
5888-87-9	5888879	3258	N,N'-hexane-1,6-diylbis(hexahydro-2-oxo-1H-azepine-1-carboxamide)	394.52	3_REACH			1	0.3	7.6042E-07			1	0.03	7.6042E-08			1	0.03	7.60418E-08
591-27-5	591275	734	3-aminoacetonitrile	109.13	3_REACH	366.6666667	366.6666667	0	366.6666667	0.00335991			1	0.03	2.7495E-07			1	0.03	2.74901E-07
59227-88-2	59227882	4300	1-octylazepin-2-one	225.38	3_REACH			1	0.3	1.3311E-06			1	0.03	1.3311E-07			1	0.03	1.33109E-07
59447-55-1	59447551	3278	(pentabromophenyl)methyl acrylate	556.7	3_REACH			1	0.3	5.3869E-07			1	0.03	5.3869E-08			1	0.03	5.3869E-08
59487-23-9	59487239	3279	4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide	654.08	3_REACH			1	0.3	4.5866E-07			1	0.03	4.5866E-08			1	0.03	4.58659E-08
59-50-7	59507	737	chlorocresol	142.59	3_REACH	500	500	0	500	0.00350956	1300	1300	0	1300	0.00911705	1300	1300	0	1300	0.009117049
59719-67-4	59719674	3284	bis[2-(2-(1-methylethyl)-3-oxazolidinyl)ethyl] hexan-1,6-diylbiscarbamate	486.66	3_REACH			1	0.3	6.1645E-07			1	0.03	6.1645E-08			1	0.03	6.16447E-08
5989-27-5	5989275	743	(R)-Limonene	136.24	3_REACH	282.5	282.5	0	282.5	0.00207855			1	0.03	2.202E-07			1	0.03	2.2025E-07
5989-54-8	5989548	744	(S)-Limonene	136.24	3_REACH	2406.666667	2406.666667	0	2406.666667	0.01769491			1	0.03	2.202E-07			1	0.03	2.2025E-07
599-04-2	599042	3296	2,4-dihydroxy-3,3-dimethylbutyric acid gamma lactone	130.14	3_REACH			1	0.3	2.3052E-06			1	0.03	2.3052E-07			1	0.03	2.30521E-07
599-61-1	599611	3298	3,3'-sulfonylbis(aniline)	248.31	3_REACH			1	0.3	1.2062E-06			1	0.03	1.2062E-07			1	0.03	1.20617E-07
599-64-4	599644	3299	P-Cumylphenol	212.29	3_REACH			1	0.3	1.4132E-06			1	0.03	1.4132E-07			1	0.03	1.41316E-07
60-00-4	60004	71	edetic acid	292.25	3_REACH	37666.66667	37666.66667	0	37666.6667	0.12889509			1	0.03	1.0265E-07			1	0.03	1.02652E-07
60-09-3	60093	746	4-aminoazobenzene	197.24	3_REACH			1	0.3	1.521E-06			1	0.03	1.521E-07			1	0.03	1.52099E-07
60111-54-8	60111548	3304	3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-diphenylsilazane	432.89	3_REACH			1	0.3	6.9302E-07			1	0.03	6.9302E-08			1	0.03	6.93017E-08
60-12-8	60128	3306	2-phenylethanol	122.17	3_REACH			1	0.3	2.4556E-06			1	0.03	2.4556E-07			1	0.03	2.45559E-07
603-35-0	603350	751	triphenylphosphine	262.29	3_REACH			1	0.3	1.1438E-06			1	0.03	1.1438E-07			1	0.03	1.14377E-07
6041-94-7	6041947	3310	4-[[2,5-dichlorophenyl]azo]-3-hydroxy-N-phenylnaphthalene-2-carboxamide	436.3	3_REACH			1	0.3	6.876E-07			1	0.03	6.876E-08			1	0.03	6.8765E-08
60658-04-0	60658040	4438	Ethyl 2-(3-benzoylphenyl)propanoate	282.34	3_REACH			1	0.3	1.0625E-06			1	0.03	1.0625E-07			1	0.03	1.06255E-07
608-25-3	608253	3317	2-methylresorcinol	124.14	3_REACH			1	0.3	2.4166E-06			1	0.03	2.4166E-07			1	0.03	2.41663E-07
611-06-3	611063	755	1,3-dichloro-4-nitrobenzene	192	3_REACH	1400	1400	0	1400	0.00729167			1	0.03	1.5625E-07			1	0.03	1.56255E-07
611-19-8	611198	3326	2,4-dichlorobenzyl chloride	161.03	3_REACH			1	0.3	1.8635E-06			1	0.03	1.8635E-07			1	0.03	1.86351E-07
611-70-1	611701	3328	isobutylbenzene	148.21	3_REACH			1	0.3	2.0242E-06			1	0.03	2.0242E-07			1	0.03	2.02416E-07
61260-55-7	61260557	3330	N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine	394.7	3_REACH			1	0.3	7.6007E-07			1	0.03	7.6007E-08			1	0.03	7.60071E-08
613-62-7	613627	4310	2-(phenylmethoxy)naphthalene	234.3	3_REACH			1	0.3	1.2804E-06			1	0.03	1.2804E-07			1	0.03	1.28041E-07
614-45-9	614459	3334	tert-butyl methanoate	194.23	3_REACH			1	0.3	1.5446E-06			1	0.03	1.5446E-07			1	0.03	1.54455E-07
615-20-3	615203	3338	2-chlorobenzonitrile	169.63	3_REACH			1	0.3	1.7886E-06			1	0.03	1.7886E-07			1	0.03	1.78865E-07
615-60-1	615601	3339	4-chloro-o-cresol	142.61	3_REACH			1	0.3	2.1336E-06			1	0.03	2.1336E-07			1	0.03	2.13355E-07
61597-98-6	61597986	3340	4-Methyl lactate	208.33	3_REACH			1	0.3	1.3136E-06			1	0.03	1.3136E-07			1	0.03	1.31365E-07
616-45-5	616455	757	2-pyrrolidone	85.107	3_REACH	4403.333333	4403.333333	0	4403.33333	0.05173679			1	0.03	3.5256E-07			1	0.03	3.52497E-07
616-47-7	616477	3346	1-methylimidazole	82.108	3_REACH			1	0.3	3.6537E-06			1	0.03	3.6537E-07			1	0.03	3.65372E-07
6166-86-5	6166865	3347	pentamethylcyclopentasiloxane	295.6	3_REACH			1	0.3	1.0149E-06			1	0.03	1.0149E-07			1	0.03	1.01488E-07
61826-76-4	61826764	4625	(S)-2-Hydroxy-2-(3-phenoxyphenyl)acetonitrile	225.25	3_REACH			1	0.3	1.3319E-06			1	0.03	1.3319E-07			1	0.03	1.33185E-07
61847-48-1	61847481	3356	methyl 4-[[[2,5-dichlorophenyl]amino]carbonyl]-2-[[2-hydroxy-3-[[(2-methoxyphenyl)amino]carbonyl]-1-naphthyl]azo]benzoate	643.49	3_REACH			1	0.3	4.6621E-07			1	0.03	4.6621E-08			1	0.03	4.66208E-08
618-62-2	618622	759	3,5-dichloronitrobenzene	192	3_REACH	2500	2500	0	2500	0.01302083			1	0.03	1.5625E-07			1	0.03	1.56255E-07
618-88-2	618882	3358	5-nitroisophthalic acid	211.13	3_REACH			1	0.3	1.4206E-06			1	0.03	1.4206E-07			1	0.03	1.42093E-07
6197-30-4	6197304	3360	octocrylene	361.49	3_REACH			1	0.3	8.2966E-07			1	0.03	8.2966E-08			1	0.03	8.29665E-08
621-29-4	621294	3362	methyl isovalerate	133.15	3_REACH			1	0.3	2.2531E-06			1	0.03	2.2531E-07			1	0.03	2.25315E-07
62-23-7	62237	761	4-nitrobenzoic acid	167.12	3_REACH			1	0.3	1.7561E-06			1	0.03	1.7561E-07			1	0.03	1.75612E-07
622-40-2	622402	762	2-methylbutanal	133.15	3_REACH			1	0.3	2.2566E-06			1	0.03	2.2566E-07			1	0.03	2.25663E-07
622-58-2	622582	3365	methyl isovalerate	133.15	3_REACH			1	0.3	2.2531E-06			1	0.03	2.2531E-07			1	0.03	2.25315E-07
623-03-0	623030	763	4-chlorobenzonitrile	137.57	3_REACH			1	0.3	2.1807E-06			1	0.03	2.1807E-07			1	0.03	2.18077E-07
623-40-5	623405	4785	2-Pentanone oxime	101.15	3_REACH			1	0.3	2.9656E-06			1	0.03	2.9656E-07			1	0.03	2.96559E-07
624-54-4	624544	3370	neptyl propionate	144.21	3_REACH			1	0.3	2.0803E-06			1	0.03	2.0803E-07			1	0.03	2.08035E-07
62-53-3	62533	765	aniline	93.13	3_REACH	26.66666667	26.66666667	0	26.6666667	0.00028634	4	4	0	4	4.2861E-05	4	4	0	4	4.28607E-05
62-56-6	62566	767	thiourea	76.123	3_REACH	3000	3000	0	3000	0.0394069			1	0.03	3.9415E-07			1	0.03	3.94069E-07
6259-76-3	6259763	3375	hexyl salicylate	222.28	3_REACH			1	0.3	1.3496E-06			1	0.03	1.3496E-07			1	0.03	1.34965E-07
626-43-7	626437	768	3,5-dichloroaniline	162.02	3_REACH	373.3333333	373.3333333	0	373.333333	0.02304244			1	0.03	1.8616E-07			1	0.03	1.86162E-07
6284-40-8	6284408	770	menthylamine	156.27	3_REACH			1	0.3	1.5367E-06			1	0.03	1.5367E-07			1	0.03	1.53673E-07
62889-66-1	62889661	3379	[illegible]	316.64	3_REACH			1	0.3	9.5076E-07			1	0.03	9.5076E-08			1	0.03	9.50761E-08
628-89-7	628897	3380	2-(2-chloroethoxy)ethanol	124.57	3_REACH			1	0.3	2.4083E-06			1	0.03	2.4083E-07			1	0.03	2.40828E-07
628-96-6	628966	3382	ethylene dinitrate	152.06	3_REACH			1	0.3	1.9729E-06			1	0.03	1.9729E-07			1	0.03	1.97291E-07
629-11-8	629118	3385	hexane-1,6-diol	118.18	3_REACH			1	0.3	2.5385E-06			1	0.03	2.5385E-07			1	0.03	2.53855E-07
6291-95-8	6291958	4276	1,3,5-tris(2-methyl-2-propenyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione	291.35	3_REACH			1	0.3	1.0297E-06			1	0.03	1.0297E-07			1	0.03	1.02969E-07
629-40-3	629403	771	suberonitrile	136.2	3_REACH			1	0.3	2.2029E-06			1	0.03	2.2029E-07			1	0.03	2.20264E-07
629-50-5	629505	3389	tridecane	184.37	3_REACH			1	0.3	1.6272E-06			1	0.03	1.6272E-07			1	0.03	1.62716E-07
629-59-4	629594	3390	tetradecane	198.39	3_REACH			1	0.3	1.5122E-06			1	0.03	1.5122E-07			1	0.03	1.51217E-07
629-62-9	629629	772	pentadecane	212.42	3_REACH			1	0.3	1.4123E-06			1	0.03	1.4123E-07			1	0.03	1.41235E-07
629-73-2	629732	3391	hexadec-1-ene	224.43	3_REACH			1	0.3	1.3357E-06			1	0.03	1.3357E-07			1	0.03	1.33672E-07
629-82-3	629823	3392	dioctyl ether	242.45	3_REACH			1	0.3	1.2374E-06			1	0.03	1.2374E-07			1	0.03	1.23757E-07
63-05-8	63058	75	androst-4-ene-3,17-dione	286.42	3_REACH			1	0.3	1.0474E-06			1	0.03	1.0474E-07			1	0.03	1.04741E-07
6309-51-9	6309519	3394	isononyl laurate	270.46	3_REACH			1	0.3	1.1092E-06			1	0.03	1.1092E-07			1	0.03	1.10922E-07
6331-96-0	6331960	3399	2-amino-4,5-dichlorobenzenesulfonic acid	242.08	3_REACH			1	0.3	1.2393E-06			1	0.03	1.2393E-07			1	0.03	1.23926E-07
63562-34-5	63562345	3405	bis(2-hydroxyethyl) (6H-dibenz[c,e][1,2]oxaphosphorin-6-ylmethyl)succinate P-oxide	434.38	3_REACH			1	0.3	6.9064E-07			1	0.03	6.9064E-08			1	0.03	6.90645E-08
6358-30-1	6358301	3406	8,18-dichloro-5,15-diethyl-5,15-dihydrodindolo[3,2-b:3',2'-m]triphenodioxazine	589.49	3_REACH			1	0.3	5.0891E-07			1	0.03	5.0891E-08			1	0.03	5.08914E-08
6358-37-8	6358378	3408	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-methylphenyl)-3-oxobutyramide]	657.56	3_REACH			1	0.3	4.5623E-07			1	0.03	4.5623E-08			1	0.03	4.56232E-08
6358-64-1	6358641	3409	4-chloro-2,5-dimethoxyaniline	187.63	3_REACH			1	0.3	1.5969E-06			1	0.03	1.5969E-07			1	0.03	1.59689E-07
6358-85-6	6358856	3410	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]	629.51	3_REACH			1	0.3	4.7656E-07			1	0.03	4.7656E-08			1	0.03	4.76561E-08
636-30-6	636306	774	2,4,5-trichloroaniline	196.47	3_REACH	1133.333333	1133.333333	0	1133.33333	0.00578846			1	0.03	1.5275E-07			1	0.03	1.52695E-07
6386-38-5	6386385	3420	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	292.42	3_REACH			1	0.3	1.0259E-06			1	0.03	1.0259E-07			1	0.03	1.02592E-07
6410-32-8	6410328	3424	3-hydroxy-4-[(2-methyl-4-nitrophenyl)azo]-N-(o-tolyl)naphthalene-2-carboxamide	440.46	3_REACH			1	0.3	6.8111E-07			1	0.03	6.8111E-08			1	0.03	6.81106E-08
6410-41-9	6410419	3425	N-[5-chloro-2,4-dimethoxyphenyl]-4-[[5-[(diethylamino)sulphonyl]-2-methoxyphenyl]azo]-3-hydroxynaphthalene-2-carboxamide	627.12	3_REACH			1	0.3	4.7638E-07			1	0.03	4.7638E-08			1	0.03	4.76377E-08
6419-19-8	6419198	3429	nitrilotrimethylenetris(phosphonic acid)	299.05	3_REACH			1	0.3	1.0032E-06			1	0.03	1.0032E-07			1	0.03	1.00318E-07
6422-86-2	6422862	3430	bis(2-ethylhexyl) terephthalate	390.56	3_REACH			1	0.3	7.6813E-07			1	0.03	7.6813E-08			1	0.03	7.68128E-08
6425-39-4	6425394	3432	2,2'-dimorpholinyldiethyl ether	244.34	3_REACH			1	0.3	1.2278E-06			1	0.03	1.2278E-07			1	0.03	1.22785E-07
64354-92-3	64354923	3434	3-(isodecyloxy)propiononitrile	211.35	3_REACH			1	0.3	1.4194E-06			1	0.03	1.4194E-07			1	0.03	1.41945E-07
6440-58-0	6440580	779	1,3-bis(hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione	188.19	3_REACH	10000	10000	0	10000	0.05313779			1	0.03	5.5941E-07			1	0.03	1.59413E-07
6448-95-9	6448959	3436	3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthalene-2-carboxamide	426.44	3_REACH			1	0.3	7.035E-07			1	0.03	7.035E-08			1	0.03	7.03499E-08
645-62-5	645625	3438	2-ethylhex-2-enal	126.2	3_REACH			1	0.3	2.3772E-06			1	0.03	2.3772E-07			1	0.03	2.37718E-07
646-24-2	646242	3439	nonamethylenediamine	158.29	3_REACH			1	0.3	1.8983E-06			1	0.03	1.8983E-07			1	0.03	1.89832E-07
6485-40-1	6485401	781	l-p-mentha-1(6),8-dien-2-one	150.22	3_REACH			1	0.3	1.9971E-06			1	0.03	1.9971E-07			1	0.03	1.99707E-07
6485-55-8	6485558	3445	cis-2,6-dimethylmorpholine	115.18	3_REACH			1	0.3	2.6046E-06			1	0.03	2.6046E-07			1	0.03	2.60462E-07
6485-67-2	6485672	4453	(2R)-2-amino-2-phenylacetamide	150.18	3_REACH			1	0.3	1.9976E-06			1	0.03	1.9976E-07			1	0.03	1.99765E-07
6486-23-3	6486233	3446	2-[(4-chloro-2-nitrophenyl)azo]-N-(2-chlorophenyl)-3-oxobutyramide	395.21	3_REACH			1	0.3	7.5909E-07			1	0.03	7.5909E-08			1	0.03	7.5909E-08
6528-34-3	6528343	3450	2-[(4-methoxy-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide	386.37	3_REACH			1	0.3	7.7646E-07			1	0.03	7.7646E-08			1	0.03	7.76458E-08
65405-77-8	65405778	3452	(Z)-3-hexenyl salicylate	220.27	3_REACH			1	0.3	1.362E-06			1	0.03	1.362E-07			1	0.03	1.36196E-07
65-45-2	65452	784	salicylamide	137.14	3_REACH			1	0.3	2.1876E-06			1	0.03	2.1876E-07			1	0.03	2.18765E-07

65520-46-9	**65520469**	3455	bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] adipate	522.68	3_REACH			**1**	**0.3**	**5.7396E-07**			**1**	**0.03**	**5.7396E-08**			**1**	**0.03**	**5.73965E-08**
65-85-0	**65850**	785	benzoic acid	122.12	3_REACH	100000	100000	**0**	**100000**	**0.81886669**			**1**	**0.03**	**2.4566E-07**			**1**	**0.03**	**2.4566E-07**
65855-02-9	**65855029**	4291	1-benzyl-5-ethoxyimidazolidine-2,4-dione	234.26	3_REACH			**1**	**0.3**	**1.2806E-06**			**1**	**0.03**	**1.2806E-07**			**1**	**0.03**	**1.28063E-07**
6600-31-3	**6600313**	3458	3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane	320.43	3_REACH			**1**	**0.3**	**9.3624E-07**			**1**	**0.03**	**9.3624E-08**			**1**	**0.03**	**9.36242E-08**
66063-15-8	**66063158**	3459	4-chloro-N-cyclopentylbenzylamine	209.72	3_REACH			**1**	**0.3**	**1.4305E-06**			**1**	**0.03**	**1.4305E-07**			**1**	**0.03**	**1.43048E-07**
66068-84-6	**66068846**	3460	4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	236.4	3_REACH			**1**	**0.3**	**1.269E-06**			**1**	**0.03**	**1.269E-07**			**1**	**0.03**	**1.26904E-07**
6610-29-3	**6610293**	3462	4-methylthiosemicarbazide	105.17	3_REACH			**1**	**0.3**	**2.8525E-06**			**1**	**0.03**	**2.8525E-07**			**1**	**0.03**	**2.85252E-07**
66423-13-0	**66423130**	3473	octyl (R)-2-(4-chloro-2-methylphenoxy)propionate	326.86	3_REACH			**1**	**0.3**	**9.1782E-07**			**1**	**0.03**	**9.1782E-08**			**1**	**0.03**	**9.17824E-08**
66492-51-1	**66492511**	3475	(5-ethyl-1,3-dioxan-5-yl)methyl acrylate	200.23	3_REACH			**1**	**0.3**	**1.4983E-06**			**1**	**0.03**	**1.4983E-07**			**1**	**0.03**	**1.49828E-07**
6674-22-2	**6674222**	3481	1,8-diazabicyclo[5.4.0]undec-7-ene	152.24	3_REACH			**1**	**0.3**	**1.9706E-06**			**1**	**0.03**	**1.9706E-07**			**1**	**0.03**	**1.97057E-07**
67075-37-0	**67075370**	3484	2,9-bis(2-phenylethyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone	598.66	3_REACH			**1**	**0.3**	**5.0112E-07**			**1**	**0.03**	**5.0112E-08**			**1**	**0.03**	**5.01119E-08**
6711-48-4	**6711484**	3485	N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamine	187.33	3_REACH			**1**	**0.3**	**1.6015E-06**			**1**	**0.03**	**1.6015E-07**			**1**	**0.03**	**1.60145E-07**
6712-98-7	**6712987**	3486	1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol	163.22	3_REACH			**1**	**0.3**	**1.838E-06**			**1**	**0.03**	**1.838E-07**			**1**	**0.03**	**1.83801E-07**
67151-63-7	**67151637**	3487	1-[bis[3-(dimethylamino)propyl]amino]propan-2-ol	245.41	3_REACH			**1**	**0.3**	**1.2224E-06**			**1**	**0.03**	**1.2224E-07**			**1**	**0.03**	**1.22244E-07**
6731-36-8	**6731368**	3488	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	302.45	3_REACH			**1**	**0.3**	**9.919E-07**			**1**	**0.03**	**9.919E-08**			**1**	**0.03**	**9.91899E-08**
67-43-6	**67436**	82	N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)	393.35	3_REACH	81666.66667	81666.66667	**0**	**81666.6667**	**0.20761832**	1000	1000	**0**	**1000**	**0.00254227**	1000	1000	**0**	**1000**	**0.002542265**
674-82-8	**674828**	3493	but-3-en-3-olide	84.074	3_REACH			**1**	**0.3**	**3.5683E-06**			**1**	**0.03**	**3.5683E-07**			**1**	**0.03**	**3.56829E-07**
67801-15-4	**67801154**	3500	3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one	206.33	3_REACH			**1**	**0.3**	**1.454E-06**			**1**	**0.03**	**1.454E-07**			**1**	**0.03**	**1.45398E-07**
6786-83-0	**6786830**	3502	alpha,alpha-Bis[4-(dimethylamino)phenyl]-4-(phenylamino)naphthalene-1-methanol	487.65	3_REACH			**1**	**0.3**	**6.152E-07**			**1**	**0.03**	**6.152E-08**			**1**	**0.03**	**6.15195E-08**
67990-05-0	**67990050**	3504	N-(5-chloro-2-methoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide	581.03	3_REACH			**1**	**0.3**	**5.1632E-07**			**1**	**0.03**	**5.1632E-08**			**1**	**0.03**	**5.16324E-08**
68-11-1	**68111**	798	mercaptoacetic acid	92.116	3_REACH			**1**	**0.3**	**3.2568E-06**			**1**	**0.03**	**3.2568E-07**			**1**	**0.03**	**3.25676E-07**
68134-22-5	**68134225**	3507	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo-2-[[2-(trifluoromethyl)phenyl]azo]butyramide	405.34	3_REACH			**1**	**0.3**	**7.4012E-07**			**1**	**0.03**	**7.4012E-08**			**1**	**0.03**	**7.40119E-08**
682-01-9	**682019**	3509	tetrapropyl orthosilicate	264.44	3_REACH			**1**	**0.3**	**1.1345E-06**			**1**	**0.03**	**1.1345E-07**			**1**	**0.03**	**1.13447E-07**
682-09-7	**682097**	3510	2,2-bis(allyloxymethyl)butan-1-ol	214.31	3_REACH			**1**	**0.3**	**1.3998E-06**			**1**	**0.03**	**1.3998E-07**			**1**	**0.03**	**1.39984E-07**
682-11-1	**682111**	3511	2-allyloxymethyl-2-ethylpropanediol	174.24	3_REACH			**1**	**0.3**	**1.7218E-06**			**1**	**0.03**	**1.7218E-07**			**1**	**0.03**	**1.72176E-07**
68227-78-1	**68227781**	3512	N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide	565.03	3_REACH			**1**	**0.3**	**5.3095E-07**			**1**	**0.03**	**5.3095E-08**			**1**	**0.03**	**5.30945E-08**
68-26-8	**68268**	3514	retinol	286.46	3_REACH			**1**	**0.3**	**1.0473E-06**			**1**	**0.03**	**1.0473E-07**			**1**	**0.03**	**1.04727E-07**
6842-62-2	**6842622**	3515	614-477-3	239.1	3_REACH			**1**	**0.3**	**1.2547E-06**			**1**	**0.03**	**1.2547E-07**			**1**	**0.03**	**1.25471E-07**
6843-66-9	**6843669**	3516	dimethoxydiphenylsilane	244.37	3_REACH			**1**	**0.3**	**1.2276E-06**			**1**	**0.03**	**1.2276E-07**			**1**	**0.03**	**1.22765E-07**
6850-63-1	**6850631**	801	2,6-dimethylcyclohexylamine	127.23	3_REACH			**1**	**0.3**	**2.3579E-06**			**1**	**0.03**	**2.3579E-07**			**1**	**0.03**	**2.35793E-07**
68516-73-4	**68516734**	3518	tetramethyl 2,2'-[1,4-phenylenebis[imino(1-acetyl-2-oxoethane-1,2-diyl)azo]]bisterephthalate	716.67	3_REACH			**1**	**0.3**	**4.186E-07**			**1**	**0.03**	**4.186E-08**			**1**	**0.03**	**4.18603E-08**
68610-86-6	**68610866**	3522	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-	687.59	3_REACH			**1**	**0.3**	**4.3631E-07**			**1**	**0.03**	**4.3631E-08**			**1**	**0.03**	**4.36307E-08**
687-47-8	**687478**	3526	ethyl (S)-2-hydroxypropionate	118.13	3_REACH			**1**	**0.3**	**2.5396E-06**			**1**	**0.03**	**2.5396E-07**			**1**	**0.03**	**2.53958E-07**
68855-18-5	**68855185**	3527	(3-Hydroxy-2,2-dimethylpropyl) heptanoate	216.32	3_REACH			**1**	**0.3**	**1.3868E-06**			**1**	**0.03**	**1.3868E-07**			**1**	**0.03**	**1.38683E-07**
688-84-6	**688846**	3529	2-ethylhexyl methacrylate	198.31	3_REACH			**1**	**0.3**	**1.5128E-06**			**1**	**0.03**	**1.5128E-07**			**1**	**0.03**	**1.51278E-07**
69045-84-7	**69045847**	4322	2,3-dichloro-5-trifluoromethylpyridine	215.99	3_REACH			**1**	**0.3**	**1.389E-06**			**1**	**0.03**	**1.389E-07**			**1**	**0.03**	**1.38895E-07**
6925-69-5	**6925695**	3537	12H-phthaloperin-12-one	270.29	3_REACH			**1**	**0.3**	**1.1099E-06**			**1**	**0.03**	**1.1099E-07**			**1**	**0.03**	**1.10992E-07**
693-21-0	**693210**	804	oxydiethylene dinitrate	196.12	3_REACH	30033.33333	30033.33333	**0**	**30033.3333**	**0.15313753**			**1**	**0.03**	**1.5297E-07**			**1**	**0.03**	**1.52968E-07**
693-23-2	**693232**	3538	dodecanedioic acid	230.3	3_REACH			**1**	**0.3**	**1.3026E-06**			**1**	**0.03**	**1.3026E-07**			**1**	**0.03**	**1.30265E-07**
693-36-7	**693367**	3539	dioctadecyl 3,3'-thiodipropionate	683.18	3_REACH			**1**	**0.3**	**4.3912E-07**			**1**	**0.03**	**4.3912E-08**			**1**	**0.03**	**4.39123E-08**
693-57-2	**693572**	3540	12-aminododecanoic acid	215.34	3_REACH			**1**	**0.3**	**1.3931E-06**			**1**	**0.03**	**1.3931E-07**			**1**	**0.03**	**1.39315E-07**
6938-94-9	**6938949**	3541	diisopropyl adipate	230.3	3_REACH			**1**	**0.3**	**1.3026E-06**			**1**	**0.03**	**1.3026E-07**			**1**	**0.03**	**1.30265E-07**
693-98-1	**693981**	806	2-methylimidazole	82.108	3_REACH			**1**	**0.3**	**3.6537E-06**			**1**	**0.03**	**3.6537E-07**			**1**	**0.03**	**3.65372E-07**
6940-53-0	**6940530**	3543	1-chloro-2,5-dimethoxy-4-nitrobenzene	217.61	3_REACH			**1**	**0.3**	**1.3786E-06**			**1**	**0.03**	**1.3786E-07**			**1**	**0.03**	**1.37861E-07**
694-83-7	**694837**	807	cyclohex-1,2-ylenediamine	114.19	3_REACH			**1**	**0.3**	**2.6272E-06**			**1**	**0.03**	**2.6272E-07**			**1**	**0.03**	**2.6272E-07**
700-13-0	**700130**	3554	2,3,5-trimethylhydroquinone	152.19	3_REACH			**1**	**0.3**	**1.9712E-06**			**1**	**0.03**	**1.9712E-07**			**1**	**0.03**	**1.97122E-07**
70356-09-1	**70356091**	3560	1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-1,3-dione	310.39	3_REACH			**1**	**0.3**	**9.6653E-07**			**1**	**0.03**	**9.6653E-08**			**1**	**0.03**	**9.66526E-08**
70445-33-9	**70445339**	4370	3-(2-ethylhexyloxy)propane-1,2-diol	204.31	3_REACH			**1**	**0.3**	**1.4684E-06**			**1**	**0.03**	**1.4684E-07**			**1**	**0.03**	**1.46836E-07**
70516-41-5	**70516415**	3563	2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one	518.66	3_REACH			**1**	**0.3**	**5.7841E-07**			**1**	**0.03**	**5.7841E-08**			**1**	**0.03**	**5.78414E-08**
70-55-3	**70553**	85	toluene-4-sulphonamide	171.22	3_REACH			**1**	**0.3**	**1.7521E-06**			**1**	**0.03**	**1.7521E-07**			**1**	**0.03**	**1.75213E-07**
706-14-9	**706149**	813	decan-4-olide	170.25	3_REACH			**1**	**0.3**	**1.7621E-06**			**1**	**0.03**	**1.7621E-07**			**1**	**0.03**	**1.76211E-07**
7069-42-3	**7069423**	3567	retinyl propionate	342.52	3_REACH			**1**	**0.3**	**8.7586E-07**			**1**	**0.03**	**8.7586E-08**			**1**	**0.03**	**8.75861E-08**
70969-58-3	**70969583**	815	diisobutyl hexahydrophthalate	284.4	3_REACH			**1**	**0.3**	**1.0549E-06**			**1**	**0.03**	**1.0549E-07**			**1**	**0.03**	**1.05485E-07**
71048-82-3	**71048823**	3577	(2E)-1-[(1R,2S)-2,6,6-Trimethylcyclohex-3-en-1-yl]but-2-en-1-one	192.3	3_REACH			**1**	**0.3**	**1.5601E-06**			**1**	**0.03**	**1.5601E-07**			**1**	**0.03**	**1.56006E-07**
712-50-5	**712505**	818	cyclohexyl phenyl ketone	188.27	3_REACH			**1**	**0.3**	**1.5935E-06**			**1**	**0.03**	**1.5935E-07**			**1**	**0.03**	**1.59346E-07**
713-95-1	**713951**	3581	dodecan-5-olide	198.31	3_REACH			**1**	**0.3**	**1.5128E-06**			**1**	**0.03**	**1.5128E-07**			**1**	**0.03**	**1.51278E-07**
71604-74-5	**71604745**	3586	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	277.32	3_REACH			**1**	**0.3**	**1.0818E-06**			**1**	**0.03**	**1.0818E-07**			**1**	**0.03**	**1.08178E-07**
71617-10-2	**71617102**	3587	isopentyl p-methoxycinnamate	248.32	3_REACH			**1**	**0.3**	**1.2081E-06**			**1**	**0.03**	**1.2081E-07**			**1**	**0.03**	**1.20812E-07**
71735-74-5	**71735745**	3588	ethyl 3-[[bis(1-methylethoxy)phosphinothioyl]thio]propionate	314.4	3_REACH			**1**	**0.3**	**9.542E-07**			**1**	**0.03**	**9.542E-08**			**1**	**0.03**	**9.54198E-08**
7173-62-8	**7173628**	3589	(Z)-N-9-octadecenylpropane-1,3-diamine	324.6	3_REACH			**1**	**0.3**	**9.2421E-07**			**1**	**0.03**	**9.2421E-08**			**1**	**0.03**	**9.24214E-08**
71902-23-3	**71902233**	3594	6-[(1-oxomethyloctyl)amino]hexanoic acid	271.4	3_REACH			**1**	**0.3**	**1.1054E-06**			**1**	**0.03**	**1.1054E-07**			**1**	**0.03**	**1.10538E-07**
7195-44-0	**7195440**	3595	bis(2,3-epoxypropyl) terephthalate	278.26	3_REACH			**1**	**0.3**	**1.0781E-06**			**1**	**0.03**	**1.0781E-07**			**1**	**0.03**	**1.07813E-07**
72361-35-4	**72361354**	3603	triisotridecyl benzene-1,2,4-tricarboxylate	757.19	3_REACH			**1**	**0.3**	**3.962E-07**			**1**	**0.03**	**3.962E-08**			**1**	**0.03**	**3.96202E-08**
7300-34-7	**7300347**	3612	3,3'-[butane-1,4-diylbis(oxy)]bispropanamine	204.32	3_REACH			**1**	**0.3**	**1.4683E-06**			**1**	**0.03**	**1.4683E-07**			**1**	**0.03**	**1.46829E-07**
7305-71-7	**7305717**	4342	2-amino-5-methylthiazole	114.17	3_REACH			**1**	**0.3**	**2.6277E-06**			**1**	**0.03**	**2.6277E-07**			**1**	**0.03**	**2.62766E-07**
732-26-3	**732263**	829	2,4,6-tri-tert-butylphenol	262.44	3_REACH			**1**	**0.3**	**1.1431E-06**			**1**	**0.03**	**1.1431E-07**			**1**	**0.03**	**1.14312E-07**
7328-22-5	**7328225**	3618	2-(2-butoxyethoxy)ethyl methacrylate	230.3	3_REACH			**1**	**0.3**	**1.3026E-06**			**1**	**0.03**	**1.3026E-07**			**1**	**0.03**	**1.30265E-07**
7381-13-7	**7381137**	3627	1,1'-(1,3-Phenylenedicarbonyl)diazepan-2-one	356.42	3_REACH			**1**	**0.3**	**8.417E-07**			**1**	**0.03**	**8.417E-08**			**1**	**0.03**	**8.41704E-08**
7396-58-9	**7396589**	3629	N-methyldidecylamine	311.6	3_REACH			**1**	**0.3**	**9.6277E-07**			**1**	**0.03**	**9.6277E-08**			**1**	**0.03**	**9.62773E-08**
7397-62-8	**7397628**	3630	butyl glycollate	132.16	3_REACH			**1**	**0.3**	**2.27E-06**			**1**	**0.03**	**2.27E-07**			**1**	**0.03**	**2.26998E-07**
74338-72-0	**74338720**	4323	2,4,4,7-tetramethyl-6-octen-3-one	182.31	3_REACH			**1**	**0.3**	**1.6455E-06**			**1**	**0.03**	**1.6455E-07**			**1**	**0.03**	**1.64555E-07**
74441-05-7	**74441057**	3635	N-[4-(aminocarbonyl)phenyl]-4-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzamide	499.49	3_REACH			**1**	**0.3**	**6.0061E-07**			**1**	**0.03**	**6.0061E-08**			**1**	**0.03**	**6.00613E-08**
7473-98-5	**7473985**	3642	2-hydroxy-2-methylpropiophenone	164.2	3_REACH			**1**	**0.3**	**1.827E-06**			**1**	**0.03**	**1.827E-07**			**1**	**0.03**	**1.82704E-07**
75-12-7	**75127**	851	formamide	45.042	3_REACH			**1**	**0.3**	**6.6605E-06**			**1**	**0.03**	**6.6605E-07**			**1**	**0.03**	**6.66045E-07**
7526-26-3	**7526263**	3659	diphenyl methylphosphonate	248.22	3_REACH			**1**	**0.3**	**1.2086E-06**			**1**	**0.03**	**1.2086E-07**			**1**	**0.03**	**1.20861E-07**
7534-94-3	**7534943**	3668	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate	222.33	3_REACH			**1**	**0.3**	**1.3493E-06**			**1**	**0.03**	**1.3493E-07**			**1**	**0.03**	**1.34935E-07**
75490-39-0	**75490390**	4313	2,2,4-trimethyl-4-phenyl-butane-nitrile	187.29	3_REACH			**1**	**0.3**	**1.6018E-06**			**1**	**0.03**	**1.6018E-07**			**1**	**0.03**	**1.60179E-07**
756-80-9	**756809**	864	O,O-dimethyl hydrogen dithiophosphate	158.18	3_REACH			**1**	**0.3**	**1.8966E-06**			**1**	**0.03**	**1.8966E-07**			**1**	**0.03**	**1.89657E-07**
75-75-2	**75752**	3683	methanesulphonic acid	96.104	3_REACH			**1**	**0.3**	**3.1216E-06**			**1**	**0.03**	**3.1216E-07**			**1**	**0.03**	**3.12162E-07**
7575-23-7	**7575237**	3684	pentaerythritol tetrakis(3-mercaptopropionate)	488.66	3_REACH			**1**	**0.3**	**6.1392E-07**			**1**	**0.03**	**6.1392E-08**			**1**	**0.03**	**6.13924E-08**
75980-60-8	**75980608**	3692	diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	348.38	3_REACH			**1**	**0.3**	**8.6113E-07**			**1**	**0.03**	**8.6113E-08**			**1**	**0.03**	**8.61129E-08**
75-98-9	**75989**	868	pivalic acid	102.13	3_REACH			**1**	**0.3**	**2.9374E-06**			**1**	**0.03**	**2.9374E-07**			**1**	**0.03**	**2.93743E-07**
76-03-9	**76039**	90	trichloroacetic acid	163.39	3_REACH	48666.66667	48666.66667	**0**	**48666.6667**	**0.29785585**			**1**	**0.03**	**1.8361E-07**			**1**	**0.03**	**1.8361E-07**
7605-52-9	**7605529**	3696	methyl cis-3-methylcyclohexanecarboxylate	156.22	3_REACH			**1**	**0.3**	**1.9204E-06**			**1**	**0.03**	**1.9204E-07**			**1**	**0.03**	**1.92037E-07**
760-67-8	**760678**	3697	2-ethylhexanoyl chloride	162.66	3_REACH			**1**	**0.3**	**1.8443E-06**			**1**	**0.03**	**1.8443E-07**			**1**	**0.03**	**1.84434E-07**
76114-73-3	**76114733**	3699	2-Propynyl butylcarbamate	155.2	3_REACH			**1**	**0.3**	**1.933E-06**			**1**	**0.03**	**1.933E-07**			**1**	**0.03**	**1.93299E-07**
76201-56-4	**76201564**	3704	3-[dimethyl(3-{[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino}propyl)ammonio]-2-hydroxypropane-1-sulfonate	650.47	3_REACH			**1**	**0.3**	**4.612E-07**			**1**	**0.03**	**4.612E-08**			**1**	**0.03**	**4.61205E-08**
762-04-9	**762049**	3705	diethyl phosphonate	138.1	3_REACH			**1**	**0.3**	**2.1723E-06**			**1**	**0.03**	**2.1723E-07**			**1**	**0.03**	**2.17234E-07**
76-22-2	**76222**	872	bornan-2-one	152.24	3_REACH			**1**	**0.3**	**1.9706E-06**			**1**	**0.03**	**1.9706E-07**			**1**	**0.03**	**1.97057E-07**
763-69-9	**763699**	3710	ethyl 3-ethoxypropionate	146.19	3_REACH			**1**	**0.3**	**2.0521E-06**			**1**	**0.03**	**2.0521E-07**			**1**	**0.03**	**2.05212E-07**

764-99-8	**764998**	3714	1,1'-[oxybis(ethyleneoxy)]diethylene	158.2	3_REACH			**1**	**0.3**	**1.8963E-06**			**1**	**0.03**	**1.8963E-07**			**1**	**0.03**	**1.89633E-07**
76524-94-2	**76524942**	3715	N-[3-(Triethoxysilyl)propyl]formamide	249.38	3_REACH			**1**	**0.3**	**1.203E-06**			**1**	**0.03**	**1.203E-07**			**1**	**0.03**	**1.20298E-07**
7659-86-1	**7659861**	3721	2-ethylhexyl mercaptoacetate	204.33	3_REACH			**1**	**0.3**	**1.4682E-06**			**1**	**0.03**	**1.4682E-07**			**1**	**0.03**	**1.46821E-07**
76855-69-1	**76855691**	4234	Azetidon	287.43	3_REACH			**1**	**0.3**	**1.0437E-06**			**1**	**0.03**	**1.0437E-07**			**1**	**0.03**	**1.04373E-07**
768-94-5	**768945**	878	amantadine	151.25	3_REACH			**1**	**0.3**	**1.9835E-06**			**1**	**0.03**	**1.9835E-07**			**1**	**0.03**	**1.98347E-07**
7695-91-2	**7695912**	3727	3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-yl acetate	472.75	3_REACH			**1**	**0.3**	**6.3458E-07**			**1**	**0.03**	**6.3458E-08**			**1**	**0.03**	**6.34585E-08**
770-35-4	**770354**	3730	1-phenoxypropan-2-ol	152.19	3_REACH			**1**	**0.3**	**1.9712E-06**			**1**	**0.03**	**1.9712E-07**			**1**	**0.03**	**1.97122E-07**
77-09-8	**77098**	879	phenolphthalein	318.33	3_REACH	2980	2980	**0**	**2980**	**0.00936135**			**1**	**0.03**	**9.4242E-08**			**1**	**0.03**	**9.42418E-08**
7747-35-5	**7747355**	880	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	143.19	3_REACH	32000	32000	**0**	**32000**	**0.22347929**			**1**	**0.03**	**2.0951E-07**			**1**	**0.03**	**2.09512E-07**
77501-63-4	**77501634**	882	Lactofen	461.78	3_REACH	33.33333333	33.33333333	**0**	**33.3333333**	**7.2184E-05**			**1**	**0.03**	**6.4966E-08**			**1**	**0.03**	**6.4966E-08**
77-71-4	**77714**	883	5,5-dimethylhydantoin	128.13	3_REACH			**1**	**0.3**	**2.3414E-06**			**1**	**0.03**	**2.3414E-07**			**1**	**0.03**	**2.34137E-07**
77-73-6	**77736**	884	3a,4,7,7a-tetrahydro-4,7-methanoindene	132.21	3_REACH	1400	1400	**0**	**1400**	**0.01058921**			**1**	**0.03**	**2.2691E-07**			**1**	**0.03**	**2.26912E-07**
77-78-1	**77781**	886	dimethyl sulphate	126.13	3_REACH			**1**	**0.3**	**2.3785E-06**			**1**	**0.03**	**2.3785E-07**			**1**	**0.03**	**2.3785E-07**
77804-81-0	**77804810**	3736	2,2'-[ethylenebis(oxyphenyl-2,1-eneazo)]bis[N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide	732.72	3_REACH			**1**	**0.3**	**4.0943E-07**			**1**	**0.03**	**4.0943E-08**			**1**	**0.03**	**4.09433E-08**
77-83-8	**77838**	3738	ethyl 2,3-epoxy-3-phenylbutyrate	206.24	3_REACH			**1**	**0.3**	**1.4546E-06**			**1**	**0.03**	**1.4546E-07**			**1**	**0.03**	**1.45462E-07**
7785-26-4	**7785264**	887	(-)-pin-2(3)-ene	136.24	3_REACH			**1**	**0.3**	**2.202E-06**			**1**	**0.03**	**2.202E-07**			**1**	**0.03**	**2.202E-07**
7785-70-8	**7785708**	888	(+)-pin-2(3)-ene	136.24	3_REACH	380	380	**0**	**380**	**0.0027892**			**1**	**0.03**	**2.202E-07**			**1**	**0.03**	**2.202E-07**
77-86-1	**77861**	3739	trometamol	121.14	3_REACH			**1**	**0.3**	**2.4765E-06**			**1**	**0.03**	**2.4765E-07**			**1**	**0.03**	**2.47647E-07**
7787-93-1	**7787931**	3741	dichloro(3-chloropropyl)methylsilane	191.56	3_REACH			**1**	**0.3**	**1.5661E-06**			**1**	**0.03**	**1.5661E-07**			**1**	**0.03**	**1.56609E-07**
778-94-9	**778949**	3743	2-nitro-4-(trifluoromethyl)benzonitrile	216.12	3_REACH			**1**	**0.3**	**1.3881E-06**			**1**	**0.03**	**1.3881E-07**			**1**	**0.03**	**1.38812E-07**
77-90-7	**77907**	3744	tributyl O-acetylcitrate	402.48	3_REACH			**1**	**0.3**	**7.4538E-07**			**1**	**0.03**	**7.4538E-08**			**1**	**0.03**	**7.45379E-08**
77-92-9	**77929**	889	citric acid	192.12	3_REACH	511666.6667	511666.6667	**0**	**511666.667**	**2.66326601**			**1**	**0.03**	**1.5615E-07**			**1**	**0.03**	**1.56152E-07**
77-93-0	**77930**	92	triethyl citrate	276.29	3_REACH			**1**	**0.3**	**1.0858E-06**			**1**	**0.03**	**1.0858E-07**			**1**	**0.03**	**1.08582E-07**
77-94-1	**77941**	3745	tributyl citrate	360.45	3_REACH			**1**	**0.3**	**8.3229E-07**			**1**	**0.03**	**8.3229E-08**			**1**	**0.03**	**8.32293E-08**
77-99-6	**77996**	890	propylidynetrimethanol	134.18	3_REACH			**1**	**0.3**	**2.2358E-06**			**1**	**0.03**	**2.2358E-07**			**1**	**0.03**	**2.2358E-07**
780-69-8	**780698**	891	triethoxy(phenyl)silane	240.38	3_REACH	3940	3940	**0**	**3940**	**0.01639071**			**1**	**0.03**	**1.248E-07**			**1**	**0.03**	**1.24802E-07**
78-08-0	**78080**	3746	triethoxy(vinyl)silane	190.32	3_REACH			**1**	**0.3**	**1.5763E-06**			**1**	**0.03**	**1.5763E-07**			**1**	**0.03**	**1.57629E-07**
78-11-5	**78115**	892	pentaerithrityl tetranitrate	316.14	3_REACH	16333.33333	16333.33333	**0**	**16333.3333**	**0.05166487**			**1**	**0.03**	**9.4895E-08**			**1**	**0.03**	**9.48947E-08**
78-27-3	**78273**	893	1-ethynylcyclohexanol	124.18	3_REACH			**1**	**0.3**	**2.4158E-06**			**1**	**0.03**	**2.4158E-07**			**1**	**0.03**	**2.41585E-07**
78-40-0	**78400**	894	triethyl phosphate	182.16	3_REACH	33333.33333	33333.33333	**0**	**33333.3333**	**0.18298931**	190000	190000	**0**	**190000**	**1.04303909**	190000	190000	**0**	**190000**	**1.043039087**
78-42-2	**78422**	895	tris(2-ethylhexyl) phosphate	434.64	3_REACH			**1**	**0.3**	**6.9023E-07**			**1**	**0.03**	**6.9023E-08**			**1**	**0.03**	**6.90226E-08**
78-51-3	**78513**	93	tris(2-butoxyethyl) phosphate	398.48	3_REACH	32000	32000	**0**	**32000**	**0.08030516**			**1**	**0.03**	**7.5286E-08**			**1**	**0.03**	**7.52861E-08**
78521-39-8	**78521398**	3751	6-[[(4-methylphenyl)sulphonyl]amino]hexanoic acid	285.36	3_REACH			**1**	**0.3**	**1.0513E-06**			**1**	**0.03**	**1.0513E-07**			**1**	**0.03**	**1.0513E-07**
78531-61-0	**78531610**	4400	4-(trans-4-propylcyclohexyl)acetophenone	244.38	3_REACH			**1**	**0.3**	**1.2276E-06**			**1**	**0.03**	**1.2276E-07**			**1**	**0.03**	**1.2276E-07**
78-59-1	**78591**	897	3,5,5-trimethylcyclohex-2-enone	138.21	3_REACH	40000	40000	**0**	**40000**	**0.28941466**			**1**	**0.03**	**2.1706E-07**			**1**	**0.03**	**2.17061E-07**
78605-96-6	**78605966**	3752	alpha-Amylcinnamaldehyde	202.3	3_REACH			**1**	**0.3**	**1.4829E-06**			**1**	**0.03**	**1.4829E-07**			**1**	**0.03**	**1.48295E-07**
78-63-7	**78637**	3753	di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide	290.44	3_REACH			**1**	**0.3**	**1.0329E-06**			**1**	**0.03**	**1.0329E-07**			**1**	**0.03**	**1.03292E-07**
78-67-1	**78671**	3754	2,2'-dimethyl-2,2'-azodipropiononitrile	164.22	3_REACH			**1**	**0.3**	**1.8268E-06**			**1**	**0.03**	**1.8268E-07**			**1**	**0.03**	**1.82682E-07**
78-69-3	**78693**	3755	3,7-dimethyloctan-3-ol	158.29	3_REACH			**1**	**0.3**	**1.8953E-06**			**1**	**0.03**	**1.8953E-07**			**1**	**0.03**	**1.89526E-07**
78-70-6	**78706**	899	linalool	154.25	3_REACH	12233.33333	12233.33333	**0**	**12233.3333**	**0.07930848**			**1**	**0.03**	**1.9449E-07**			**1**	**0.03**	**1.94489E-07**
78850-37-0	**78850370**	5023	methyl (3aR,4R,7aR)-2-methyl-4-(1S,2R,3-triacetoxypropyl)-3a,7a-dihydro-4H-pyrano[3,4-d]oxazole-6-carboxylate	413.38	3_REACH			**1**	**0.3**	**7.2572E-07**			**1**	**0.03**	**7.2572E-08**			**1**	**0.03**	**7.25725E-08**
78-97-7	**78977**	3762	lactonitrile	71.08	3_REACH			**1**	**0.3**	**4.2206E-06**			**1**	**0.03**	**4.2206E-07**			**1**	**0.03**	**4.2206E-07**
79-06-1	**79061**	911	acrylamide	71.08	3_REACH	32666.66667	32666.66667	**0**	**32666.6667**	**0.45957606**			**1**	**0.03**	**4.2206E-07**			**1**	**0.03**	**4.2206E-07**
79-07-2	**79072**	3765	2-chloroacetamide	93.514	3_REACH			**1**	**0.3**	**3.2081E-06**			**1**	**0.03**	**3.2081E-07**			**1**	**0.03**	**3.20808E-07**
79-08-3	**79083**	912	bromoacetic acid	138.95	3_REACH	21666.66667	21666.66667	**0**	**21666.6667**	**0.15593139**	1600	1600	**0**	**1600**	**0.01151493**	1600	1600	**0**	**1600**	**0.011514933**
79-11-8	**79118**	915	chloroacetic acid	94.497	3_REACH	25666.66667	25666.66667	**0**	**25666.6667**	**0.27161356**	32000	32000	**0**	**32000**	**0.33863509**	32000	32000	**0**	**32000**	**0.338635089**
791-28-6	**791286**	95	triphenylphosphine oxide	278.29	3_REACH			**1**	**0.3**	**1.078E-06**			**1**	**0.03**	**1.078E-07**			**1**	**0.03**	**1.07801E-07**
79-14-1	**79141**	3766	glycollic acid	76.051	3_REACH			**1**	**0.3**	**3.9447E-06**			**1**	**0.03**	**3.9447E-07**			**1**	**0.03**	**3.94472E-07**
79-16-3	**79163**	3767	N-methylacetamide	73.096	3_REACH			**1**	**0.3**	**4.1042E-06**			**1**	**0.03**	**4.1042E-07**			**1**	**0.03**	**4.10419E-07**
793-24-8	**793248**	3771	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	268.41	3_REACH			**1**	**0.3**	**1.1177E-06**			**1**	**0.03**	**1.1177E-07**			**1**	**0.03**	**1.11769E-07**
79-33-4	**79334**	920	L-(+)-lactic acid	90.078	3_REACH	320000	320000	**0**	**320000**	**3.55247674**			**1**	**0.03**	**3.3304E-07**			**1**	**0.03**	**3.33045E-07**
79-41-4	**79414**	3776	methacrylic acid	86.09	3_REACH			**1**	**0.3**	**3.4847E-06**			**1**	**0.03**	**3.4847E-07**			**1**	**0.03**	**3.48473E-07**
79456-26-1	**79456261**	4391	3-chloro-5-trifluoromethyl-2-pyridylamine	196.56	3_REACH			**1**	**0.3**	**1.5263E-06**			**1**	**0.03**	**1.5263E-07**			**1**	**0.03**	**1.52625E-07**
79-74-3	**79743**	3781	2,5-di-tert-pentylhydroquinone	250.38	3_REACH			**1**	**0.3**	**1.1982E-06**			**1**	**0.03**	**1.1982E-07**			**1**	**0.03**	**1.19818E-07**
79-77-6	**79776**	926	(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	192.3	3_REACH			**1**	**0.3**	**1.5601E-06**			**1**	**0.03**	**1.5601E-07**			**1**	**0.03**	**1.56006E-07**
79815-20-6	**79815206**	4252	(S)-2,3-dihydro-1H-indole-2-carboxylic acid	163.18	3_REACH			**1**	**0.3**	**1.8385E-06**			**1**	**0.03**	**1.8385E-07**			**1**	**0.03**	**1.83846E-07**
79-94-7	**79947**	929	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	543.9	3_REACH	2633.333333	2633.333333	**0**	**2633.33333**	**0.00484158**			**1**	**0.03**	**5.5157E-08**			**1**	**0.03**	**5.51572E-08**
80-04-6	**80046**	931	4,4'-isopropylidenedicyclohexanol	240.39	3_REACH			**1**	**0.3**	**1.248E-06**			**1**	**0.03**	**1.248E-07**			**1**	**0.03**	**1.24797E-07**
80-05-7	**80057**	96	4,4'-isopropylidenediphenol	228.29	3_REACH	0.3	0.3	**0**	**0.3**	**1.3141E-06**	30	30	**0**	**30**	**0.00013141**	30	30	**0**	**30**	**0.000131412**
80-07-9	**80079**	3786	bis(4-chlorophenyl) sulphone	287.16	3_REACH			**1**	**0.3**	**1.0447E-06**			**1**	**0.03**	**1.0447E-07**			**1**	**0.03**	**1.04471E-07**
80-10-4	**80104**	3788	dichloro(diphenyl)silane	253.2	3_REACH			**1**	**0.3**	**1.1848E-06**			**1**	**0.03**	**1.1848E-07**			**1**	**0.03**	**1.18483E-07**
80-15-9	**80159**	932	Cumene hydroperoxide	152.19	3_REACH	2333.333333	2333.333333	**0**	**2333.33333**	**0.01533171**			**1**	**0.03**	**1.9712E-07**			**1**	**0.03**	**1.97122E-07**
80-26-2	**80262**	934	p-menth-1-en-8-yl acetate	196.29	3_REACH			**1**	**0.3**	**1.5284E-06**			**1**	**0.03**	**1.5284E-07**			**1**	**0.03**	**1.52835E-07**
80-43-3	**80433**	3791	Dicumyl peroxide	270.37	3_REACH			**1**	**0.3**	**1.1096E-06**			**1**	**0.03**	**1.1096E-07**			**1**	**0.03**	**1.10959E-07**
80-46-6	**80466**	936	p-(1,1-dimethylpropyl)phenol	164.25	3_REACH			**1**	**0.3**	**1.8265E-06**			**1**	**0.03**	**1.8265E-07**			**1**	**0.03**	**1.82648E-07**
80-51-3	**80513**	3792	4,4'-oxydi(benzenesulphonohydrazide)	358.4	3_REACH			**1**	**0.3**	**8.3705E-07**			**1**	**0.03**	**8.3705E-08**			**1**	**0.03**	**8.37054E-08**
80-54-6	**80546**	3794	2-(4-tert-butylbenzyl)propionaldehyde	204.31	3_REACH			**1**	**0.3**	**1.4684E-06**			**1**	**0.03**	**1.4684E-07**			**1**	**0.03**	**1.46836E-07**
80-56-8	**80568**	937	pin-2(3)-ene	136.24	3_REACH	13666.66667	13666.66667	**0**	**13666.6667**	**0.10031317**			**1**	**0.03**	**2.202E-07**			**1**	**0.03**	**2.202E-07**
80-73-9	**80739**	3797	1,3-dimethylimidazolidin-2-one	114.15	3_REACH			**1**	**0.3**	**2.6281E-06**			**1**	**0.03**	**2.6281E-07**			**1**	**0.03**	**2.62812E-07**
81-07-2	**81072**	98	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	183.19	3_REACH			**1**	**0.3**	**1.6376E-06**			**1**	**0.03**	**1.6376E-07**			**1**	**0.03**	**1.63764E-07**
81-19-6	**81196**	939	1,3-Dichloro-2-(dichloromethyl)benzene	229.92	3_REACH			**1**	**0.3**	**1.3048E-06**			**1**	**0.03**	**1.3048E-07**			**1**	**0.03**	**1.3048E-07**
81-25-4	**81254**	100	cholic acid	408.58	3_REACH			**1**	**0.3**	**7.3425E-07**			**1**	**0.03**	**7.3425E-08**			**1**	**0.03**	**7.3425E-08**
81-33-4	**81334**	3804	perylene-3,4:9,10-tetracarboxydiimide	390.36	3_REACH			**1**	**0.3**	**7.6852E-07**			**1**	**0.03**	**7.6852E-08**			**1**	**0.03**	**7.68521E-08**
81782-77-6	**81782776**	3814	4-methyl-3-decen-5-ol	170.3	3_REACH			**1**	**0.3**	**1.7616E-06**			**1**	**0.03**	**1.7616E-07**			**1**	**0.03**	**1.7616E-07**
818-61-1	**818611**	943	2-hydroxyethyl acrylate	116.12	3_REACH			**1**	**0.3**	**2.5835E-06**			**1**	**0.03**	**2.5835E-07**			**1**	**0.03**	**2.58353E-07**
82199-12-0	**82199120**	3820	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(2-methoxyphenyl)azo]-3-oxobutyramide	367.37	3_REACH			**1**	**0.3**	**8.1662E-07**			**1**	**0.03**	**8.1662E-08**			**1**	**0.03**	**8.16615E-08**
822-06-0	**822060**	3822	hexamethylene diisocyanate	168.2	3_REACH			**1**	**0.3**	**1.7836E-06**			**1**	**0.03**	**1.7836E-07**			**1**	**0.03**	**1.78359E-07**
826-36-8	**826368**	3834	2,2,6,6-tetramethyl-4-piperidone	155.24	3_REACH			**1**	**0.3**	**1.9325E-06**			**1**	**0.03**	**1.9325E-07**			**1**	**0.03**	**1.93249E-07**
82985-35-1	**82985351**	3839	bis(trimethoxysilylpropyl)amine	341.55	3_REACH			**1**	**0.3**	**8.7835E-07**			**1**	**0.03**	**8.7835E-08**			**1**	**0.03**	**8.78349E-08**
830-13-7	**830137**	3840	cyclododecanone	182.31	3_REACH			**1**	**0.3**	**1.6455E-06**			**1**	**0.03**	**1.6455E-07**			**1**	**0.03**	**1.64555E-07**
83066-88-0	**83066880**	950	(2R)-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoic acid	327.26	3_REACH			**1**	**0.3**	**9.167E-07**			**1**	**0.03**	**9.167E-08**			**1**	**0.03**	**9.16702E-08**
83261-15-8	**83261158**	3844	isobutyl (S)-2-chloropropionate	164.63	3_REACH			**1**	**0.3**	**1.8223E-06**			**1**	**0.03**	**1.8223E-07**			**1**	**0.03**	**1.82227E-07**
83-32-9	**83329**	952	acenaphthene	154.21	3_REACH	425	425	**0**	**425**	**0.00275598**			**1**	**0.03**	**1.9454E-07**			**1**	**0.03**	**1.9454E-07**
83-42-1	**83421**	954	2-chloro-6-nitrotoluene	171.58	3_REACH	1333.333333	1333.333333	**0**	**1333.33333**	**0.00777091**	630	630	**0**	**630**	**0.00367176**	630	630	**0**	**630**	**0.003671757**
83524-75-8	**83524758**	3848	2,9-bis(p-methoxybenzyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone	630.66	3_REACH			**1**	**0.3**	**4.7569E-07**			**1**	**0.03**	**4.7569E-08**			**1**	**0.03**	**4.75692E-08**
83-73-8	**83738**	3850	diiodohydroxyquinoline	396.95	3_REACH			**1**	**0.3**	**7.5576E-07**			**1**	**0.03**	**7.5576E-08**			**1**	**0.03**	**7.55763E-08**
83926-73-2	**83926732**	4796	4-cyclohexyl-2-methyl-2-butanol	170.3	3_REACH			**1**	**0.3**	**1.7616E-06**			**1**	**0.03**	**1.7616E-07**			**1**	**0.03**	**1.7616E-07**
84170-74-1	**84170741**	3857	(2,2-Dimethyl-1,3-propanediyl)bis(oxy-3,1-propanediyl) bisacrylate	328.4	3_REACH			**1**	**0.3**	**9.1352E-07**			**1**	**0.03**	**9.1352E-08**			**1**	**0.03**	**9.1352E-08**
84281-74-3	**84281743**	3859	1,3-Benzenediamine, coupled with diazotized m-phenylenediamine, acetates	346.41	3_REACH			**1**	**0.3**	**8.6603E-07**			**1**	**0.03**	**8.6603E-08**			**1**	**0.03**	**8.66026E-08**
84418-63-3	**84418633**	3863	Isononanoic acid, mixed esters with dipentaerythritol, heptanoic acid and pentaerythritol	328.4	3_REACH			**1**	**0.3**	**9.1352E-07**			**1**	**0.03**	**9.1352E-08**			**1**	**0.03**	**9.1352E-08**
84434-11-7	**84434117**	3864	ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate	316.34	3_REACH			**1**	**0.3**	**9.4835E-07**			**1**	**0.03**	**9.4835E-08**			**1**	**0.03**	**9.48347E-08**
84583-68-6	**84583686**	3868	2-Butenoic acid, 4-oxo-4-(tridecylamino)-, (Z)-, branched	297.44	3_REACH			**1**	**0.3**	**1.0086E-06**			**1**	**0.03**	**1.0086E-07**			**1**	**0.03**	**1.00861E-07**
84-65-1	**84651**	960	anthraquinone	208.22	3_REACH	3333.333333	3333.333333	**0**	**3333.33333**	**0.01600871**			**1**	**0.03**	**1.4408E-07**			**1**	**0.03**	**1.44078E-07**
84-66-2	**84662**	961	diethyl phthalate	222.24	3_REACH	13666.66667	13666.66667	**0**	**13666.6667**	**0.06149508**	3800	3800	**0**	**3800**	**0.01709863**	3800	3800	**0**	**3800**	**0.017098632**
84-69-5	**84695**	962	diisobutyl phthalate	278.35	3_REACH			**1**	**0.3**	**1.0778E-06**			**1**	**0.03**	**1.0778E-07**			**1**	**0.03**	**1.07778E-07**
84713-17-7	**84713177**	3874	2,2,4(or 2,4,4)-trimethylhexanedinitrile	150.23	3_REACH			**1**	**0.3**	**1.9969E-06**			**1**	**0.03**	**1.9969E-07**			**1**	**0.03**	**1.99694E-07**
84-74-2	**84742**	963	dibutyl phthalate	278.35	3_REACH	996.6666667	996.6666667	**0**	**996.666667**	**0.00358062**	500	500	**0**	**500**	**0.0017963**	500	500	**0**	**500**	**0.0017963**
84852-15-3	**84852153**	964	Phenol, 4-nonyl-, branched	220.36	3_REACH			**1**	**0.3**	**1.3614E-06**			**1**	**0.03**	**1.3614E-07**			**1**	**0.03**	**1.36141E-07**
84852-53-9	**84852539**	3878	1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]	971.29	3_REACH			**1**	**0.3**	**3.0887E-07**			**1**	**0.03**	**3.0887E-08**			**1**	**0.03**	**3.08868E-08**
85-41-6	**85416**	965	phthalimide	147.13	3_REACH			**1**	**0.3**	**2.039E-06**			**1**	**0.03**	**2.039E-07**			**1**	**0.03**	**2.03901E-07**
85-42-7	**85427**	3889	cyclohexane-1,2-dicarboxylic anhydride	154.16	3_REACH			**1**	**0.3**	**1.946E-06**			**1**	**0.03**	**1.946E-07**			**1**	**0.03**	**1.94603E-07**
85-68-7	**85687**	968	benzyl butyl phthalate	312.37	3_REACH	333.3333333	333.3333333	**0**	**333.333333**	**0.00106711**	280	280	**0**	**280**	**0.00089637**	280	280	**0**	**280**	**0.000896373**
85702-79-0	**85702790**	3896	6-(isononanoylamino)hexanoic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	271.4	3_REACH			**1**	**0.3**	**1.1054E-06**			**1**	**0.03**	**1.1054E-07**			**1**	**0.03**	**1.10538E-07**
85-73-4	**85734**	3897	phthalylsulfathiazole	403.44	3_REACH			**1**	**0.3**	**7.436E-07**			**1**	**0.03**	**7.436E-08**			**1**	**0.03**	**7.43605E-08**
86261-90-7	**86261907**	3902	2-(2-oxoimidazolidin-1-yl)ethyl methacrylate	198.22	3_REACH			**1**	**0.3**	**1.5135E-06**			**1**	**0.03**	**1.5135E-07**			**1**	**0.03**	**1.51347E-07**
867-13-0	**867130**	3910	triethyl phosphonoacetate	224.19	3_REACH			**1**	**0.3**	**1.3382E-06**			**1**	**0.03**	**1.3382E-07**			**1**	**0.03**	**1.33815E-07**
86-73-7	**86737**	973	fluorene	166.22	3_REACH	70.66666667	70.66666667	**0**	**70.6666667**	**0.00042514**			**1**	**0.03**	**1.8048E-07**			**1**	**0.03**	**1.80484E-07**
86-74-8	**86748**	974	carbazole	167.21	3_REACH	1116.666667	1116.666667	**0**	**1116.66667**	**0.00667823**			**1**	**0.03**	**1.7942E-07**			**1**	**0.03**	**1.79415E-07**
868-77-9	**868779**	975	2-hydroxyethyl methacrylate	130.14	3_REACH			**1**	**0.3**	**2.3052E-06**			**1**	**0.03**	**2.3052E-07**			**1**	**0.03**	**2.30521E-07**
86960-46-5	**86960465**	3914	4-(decanoyloxy)benzoic acid	292.38	3_REACH			**1**	**0.3**	**1.0261E-06**			**1**	**0.03**	**1.0261E-07**			**1**	**0.03**	**1.02606E-07**
872-05-9	**872059**	3921	dec-1-ene	140.27	3_REACH			**1**	**0.3**	**2.1387E-06**			**1**	**0.03**	**2.1387E-07**			**1**	**0.03**	**2.13873E-07**
872-36-6	**872366**	3923	vinylene carbonate	86.046	3_REACH			**1**	**0.3**	**3.4865E-06**			**1**	**0.03**	**3.4865E-07**			**1**	**0.03**	**3.48651E-07**
872-50-4	**872504**	977	1-methyl-2-pyrrolidone	99.134	3_REACH			**1**	**0.3**	**3.0262E-06**			**1**	**0.03**	**3.0262E-07**			**1**	**0.03**	**3.02621E-07**

87305-03-1	87305031	3924	(1R,4R,5S)-6,6-Dimethyl-4-(tribromomethyl)-3-oxabicyclo[3.1.0]hexan-2-one	376.89	3_REACH			1	0.3	7.9599E-07			1	0.03	7.9599E-08			1	0.03	7.95988E-08
873-32-5	873325	3927	2-chlorobenzonitrile	137.57	3_REACH			1	0.3	2.1807E-06			1	0.03	2.1807E-07			1	0.03	2.18071E-07
87333-22-0	87333220	4632	methyl 2-(acetylamino)-3-chloropropionate	195.599	3_REACH			1	0.3	1.5338E-06			1	0.03	1.5338E-07			1	0.03	1.53375E-07
87-59-2	87592	978	2,3-xylidine	121.18	3_REACH	3333.333333	3333.333333	0	3333.33333	0.02750729	100	100	0	100	0.00082522	100	100	0	100	0.000825219
87-61-6	87616	979	1,2,3-trichlorobenzene	181.45	3_REACH	116.6666667	116.6666667	0	116.666667	0.00064297	30	30	0	30	0.00016533	30	30	0	30	0.000165335
87-62-7	87627	980	2,6-xylidine	121.18	3_REACH			1	0.3	2.4757E-06			1	0.03	2.4757E-07			1	0.03	2.47566E-07
87-99-0	87990	3944	xylitol	152.15	3_REACH			1	0.3	1.9717E-06			1	0.03	1.9717E-07			1	0.03	1.97174E-07
88-12-0	88120	3948	1-vinyl-2-pyrrolidone	111.15	3_REACH			1	0.3	2.6991E-06			1	0.03	2.6991E-07			1	0.03	2.69906E-07
88150-62-3	88150623	4393	3-ethyl 5-methyl 4-(2-chlorophenyl)-1,4-dihydro-2[2-(1,3-dihydro-1,3-dioxo-(2H)isoindol-2-yl)-ethoxymethyl]-6-methyl-3,5-pyridinedicarboxylate	538.99	3_REACH			1	0.3	5.566E-07			1	0.03	5.566E-08			1	0.03	5.56597E-08
88-18-6	88186	983	2-tert-butylphenol	150.22	3_REACH			1	0.3	1.9971E-06			1	0.03	1.9971E-07			1	0.03	1.99707E-07
88-27-7	88277	3954	2,6-DI-Tert-butyl-4-(dimethylamino)methylphenol	263.43	3_REACH			1	0.3	1.1388E-06			1	0.03	1.1388E-07			1	0.03	1.13882E-07
88374-05-4	88374054	3955	2-(2-Fluorophenyl)-2-(4-fluorophenyl)oxirane	232.23	3_REACH			1	0.3	1.2918E-06			1	0.03	1.2918E-07			1	0.03	1.29182E-07
88-44-8	88448	3956	4-aminotoluene-3-sulphonic acid	187.22	3_REACH			1	0.3	1.6024E-06			1	0.03	1.6024E-07			1	0.03	1.60239E-07
88-45-9	88459	3957	2,5-diaminobenzenesulphonic acid	188.21	3_REACH			1	0.3	1.594E-06			1	0.03	1.594E-07			1	0.03	1.59396E-07
88-51-7	88517	3959	4-amino-6-chlorotoluene-3-sulphonic acid	221.66	3_REACH			1	0.3	1.3534E-06			1	0.03	1.3534E-07			1	0.03	1.35342E-07
88-60-8	88608	3961	6-tert-butyl-m-cresol	164.25	3_REACH			1	0.3	1.8265E-06			1	0.03	1.8265E-07			1	0.03	1.82648E-07
88-72-2	88722	985	2-nitrotoluene	137.14	3_REACH	1800	1800	0	1800	0.01312527			1	0.03	2.1875E-07			1	0.03	2.18755E-07
88-73-3	88733	986	1-chloro-2-nitrobenzene	157.56	3_REACH	1066.666667	1066.666667	0	1066.66667	0.00676991	3000	3000	0	3000	0.01904037	3000	3000	0	3000	0.019040366
88-74-4	88744	987	2-nitroaniline	138.13	3_REACH			1	0.3	2.1719E-06			1	0.03	2.1719E-07			1	0.03	2.17187E-07
88-75-5	88755	988	2-nitrophenol	139.11	3_REACH	5666.666667	5666.666667	0	5666.66667	0.04073515			1	0.03	2.1566E-07			1	0.03	2.15657E-07
88-85-7	88857	989	dinoseb	240.22	3_REACH	80	80	0	80	0.00033303			1	0.03	1.2489E-07			1	0.03	1.24886E-07
88-99-3	88993	990	phthalic acid	166.13	3_REACH			1	0.3	1.8058E-06			1	0.03	1.8058E-07			1	0.03	1.80581E-07
89182-60-5	89182605	3969	D-Glucitol, 1-deoxy-1-(formylamino)	209.2	3_REACH			1	0.3	1.434E-06			1	0.03	1.434E-07			1	0.03	1.43403E-07
89-48-5	89485	3976	menthyl acetate	198.31	3_REACH			1	0.3	1.5128E-06			1	0.03	1.5128E-07			1	0.03	1.51278E-07
89604-91-1	89604911	4680	3-[2-(1,3-benzothiazol-2-ylsulfanyl)-1-(methoxyimino)-2-oxoethyl]-1,2,4-thiadiazol-5-amine	351.43	3_REACH			1	0.3	8.5366E-07			1	0.03	8.5366E-08			1	0.03	8.53655E-08
89-62-3	89623	991	2-nitro-p-toluidine	152.16	3_REACH			1	0.3	1.9716E-06			1	0.03	1.9716E-07			1	0.03	1.97161E-07
89-63-4	89634	992	4-chloro-2-nitroaniline	172.57	3_REACH	1066.666667	1066.666667	0	1066.66667	0.00618107			1	0.03	1.7384E-07			1	0.03	1.73842E-07
89-72-5	89725	993	2-sec-butylphenol	150.22	3_REACH			1	0.3	1.9971E-06			1	0.03	1.9971E-07			1	0.03	1.99707E-07
89-83-8	89838	996	thymol	150.22	3_REACH	566.6666667	566.6666667	0	566.666667	0.00377225			1	0.03	1.9971E-07			1	0.03	1.99707E-07
89-98-5	89985	997	2-chlorobenzaldehyde	140.57	3_REACH			1	0.3	2.1342E-06			1	0.03	2.1342E-07			1	0.03	2.13417E-07
90-02-8	90028	998	salicylaldehyde	122.12	3_REACH	1033.333333	1033.333333	0	1033.33333	0.00846162	380	380	0	380	0.00311169	380	380	0	380	0.003111693
90-04-0	90040	999	o-anisidine	123.16	3_REACH	2266.666667	2266.666667	0	2266.66667	0.01840424			1	0.03	2.4359E-07			1	0.03	2.43586E-07
90-05-1	90051	3990	guaiacol	124.14	3_REACH			1	0.3	2.4166E-06			1	0.03	2.4166E-07			1	0.03	2.41663E-07
90-12-0	90120	1000	1-methylnaphthalene	142.2	3_REACH			1	0.3	2.1097E-06			1	0.03	2.1097E-07			1	0.03	2.1097E-07
901-44-0	901440	3991	2,2'-isopropylidenebis(p-phenyleneoxy)diethanol	316.4	3_REACH			1	0.3	9.4817E-07			1	0.03	9.4817E-08			1	0.03	9.48167E-08
9016-45-9	9016459	1001	Nonylphenol, ethoxylated	308.462	3_REACH	49.33333333	49.33333333	0	49.3333333	0.00015993			1	0.03	9.7257E-08			1	0.03	9.72567E-08
90-17-5	90175	3992	2,2,2-trichloro-1-phenylethyl acetate	267.54	3_REACH			1	0.3	1.1213E-06			1	0.03	1.1213E-07			1	0.03	1.12133E-07
90268-23-8	90268238	3995	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(p-anisyl and Ph) derivs	659.54	3_REACH			1	0.3	4.5486E-07			1	0.03	4.5486E-08			1	0.03	4.54862E-08
90268-24-9	90268249	3996	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxyphenyl and 2,4-xylyl) derivs	752.06	3_REACH			1	0.3	3.989E-07			1	0.03	3.989E-08			1	0.03	3.98904E-08
90-30-2	90302	1002	N-1-naphthylaniline	219.29	3_REACH			1	0.3	1.3681E-06			1	0.03	1.3681E-07			1	0.03	1.36805E-07
90-43-7	90437	106	biphenyl-2-ol	170.21	3_REACH	236.6666667	236.6666667	0	236.666667	0.00139044			1	0.03	1.7625E-07			1	0.03	1.76253E-07
90474-13-8	90474138	4000	diethyl 1,2-cyclopentanedicarboxylate	214.26	3_REACH			1	0.3	1.4002E-06			1	0.03	1.4002E-07			1	0.03	1.40017E-07
90498-90-1	90498901	4387	3,9-bis(2-(3-(3-tert-butyl-4-hydroxy-5-	740.98	3_REACH			1	0.3	4.0487E-07			1	0.03	4.0487E-08			1	0.03	4.04869E-08
90-51-7	90517	4001	6-amino-4-hydroxynaphthalene-2-sulphonic acid	239.25	3_REACH			1	0.3	1.2539E-06			1	0.03	1.2539E-07			1	0.03	1.25392E-07
90-72-2	90722	4003	2,4,6-tris(dimethylaminomethyl)phenol	265.4	3_REACH			1	0.3	1.1304E-06			1	0.03	1.1304E-07			1	0.03	1.13037E-07
90-80-2	90802	4006	D-glucono-1,5-lactone	178.14	3_REACH			1	0.3	1.6841E-06			1	0.03	1.6841E-07			1	0.03	1.68407E-07
91-15-6	91156	1004	phthalonitrile	128.14	3_REACH			1	0.3	2.3412E-06			1	0.03	2.3412E-07			1	0.03	2.34119E-07
91-17-8	91178	1005	decahydronaphthalene	138.25	3_REACH	830	830	0	830	0.00600362			1	0.03	2.17E-07			1	0.03	2.16998E-07
91-20-3	91203	107	naphthalene	128.17	3_REACH	480	480	0	480	0.00374503			1	0.03	2.3406E-07			1	0.03	2.34064E-07
91-22-5	91225	1006	quinoline	129.16	3_REACH	11500	11500	0	11500	0.08903685	800	800	0	800	0.00619387	800	800	0	800	0.006193868
91273-04-0	91273040	4271	1-(N,N-bis(2-ethylhexyl)aminomethyl)-1,2,4-triazole	322.55	3_REACH			1	0.3	9.3009E-07			1	0.03	9.3009E-08			1	0.03	9.30088E-08
91-57-6	91576	1007	2-methylnaphthalene	142.2	3_REACH			1	0.3	2.1097E-06			1	0.03	2.1097E-07			1	0.03	2.1097E-07
91-64-5	91645	1008	coumarin	146.15	3_REACH	4500	4500	0	4500	0.03079028			1	0.03	2.0527E-07			1	0.03	2.05269E-07
91-66-7	91667	1009	N,N-diethylaniline	149.24	3_REACH			1	0.3	2.0102E-06			1	0.03	2.0102E-07			1	0.03	2.01018E-07
91-68-9	91689	4019	3-diethylaminophenol	165.24	3_REACH			1	0.3	1.8155E-06			1	0.03	1.8155E-07			1	0.03	1.81554E-07
91-76-9	91769	4021	6-phenyl-1,3,5-triazine-2,4-diyldiamine	187.21	3_REACH			1	0.3	1.6025E-06			1	0.03	1.6025E-07			1	0.03	1.60248E-07
919-30-2	919302	4023	3-aminopropyltriethoxysilane	221.37	3_REACH			1	0.3	1.3552E-06			1	0.03	1.3552E-07			1	0.03	1.3552E-07
91-97-4	91974	4025	3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate	264.29	3_REACH			1	0.3	1.1351E-06			1	0.03	1.1351E-07			1	0.03	1.13512E-07
923-02-4	923024	4030	N-(hydroxymethyl)methacrylamide	115.13	3_REACH			1	0.3	2.6058E-06			1	0.03	2.6058E-07			1	0.03	2.60575E-07
925-21-3	925213	4038	butyl hydrogen maleate	172.18	3_REACH			1	0.3	1.7424E-06			1	0.03	1.7424E-07			1	0.03	1.74236E-07
92-52-4	92524	1012	biphenyl	154.21	3_REACH	120	120	0	120	0.00077816	230	230	0	230	0.00149147	230	230	0	230	0.001491473
92-69-3	92693	1013	biphenyl-4-ol	170.21	3_REACH			1	0.3	1.7625E-06			1	0.03	1.7625E-07			1	0.03	1.76253E-07
92-70-6	92706	4045	3-hydroxy-2-naphthoic acid	188.18	3_REACH			1	0.3	1.5942E-06			1	0.03	1.5942E-07			1	0.03	1.59422E-07
927-07-1	927071	4046	tert-butyl peroxypivalate	174.24	3_REACH			1	0.3	1.7218E-06			1	0.03	1.7218E-07			1	0.03	1.72176E-07
92-84-2	92842	4051	phenothiazine	199.28	3_REACH			1	0.3	1.5054E-06			1	0.03	1.5054E-07			1	0.03	1.50542E-07
92-88-6	92886	1015	biphenyl-4,4'-diol	186.21	3_REACH			1	0.3	1.6111E-06			1	0.03	1.6111E-07			1	0.03	1.61108E-07
928-96-1	928961	1016	cis-hex-3-en-1-ol	100.16	3_REACH			1	0.3	2.9952E-06			1	0.03	2.9952E-07			1	0.03	2.99521E-07
929-06-6	929066	4053	2-(2-aminoethoxy)ethanol	105.14	3_REACH			1	0.3	2.8533E-06			1	0.03	2.8533E-07			1	0.03	2.85334E-07
92952-81-3	92952813	4412	4-[(3-hydroxypropyl)amino]-3-nitrophenol	212.21	3_REACH			1	0.3	1.4137E-06			1	0.03	1.4137E-07			1	0.03	1.41369E-07
93-04-9	93049	1017	methyl 2-naphthyl ether	158.2	3_REACH	1346.666667	1346.666667	0	1346.66667	0.00851243			1	0.03	1.8963E-07			1	0.03	1.89633E-07
931-36-2	931362	4059	2-ethyl-4-methylimidazole	110.16	3_REACH			1	0.3	2.7233E-06			1	0.03	2.7233E-07			1	0.03	2.72331E-07
93-17-4	93174	4063	3,4-dimethoxyphenylacetonitrile	177.2	3_REACH			1	0.3	1.693E-06			1	0.03	1.693E-07			1	0.03	1.693E-07
93-20-9	93209	4065	2-(2-naphthyloxy)ethanol	188.23	3_REACH			1	0.3	1.5938E-06			1	0.03	1.5938E-07			1	0.03	1.59379E-07
932-64-9	932649	4066	1,2-dihydro-5-nitro-3H-1,2,4-triazol-3-one	130.07	3_REACH			1	0.3	2.3065E-06			1	0.03	2.3065E-07			1	0.03	2.30645E-07
93413-62-8	93413628	4069	4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol	263.38	3_REACH			1	0.3	1.139E-06			1	0.03	1.139E-07			1	0.03	1.13904E-07
93-58-3	93583	4073	methyl benzoate	136.15	3_REACH			1	0.3	2.2035E-06			1	0.03	2.2035E-07			1	0.03	2.20345E-07
936-49-2	936492	4076	2-phenyl-2-imidazoline	146.19	3_REACH			1	0.3	2.0521E-06			1	0.03	2.0521E-07			1	0.03	2.05212E-07
93-69-6	93696	4079	1-o-tolylbiguanide	191.24	3_REACH			1	0.3	1.5687E-06			1	0.03	1.5687E-07			1	0.03	1.56871E-07
93-70-9	93709	4080	2'-chloroacetoacetanilide	211.65	3_REACH			1	0.3	1.4174E-06			1	0.03	1.4174E-07			1	0.03	1.41743E-07
93-92-5	93925	4093	1-phenylethyl acetate	164.2	3_REACH			1	0.3	1.827E-06			1	0.03	1.827E-07			1	0.03	1.82704E-07
93957-50-7	93957507	4490	3-[3-(4-fluorophenyl)-1-(1-methylethyl)-1H-indol-2-yl]-(E)-2-propenal	307.37	3_REACH			1	0.3	9.7602E-07			1	0.03	9.7602E-08			1	0.03	9.76022E-08
939-97-9	939979	4095	4-tert-butylbenzaldehyde	162.23	3_REACH			1	0.3	1.8492E-06			1	0.03	1.8492E-07			1	0.03	1.84923E-07
94-04-2	94042	4096	vinyl 2-ethylhexanoate	170.25	3_REACH			1	0.3	1.7621E-06			1	0.03	1.7621E-07			1	0.03	1.76211E-07
94050-90-5	94050905	4248	(R)-2-(4-hydroxyphenoxy)propanoic acid	182.18	3_REACH			1	0.3	1.6467E-06			1	0.03	1.6467E-07			1	0.03	1.64672E-07
94-13-3	94133	109	propyl 4-hydroxybenzoate	180.2	3_REACH			1	0.3	1.6648E-06			1	0.03	1.6648E-07			1	0.03	1.66482E-07
941-69-5	941695	4098	N-phenylmaleimide	173.17	3_REACH			1	0.3	1.7324E-06			1	0.03	1.7324E-07			1	0.03	1.7324E-07
947-04-6	947046	4110	dodecane-12-lactam	197.32	3_REACH			1	0.3	1.5204E-06			1	0.03	1.5204E-07			1	0.03	1.52037E-07
947-19-3	947193	4112	hydroxycyclohexyl phenyl ketone	204.27	3_REACH			1	0.3	1.4686E-06			1	0.03	1.4686E-07			1	0.03	1.46864E-07
94723-86-1	94723861	4485	2-butanoyl-3-hydroxy-5-(thian-3-yl)cyclohex-2-en-1-one	282.4	3_REACH			1	0.3	1.0623E-06			1	0.03	1.0623E-07			1	0.03	1.06232E-07
947753-66-4	947753664	4115	2-Ethylhexyl-2-cyano-3-(4-methoxyphenyl)-3-phenylprop-2-enoate	391.51	3_REACH			1	0.3	7.6626E-07			1	0.03	7.6626E-08			1	0.03	7.66264E-08
94-91-7	94917	4116	N,N'-Bis(salicylidene)-1,2-propanediamine	282.35	3_REACH			1	0.3	1.0625E-06			1	0.03	1.0625E-07			1	0.03	1.06251E-07
94-96-2	94962	1024	2-ethylhexane-1,3-diol	146.23	3_REACH			1	0.3	2.0516E-06			1	0.03	2.0516E-07			1	0.03	2.05156E-07
95-14-7	95147	112	benzotriazole	119.13	3_REACH	63000	63000	0	63000	0.52883405	3000	3000	0	3000	0.02518257	3000	3000	0	3000	0.025182574
95-16-9	95169	113	benzothiazole	135.19	3_REACH	12400	12400	0	12400	0.09172276			1	0.03	2.2191E-07			1	0.03	2.2191E-07
95235-30-6	95235306	4398	4-(4-isopropoxyphenylsulfonyl)phenol	292.35	3_REACH			1	0.3	1.0262E-06			1	0.03	1.0262E-07			1	0.03	1.02617E-07
95-31-8	95318	4124	N-tert-butylbenzothiazole-2-sulphenamide	238.38	3_REACH			1	0.3	1.2585E-06			1	0.03	1.2585E-07			1	0.03	1.25849E-07
95-33-0	95330	4125	N-cyclohexylbenzothiazole-2-sulfenamide	264.42	3_REACH			1	0.3	1.1346E-06			1	0.03	1.1346E-07			1	0.03	1.13456E-07
95-38-5	95385	4126	2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol	350.59	3_REACH			1	0.3	8.557E-07			1	0.03	8.557E-08			1	0.03	8.557E-08
95-48-7	95487	1029	o-cresol	108.14	3_REACH	1666.666667	1666.666667	0	1666.66667	0.01541212			1	0.03	2.7742E-07			1	0.03	2.77418E-07
95-49-8	95498	1030	2-chlorotoluene	126.59	3_REACH	3000	3000	0	3000	0.02369855	140	140	0	140	0.00110593	140	140	0	140	0.001105933
95-51-2	95512	1031	2-chloroaniline	127.58	3_REACH	43.33333333	43.33333333	0	43.3333333	0.00033966	32	32	0	32	0.00025082	32	32	0	32	0.000250823
95-53-4	95534	1032	o-toluidine	107.16	3_REACH	173.3333333	173.3333333	0	173.333333	0.00161752			1	0.03	2.7996E-07			1	0.03	2.79955E-07
95-54-5	95545	1033	o-phenylenediamine	108.15	3_REACH			1	0.3	2.7739E-06			1	0.03	2.7739E-07			1	0.03	2.77393E-07
95-63-6	95636	1035	1,2,4-trimethylbenzene	120.19	3_REACH			1	0.3	2.496E-06			1	0.03	2.496E-07			1	0.03	2.49605E-07
95-68-1	95681	1036	2,4-xylidine	121.18	3_REACH	3300	3300	0	3300	0.02723222			1	0.03	2.4757E-07			1	0.03	2.47566E-07
95-74-9	95749	1037	3-chloro-p-toluidine	141.6	3_REACH	206.6666667	206.6666667	0	206.666667	0.00145951			1	0.03	2.1186E-07			1	0.03	2.11864E-07
95-80-7	95807	1039	4-methyl-m-phenylenediamine	122.17	3_REACH			1	0.3	2.4556E-06			1	0.03	2.4556E-07			1	0.03	2.45559E-07
95-82-9	95829	1040	2,5-dichloroaniline	162.02	3_REACH	973.3333333	973.3333333	0	973.333333	0.00600749			1	0.03	1.8516E-07			1	0.03	1.85162E-07
95962-14-4	95962144	4305	2-(2-(4-methyl-3-cyclohexen-1-yl)propyl)cyclopentanone	220.36	3_REACH			1	0.3	1.3614E-06			1	0.03	1.3614E-07			1	0.03	1.36141E-07
95-96-5	95965	4140	dilactide	144.13	3_REACH			1	0.3	2.0815E-06			1	0.03	2.0815E-07			1	0.03	2.08145E-07
96-09-3	96093	1044	(epoxyethyl)benzene	120.15	3_REACH	3866.666667	3866.666667	0	3866.66667	0.03218199			1	0.03	2.4969E-07			1	0.03	2.49688E-07
96-12-8	96128	1045	1,2-dibromo-3-chloropropane	236.35	3_REACH			1	0.3	1.2693E-06			1	0.03	1.2693E-07			1	0.03	1.2693E-07
96-18-4	96184	1047	1,2,3-trichloropropane	147.43	3_REACH	11266.66667	11266.66667	0	11266.6667	0.07642045			1	0.03	2.0349E-07			1	0.03	2.03486E-07
96-23-1	96231	1049	1,3-dichloropropan-2-ol	128.99	3_REACH	327666.6667	327666.6667	0	327666.667	2.5402486	10400	10400	0	10400	0.08062641	10400	10400	0	10400	0.080626405
96-24-2	96242	1050	3-chloropropane-1,2-diol	110.54	3_REACH			1	0.3	2.7139E-06			1	0.03	2.7139E-07			1	0.03	2.71395E-07
96-29-7	96297	1051	butanone oxime	87.123	3_REACH			1	0.3	3.4434E-06			1	0.03	3.4434E-07			1	0.03	3.44341E-07
96-31-1	96311	1052	1,3-dimethylurea	88.112	3_REACH			1	0.3	3.4048E-06			1	0.03	3.4048E-07			1	0.03	3.40476E-07
96-45-7	96457	1054	imidazolidine-2-thione	102.16	3_REACH	6510	6510	0	6510	0.06372357			1	0.03	2.9366E-07			1	0.03	2.93657E-07
96-48-0	96480	4148	Butyrolactone	86.09	3_REACH			1	0.3	3.4847E-06			1	0.03	3.4847E-07			1	0.03	3.48473E-07
96-49-1	96491	4149	ethylene carbonate	88.062	3_REACH			1	0.3	3.4067E-06			1	0.03	3.4067E-07			1	0.03	3.40669E-07

96-67-3	**96673**	4151	3-amino-2-hydroxy-5-nitrobenzenesulphonic acid	234.19	3_REACH			1	0.3	1.281E-06			1	0.03	1.281E-07			1	0.03	1.281015-07
96-69-5	**96695**	4152	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	358.54	3_REACH			1	0.3	8.3673E-07			1	0.03	8.3673E-08			1	0.03	8.367275-08
96-76-4	**96764**	4153	2,4-di-tert-butylphenol	206.33	3_REACH			1	0.3	1.454E-06			1	0.03	1.454E-07			1	0.03	1.453998-07
96-93-5	**96935**	4156	3-amino-4-hydroxy-5-nitrobenzenesulphonic acid	234.19	3_REACH			1	0.3	1.281E-06			1	0.03	1.281E-07			1	0.03	1.281015-07
96-96-8	**96968**	4157	2-nitro-p-anisidine	168.15	3_REACH			1	0.3	1.7841E-06			1	0.03	1.7841E-07			1	0.03	1.784125-07
96-97-9	**96979**	4158	5-nitrosalicylic acid	183.12	3_REACH			1	0.3	1.6383E-06			1	0.03	1.638375-07			1	0.03	1.638375-07
97-00-7	**97007**	1056	1-chloro-2,4-dinitrobenzene	202.56	3_REACH	163.3333333	163.3333333	0	163.333333	0.00080935			1	0.03	1.481E-07			1	0.03	1.481045-07
97-39-2	**97392**	4164	1-Octadecylpyridinium	239.32	3_REACH			1	0.3	1.2636E-06			1	0.03	1.2636E-07			1	0.03	1.263555-07
97-52-9	**97529**	4165	4-nitro-p-anisidine	168.15	3_REACH			1	0.3	1.7841E-06			1	0.03	1.7841E-07			1	0.03	1.784125-07
97-53-0	**97530**	1057	eugenol	164.2	3_REACH			1	0.3	1.827E-06			1	0.03	1.827E-07			1	0.03	1.827045-07
97-65-4	**97654**	4168	itaconic acid	130.1	3_REACH			1	0.3	2.3059E-06			1	0.03	2.3059E-07			1	0.03	2.305925-07
976-71-6	**976716**	4170	carvone	150.26	3_REACH			1	0.3	8.8116E-07			1	0.03	8.8116E-08			1	0.03	8.811615-08
97-74-5	**97745**	1059	tetramethylthiuram monosulphide	208.37	3_REACH	966.6666667	966.6666667	0	966.666667	0.00463918			1	0.03	1.439E-07			1	0.03	1.439765-07
97-78-9	**97789**	4172	N-lauroylsarcosine	271.4	3_REACH			1	0.3	1.1054E-06			1	0.03	1.1054E-07			1	0.03	1.105338-07
97-88-1	**97881**	1061	butyl methacrylate	142.2	3_REACH			1	0.3	2.1097E-06			1	0.03	2.1097E-07			1	0.03	2.109775-07
97-90-5	**97905**	4175	ethylene dimethacrylate	198.22	3_REACH			1	0.3	1.5135E-06			1	0.03	1.5135E-07			1	0.03	1.513475-07
98-00-0	**98000**	1063	furfuryl alcohol	98.101	3_REACH	38333.33333	38333.33333	0	38333.3333	0.39075375			1	0.03	3.0581E-07			1	0.03	3.058075-07
980-26-7	**980267**	4177	5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione	340.38	3_REACH			1	0.3	8.5137E-08			1	0.03	8.5137E-09			1	0.03	8.513685-09
98-07-7	**98077**	1065	Benzotrichloride	195.48	3_REACH	16666.66667	16666.66667	0	16666.6667	0.08528021			1	0.03	1.5347E-07			1	0.03	1.534685-07
98-09-9	**98099**	1066	benzenesulphonyl chloride	176.62	3_REACH			1	0.3	1.6986E-06			1	0.03	1.6986E-07			1	0.03	1.698565-07
98-13-5	**98135**	1067	triphenylphenylsilane	311.55	3_REACH			1	0.3	1.4181E-06			1	0.03	1.4181E-07			1	0.03	1.41815-07
98-16-8	**98168**	1068	3,Trifluoromethylaniline	161.13	3_REACH	900	900	0	900	0.00558656			1	0.03	1.8619E-07			1	0.03	1.861855-07
98-17-9	**98179**	1069	3,Trifluoromethylphenol	162.11	3_REACH	3666.666667	3666.666667	0	3666.6667	0.02281839			1	0.03	1.8506E-07			1	0.03	1.85065-07
98-29-3	**98293**	4181	4-tert-butylpyrocatechol	166.22	3_REACH			1	0.3	1.8048E-06			1	0.03	1.8048E-07			1	0.03	1.804845-07
98-37-3	**98373**	4183	3-amino-4-hydroxybenzenesulphonic acid	189.19	3_REACH			1	0.3	1.5857E-06			1	0.03	1.5857E-07			1	0.03	1.585715-07
98377-35-6	**98377356**	4501	1-(2-chlorophenyl)-1,2-dihydro-5H-tetrazol-5-one	196.6	3_REACH			1	0.3	1.5259E-06			1	0.03	1.5259E-07			1	0.03	1.525945-07
98-44-2	**98442**	4185	2-aminobenzene-1,4-disulphonic acid	253.25	3_REACH			1	0.3	1.1846E-06			1	0.03	1.1846E-07			1	0.03	1.18465-07
98-51-1	**98511**	1071	4-tert-butylbenzene	148.25	3_REACH			1	0.3	2.0236E-06			1	0.03	2.0236E-07			1	0.03	2.023615-07
98-52-2	**98522**	1072	4-tert-butylcyclohexanol	156.27	3_REACH			1	0.3	1.9196E-06			1	0.03	1.9196E-07			1	0.03	1.919655-07
98-53-3	**98533**	4186	4-tert-butylcyclohexanone	154.25	3_REACH			1	0.3	1.9446E-06			1	0.03	1.9446E-07			1	0.03	1.944695-07
98-54-4	**98544**	1073	4-tert-butylphenol	150.22	3_REACH	1300	1300	0	1300	0.00866367			1	0.03	1.9971E-07			1	0.03	1.997075-07
98-55-5	**98555**	1074	p-menth-1-en-8-ol	154.25	3_REACH			1	0.3	1.9446E-06			1	0.03	1.9446E-07			1	0.03	1.944695-07
98-59-9	**98599**	4188	tosyl chloride	190.65	3_REACH			1	0.3	1.5736E-06			1	0.03	1.5736E-07			1	0.03	1.573565-07
98730-04-2	**98730042**	4191	2,2-Dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)ethanone	260.12	3_REACH			1	0.3	1.1633E-06			1	0.03	1.1633E-07			1	0.03	1.163315-07
98-73-7	**98737**	1075	4-tert-butylbenzoic acid	178.23	3_REACH			1	0.3	1.6832E-06			1	0.03	1.6832E-07			1	0.03	1.683225-07
98-82-8	**98828**	1076	cumene	120.19	3_REACH	466.6666667	466.6666667	0	466.666667	0.00388274			1	0.03	2.496E-07			1	0.03	2.496005-07
98-83-9	**98830**	4193	2-phenylpropene	118.18	3_REACH			1	0.3	2.5385E-06			1	0.03	2.5385E-07			1	0.03	2.538505-07
98-85-1	**98851**	4194	1-phenylethanol	122.17	3_REACH			1	0.3	2.4558E-06			1	0.03	2.4558E-07			1	0.03	2.455595-07
98-86-2	**98862**	1077	acetophenone	120.15	3_REACH			1	0.3	2.4969E-06			1	0.03	2.4969E-07			1	0.03	2.496885-07
98967-40-9	**98967409**	1081	N-(2,6-diflurophenyl)-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine-2-sulfonamide Flumetsulam	325.3	3_REACH	174000	174000	0	174000	0.53489087	111000	111000	0	111000	0.34122349			1	0.03	9.222225-08
99-08-1	**99081**	1082	3-nitrotoluene	137.14	3_REACH	2466.666667	2466.666667	0	2466.66667	0.01796849			1	0.03	2.187E-07			1	0.03	2.187555-07
99189-60-3	**99189603**	4198	2-[1-(2-Amino-2-oxoethyl)cyclohexyl]acetic acid	199.25	3_REACH			1	0.3	1.8056E-06			1	0.03	1.8056E-07			1	0.03	1.805665-07
993-13-5	**993135**	4203	methylphosphonic acid	96.022	3_REACH			1	0.3	3.1243E-06			1	0.03	3.1243E-07			1	0.03	3.124325-07
99-34-3	**99343**	4204	3,5dinitrobenzoic acid	212.12	3_REACH			1	0.3	1.4143E-06			1	0.03	1.4143E-07			1	0.03	1.414325-07
99-54-7	**99547**	1087	1,2-dichloro-4-nitrobenzene	192	3_REACH	1000	1000	0	1000	0.00520833			1	0.03	1.5625E-07			1	0.03	1.56255-07
99-55-8	**99558**	1088	5-nitro-o-toluidine	152.16	3_REACH	1700	1700	0	1700	0.01117245			1	0.03	1.9716E-07			1	0.03	1.971615-07
99-57-0	**99570**	4206	2-amino-4-nitrophenol	154.13	3_REACH			1	0.3	1.9464E-06			1	0.03	1.9464E-07			1	0.03	1.946415-07
99591-74-9	**99591749**	4207	1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide	188.18	3_REACH			1	0.3	1.5942E-06			1	0.03	1.5942E-07			1	0.03	1.594225-07
99607-70-2	**99607702**	1089	Heptan-2-yl [(5-chloroquinolin-8-yl)oxy]acetate	335.83	3_REACH	820	820	0	820	0.00244171			1	0.03	8.9331E-08			1	0.03	8.933095-08
99-62-7	**99627**	4210	1,3-diisopropylbenzene	162.28	3_REACH			1	0.3	1.8487E-06			1	0.03	1.8487E-07			1	0.03	1.848665-07
99-63-8	**99638**	4214	isophthaloyl dichloride	203.02	3_REACH			1	0.3	1.4777E-06			1	0.03	1.4777E-07			1	0.03	1.477665-07
99-75-2	**99752**	4215	methyl nicotinate	136.15	3_REACH			1	0.3	1.9976E-06			1	0.03	1.9976E-07			1	0.03	1.99765-07
99-76-3	**99763**	4216	methyl 4-hydroxybenzoate	152.15	3_REACH			1	0.3	1.9717E-06			1	0.03	1.9717E-07			1	0.03	1.971745-07
99817-36-4	**99817364**	4328	2,4-dichloro-3-ethyl-6-nitrophenol	236.06	3_REACH			1	0.3	1.2709E-06			1	0.03	1.2709E-07			1	0.03	1.270965-07
99-87-6	**99876**	1092	p-cymene	134.22	3_REACH	1180	1180	0	1180	0.00879154			1	0.03	2.2261E-07			1	0.03	2.226145-07
99-88-7	**99887**	4221	4-isopropylaniline	135.21	3_REACH			1	0.3	2.2188E-06			1	0.03	2.2188E-07			1	0.03	2.218775-07
99-93-4	**99934**	4222	4'-hydroxyacetophenone	136.15	3_REACH			1	0.3	2.2035E-06			1	0.03	2.2035E-07			1	0.03	2.203455-07
99-96-7	**99967**	1093	4-hydroxybenzoic acid	138.12	3_REACH	57666.66667	57666.66667	0	57666.6667	0.41751134			1	0.03	2.172E-07			1	0.03	2.172025-07
99-97-8	**99978**	1094	N,N-dimethyl-o-toluidine	135.21	3_REACH			1	0.3	2.2188E-06			1	0.03	2.2188E-07			1	0.03	2.218775-07
99-99-0	**99990**	1095	4-nitrotoluene	137.14	3_REACH	2500	2500	0	2500	0.01822965			1	0.03	2.187E-07			1	0.03	2.187555-07

						fish, acute						fish, chronic						fish, chronic reproduction						Algae					
CAS	CAS_NR	ID	Compound	MW	Emissions	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value	Final Tox conc (ug/l)	Final Tox conc (mol/m3)	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value	Final Tox conc (ug/l)	Final Tox conc (mol/m3)	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value	Final Tox conc (ug/l)	Final Tox conc (mol/m3)	Tox Conc (MIN, ug/l)	Tox Conc (5%, ug/l)	Tox Conc (P5 preferred)	missing value	Final Tox conc (ug/l)	Final Tox conc
100986-85-4	100986854	139	Levofloxacin	361.38	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.09223901				1	0.039	1.0792E-07				1	0.039	1.0792E-07				1	1	2.7672E-06
10238-21-8	10238218	152	Glibenklamid	494.01	1_Pharma	33333.71795		33333.71795	0	33333.71795	0.067475796				1	0.039	7.89458E-08				1	0.039	7.89458E-08	33333.71795		33333.71795	0	33333.7179	0.0674758
103-90-2	103902	165	paracetamol	151.17	1_Pharma	1		1	0	1	6.61507E-06				1	0.039	2.57988E-07				1	0.039	2.57988E-07	5		5	0	5	3.3075E-05
114-07-8	114078	336	erythromycin	733.94	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.045416973	100000		100000	0	100000	0.13625092				1	0.039	5.31379E-08	2		2	0	2	2.725E-06
114798-26-4	114798264	1626	Losartan	422.93	1_Pharma	929000		929000	0	929000	2.196580994				1	0.039	9.22138E-08				1	0.039	9.22138E-08	143000		143000	0	143000	0.33811742
120-51-4	120514	359	benzyl benzoate	212.25	1_Pharma	950		950	0	950	0.004475854	237		237	0	237	0.001116608				1	0.039	1.83746E-07	64.7		64.7	0	64.7	0.00030483
121-75-5	121755	374	Malathion	330.36	1_Pharma	1.5		1.5	0	1.5	4.5405E-06	0.45	2	2	0	2	6.054E-06				1	0.039	1.18053E-07	3.1		3.1	0	3.1	9.3837E-06
123-99-9	123999	1782	azelaic acid	188.22	1_Pharma				1	0.39	2.07204E-06	2000		2000	0	2000	0.010625863				1	0.039	2.07204E-07	70		70	0	70	0.00037191
126-07-8	126078	1144	Griseofulvin	352.77	1_Pharma				1	0.39	1.10554E-06				1	0.039	1.10554E-07				1	0.039	1.10554E-07				1	1	2.8347E-06
127-07-1	127071	411	Hydroxikarbamid	76.057	1_Pharma	423345		423345	0	423345	5.566154332				1	0.039	5.12773E-07				1	0.039	5.12773E-07				1	1	1.3148E-05
128-13-2	128132	1816	Ursodiol	392.58	1_Pharma	70290		70290	0	70290	0.179046309				1	0.039	9.93428E-08				1	0.039	9.93428E-08	30640		30640	0	30640	0.07804779
130-26-7	130267	1834	Clioquinol	305.5	1_Pharma	3333.333333		3333.333333	0	3333.333333	0.010911075				1	0.039	1.2766E-07				1	0.039	1.2766E-07	4034.495		4034.495	0	4034.495	0.0132062
13311-84-7	13311847	427	Flutamid	276.22	1_Pharma	50		50	0	50	0.000181015	14.5		14.5	0	14.5	5.24944E-05				1	0.039	1.41192E-07				1	1	3.6203E-06
134523-00-5	134523005	431	Atorvastatin	558.65	1_Pharma				1	0.39	6.98112E-07	0.013		0.013	0	0.013	2.32704E-08				1	0.039	6.98112E-08				1	1	1.79E-06
137862-53-4	137862534	442	Valsartan	435.53	1_Pharma				1	0.39	8.95461E-07				1	0.039	8.95461E-08				1	0.039	8.95461E-08	17666.66667		17666.66667	0	17666.6667	0.0405636
138402-11-6	138402116	444	Irbesartan	428.55	1_Pharma	7040		7040	0	7040	0.016427488				1	0.039	9.10046E-08				1	0.039	9.10046E-08	7200		7200	0	7200	0.01680084
139481-59-7	139481597	447	Candesartan	440.47	1_Pharma				1	0.39	8.85418E-07	1000		1000	0	1000	0.002270302				1	0.039	8.85418E-08	32000		32000	0	32000	0.07264967
15307-86-5	15307865	31	diclofenac	296.15	1_Pharma	1		1	0	1	3.37667E-06	0.5		0.5	0	0.5	1.68833E-06				1	0.039	1.3169E-07	5		5	0	5	1.6883E-05
15687-27-1	15687271	493	ibuprofen	206.29	1_Pharma	1		1	0	1	4.84754E-06	0.01		0.01	0	0.01	4.84754E-08				1	0.039	1.89054E-07	10		10	0	10	4.8475E-05
20830-75-5	20830755	529	Digoxin	780.95	1_Pharma				1	0.39	4.99392E-07				1	0.039	4.99392E-08				1	0.039	4.99392E-08				1	1	1.2805E-06
22204-53-1	22204531	539	Naproxen	230.26	1_Pharma	186672.5035		186672.5035	0	186672.5035	0.810703133				1	0.039	1.69374E-07				1	0.039	1.69374E-07	7000.21888		7000.21888	0	7000.21888	0.03040137
23593-75-1	23593751	553	Klotrimazol	344.85	1_Pharma	63		63	0	63	0.000182688				1	0.039	1.13093E-07				1	0.039	1.13093E-07	5.3141385		5.3141385	0	5.3141385	0.00001541
25812-30-0	25812300	570	Gemfibrozil	250.34	1_Pharma				1	0.39	1.55788E-06	0.38		0.38	0	0.38	1.51794E-06				1	0.039	1.55788E-07	3125		3125	0	3125	0.01248302
26787-78-0	26787780	574	amoxicillin	365.41	1_Pharma	333333.3333		333333.3333	0	333333.3333	0.912217327				1	0.039	1.06729E-07				1	0.039	1.06729E-07	733.3469804		733.3469804	0	733.34698	0.00200692
29122-68-7	29122687	44	Atenolol	266.34	1_Pharma	11.08		11.08	0	11.08	4.1601E-05				1	0.039	1.46429E-07				1	0.039	1.46429E-07	206666.6667		206666.6667	0	206666.667	0.77595054
298-46-4	298464	45	Carbamazepine	236.28	1_Pharma	7.85		7.85	0	7.85	3.32233E-05	0.89		0.89	0	0.89	3.76672E-06	1780		1780	0	1780	0.007533435	10		10	0	10	4.2323E-05
3380-34-5	3380345	48	triclosan	289.55	1_Pharma	100		100	0	100	0.000345363	0.45		0.45	0	0.45	1.55414E-06	57.9		57.9	0	57.9	0.000199965	0.146666667		0.146666667	0	0.14666667	5.0653E-07
37350-58-6	37350586	50	Metoprolol	267.37	1_Pharma				1	0.39	1.45865E-06	5		5	0	5	1.87007E-05				1	0.039	1.45865E-07	2433.333333		2433.333333	0	2433.33333	0.009101
3930-20-9	3930209	51	Sotalol	272.37	1_Pharma				1	0.39	1.43188E-06				1	0.039	1.43188E-07				1	0.039	1.43188E-07	220666.6667		220666.6667	0	220666.667	0.81017244
41859-67-0	41859670	53	Bezafibrat	361.83	1_Pharma	33333.85845		33333.85845	0	33333.85845	0.092125745	0.03386		0.03386	0	0.03386	9.35799E-08				1	0.039	1.07785E-07	2540		2540	0	2540	0.00701987
42200-33-9	42200339	1154	Nadolol	309.41	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.10773192				1	0.039	1.26046E-07				1	0.039	1.26046E-07				1	1	3.232E-06
439-14-5	439145	640	Diazepam	284.75	1_Pharma	4233.415103		4233.415103	0	4233.415103	0.014867129	72000		72000	0	72000	0.25285338				1	0.039	1.36962E-07	1033.353293		1033.353293	0	1033.35329	0.00362898
443-48-1	443481	642	Metronidazol	171.16	1_Pharma	40000		40000	0	40000	0.233699462				1	0.039	2.27857E-07				1	0.039	2.27857E-07	4166.666667		4166.666667	0	4166.66667	0.02434369
49562-28-9	49562289	649	fenofibrate	360.84	1_Pharma				1	0.39	1.08081E-06				1	0.039	1.08081E-07				1	0.039	1.08081E-07	3120		3120	0	3120	0.00864649
50-02-2	50022	652	Dexametason	392.47	1_Pharma	1000		1000	0	1000	0.002547965	42.7		42.7	0	42.7	0.000108798				1	0.039	9.93707E-08				1	1	2.548E-06
50-06-6	50066	4945	phenobarbital	232.24	1_Pharma	161333.3333		161333.3333	0	161333.3333	0.694683661				1	0.039	1.6793E-07				1	0.039	1.6793E-07				1	1	4.3059E-06
50-18-0	50180	1131	Cyclophosphamid	261.09	1_Pharma	4000		4000	0	4000	0.015320388				1	0.039	1.49374E-07				1	0.039	1.49374E-07				1	1	3.8301E-06
50-24-8	50248	656	prednisolone	360.45	1_Pharma				1	0.39	1.08198E-06				1	0.039	1.08198E-07				1	0.039	1.08198E-07	160000		160000	0	160000	0.44388958
50-28-2	50282	55	estradiol	272.39	1_Pharma	0.001		0.001	0	0.001	3.67121E-09	0.0005	0.005	0.005	0	0.005	1.8356E-08	0.0066		0.0066	0	0.0066	2.423E-08	523		523	0	523	0.00192004
50-78-2	50782	666	O-acetylsalicylic acid	180.16	1_Pharma	16034.25068		16034.25068	0	16034.25068	0.089000059				1	0.039	2.16474E-07				1	0.039	2.16474E-07	90600		90600	0	90600	0.50288632
51-21-8	51218	668	fluorouracil	130.08	1_Pharma	133333.3333		133333.3333	0	133333.3333	1.02501025				1	0.039	2.99815E-07				1	0.039	2.99815E-07	36.66714587		36.66714587	0	36.6671459	0.00028188
51481-61-9	51481619	1129	Cimetidin	252.35	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.132091672				1	0.039	1.54547E-07				1	0.039	1.54547E-07				1	1	3.9628E-06
51-52-5	51525	5108	propylthiouracil	170.24	1_Pharma	100		100	0	100	0.000587406				1	0.039	2.29088E-07				1	0.039	2.29088E-07	3333.356831		3333.356831	0	3333.35683	0.01958034
525-66-6	525666	59	Propranolol	259.35	1_Pharma	618.5086105		618.5086105	0	618.5086105	0.002384841	1		1	0	1	3.85579E-06				1	0.039	1.50376E-07	21.642294		21.642294	0	21.642294	8.3448E-05
52645-53-1	52645531	676	Permethrin	391.29	1_Pharma	0.1	0.48	0.48	0	0.48	1.22671E-06	0.3		0.3	0	0.3	7.66695E-07				1	0.039	9.96703E-08	0.87		0.87	0	0.87	2.2234E-06
53-86-1	53861	1101	Indometacin	357.79	1_Pharma	27306.66667		27306.66667	0	27306.66667	0.076320374				1	0.039	1.09002E-07				1	0.039	1.09002E-07				1	1	2.7949E-06
54-11-5	54115	5067	nicotine	162.24	1_Pharma	3200		3200	0	3200	0.019723866	2900		2900	0	2900	0.017874753				1	0.039	2.40385E-07				1	1	6.1637E-06
54-31-9	54319	62	Furosemid	330.75	1_Pharma				1	0.39	1.17914E-06	0.61108		0.61108	0	0.61108	1.84756E-06				1	0.039	1.17914E-07	10		10	0	10	3.0234E-05
54739-18-3	54739183	689	Fluvoxamin	318.34	1_Pharma	432		432	0	432	0.00135704				1	0.039	1.22511E-07				1	0.039	1.22511E-07	1662.91		1662.91	0	1662.91	0.00522369
54-85-3	54853	691	Isoniazid	137.15	1_Pharma	14130.10261		14130.10261	0	14130.10261	0.103026632				1	0.039	2.8436E-07				1	0.039	2.8436E-07				1	1	7.2913E-06
54910-89-3	54910893	692	Fluoxetin	309.33	1_Pharma	0.32		0.32	0	0.32	1.03449E-06	0.54		0.54	0	0.54	1.74571E-06				1	0.039	1.26079E-07	7.999987069		7.999987069	0	7.99998707	2.5862E-05
55-56-1	55561	3175	chlorhexidine	505.47	1_Pharma	1000		1000	0	1000	0.001978357				1	0.039	7.71559E-08				1	0.039	7.71559E-08	4.2		4.2	0	4.2	8.3091E-06
55-63-0	55630	702	glycerol trinitrate	227.09	1_Pharma	2.309401077		2.309401077	0	2.309401077	1.01695E-05	30		30	0	30	0.000132106				1	0.039	1.71738E-07	370		370	0	370	0.00162931
56-75-7	56757	64	Chloramphenicol	323.13	1_Pharma	609333.3333		609333.3333	0	609333.3333	1.885721949				1	0.039	1.20694E-07				1	0.039	1.20694E-07	33.33333333		33.33333333	0	33.3333333	0.00010316
56-81-5	56815	716	glycerol	92.094	1_Pharma	295000		295000	0	295000	3.203248854				1	0.039	4.2348E-07				1	0.039	4.2348E-07	2900000		2900000	0	2900000	31.489565
56-86-0	56860	3214	glutamic acid	147.13	1_Pharma	100000		100000	0	100000	0.679671039				1	0.039	2.65072E-07				1	0.039	2.65072E-07	16000		16000	0	16000	0.10874737
57-13-6	57136	719	urea	60.058	1_Pharma	1666.666667		1666.666667	0	1666.666667	0.027750952	2000000		2000000	0	2000000	33.30114223				1	0.039	6.49372E-07	47000		47000	0	47000	0.78257684
57-63-6	57636	724	Etinylestradiol	296.41	1_Pharma	0.0005	0.00065	0.00065	0	0.00065	2.19291E-09	0.00004	0.0001	0.0001	0	0.0001	3.37371E-10	0.0003		0.0003	0	0.0003	1.01211E-09	54		54	0	54	0.00018218
58-08-2	58082	66	caffeine	194.2	1_Pharma	3.2		3.2	0	3.2	1.64779E-05				1	0.039	2.00824E-07				1	0.039	2.00824E-07	5		5	0	5	2.5747E-05
58-22-0	58220	67	testosterone	288.43	1_Pharma	5		5	0	5	1.73352E-05				1	0.039	1.35215E-07				1	0.039	1.35215E-07	166.6666667		166.6666667	0	166.666667	0.00057784
58-55-9	58559	730	theophylline	180.17	1_Pharma	46400		46400	0	46400	0.257534551				1	0.039	2.16462E-07				1	0.039	2.16462E-07	12500		12500	0	12500	0.06937892
59-05-2	59052	732	Metotrexat	454.45	1_Pharma	28333.68248		28333.68248	0	28333.68248	0.062347194				1	0.039	8.5818E-08				1	0.039	8.5818E-08	86667.73464		86667.73464	0	86667.7346	0.19070907
59277-89-3	59277893	735	Aciklovir	225.21	1_Pharma	31667.14475		31667.14475	0	31667.14475	0.140611628				1	0.039	1.73172E-07				1	0.039	1.73172E-07	33000.49821		33000.49821	0	33000.4982	0.14653212
59467-70-8	59467708	736	Midazolam	325.78	1_Pharma	1433.367652		1433.367652	0	1433.367652	0.004399802				1	0.039	1.19713E-07				1	0.039	1.19713E-07	3800.090984		3800.090984	0	3800.09098	0.01166459
59-67-6	59676	739	Niacin	123.11	1_Pharma	3333.306257		3333.306257	0	3333.306257	0.027075837				1	0.039	3.1679E-07				1	0.039	3.1679E-07	4253		4253	0	4253	0.03454634
59-92-7	59927	745	Levodopa	197.19	1_Pharma	33333.29953		33333.29953	0	33333.29953	0.169041531				1	0.039	1.97779E-07				1	0.039	1.97779E-07	499.9994929		499.9994929	0	499.999493	0.00253562
60-54-8	60548	754	Tetracycline	444.44	1_Pharma	1000		1000	0	1000	0.002250023				1	0.039	8.77509E-08				1	0.039	8.77509E-08	0.44		0.44	0	0.44	9.9001E-07
61-68-7	61687	1150	Mefenamic acid	241.29	1_Pharma	5		5	0	5	2.0722E-05				1	0.039	1.61631E-07				1	0.039	1.61631E-07	2083		2083	0	2083	0.00863277
61869-08-7	61869087	760	Paroxetin	329.37	1_Pharma	666.6660594		666.6660594	0	666.6660594	0.002024064				1	0.039	1.18408E-07				1	0.039	1.18408E-07				1	1	3.0361E-06
62571-86-2	62571862	1103	Captopril	217.29	1_Pharma				1	0.39	1.79484E-06				1	0.039	1.79484E-07				1	0.039	1.79484E-07	56000		56000	0	56000	0.2577201
657-24-9	657249	79	Metformin	129.17	1_Pharma				1	0.39	3.01928E-06				1	0.039	3.01928E-07				1	0.039	3.01928E-07	106666.6667		106666.6667	0	106666.667	0.82578514
66357-35-5	66357355	789	ranitidine	314.41	1_Pharma				1	0.39	1.24042E-06	0.24555		0.24555	0	0.24555	7.80987E-07				1	0.039	1.24042E-07				1	1	3.1806E-06
67-20-9	67209	791	Nitrofurantoin	238.16	1_Pharma	3333.34453		3333.34453	0	3333.34453	0.01399624				1	0.039	1.63755E-07				1	0.039	1.63755E-07	15066.71728		15066.71728	0	15066.7173	0.06326301
68-35-9	68359	1165	Sulfadiazin	250.28	1_Pharma				1	0.39	1.55825E-06				1	0.039	1.55825E-07				1	0.039	1.55825E-07	1000		1000	0	1000	0.00399553
69-53-4	69534	808	ampicillin	349.41	1_Pharma	333333.3333		333333.3333	0	333333.3333	0.953989105				1	0.039	1.11617E-07				1	0.039	1.11617E-07	10		10	0	10	2.862E-05
69-72-7	69727	84	salicylic acid	138.12	1_Pharma	7596.6		7596.6	0	7596.6	0.055				1	0.039	2.82363E-07				1	0.039	2.82363E-07	18856.18083		18856.18083	0	18856.1808	0.13652028
70458-96-7	70458967	812	Norfloxacin	319.34	1_Pharma				1	0.39	1.22127E-06				1	0.039	1.22127E-07				1	0.039	1.22127E-07	1.6		1.6	0	1.6	5.0103E-06
723-46-6	723466	86	Sulfametoxazol	253.28	1_Pharma	16		16	0	16	6.31712E-05	533		533	0	533	0.00210439				1	0.039	1.5398E-07	10.00018952		10.00018952	0	10.0001895	3.9483E-05
72956-09-3	72956093	826	Carvedilol	406.48	1_Pharma	25		25	0	25	6.15036E-05				1	0.039	9.59457E-08				1	0.039	9.59457E-08	56.66800498		56.66800498	0	56.668005	0.00013941
73334-07-3	73334073	4988	Iopromide	791.11	1_Pharma	320668.1259		320668.1259	0	320668.1259	0.405339492				1	0.039	4.92978E-08				1	0.039	4.92978E-08	45666.87447		45666.87447	0	45666.8745	0.05772506
738-70-5	738705	89	Trimetoprim	290.33	1_Pharma	33333.19555		33333.19555	0	33333.19555	0.114811406	157		157	0	157	0.000540764	157		157	0	157	0.000540764	3100		3100	0	3100	0.0106775
76824-35-6	76824356	1100	Famotidine	337.45	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.098780066				1	0.039	1.15573E-07				1	0.039	1.15573E-07				1	1	2.9634E-06
78439-06-2	78439062	896	Ceftazidim	546.59	1_Pharma	35268.82632		35268.82632	0	35268.82632	0.064525195				1	0.039	7.13515E-08				1	0.039	7.13515E-08	8.318119414		8.318119414	0	8.31811941	1.5218E-05
79-57-2	79572	923	Oxitetracyklin	460.44	1_Pharma	1000		1000	0	1000	0.002171836	80000		80000	0	80000	0.173746851				1	0.039	8.47016E-08	100		100	0	100	0.00021718
79617-96-2	79617962	924	Sertraline	306.24	1_Pharma	91		91	0	91	0.000297153				1	0.039	1.27351E-07				1	0.039	1.27351E-07	4.57		4.57	0	4.57	1.4923E-05
80-08-0	80080	3787	dapsone	248.31	1_Pharma	100000		100000	0	100000	0.402722403				1	0.039	1.57062E-07				1	0.039	1.57062E-07	173.3333333		173.3333333	0	173.333333	0.00069805
81103-11-9	81103119	99	Claritromycin	747.97	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.044565067				1	0.039	5.21411E-08				1	0.039	5.21411E-08	0.666666667		0.666666667	0	0.66666667	8.913E-07
81-13-0	81130	3802	dexpanthenol	205.26	1_Pharma	10000000		10000000	0	10000000	48.71869824				1	0.039	1.90003E-07				1	0.039	1.90003E-07	100000		100000	0	100000	0.48718698
81-81-2	81812	942	warfarin	308.33	1_Pharma	11.43333333		11.43333333	0	11.43333333	3.70815E-05	2000		2000	0	2000	0.006486557				1	0.039	1.26488E-07	8500		8500	0	8500	0.02756787
82419-36-1	82419361	945	Ofloxacin	361.38	1_Pharma				1	0.39	1.0792E-06				1	0.039	1.0792E-07				1	0.039	1.0792E-07	480		480	0	480	0.00132824
83799-24-0	83799240	956	Fexofenadine	501.67	1_Pharma	313333.3333		313333.3333	0	313333.3333	0.624580568				1	0.039	7.77403E-08				1	0.039	7.77403E-08	66666.66667		66666.66667	0	66666.6667	0.13288948
83905-01-5	83905015	957	Azithromycin	749	1_Pharma				1	0.39	5.20694E-07				1	0.039	5.20694E-08				1	0.039	5.20694E-08	0.313333333		0.313333333	0	0.31333333	4.1834E-07
84057-84-1	84057841	102	Lamotrigin	256.1	1_Pharma	28333.33333		28333.33333	0	28333.33333	0.110633867				1	0.039	1.52284E-07				1	0.039	1.52284E-07	13233.33333		13233.33333	0	13233.3333	0.05167252
85721-33-1	85721331	969	Ciprofloxacin	331.35	1_Pharma				1	0.39	1.177E-06				1	0.039	1.177E-07				1	0.039	1.177E-07	500		500	0	500	0.00150898
86386-73-4	86386734	970	Fluconazole	306.28	1_Pharma	33333.33333		33333.33333	0	33333.33333	0.108832876				1	0.039	1.27334E-07				1	0.039	1.27334E-07	7700		7700	0	7700	0.02514039
88150-42-9	88150429	982	Amlodipine	408.88	1_Pharma	1000		1000	0	1000	0.002445705				1	0.039	9.53825E-08				1	0.039	9.53825E-08	10		10	0	10	2.4457E-05
89-57-6	89576	3980	Mesalamine	153.14	1_Pharma	49333.33333		49333.33333	0	49333.33333	0.322145314	9712		9712	0	9712	0.063419094				1	0.039	2.54669E-07	21250.33333		21250.33333	0	21250.3333	0.13876409
89-78-1	89781	994	menthol	156.27	1_Pharma	16000		16000	0	16000	0.102386894				1	0.039	2.49568E-07				1	0.039	2.49568E-07	4600		4600	0	4600	0.02943623
90-82-4	90824	4008	pseudoephedrine	165.24	1_Pharma	220000		220000	0	220000	1.331396756				1	0.039	2.3602E-07				1	0.039	2.3602E-07	11500		11500	0	11500	0.06959574
93413-69-5	93413695	1019	Venlafaxine	277.41	1_Pharma				1	0.39	1.40586E-06	28.74		28.74	0	28.74	0.000103601				1	0.039	1.40586E-07				1	1	3.6048E-06
94-09-7	94097	1020	Bensokain	165.19	1_Pharma	2400		2400	0	2400	0.014528724				1	0.039	2.36092E-07				1	0.039	2.36092E-07				1	1	6.0536E-06
94-36-0	94360	4103	dibenzoyl peroxide	242.23	1_Pharma	31.6		31.6	0	31.6	0.000130455				1	0.039	1.61004E-07				1	0.039	1.61004E-07	20		20	0	20	8.2566E-05
97-77-8	97778	1060	disulfiram	296.54	1_Pharma	22.33333333		22.33333333	0	22.33333333	7.53131E-05	1.8		1.8	0	1.8	6.07001E-06				1	0.039	1.31517E-07	21.66666667		21.66666667	0	21.6666667	7.3065E-05
98-92-0	98920	1079	nicotinamide	122.13	1_Pharma	1000000		1000000	0	1000000	8.187996397				1	0.039	3.19332E-07				1	0.039	3.19332E-07	560000		560000	0	560000	4.58527798
99-66-1	99661	1091	Valproic acid	144.21	1_Pharma	6729.8		6729.8	0	6729.8	0.046666667				1	0.039	2.70439E-07				1	0.039	2.70439E-07	100000		100000	0	100000	0.69343319
2164-08-1	2164081	114	Lenacil	234.3	2_Pest	666.6666667		666.6666667	0	666.6666667	0.002845355				1	0.039	1.66453E-07				1	0.039	1.66453E-07	4		4	0	4	1.7072E-05
2439-01-2	2439012	5114	Quinomethionate	234.3	2_Pest	15.6		15.6	0	15.6	6.65813E-05	2		2	0	2	8.53606E-06	3.8		3.8	0	3.8	1.62185E-05	3.2		3.2	0	3.2	1.3658E-05
3813-05-6	3813056	116	Benazolin	243.67	2_Pest	9000		9000	0	9000	0.036935199				1	0.039	1.60053E-07				1	0.039	1.60053E-07				1	1	4.1039E-06
10004-44-1	10004441	121	Hymexazol	99.09	2_Pest	13333.33333		13333.33333	0	13333.33333	0.134557809				1	0.039	3.93582E-07				1	0.039	3.93582E-07	12.5		12.5	0	12.5	0.00012615
100646-51-3	100646513	5117	Quizalofop-P-ethyl	372.81	2_Pest	91		91	0	91	0.000244092	44		44	0	44	0.000118023				1	0.039	1.04611E-07	10		10	0	10	2.6823E-05
101-05-3	101053	141	Anilazine	275.53	2_Pest	2.833333333		2.833333333	0	2.833333333	1.02832E-05	9		9	0	9	3.26643E-05				1	0.039	1.41545E-07	200		200	0	200	0.00072587
101200-48-0	101200480	142	Tribenuron-methyl	395.4	2_Pest	132000		132000	0	132000	0.33383915	11800		11800	0	11800	0.029843197				1	0.039	9.86343E-08	4.3		4.3	0	4.3	1.0875E-05
101205-02-1	101205021	144	Cycloxydim	325.47	2_Pest	33333.33333		33333.33333	0	33333.33333	0.102415993				1	0.039	1.19827E-07				1	0.039	1.19827E-07	10666.66667		10666.66667	0	10666.6667	0.03277312
101-21-3	101213	145	Chlorpropham	213.66	2_Pest	560		560	0	560	0.002620987				1	0.039	1.82533E-07				1	0.039	1.82533E-07	1100		1100	0	1100	0.00514837
101-42-8	101428	147	Fenuron	164.21	2_Pest	68000		68000	0	68000	0.414103891				1	0.039	2.37501E-07				1	0.039	2.37501E-07				1	1	6.0898E-06
101463-69-8	101463698	148	Flufenoxuron	488.77	2_Pest	4.9		4.9	0	4.9	1.00252E-05	0.82		0.82	0	0.82	1.67768E-06				1	0.039	7.97921E-08	3.95		3.95	0	3.95	8.0815E-06
1014-69-3	1014693	149	Desmetryn	213.31	2_Pest	733.3333333		733.3333333	0	733.3333333	0.003437876				1	0.039	1.82832E-07				1	0.039	1.82832E-07	8.333333333		8.333333333	0	8.33333333	3.9067E-05
10265-92-6	10265926	153	Methamidophos	141.13	2_Pest	426.6666667		426.6666667	0	426.6666667	0.003023217				1	0.039	2.76341E-07				1	0.039	2.76341E-07	100		100	0	100	0.00070857
102851-06-9	102851069	157	Tau-fluvalinate	502.92	2_Pest	0.21		0.21	0	0.21	4.17561E-07				1	0.039	7.75471E-08				1	0.039	7.75471E-08				1	1	1.9884E-06
103055-07-8	103055078	158	Lufenuron	511.15	2_Pest	73000		73000	0	73000	0.142815221				1	0.039	7.62985E-08				1	0.039	7.62985E-08				1	1	1.9564E-06
10311-84-9	10311849	4894	Dialifos	393.85	2_Pest				1	0.39	9.90225E-07				1	0.039	9.90225E-08				1	0.039	9.90225E-08				1	1	2.539E-06
104040-78-0	104040780	166	Flazasulfuron	407.33	2_Pest	27000		27000	0	27000	0.066285321	17000		17000	0	17000	0.041735202				1	0.039	9.57455E-08	0.59		0.59	0	0.59	1.4485E-06
104206-82-8	104206828	167	Mesotrione	339.32	2_Pest	7.5		7.5	0	7.5	2.2103E-05	11000		11000	0	11000	0.032417777				1	0.039	1.14936E-07	500		500	0	500	0.00147354
10453-86-8	10453868	1114	Resmethrin	338.45	2_Pest	0.25		0.25	0	0.25	7.38662E-07	0.3		0.3	0	0.3	8.86394E-07				1	0.039	1.15231E-07				1	1	2.9546E-06
10552-74-6	10552746	176	Nitrothal-isopropyl	295.29	2_Pest	186.6666667		186.6666667	0	186.6666667	0.000632147				1	0.039	1.32074E-07				1	0.039	1.32074E-07	693.3333333		693.3333333	0	693.333333	0.00234797
10605-21-7	10605217	3	Carbendazim	191.19	2_Pest	2.333333333	2.47	2.47	0	2.47	1.29191E-05				1	0.039	2.03986E-07				1	0.039	2.03986E-07	113.3333333		113.3333333	0	113.333333	0.00059278
1071-83-6	1071836	212	Glyphosate	169.07	2_Pest	17.9		17.9	0	17.9	0.000105873	10		10	0	10	5.91471E-05				1	0.039	2.30674E-07	3.55	100	100	0	100	0.00059147
107534-96-3	107534963	221	Tebuconazole	307.83	2_Pest	230		230	0	230	0.000747166	12		12	0	12	3.89826E-05				1	0.039	1.26693E-07	36.66666667		36.66666667	0	36.6666667	0.00011911
1085-98-9	1085989	241	Dichlofluanid	333.23	2_Pest	3.333333333		3.333333333	0	3.333333333	1.00031E-05				1	0.039	1.17036E-07				1	0.039	1.17036E-07	50		50	0	50	0.00015005
110488-70-5	110488705	4906	Dimethomorph	387.86	2_Pest	1000		1000	0	1000	0.00257825	107		107	0	107	0.000275873	900		900	0	900	0.002320425	16300		16300	0	16300	0.04202547
1113-02-6	1113026	295	Omethoate	213.19	2_Pest	2900		2900	0	2900	0.013602889				1	0.039	1.82935E-07				1	0.039	1.82935E-07	41666.66667		41666.66667	0	41666.6667	0.19544381
111479-05-1	111479051	303	Propaquizafop	443.89	2_Pest	63.33333333		63.33333333	0	63.33333333	0.000142678				1	0.039	8.78596E-08				1	0.039	8.78596E-08	700		700	0	700	0.00157697
111988-49-9	111988499	6	Thiacloprid	252.73	2_Pest	3500		3500	0	3500	0.013848771	170		170	0	170	0.000672655	3900		3900	0	3900	0.015431488	16800		16800	0	16800	0.0664741
111991-09-4	111991094	319	Nicosulfuron	410.42	2_Pest	10		10	0	10	2.43653E-05				1	0.039	9.50246E-08				1	0.039	9.50246E-08	477.1666667		477.1666667	0	477.166667	0.00116263
112281-77-3	112281773	323	Tetraconazole	372.15	2_Pest	600		600	0	600	0.001612253	300		300	0	300	0.000806127	3100		3100	0	3100	0.008329974	950		950	0	950	0.00255273
112410-23-8	112410238	328	Tebufenozide	352.48	2_Pest	390		390	0	390	0.001106446	180		180	0	180	0.000510667	180		180	0	180	0.000510667	50		50	0	50	0.00014185
113136-77-9	113136779	334	Cyclanilide	274.1	2_Pest	11000		11000	0	11000	0.040131339				1	0.039	1.42284E-07				1	0.039	1.42284E-07	9.7		9.7	0	9.7	3.5389E-05
113158-40-0	113158400	335	Fenoxaprop-P	333.73	2_Pest	80		80	0	80	0.000239715				1	0.039	1.16861E-07				1	0.039	1.16861E-07	0.32		0.32	0	0.32	9.5886E-07
1134-23-2	1134232	4878	Cycloate	215.36	2_Pest	300		300	0	300	0.001393016				1	0.039	1.81092E-07				1	0.039	1.81092E-07				1	1	4.6434E-06
114-26-1	114261	337	Propoxur	209.25	2_Pest	1000		1000	0	1000	0.004778973	141		141	0	141	0.000673835				1	0.039	1.8638E-07	1000		1000	0	1000	0.00477897
114369-43-6	114369436	338	Fenbuconazole	336.83	2_Pest	420		420	0	420	0.00124692	5		5	0	5	1.48443E-05	27		27	0	27	8.01591E-05	30.33333333		30.33333333	0	30.3333333	9.0055E-05
115-29-7	115297	4921	Endosulfan	406.93	2_Pest	0.004		0.004	0	0.004	9.8297E-09	0.03		0.03	0	0.03	7.37228E-08	0.03		0.03	0	0.03	7.37228E-08				1	1	2.4574E-06
115-32-2	115322	340	Dicofol	370.49	2_Pest	19		19	0	19	5.12834E-05	4.4		4.4	0	4.4	1.18762E-05	125		125	0	125	0.000337391	24.33333333		24.33333333	0	24.3333333	6.5679E-05
116-06-3	116063	342	Aldicarb	190.27	2_Pest	31.3		31.3	0	31.3	0.000164503	78		78	0	78	0.000409944				1	0.039	2.04972E-07	16666.66667		16666.66667	0	16666.6667	0.08759482
116255-48-2	116255482	343	Bromuconazole	377.08	2_Pest	21.66666667		21.66666667	0	21.66666667	5.74591E-05	34		34	0	34	9.01665E-05				1	0.039	1.03426E-07	7		7	0	7	1.8564E-05
116-29-0	116290	344	Tetradifon	356.05	2_Pest	293.3333333		293.3333333	0	293.3333333	0.000823854				1	0.039	1.09535E-07				1	0.039	1.09535E-07				1	1	2.8086E-06

118134-30-8	118134308	347	Spiroxamine	297.48	2_Pest	11		11	0	11	3.69773E-05	2.6		2.6	0	2.6	8.74008E-06	14.9		14.9	0	14.9	5.00874E-05	0.32		0.32	0	0.32	1.0757E-06
119168-77-3	119168773	350	Tebufenpyrad	333.87	2_Pest	13		13	0	13	3.89373E-05				1	0.039	1.16812E-07				1	0.039	1.16812E-07				1	1	2.9952E-06
119446-68-3	119446683	351	Difenoconazole	406.27	2_Pest	270		270	0	270	0.000664583	1.9		1.9	0	1.9	4.67669E-06				1	0.039	9.59953E-08	6.3		6.3	0	6.3	1.5507E-05
1194-65-6	1194656	352	dichlobenil	172.01	2_Pest	2600		2600	0	2600	0.0151154	110		110	0	110	0.000639498				1	0.039	2.26731E-07	82		82	0	82	0.00047672
120068-37-3	120068373	11	Fipronil	437.15	2_Pest	33		33	0	33	7.5489E-05	0.05		0.05	0	0.05	1.14377E-07	0.24		0.24	0	0.24	5.49011E-07	40		40	0	40	9.1502E-05
120-36-5	120365	4895	Dichlorprop	235.07	2_Pest	166.6666667		166.6666667	0	166.6666667	0.000709009				1	0.039	1.65908E-07				1	0.039	1.65908E-07	180000		180000	0	180000	0.76572936
120928-09-8	120928098	366	Fenazaquin	306.41	2_Pest	2.9		2.9	0	2.9	9.46444E-06	0.95		0.95	0	0.95	3.10042E-06				1	0.039	1.2728E-07	45.4		45.4	0	45.4	0.00014817
121552-61-2	121552612	371	Cyprodinil	225.3	2_Pest	445		445	0	445	0.001975144	83		83	0	83	0.000368398				1	0.039	1.73103E-07	538		538	0	538	0.00238793
122-14-5	122145	378	Fenitrothion	277.24	2_Pest	0.55	113.333333	113.3333333	0	113.3333333	0.000408791	10.75		10.75	0	10.75	3.87751E-05	100		100	0	100	0.000360698	100		100	0	100	0.0003607
122-34-9	122349	15	Simazine	201.67	2_Pest	46.66666667	83.3333333	83.33333333	0	83.33333333	0.000413216	0.06		0.06	0	0.06	2.97516E-07				1	0.039	1.93385E-07	0.746666667		0.746666667	0	0.74666667	3.7024E-06
122-42-9	122429	5107	Propham	179.22	2_Pest	7833.333333		7833.333333	0	7833.333333	0.04370792				1	0.039	2.1761E-07				1	0.039	2.1761E-07	166.6666667		166.6666667	0	166.666667	0.00092996
122453-73-0	122453730	380	Chlorfenapyr	407.63	2_Pest	2.61		2.61	0	2.61	6.40287E-06				1	0.039	9.5675E-08				1	0.039	9.5675E-08				1	1	2.4532E-06
122931-48-0	122931480	383	Rimsulfuron	431.45	2_Pest	110000		110000	0	110000	0.254954224				1	0.039	9.03929E-08				1	0.039	9.03929E-08	29		29	0	29	6.7215E-05
123312-89-0	123312890	387	Pymetrozine	217.24	2_Pest	117000		117000	0	117000	0.538574848	11700		11700	0	11700	0.053857485				1	0.039	1.79525E-07	6300		6300	0	6300	0.02900018
123-33-1	123331	389	Maleic hydrazide	112.09	2_Pest	5000		5000	0	5000	0.044607012				1	0.039	3.47935E-07				1	0.039	3.47935E-07	9840		9840	0	9840	0.0877866
125116-23-6	125116236	405	Metconazole	319.84	2_Pest	814		814	0	814	0.002545023				1	0.039	1.21936E-07				1	0.039	1.21936E-07				1	1	3.1266E-06
126833-17-8	126833178	409	Fenhexamid	302.2	2_Pest	940		940	0	940	0.003110523	100		100	0	100	0.000330907	780		780	0	780	0.002581072	25		25	0	25	8.2727E-05
13071-79-9	13071799	416	Terbufos	288.43	2_Pest	0.18		0.18	0	0.18	6.24068E-07	0.34		0.34	0	0.34	1.1788E-06				1	0.039	1.35215E-07	0.1		0.1	0	0.1	3.467E-07
13121-70-5	13121705	419	Cyhexatin	385.16	2_Pest	0.65		0.65	0	0.65	1.68761E-06				1	0.039	1.01257E-07				1	0.039	1.01257E-07				1	1	2.5963E-06
131341-86-1	131341861	420	Fludioxonil	248.19	2_Pest	140		140	0	140	0.000564084	6.2		6.2	0	6.2	2.49809E-05	6.2		6.2	0	6.2	2.49809E-05	4.66		4.66	0	4.66	1.8776E-05
13171-21-6	13171216	5093	Phosphamidon	299.69	2_Pest	36.66666667	333.333333	333.3333333	0	333.3333333	0.00111226	1100		1100	0	1100	0.003670459				1	0.039	1.30134E-07	86666.66667		86666.66667	0	86666.6667	0.28918772
131807-57-3	131807573	421	Famoxadone	374.4	2_Pest	5.2		5.2	0	5.2	1.38889E-05	1.4		1.4	0	1.4	3.73932E-06	5.58		5.58	0	5.58	1.49038E-05	3.08		3.08	0	3.08	8.2265E-06
13181-17-4	13181174	422	Bromofenoxim	461.04	2_Pest	29.33333333		29.33333333	0	29.33333333	6.36243E-05				1	0.039	8.45914E-08				1	0.039	8.45914E-08	733.3333333		733.3333333	0	733.333333	0.00159061
131860-33-8	131860338	423	Azoxystrobin	403.4	2_Pest	68		68	0	68	0.000168567	147		147	0	147	0.000364403				1	0.039	9.66782E-08	8.15		8.15	0	8.15	2.0203E-05
13194-48-4	13194484	4930	Ethoprophos	242.34	2_Pest	1.8		1.8	0	1.8	7.42758E-06	2		2	0	2	8.25287E-06	15		15	0	15	6.18965E-05	3200		3200	0	3200	0.01320459
131983-72-7	131983727	424	Triticonazole	317.82	2_Pest	1400		1400	0	1400	0.004405009	8.7		8.7	0	8.7	2.7374E-05				1	0.039	1.22711E-07	33		33	0	33	0.00010383
132-66-1	132661	5059	Naptalam	291.31	2_Pest	25366.66667		25366.66667	0	25366.66667	0.087077912				1	0.039	1.33878E-07				1	0.039	1.33878E-07				1	1	3.4328E-06
133-06-2	133062	425	Captan	300.59	2_Pest	8.666666667	8.73333333	8.733333333	0	8.733333333	2.9054E-05	1.1		1.1	0	1.1	3.65947E-06	1.1		1.1	0	1.1	3.65947E-06	62		62	0	62	0.00020626
133-07-3	133073	426	Folpet	296.56	2_Pest	2.2		2.2	0	2.2	7.4184E-06	8.81		8.81	0	8.81	2.97073E-05				1	0.039	1.31508E-07	30		30	0	30	0.00010116
13360-45-7	13360457	428	Chlorbromuron	293.56	2_Pest	466.6666667		466.6666667	0	466.6666667	0.001589681				1	0.039	1.32852E-07				1	0.039	1.32852E-07	5.666666667		5.666666667	0	5.66666667	1.9303E-05
134098-61-6	134098616	429	Fenpyroximate	421.5	2_Pest	0.27		0.27	0	0.27	6.40569E-07	0.11		0.11	0	0.11	2.60973E-07				1	0.039	9.25267E-08	0.01		0.01	0	0.01	2.3725E-08
13457-18-6	13457186	432	Pyrazophos	373.37	2_Pest	5.333333333		5.333333333	0	5.333333333	1.42843E-05				1	0.039	1.04454E-07				1	0.039	1.04454E-07	21666.66667		21666.66667	0	21666.6667	0.05803001
13593-03-8	13593038	437	Quinalphos	298.3	2_Pest	1		1	0	1	3.35233E-06				1	0.039	1.30741E-07				1	0.039	1.30741E-07				1	1	3.3523E-06
136426-54-5	136426545	438	Fluquinconazole	376.18	2_Pest	78		78	0	78	0.000207348	300		300	0	300	0.000797491				1	0.039	1.03674E-07	3.2		3.2	0	3.2	8.5066E-06
13684-56-5	13684565	439	Desmedipham	300.32	2_Pest	1000		1000	0	1000	0.003329782				1	0.039	1.29861E-07				1	0.039	1.29861E-07	30		30	0	30	9.9893E-05
13684-63-4	13684634	440	Phenmedipham	300.32	2_Pest	1000		1000	0	1000	0.003329782				1	0.039	1.29861E-07				1	0.039	1.29861E-07	180		180	0	180	0.00059936
137-26-8	137268	441	thiram	240.43	2_Pest	0.223333333	1.12	1.12	0	1.12	4.65832E-06	0.32		0.32	0	0.32	1.33095E-06	1.1		1.1	0	1.1	4.57514E-06	10		10	0	10	4.1592E-05
138261-41-3	138261413	443	Imidacloprid	255.67	2_Pest	25000		25000	0	25000	0.097782297	79.66666667		79.66666667	0	79.66666667	0.0003116				1	0.039	1.5254E-07	10000		10000	0	10000	0.03911292
139-40-2	139402	446	propazine	229.72	2_Pest	4500		4500	0	4500	0.019589065	1340		1340	0	1340	0.005833188	1340		1340	0	1340	0.005833188	6.5		6.5	0	6.5	2.8295E-05
139528-85-1	139528851	1922	Metosulam	419.27	2_Pest	53200		53200	0	53200	0.126887209				1	0.039	9.30188E-08				1	0.039	9.30188E-08	17.3		17.3	0	17.3	4.1262E-05
140923-17-7	140923177	453	Iprovalicarb	320.44	2_Pest				1	0.39	1.21708E-06	5000		5000	0	5000	0.015603545				1	0.039	1.21708E-07				1	1	3.1207E-06
141517-21-7	141517217	5178	Trifloxystrobine	408.38	2_Pest	7.2		7.2	0	7.2	1.76306E-05	4.3		4.3	0	4.3	1.05294E-05	15		15	0	15	3.67305E-05	5.7		5.7	0	5.7	1.3958E-05
141776-32-1	141776321	457	Sulfosulfuron	470.49	2_Pest	95000		95000	0	95000	0.20191715	100000		100000	0	100000	0.212544369				1	0.039	8.28923E-08	120		120	0	120	0.00025505
1420-07-1	1420071	4911	Dinoterb	240.22	2_Pest	1.133333333		1.133333333	0	1.133333333	4.7179E-06				1	0.039	1.62351E-07				1	0.039	1.62351E-07	1010		1010	0	1010	0.00420448
14214-32-5	14214325	4902	Difenoxuron	286.33	2_Pest	2500		2500	0	2500	0.008731184				1	0.039	1.36206E-07				1	0.039	1.36206E-07	10		10	0	10	3.4925E-05
142459-58-3	142459583	461	Flufenacet	363.34	2_Pest	470		470	0	470	0.001293554	179		179	0	179	0.000492652	735		735	0	735	0.002022899	0.7		0.7	0	0.7	1.9266E-06
143390-89-0	143390890	470	Kresoxim-Methyl	313.35	2_Pest	104		104	0	104	0.000331897	13		13	0	13	4.14872E-05				1	0.039	1.24461E-07	7		7	0	7	2.2339E-05
145701-23-1	145701231	473	Florasulam	359.283	2_Pest	5720		5720	0	5720	0.015920597				1	0.039	1.0855E-07				1	0.039	1.0855E-07	49.3		49.3	0	49.3	0.00013722
14816-18-3	14816183	475	Phoxim	298.3	2_Pest	27.33333333		27.33333333	0	27.33333333	9.16303E-05				1	0.039	1.30741E-07				1	0.039	1.30741E-07	83.884943		83.884943	0	83.884943	0.00028121
148-79-8	148798	476	Thiabendazole	201.25	2_Pest	45		45	0	45	0.000223602	12		12	0	12	5.96273E-05				1	0.039	1.93789E-07				1	1	4.9689E-06
149961-52-4	149961524	481	Dimoxystrobin	326.4	2_Pest	14.46666667		14.46666667	0	14.46666667	4.43219E-05	1		1	0	1	3.06373E-06				1	0.039	1.19485E-07	5.666666667		5.666666667	0	5.66666667	1.7361E-05
149979-41-9	149979419	5148	Tepraloxydim	341.84	2_Pest	450		450	0	450	0.001316405				1	0.039	1.14088E-07				1	0.039	1.14088E-07	92		92	0	92	0.00026913
150-68-5	150685	482	Monuron	198.66	2_Pest	1100		1100	0	1100	0.005537099				1	0.039	1.96315E-07				1	0.039	1.96315E-07				1	1	5.0337E-06
15165-67-0	15165670	4896	Dichlorprop-P	235.07	2_Pest	23000		23000	0	23000	0.097843196	100000		100000	0	100000	0.425405198				1	0.039	1.65908E-07	38500		38500	0	38500	0.163781
15299-99-7	15299997	5058	Napropamide	271.36	2_Pest	3200		3200	0	3200	0.011792453				1	0.039	1.43721E-07				1	0.039	1.43721E-07	1200		1200	0	1200	0.00442217
153719-23-4	153719234	487	Thiamethoxam	291.72	2_Pest	38260		38260	0	38260	0.131153161	20000		20000	0	20000	0.068558892				1	0.039	1.3369E-07	81800		81800	0	81800	0.28040587
15457-05-3	15457053	4958	Fluorodifen	328.2	2_Pest				1	0.39	1.1883E-06				1	0.039	1.1883E-07				1	0.039	1.1883E-07				1	1	3.0469E-06
15545-48-9	15545489	32	Chlorotoluron	212.68	2_Pest	2056.666667		2056.666667	0	2056.666667	0.00967024				1	0.039	1.83374E-07				1	0.039	1.83374E-07	2.833333333		2.833333333	0	2.83333333	1.3322E-05
156052-68-5	156052685	490	Zoxamide	336.65	2_Pest	5.1		5.1	0	5.1	1.51493E-05	0.007		0.007	0	0.007	2.07931E-08	250		250	0	250	0.000742611	4.1		4.1	0	4.1	1.2179E-05
1563-66-2	1563662	491	Carbofuran	221.26	2_Pest	2.5		2.5	0	2.5	1.12989E-05	2.6		2.6	0	2.6	1.17509E-05				1	0.039	1.76263E-07	1066.666667		1066.666667	0	1066.66667	0.00482087
1582-09-8	1582098	496	Trifluralin	335.29	2_Pest	1.666666667	3.33333333	3.333333333	0	3.333333333	9.94164E-06	0.3		0.3	0	0.3	8.94748E-07	1.3		1.3	0	1.3	3.87724E-06	3.32		3.32	0	3.32	9.9019E-06
15972-60-8	15972608	497	Alachlor	269.77	2_Pest	80	80	80	0	80	0.000296549	187		187	0	187	0.000693183				1	0.039	1.44568E-07	0.35		0.35	0	0.35	1.2974E-06
161050-58-4	161050584	5021	Methoxyfenozide	368.48	2_Pest	2800		2800	0	2800	0.007598784	530		530	0	530	0.001438341				1	0.039	1.0584E-07	3400		3400	0	3400	0.0092271
161326-34-7	161326347	499	Fenamidone	311.41	2_Pest	350		350	0	350	0.00112392	8.6		8.6	0	8.6	2.76163E-05	8.6		8.6	0	8.6	2.76163E-05	12		12	0	12	3.8534E-05
163515-14-8	163515148	502	Dimethenamid-P	275.8	2_Pest	3700		3700	0	3700	0.013415518				1	0.039	1.41407E-07				1	0.039	1.41407E-07	28		28	0	28	0.00010152
16672-87-0	16672870	505	Ethephon	144.49	2_Pest	38333.33333		38333.33333	0	38333.33333	0.265300944				1	0.039	2.69915E-07				1	0.039	2.69915E-07	466.6666667		466.6666667	0	466.666667	0.00322975
16752-77-5	16752775	506	Methomyl	162.21	2_Pest	33.33333333	106.666667	106.6666667	0	106.6666667	0.000657584	46		46	0	46	0.000283583	1000		1000	0	1000	0.006164848				1	1	6.1648E-06
1689-83-4	1689834	507	Ioxynil	370.91	2_Pest	1100		1100	0	1100	0.002965679				1	0.039	1.05147E-07				1	0.039	1.05147E-07	3333.333333		3333.333333	0	3333.33333	0.00898691
1689-84-5	1689845	34	Bromoxynil	276.93	2_Pest	21		21	0	21	7.58314E-05				1	0.039	1.4083E-07				1	0.039	1.4083E-07	240		240	0	240	0.00086665
1698-60-8	1698608	35	Chloridazon	221.65	2_Pest	10666.66667		10666.66667	0	10666.66667	0.048123919	3200		3200	0	3200	0.014437176				1	0.039	1.75953E-07	60		60	0	60	0.0002707
1702-17-6	1702176	509	Clopyralid	192	2_Pest	34500		34500	0	34500	0.1796875	68000		68000	0	68000	0.354166667				1	0.039	2.03125E-07	1800		1800	0	1800	0.009375
173159-57-4	173159574	510	Foramsulfuron	452.45	2_Pest	93600		93600	0	93600	0.206873688	10500		10500	0	10500	0.023206984				1	0.039	8.61974E-08	1100		1100	0	1100	0.00243121
1746-81-2	1746812	511	Monolinuron	214.65	2_Pest	1033.333333		1033.333333	0	1033.333333	0.004814038				1	0.039	1.81691E-07				1	0.039	1.81691E-07	0.333333333		0.333333333	0	0.33333333	1.5529E-06
175013-18-0	175013180	512	Pyraclostrobin	387.83	2_Pest	3.6		3.6	0	3.6	9.28242E-06	2.35		2.35	0	2.35	6.05936E-06	4.14		4.14	0	4.14	1.06748E-05	1.1		1.1	0	1.1	2.8363E-06
17804-35-2	17804352	513	Benomyl	290.33	2_Pest	1.866666667	3.33333333	3.333333333	0	3.333333333	1.14812E-05	1.5		1.5	0	1.5	5.16653E-06	1.5		1.5	0	1.5	5.16653E-06	366.6666667		366.6666667	0	366.666667	0.00126293
18181-80-1	18181801	4865	Bromopropylate	428.13	2_Pest	116.6666667		116.6666667	0	116.6666667	0.000272503				1	0.039	9.10938E-08				1	0.039	9.10938E-08	306.6666667		306.6666667	0	306.666667	0.00071629
1861-40-1	1861401	514	Benfluralin	335.29	2_Pest	1.666666667		1.666666667	0	1.666666667	4.97082E-06	1.9		1.9	0	1.9	5.66674E-06				1	0.039	1.16317E-07	833.3333333		833.3333333	0	833.333333	0.00248541
18691-97-9	18691979	515	Methabenzthiazuron	221.29	2_Pest	2800		2800	0	2800	0.01265308				1	0.039	1.76239E-07				1	0.039	1.76239E-07	18		18	0	18	8.1341E-05
188425-85-6	188425856	36	Boscalid	343.21	2_Pest	1880		1880	0	1880	0.005477696	116		116	0	116	0.000337985	890		890	0	890	0.002593165	140		140	0	140	0.00040791
1897-45-6	1897456	516	Chlorothalonil	265.92	2_Pest	0.37		0.37	0	0.37	1.3914E-06	0.06		0.06	0	0.06	2.25632E-07				1	0.039	1.46661E-07	0.033333333	0.0333333	0.033333333	0	0.03333333	1.2535E-07
19044-88-3	19044883	517	Oryzalin	346.37	2_Pest	1000		1000	0	1000	0.002887086	220		220	0	220	0.000635159				1	0.039	1.12596E-07	8.05		8.05	0	8.05	2.3241E-05
1912-24-9	1912249	37	atrazine	215.69	2_Pest	0.3		0.3	0	0.3	1.39089E-06	0.26	0.3	0.3	0	0.3	1.39089E-06	0.26		0.26	0	0.26	1.20543E-06	0.016	2.75	2.75	0	2.75	1.275E-05
1918-00-9	1918009	519	Dicamba	221.04	2_Pest	333.3333333		333.3333333	0	333.3333333	0.001508023				1	0.039	1.76439E-07				1	0.039	1.76439E-07	5		5	0	5	2.262E-05
1918-16-7	1918167	520	Propachlor	211.69	2_Pest	100		100	0	100	0.000472389	19		19	0	19	8.97539E-05				1	0.039	1.84232E-07	3.48		3.48	0	3.48	1.6439E-05
1929-77-7	1929777	521	Vernolate	203.35	2_Pest	960		960	0	960	0.004720925				1	0.039	1.91788E-07				1	0.039	1.91788E-07	230		230	0	230	0.00113105
19666-30-9	19666309	526	Oxadiazon	345.23	2_Pest	210		210	0	210	0.00060829	0.88		0.88	0	0.88	2.54903E-06	0.88		0.88	0	0.88	2.54903E-06	1.4		1.4	0	1.4	4.0553E-06
1967-16-4	1967164	4870	Chlorbufam	223.66	2_Pest				1	0.39	1.74372E-06				1	0.039	1.74372E-07				1	0.039	1.74372E-07				1	1	4.4711E-06
19937-59-8	19937598	527	Metoxuron	228.68	2_Pest	6600		6600	0	6600	0.028861291				1	0.039	1.70544E-07				1	0.039	1.70544E-07	21.33333333		21.33333333	0	21.3333333	9.3289E-05
2032-65-7	2032657	528	Methiocarb	225.31	2_Pest	0.25	36.6666667	36.66666667	0	36.66666667	0.000162739	50		50	0	50	0.000221916				1	0.039	1.73095E-07				1	1	4.4383E-06
208465-21-8	208465218	5020	Mesosulfuron-methyl	503.51	2_Pest	91500		91500	0	91500	0.181724295	29600		29600	0	29600	0.058787313				1	0.039	7.74563E-08	29		29	0	29	5.7596E-05
21087-64-9	21087649	531	Metribuzin	214.29	2_Pest	1133.333333		1133.333333	0	1133.333333	0.005288783	2500		2500	0	2500	0.011666433	48000		48000	0	48000	0.22399552	2.33		2.33	0	2.33	1.0873E-05
2164-17-2	2164172	534	Fluometuron	232.21	2_Pest	200	213.333333	213.3333333	0	213.3333333	0.000918709	3100		3100	0	3100	0.013349985				1	0.039	1.67951E-07	10		10	0	10	4.3064E-05
21725-46-2	21725462	535	Cyanazine	240.7	2_Pest	6200		6200	0	6200	0.025758205				1	0.039	1.62027E-07				1	0.039	1.62027E-07	1.2		1.2	0	1.2	4.9855E-06
2212-67-1	2212671	537	Molinate	187.31	2_Pest	97		97	0	97	0.000517858	170		170	0	170	0.000907586				1	0.039	2.08211E-07	170		170	0	170	0.00090759
22224-92-6	22224926	540	Fenamiphos	303.36	2_Pest	1.7		1.7	0	1.7	5.6039E-06	3.8		3.8	0	3.8	1.25264E-05				1	0.039	1.2856E-07	1166.666667		1166.666667	0	1166.66667	0.00384582
2275-23-2	2275232	543	Vamidothion	287.34	2_Pest	196666.6667		196666.6667	0	196666.6667	0.684438876				1	0.039	1.35728E-07				1	0.039	1.35728E-07	508333.3333		508333.3333	0	508333.333	1.76910048
22781-23-3	22781233	544	Bendiocarb	223.23	2_Pest	310		310	0	310	0.001388702	300		300	0	300	0.001343905				1	0.039	1.74708E-07	570		570	0	570	0.00255342
2303-17-5	2303175	545	Tri-allate	304.67	2_Pest	270		270	0	270	0.000886205	193.3333333		193.3333333	0	193.3333333	0.000634566				1	0.039	1.28007E-07	6.3		6.3	0	6.3	2.0678E-05
2310-17-0	2310170	546	Phosalone	367.81	2_Pest	18		18	0	18	4.89383E-05				1	0.039	1.06033E-07				1	0.039	1.06033E-07	226.6666667		226.6666667	0	226.666667	0.00061626
23103-98-2	23103982	547	Pirimicarb	238.29	2_Pest	10000		10000	0	10000	0.041965672	4400		4400	0	4400	0.018464896				1	0.039	1.63666E-07	49500		49500	0	49500	0.20773008
23135-22-0	23135220	549	Oxamyl	219.27	2_Pest	760		760	0	760	0.003466046	500		500	0	500	0.002280294	770		770	0	770	0.003511652	4.58		4.58	0	4.58	2.0887E-05
23560-59-0	23560590	551	Heptenophos	250.62	2_Pest	18.66666667		18.66666667	0	18.66666667	7.4482E-05				1	0.039	1.55614E-07				1	0.039	1.55614E-07	25000		25000	0	25000	0.09975261
23564-05-8	23564058	552	Thiophanate-methyl	342.4	2_Pest	10		10	0	10	2.92056E-05				1	0.039	1.13902E-07				1	0.039	1.13902E-07	110		110	0	110	0.00032126
23947-60-6	23947606	555	Ethirimol	209.3	2_Pest	6666.666667		6666.666667	0	6666.666667	0.031852206				1	0.039	1.86335E-07				1	0.039	1.86335E-07	50000		50000	0	50000	0.23889154
23950-58-5	23950585	556	Propyzamide	256.13	2_Pest	875		875	0	875	0.003416234				1	0.039	1.52266E-07				1	0.039	1.52266E-07	260		260	0	260	0.00101511
24017-47-8	24017478	557	Triazophos	313.32	2_Pest	1730		1730	0	1730	0.005521512	0.5		0.5	0	0.5	1.59581E-06				1	0.039	1.24473E-07	100		100	0	100	0.00031916
24579-73-5	24579735	5105	Propamocarb	188.27	2_Pest	92000		92000	0	92000	0.488659903	6300		6300	0	6300	0.03346258				1	0.039	2.07149E-07	22400		22400	0	22400	0.11897806
24934-91-6	24934916	564	Chlormephos	234.7	2_Pest	2800		2800	0	2800	0.011930124				1	0.039	1.6617E-07				1	0.039	1.6617E-07				1	1	4.2608E-06
25057-89-0	25057890	39	Bentazone	240.28	2_Pest	10000		10000	0	10000	0.041618112				1	0.039	1.62311E-07				1	0.039	1.62311E-07	5.67		5.67	0	5.67	2.3597E-05
25311-71-1	25311711	567	Isofenphos	345.4	2_Pest	220		220	0	220	0.000636943	61		61	0	61	0.000176607				1	0.039	1.12913E-07	1900		1900	0	1900	0.00550087
2540-82-1	2540821	569	Formothion	257.27	2_Pest	4333.333333		4333.333333	0	4333.333333	0.016843524				1	0.039	1.51592E-07				1	0.039	1.51592E-07	14100		14100	0	14100	0.05480623
2593-15-9	2593159	571	Etridiazole	247.53	2_Pest	240		240	0	240	0.000969579	120		120	0	120	0.00048479				1	0.039	1.57557E-07	2		2	0	2	8.0798E-06
26225-79-6	26225796	573	Ethofumesate	286.35	2_Pest	166.6666667		166.6666667	0	166.6666667	0.000582038	2560		2560	0	2560	0.008940108				1	0.039	1.36197E-07	2700		2700	0	2700	0.00942902
2642-71-9	2642719	40	Azinphos-ethyl	345.38	2_Pest	0.366666667		0.366666667	0	0.366666667	1.06163E-06				1	0.039	1.12919E-07				1	0.039	1.12919E-07				1	1	2.8954E-06
26644-46-2	26644462	5180	Triforine	434.97	2_Pest	600		600	0	600	0.001379405				1	0.039	8.96614E-08				1	0.039	8.96614E-08	40000		40000	0	40000	0.09196037
27314-13-2	27314132	5073	Norflurazon	303.67	2_Pest	4580		4580	0	4580	0.015082162	770		770	0	770	0.002535647				1	0.039	1.28429E-07	3.2		3.2	0	3.2	1.0538E-05
2764-72-9	2764729	4912	Diquat	184.24	2_Pest	250		250	0	250	0.001356926				1	0.039	2.1168E-07				1	0.039	2.1168E-07	1.666666667		1.666666667	0	1.66666667	9.0462E-06
2797-51-5	2797515	5113	Quinoclamine	207.62	2_Pest				1	0.39	1.87843E-06				1	0.039	1.87843E-07				1	0.039	1.87843E-07				1	1	4.8165E-06
28249-77-6	28249776	580	Thiobencarb	257.78	2_Pest	36.66666667	66.6666667	66.66666667	0	66.66666667	0.000258618	23		23	0	23	8.92234E-05				1	0.039	1.51292E-07	5		5	0	5	1.9396E-05
28434-01-7	28434017	581	Bioresmethrin	338.45	2_Pest	0.52		0.52	0	0.52	1.53642E-06				1	0.039	1.15231E-07				1	0.039	1.15231E-07				1	1	2.9546E-06
29091-05-2	29091052	4910	Dinitramine	322.25	2_Pest	196.6666667		196.6666667	0	196.6666667	0.000610292				1	0.039	1.21024E-07				1	0.039	1.21024E-07				1	1	3.1032E-06
29104-30-1	29104301	4847	Benzoximate	363.8	2_Pest				1	0.39	1.07202E-06				1	0.039	1.07202E-07				1	0.039	1.07202E-07				1	1	2.7488E-06
2921-88-2	2921882	585	Chlorpyrifos	350.59	2_Pest	0.004	0.5	0.5	0	0.5	1.42617E-06	0.12	0.21	0.21	0	0.21	5.9899E-07				1	0.039	1.11241E-07	4.333333333		4.333333333	0	4.33333333	1.236E-05
29232-93-7	29232937	586	Pirimiphos-Methyl	305.34	2_Pest	100		100	0	100	0.000327504				1	0.039	1.27726E-07				1	0.039	1.27726E-07	318666.6667		318666.6667	0	318666.667	1.04364534
298-00-0	298000	5086	Parathion-Methyl	263.21	2_Pest	17		17	0	17	6.45872E-05	8.86		8.86	0	8.86	3.36613E-05				1	0.039	1.48171E-07	170		170	0	170	0.00064587
298-02-2	298022	589	Phorate	260.38	2_Pest	0.8		0.8	0	0.8	3.07243E-06	0.096		0.096	0	0.096	3.68692E-07				1	0.039	1.49781E-07	433.3333333		433.3333333	0	433.333333	0.00166423
298-04-4	298044	590	Disulfoton	274.4	2_Pest	35		35	0	35	0.000127551	2.9		2.9	0	2.9	1.05685E-05	2.9		2.9	0	2.9	1.05685E-05				1	1	3.6443E-06
29973-13-5	29973135	593	Ethiofencarb	225.31	2_Pest	1133.333333		1133.333333	0	1133.333333	0.005030107				1	0.039	1.73095E-07				1	0.039	1.73095E-07				1	1	4.4383E-06
300-76-5	300765	594	Naled	380.8	2_Pest	1.103333333	16.3333333	16.33333333	0	16.33333333	4.28922E-05	6.9		6.9	0	6.9	1.81197E-05				1	0.039	1.02416E-07	0.045		0.045	0	0.045	1.1817E-07
301-12-2	301122	595	Oxydemeton-methyl	246.28	2_Pest	243.3333333		243.3333333	0	243.3333333	0.000988035	1400		1400	0	1400	0.005684587				1	0.039	1.58356E-07	100000		100000	0	100000	0.4060419
30560-19-1	30560191	596	Acephate	183.17	2_Pest	5000		5000	0	5000	0.027297046				1	0.039	2.12917E-07				1	0.039	2.12917E-07	16666.66667		16666.66667	0	16666.6667	0.09099015
3060-89-7	3060897	598	Metobromuron	259.11	2_Pest	12000		12000	0	12000	0.046312377				1	0.039	1.50515E-07				1	0.039	1.50515E-07	100		100	0	100	0.00038594
314-40-9	314409	4864	Bromacil	261.13	2_Pest	16900		16900	0	16900	0.064718722	3000		3000	0	3000	0.011488531				1	0.039	1.49351E-07	1.1		1.1	0	1.1	4.2125E-06
330-54-1	330541	46	diuron	233.1	2_Pest	5		5	0	5	2.145E-05	26.4		26.4	0	26.4	0.000113256				1	0.039	1.6731E-07	0.069	0.44	0.44	0	0.44	1.8876E-06
330-55-2	330552	602	Linuron	249.1	2_Pest	498		498	0	498	0.001999197	5.95		5.95	0	5.95	2.3886E-05				1	0.039	1.56564E-07	0.454972527		0.454972527	0	0.45497253	1.8265E-06
33089-61-1	33089611	603	Amitraz	293.42	2_Pest	90		90	0	90	0.000306728	1.48		1.48	0	1.48	5.04396E-06				1	0.039	1.32915E-07	4000		4000	0	4000	0.01363234
333-41-5	333415	47	Diazinon	304.35	2_Pest	0.004	0.032	0.032	0	0.032	1.05142E-07	0.0036		0.0036	0	0.0036	1.18285E-08	0.55		0.55	0	0.55	1.80713E-06	170		170	0	170	0.00055857
3347-22-6	3347226	604	Dithianon	296.33	2_Pest	26.66666667		26.66666667	0	26.66666667	8.99898E-05				1	0.039	1.3161E-07				1	0.039	1.3161E-07	4166.666667		4166.666667	0	4166.66667	0.0140609
33629-47-9	33629479	605	Butralin	295.34	2_Pest	50		50	0	50	0.000169296				1	0.039	1.32051E-07				1	0.039	1.32051E-07	0.7		0.7	0	0.7	2.3701E-06
33693-04-8	33693048	606	Terbumeton	225.3	2_Pest	3333.333333		3333.333333	0	3333.333333	0.014795088				1	0.039	1.73103E-07				1	0.039	1.73103E-07				1	1	4.4385E-06
33820-53-0	33820530	4982	Isopropalin	309.37	2_Pest	105		105	0	105	0.000339399				1	0.039	1.26063E-07				1	0.039	1.26063E-07	26		26	0	26	8.4042E-05
34014-18-1	34014181	607	Tebuthiuron	228.32	2_Pest	13333.33333		13333.33333	0	13333.33333	0.058397571	9300		9300	0	9300	0.040732306				1	0.039	1.70813E-07	13		13	0	13	5.6938E-05
34123-59-6	34123596	49	Isoproturon	206.29	2_Pest	3000		3000	0	3000	0.014542634				1	0.039	1.89054E-07				1	0.039	1.89054E-07	0.21	3.16	3.16	0	3.16	1.5318E-05
34256-82-1	34256821	608	Acetochlor	269.77	2_Pest	170		170	0	170	0.000630166	130		130	0	130	0.000481892	130		130	0	130	0.000481892	1		1	0	1	3.7069E-06
34681-10-2	34681102	610	Butocarboxim	190.27	2_Pest	9666.666667		9666.666667	0	9666.666667	0.050804996				1	0.039	2.04972E-07				1	0.039	2.04972E-07	62500		62500	0	62500	0.32848058
35367-38-5	35367385	612	Diflubenzuron	310.69	2_Pest	13		13	0	13	4.18424E-05	20		20	0	20	6.43728E-05				1	0.039	1.25527E-07	190		190	0	190	0.00061154
35554-44-0	35554440	614	Imazalil	297.19	2_Pest	520		520	0	520	0.001749722				1	0.039	1.31229E-07				1	0.039	1.31229E-07	500		500	0	500	0.00168243
36734-19-7	36734197	616	Iprodione	330.17	2_Pest	520		520	0	520	0.001574946	260		260	0	260	0.000787473				1	0.039	1.18121E-07	13		13	0	13	3.9374E-05

3689-24-5	3689245	5137	Sulfotep	322.32	2_Pest	0.533333333		0.533333333	0	0.533333333	1.65467E-06				1	0.039	1.20998E-07				1	0.039	1.20998E-07				1	1	3.1025E-06
3878-19-1	3878191	622	Fuberidazole	184.2	2_Pest	833.3333333		833.3333333	0	833.3333333	0.004524068				1	0.039	2.11726E-07				1	0.039	2.11726E-07				1	1	5.4289E-06
39515-41-8	39515418	624	Fenpropathrin	349.43	2_Pest	1.3		1.3	0	1.3	3.72034E-06	0.013		0.013	0	0.013	3.72034E-08				1	0.039	1.1161E-07				1	1	2.8618E-06
39807-15-3	39807153	626	Oxadiargyl	341.2	2_Pest				1	0.39	1.14302E-06				1	0.039	1.14302E-07				1	0.039	1.14302E-07	14183.26667		14183.26667	0	14183.2667	0.04156878
40487-42-1	40487421	628	Pendimethalin	281.32	2_Pest	75		75	0	75	0.0002666	0.119		0.119	0	0.119	4.23006E-07				1	0.039	1.38632E-07	0.69		0.69	0	0.69	2.4527E-06
41083-11-8	41083118	630	Azocyclotin	436.21	2_Pest	1.333333333		1.333333333	0	1.333333333	3.05663E-06				1	0.039	8.94065E-08				1	0.039	8.94065E-08				1	1	2.2925E-06
41394-05-2	41394052	632	Metamitron	202.22	2_Pest	108666.6667		108666.6667	0	108666.6667	0.537368543				1	0.039	1.92859E-07				1	0.039	1.92859E-07	100		100	0	100	0.00049451
41483-43-6	41483436	633	Bupirimate	316.43	2_Pest	333.3333333		333.3333333	0	333.3333333	0.001053419				1	0.039	1.2325E-07				1	0.039	1.2325E-07	18384000		18384000	0	18384000	58.0981576
42576-02-3	42576023	4851	Bifenox	342.13	2_Pest	150		150	0	150	0.00043843				1	0.039	1.13992E-07				1	0.039	1.13992E-07	43333.33333		43333.33333	0	43333.3333	0.12665751
42874-03-3	42874033	638	Oxyfluorfen	361.7	2_Pest	14		14	0	14	3.87061E-05	1.3		1.3	0	1.3	3.59414E-06				1	0.039	1.07824E-07	0.1		0.1	0	0.1	2.7647E-07
43121-43-3	43121433	639	Triadimefon	293.76	2_Pest	710		710	0	710	0.002416939	40		40	0	40	0.000136166				1	0.039	1.32761E-07	100		100	0	100	0.00034041
4685-14-7	4685147	5085	Paraquat	186.26	2_Pest	833.3333333	1266.66667	1266.666667	0	1266.666667	0.00680053				1	0.039	2.09385E-07				1	0.039	2.09385E-07	0.033333333		0.033333333	0	0.03333333	1.7896E-07
470-90-6	470906	1098	Chlorfenvinphos	359.57	2_Pest	0.933333333		0.933333333	0	0.933333333	2.59569E-06				1	0.039	1.08463E-07				1	0.039	1.08463E-07	330		330	0	330	0.00091776
49866-87-7	49866877	4903	Difenzoquat	249.34	2_Pest	19333.33333		19333.33333	0	19333.33333	0.077538034				1	0.039	1.56413E-07				1	0.039	1.56413E-07	96.66666667		96.66666667	0	96.6666667	0.00038769
50471-44-8	50471448	661	Vinclozolin	286.12	2_Pest	1040		1040	0	1040	0.003634839	5.75		5.75	0	5.75	2.00965E-05	150		150	0	150	0.000524256	290		290	0	290	0.00101356
50563-36-5	50563365	663	Dimethachlor	255.75	2_Pest	1300		1300	0	1300	0.005083089				1	0.039	1.52493E-07				1	0.039	1.52493E-07	43.33333333		43.33333333	0	43.3333333	0.00016944
50594-66-6	50594666	4828	Acifluorfen	361.66	2_Pest	83000		83000	0	83000	0.229497318				1	0.039	1.07836E-07				1	0.039	1.07836E-07	265		265	0	265	0.00073273
51218-45-2	51218452	56	Metolachlor	283.8	2_Pest	6.866666667		6.866666667	0	6.866666667	2.41954E-05	100		100	0	100	0.000352361	1600		1600	0	1600	0.005637773	0.7	1.7	1.7	0	1.7	5.9901E-06
51276-47-2	51276472	4969	Glufosinate	181.13	2_Pest				1	0.39	2.15315E-06				1	0.039	2.15315E-07				1	0.039	2.15315E-07	933.6666667		933.6666667	0	933.666667	0.00515468
51630-58-1	51630581	1111	Fenvalerate	419.91	2_Pest	0.1	0.13	0.13	0	0.13	3.0959E-07	0.09		0.09	0	0.09	2.14332E-07	0.09		0.09	0	0.09	2.14332E-07	1		1	0	1	2.3815E-06
51707-55-2	51707552	5158	Thidiazuron	220.26	2_Pest	19000		19000	0	19000	0.086261691	5700		5700	0	5700	0.025878507				1	0.039	1.77063E-07	110		110	0	110	0.00049941
52315-07-8	52315078	1099	Cypermethrin	416.31	2_Pest	0.11	0.18	0.18	0	0.18	4.3237E-07	0.03		0.03	0	0.03	7.20617E-08	1		1	0	1	2.40206E-06	100		100	0	100	0.00024021
5234-68-4	5234684	673	Carboxin	235.31	2_Pest	560		560	0	560	0.002379839	562		562	0	562	0.002388339				1	0.039	1.65739E-07	110		110	0	110	0.00046747
52-68-6	52686	677	Trichlorfon	257.44	2_Pest	6.666666667	80	80	0	80	0.000310752				1	0.039	1.51492E-07				1	0.039	1.51492E-07	1012.722621		1012.722621	0	1012.72262	0.00393382
52888-80-9	52888809	60	Prosulfocarb	251.39	2_Pest	280		280	0	280	0.001113807	310		310	0	310	0.001233144				1	0.039	1.55137E-07	38		38	0	38	0.00015116
52918-63-5	52918635	679	Deltamethrin	505.22	2_Pest	0.01	0.1	0.1	0	0.1	1.97934E-07	0.0039		0.0039	0	0.0039	7.71941E-09				1	0.039	7.71941E-08	3033.333333		3033.333333	0	3033.33333	0.00600399
53112-28-0	53112280	681	Pyrimethanil	199.26	2_Pest	1200		1200	0	1200	0.006022282	19		19	0	19	9.53528E-05				1	0.039	1.95724E-07	330		330	0	330	0.00165613
55179-31-2	55179312	693	Bitertanol	337.43	2_Pest	700		700	0	700	0.002074504				1	0.039	1.1558E-07				1	0.039	1.1558E-07	103.3333333		103.3333333	0	103.333333	0.00030624
55219-65-3	55219653	694	Triadimenol	295.77	2_Pest	6900		6900	0	6900	0.023328938				1	0.039	1.31859E-07				1	0.039	1.31859E-07	320		320	0	320	0.00108192
55283-68-6	55283686	695	Ethalfluralin	333.27	2_Pest	0.8		0.8	0	0.8	2.40046E-06	0.4		0.4	0	0.4	1.20023E-06				1	0.039	1.17022E-07	10.9		10.9	0	10.9	3.2706E-05
55285-14-8	55285148	696	Carbosulfan	380.55	2_Pest	5		5	0	5	1.31389E-05	3		3	0	3	7.88333E-06				1	0.039	1.02483E-07	13333.33333		13333.33333	0	13333.3333	0.03503701
55335-06-3	55335063	698	Triclopyr	256.47	2_Pest	86.66666667	100	100	0	100	0.000389909				1	0.039	1.52065E-07				1	0.039	1.52065E-07	353		353	0	353	0.00137638
55-38-9	55389	699	Fenthion	278.33	2_Pest	110		110	0	110	0.000395214	7.5		7.5	0	7.5	2.69464E-05	7.5		7.5	0	7.5	2.69464E-05	80		80	0	80	0.00028743
55512-33-9	55512339	701	Pyridate	378.92	2_Pest	300		300	0	300	0.000791724				1	0.039	1.02924E-07				1	0.039	1.02924E-07	27333.33333		27333.33333	0	27333.3333	0.07213484
555-37-3	555373	5063	Neburon	275.18	2_Pest	106.6666667		106.6666667	0	106.6666667	0.000387625				1	0.039	1.41725E-07				1	0.039	1.41725E-07				1	1	3.634E-06
5598-13-0	5598130	709	Chlorpyrifos-Methyl	322.54	2_Pest	4.2		4.2	0	4.2	1.30216E-05				1	0.039	1.20915E-07				1	0.039	1.20915E-07				1	1	3.1004E-06
563-12-2	563122	711	Ethion	384.48	2_Pest	37.5		37.5	0	37.5	9.75343E-05	13		13	0	13	3.38119E-05				1	0.039	1.01436E-07				1	1	2.6009E-06
56-38-2	56382	713	Parathion	291.26	2_Pest	5.933333333	6.66666667	6.666666667	0	6.666666667	2.28891E-05	0.17		0.17	0	0.17	5.83671E-07	0.67		0.67	0	0.67	2.30035E-06	34		34	0	34	0.00011673
57018-04-9	57018049	718	Tolclofos-methyl	301.13	2_Pest	263.3333333		263.3333333	0	263.3333333	0.000874484	12		12	0	12	3.98499E-05				1	0.039	1.29512E-07	5600		5600	0	5600	0.01859662
57646-30-7	57646307	725	Furalaxyl	301.34	2_Pest	2900		2900	0	2900	0.009623681				1	0.039	1.29422E-07				1	0.039	1.29422E-07	34333.33333		34333.33333	0	34333.3333	0.11393553
57837-19-1	57837191	726	Metalaxyl	279.34	2_Pest	9000		9000	0	9000	0.032218801	9100		9100	0	9100	0.032576788				1	0.039	1.39615E-07	2000		2000	0	2000	0.00715973
57966-95-7	57966957	727	Cymoxanil	198.19	2_Pest	30		30	0	30	0.00015137	0.98		0.98	0	0.98	4.94475E-06	590		590	0	590	0.002976941	32		32	0	32	0.00016146
58138-08-2	58138082	5176	Tridiphane	320.43	2_Pest	123.3333333		123.3333333	0	123.3333333	0.000384899				1	0.039	1.21711E-07				1	0.039	1.21711E-07				1	1	3.1208E-06
58-89-9	58899	68	Lindane	290.83	2_Pest	0.5	3	3	0	3	1.03153E-05	2.8		2.8	0	2.8	9.62762E-06				1	0.039	1.34099E-07	0.8		0.8	0	0.8	2.7507E-06
5902-51-2	5902512	5149	Terbacil	216.67	2_Pest	32000		32000	0	32000	0.147690036	1200		1200	0	1200	0.005538376				1	0.039	1.79997E-07	4.4		4.4	0	4.4	2.0307E-05
5915-41-3	5915413	70	Terbuthylazine	229.72	2_Pest	533.3333333		533.3333333	0	533.3333333	0.002321667				1	0.039	1.69772E-07				1	0.039	1.69772E-07	0.6		0.6	0	0.6	2.6119E-06
60168-88-9	60168889	747	Fenarimol	331.2	2_Pest	490		490	0	490	0.001479469	177		177	0	177	0.00053442	497		497	0	497	0.001500604	323		323	0	323	0.00097524
60207-90-1	60207901	748	Propiconazole	342.23	2_Pest	80		80	0	80	0.000233761	0.18		0.18	0	0.18	5.25962E-07				1	0.039	1.13958E-07	0.266666667		0.266666667	0	0.26666667	7.792E-07
60-51-5	60515	753	Dimethoate	229.26	2_Pest	10		10	0	10	4.36186E-05	24.68		24.68	0	24.68	0.000107651	24.68		24.68	0	24.68	0.000107651	66.66666667		66.66666667	0	66.6666667	0.00029079
61213-25-0	61213250	4960	Flurochloridone	312.12	2_Pest	600		600	0	600	0.001922338				1	0.039	1.24952E-07				1	0.039	1.24952E-07	2133.333333		2133.333333	0	2133.33333	0.00683498
62-73-7	62737	4897	Dichlorvos	220.98	2_Pest	100		100	0	100	0.00045253	5.2		5.2	0	5.2	2.35315E-05				1	0.039	1.76487E-07	4700		4700	0	4700	0.02126889
62850-32-2	62850322	4946	Fenothiocarb	253.37	2_Pest	2633.333333		2633.333333	0	2633.333333	0.010393233				1	0.039	1.53925E-07				1	0.039	1.53925E-07				1	1	3.9468E-06
63-25-2	63252	76	Carbaryl	201.23	2_Pest	75.5		75.5	0	75.5	0.000375193	1		1	0	1	4.96944E-06				1	0.039	1.93808E-07	10		10	0	10	4.9694E-05
63284-71-9	63284719	773	Nuarimol	314.75	2_Pest	1853.333333		1853.333333	0	1853.333333	0.005888271				1	0.039	1.23908E-07				1	0.039	1.23908E-07	833.3333333		833.3333333	0	833.333333	0.0026476
640-15-3	640153	775	Thiometon	246.35	2_Pest	213.3333333		213.3333333	0	213.3333333	0.000865977				1	0.039	1.58311E-07				1	0.039	1.58311E-07	4266.666667		4266.666667	0	4266.66667	0.01731953
64902-72-3	64902723	783	Chlorsulfuron	357.78	2_Pest	12666.66667		12666.66667	0	12666.66667	0.035403507	31400		31400	0	31400	0.08776343				1	0.039	1.09006E-07	9.4		9.4	0	9.4	2.6273E-05
66215-27-8	66215278	4881	Cypromazine	166.19	2_Pest	50800		50800	0	50800	0.305674228	14000		14000	0	14000	0.084240929				1	0.039	2.34671E-07	41333.33333		41333.33333	0	41333.3333	0.24871131
66230-04-4	66230044	786	Esfenvalerate	419.91	2_Pest	0.026		0.026	0	0.026	6.1918E-08	0.028		0.028	0	0.028	6.6681E-08				1	0.039	9.2877E-08	0.833		0.833	0	0.833	1.9838E-06
66246-88-6	66246886	787	Penconazole	284.19	2_Pest	566.6666667		566.6666667	0	566.6666667	0.001993971				1	0.039	1.37232E-07				1	0.039	1.37232E-07	993.3333333		993.3333333	0	993.333333	0.00349531
66332-96-5	66332965	4961	Flutolanil	323.32	2_Pest	460		460	0	460	0.001422739	233		233	0	233	0.000720648				1	0.039	1.20624E-07	800		800	0	800	0.00247433
668-34-8	668348	790	Fentin	350.01	2_Pest	3.333333333		3.333333333	0	3.333333333	9.52354E-06	0.046		0.046	0	0.046	1.31425E-07				1	0.039	1.11425E-07	0.0008		0.0008	0	0.0008	2.2856E-09
66841-25-6	66841256	5167	Tralomethrin	665.04	2_Pest	0.533333333		0.533333333	0	0.533333333	8.01957E-07	0.027		0.027	0	0.027	4.05991E-08	0.027		0.027	0	0.027	4.05991E-08				1	1	1.5037E-06
67129-08-2	67129082	81	Metazachlor	277.76	2_Pest	1333.333333		1333.333333	0	1333.333333	0.004800307				1	0.039	1.40409E-07				1	0.039	1.40409E-07	14.66666667		14.66666667	0	14.6666667	5.2803E-05
67306-00-7	67306007	792	Fenpropidin	273.46	2_Pest	633.3333333		633.3333333	0	633.3333333	0.002316	320		320	0	320	0.001170189				1	0.039	1.42617E-07	0.053333333		0.053333333	0	0.05333333	1.9503E-07
67375-30-8	67375308	1108	alpha-Cypermethrin	416.31	2_Pest	0.133333333		0.133333333	0	0.133333333	3.20274E-07				1	0.039	9.36802E-08				1	0.039	9.36802E-08				1	1	2.4021E-06
67564-91-4	67564914	4949	Fenpropimorph	303.49	2_Pest	80		80	0	80	0.0002636	0.16		0.16	0	0.16	5.272E-07				1	0.039	1.28505E-07	5		5	0	5	1.6475E-05
67747-09-5	67747095	797	Prochloraz	376.67	2_Pest	3		3	0	3	7.96453E-06	16.4		16.4	0	16.4	4.35394E-05				1	0.039	1.03539E-07	12.55566667		12.55566667	0	12.5556667	3.3333E-05
68694-11-1	68694111	802	Triflumizole	345.76	2_Pest	100		100	0	100	0.000289218	33		33	0	33	9.54419E-05				1	0.039	1.12795E-07	35		35	0	35	0.00010123
6923-22-4	6923224	803	Monocrotophos	223.17	2_Pest	53.33333333	333.333333	333.3333333	0	333.3333333	0.00149363	2000		2000	0	2000	0.008961778				1	0.039	1.74755E-07				1	1	4.4809E-06
69377-81-7	69377817	805	Fluroxypyr	255.03	2_Pest	7280		7280	0	7280	0.028545661				1	0.039	1.52923E-07				1	0.039	1.52923E-07	179		179	0	179	0.00070188
69806-34-4	69806344	810	Haloxyfop	361.7	2_Pest	196000		196000	0	196000	0.541885541				1	0.039	1.07824E-07				1	0.039	1.07824E-07	5000		5000	0	5000	0.01382361
7003-89-6	7003896	4871	Chlormequat	122.62	2_Pest	33333.33333		33333.33333	0	33333.33333	0.271842549				1	0.039	3.18056E-07				1	0.039	3.18056E-07				1	1	8.1553E-06
70124-77-5	70124775	811	Flucythrinate	451.47	2_Pest	0.003333333	0.02	0.02	0	0.02	4.42997E-08	0.005		0.005	0	0.005	1.10749E-08				1	0.039	8.63845E-08				1	1	2.215E-06
70630-17-0	70630170	1113	Metalaxyl-M	279.34	2_Pest	10000		10000	0	10000	0.035798668				1	0.039	1.39615E-07				1	0.039	1.39615E-07	6650		6650	0	6650	0.02380611
709-98-8	709988	816	Propanil	218.08	2_Pest	720		720	0	720	0.003301541	0.4		0.4	0	0.4	1.83419E-06	150		150	0	150	0.000687821	6		6	0	6	2.7513E-05
71626-11-4	71626114	823	Benalaxyl	325.41	2_Pest				1	0.39	1.19849E-06				1	0.039	1.19849E-07				1	0.039	1.19849E-07	100		100	0	100	0.0003073
71751-41-2	71751412	1097	Abamectin	873.09	2_Pest	2.2		2.2	0	2.2	2.51979E-06				1	0.039	4.46689E-08				1	0.039	4.46689E-08	48000		48000	0	48000	0.05497715
72178-02-0	72178020	824	Fomesafen	438.77	2_Pest	54333.33333		54333.33333	0	54333.33333	0.123831012	54000		54000	0	54000	0.123071313				1	0.039	8.88848E-08				1	1	2.2791E-06
72490-01-8	72490018	825	Fenoxycarb	301.34	2_Pest	260		260	0	260	0.000862813	48		48	0	48	0.000159289				1	0.039	1.29422E-07				1	1	3.3185E-06
7287-19-6	7287196	87	Prometryn	241.37	2_Pest	560		560	0	560	0.002320089	620		620	0	620	0.002568671	1390		1390	0	1390	0.005758794	0.3		0.3	0	0.3	1.2429E-06
731-27-1	731271	827	Tolylfluanid	347.26	2_Pest	20		20	0	20	5.75937E-05				1	0.039	1.12308E-07				1	0.039	1.12308E-07	483.3333333		483.3333333	0	483.333333	0.00139185
732-11-6	732116	828	Phosmet	317.32	2_Pest	7.5		7.5	0	7.5	2.36354E-05	3.2		3.2	0	3.2	1.00845E-05				1	0.039	1.22904E-07				1	1	3.1514E-06
74051-80-2	74051802	834	Sethoxydim	327.49	2_Pest	120		120	0	120	0.000366423	98000		98000	0	98000	0.299245778				1	0.039	1.19088E-07	250		250	0	250	0.00076338
74070-46-5	74070465	835	Aclonifen	264.67	2_Pest	223.3333333		223.3333333	0	223.3333333	0.000843818	5		5	0	5	1.88914E-05				1	0.039	1.47353E-07	2.5		2.5	0	2.5	9.4457E-06
74223-64-6	74223646	836	Metsulfuron-methyl	381.37	2_Pest	66.66666667		66.66666667	0	66.66666667	0.000174808	2.9		2.9	0	2.9	7.60416E-06				1	0.039	1.02263E-07	10		10	0	10	2.6221E-05
74738-17-3	74738173	4948	Fenpiclonil	237.09	2_Pest	253.3333333		253.3333333	0	253.3333333	0.001068511				1	0.039	1.64494E-07				1	0.039	1.64494E-07	73.33333333		73.33333333	0	73.3333333	0.00030931
75-99-0	75990	4884	Dalapon	142.97	2_Pest	33333.33333		33333.33333	0	33333.33333	0.233149146				1	0.039	2.72785E-07				1	0.039	2.72785E-07				1	1	6.9945E-06
759-94-4	759944	869	EPTC	189.32	2_Pest	3000		3000	0	3000	0.015846186	69		69	0	69	0.000364462				1	0.039	2.06E-07	860		860	0	860	0.00454257
76578-12-6	76578126	5116	Quizalofop	344.76	2_Pest				1	0.39	1.13122E-06				1	0.039	1.13122E-07				1	0.039	1.13122E-07	5813.333333		5813.333333	0	5813.33333	0.01686197
76674-21-0	76674210	875	Flutriafol	301.3	2_Pest	5600		5600	0	5600	0.018586127	4800		4800	0	4800	0.015930966				1	0.039	1.29439E-07	100		100	0	100	0.0003319
76738-62-0	76738620	5082	Paclobutrazol	293.8	2_Pest	10000		10000	0	10000	0.03403676				1	0.039	1.32743E-07				1	0.039	1.32743E-07	910.78		910.78	0	910.78	0.0031
76-87-9	76879	1110	Fentin hydroxide	367.01	2_Pest	1.233333333	2.36666667	2.366666667	0	2.366666667	6.44851E-06	0.0065		0.0065	0	0.0065	1.77107E-08				1	0.039	1.06264E-07	0.196666667		0.196666667	0	0.19666667	5.3586E-07
77732-09-3	77732093	5080	Oxadixyl	278.31	2_Pest	100000		100000	0	100000	0.359311559	220000		220000	0	220000	0.79048543				1	0.039	1.40132E-07	15333.33333		15333.33333	0	15333.3333	0.05509444
7786-34-7	7786347	5035	Mevinphos	224.15	2_Pest	3.666666667	3.96666667	3.966666667	0	3.966666667	1.76965E-05				1	0.039	1.73991E-07				1	0.039	1.73991E-07	50000		50000	0	50000	0.22306491
78587-05-0	78587050	4974	Hexythiazox	352.89	2_Pest	240		240	0	240	0.000680099				1	0.039	1.10516E-07				1	0.039	1.10516E-07				1	1	2.8337E-06
786-19-6	786196	898	carbophenothion	342.87	2_Pest	0.093333333	0.25666667	0.256666667	0	0.256666667	7.48583E-07	1.3		1.3	0	1.3	3.79152E-06				1	0.039	1.13746E-07	10		10	0	10	2.9166E-05
79241-46-6	79241466	4954	Fluazifop-P-butyl	383.37	2_Pest	176.6666667		176.6666667	0	176.6666667	0.000460825				1	0.039	1.01729E-07				1	0.039	1.01729E-07	880		880	0	880	0.00229543
79277-27-3	79277273	918	Thifensulfuron-methyl	387.4	2_Pest	33333.33333		33333.33333	0	33333.33333	0.08604371	10600		10600	0	10600	0.0273619	10600		10600	0	10600	0.0273619	8.15		8.15	0	8.15	2.1038E-05
79538-32-2	79538322	922	Tefluthrin	418.74	2_Pest	0.03		0.03	0	0.03	7.16435E-08	0.00397		0.00397	0	0.00397	9.48082E-09				1	0.039	9.31366E-08				1	1	2.3881E-06
79622-59-6	79622596	925	Fluazinam	465.1	2_Pest	15		15	0	15	3.22511E-05	0.69		0.69	0	0.69	1.48355E-06	0.69		0.69	0	0.69	1.48355E-06	1.1		1.1	0	1.1	2.3651E-06
79983-71-4	79983714	930	Hexaconazole	314.22	2_Pest	970		970	0	970	0.003087009	600		600	0	600	0.00190949				1	0.039	1.24117E-07	20		20	0	20	6.365E-05
80-33-1	80331	935	Chlorfenson	303.16	2_Pest	206.6666667		206.6666667	0	206.6666667	0.000681708				1	0.039	1.28645E-07				1	0.039	1.28645E-07	2000		2000	0	2000	0.00659718
81335-37-7	81335377	4977	Imazaquin	311.34	2_Pest	140000		140000	0	140000	0.449669172				1	0.039	1.25265E-07				1	0.039	1.25265E-07				1	1	3.2119E-06
81777-89-1	81777891	941	Clomazone	239.7	2_Pest	8900		8900	0	8900	0.037129746	720		720	0	720	0.003003755				1	0.039	1.62703E-07	23.6		23.6	0	23.6	9.8456E-05
82097-50-5	82097505	944	Triasulfuron	401.83	2_Pest	22866.66667		22866.66667	0	22866.66667	0.05690632	68600		68600	0	68600	0.170718961				1	0.039	9.7056E-08	32		32	0	32	7.9636E-05
82558-50-7	82558507	946	Isoxaben	332.4	2_Pest	870		870	0	870	0.002617329	400		400	0	400	0.001203369				1	0.039	1.17329E-07	1400		1400	0	1400	0.00421179
82560-54-1	82560541	947	Benfuracarb	410.54	2_Pest	216.6666667		216.6666667	0	216.6666667	0.00052776				1	0.039	9.49968E-08				1	0.039	9.49968E-08	16666.66667		16666.66667	0	16666.6667	0.04059694
82657-04-3	82657043	948	Bifenthrin	422.87	2_Pest	0.03		0.03	0	0.03	7.09438E-08	0.04		0.04	0	0.04	9.45917E-08				1	0.039	9.22269E-08	10		10	0	10	2.3648E-05
82-68-8	82688	5115	Quintozene	295.34	2_Pest	23		23	0	23	7.78763E-05	13		13	0	13	4.40171E-05	52		52	0	52	0.000176068				1	1	3.3859E-06
83055-99-6	83055996	949	Bensulfuron-methyl	410.41	2_Pest	21000		21000	0	21000	0.051168344	120000		120000	0	120000	0.292390536				1	0.039	9.50269E-08	400		400	0	400	0.00097464
83121-18-0	83121180	5144	Teflubenzuron	381.11	2_Pest	166666.6667		166666.6667	0	166666.6667	0.437319059				1	0.039	1.02333E-07				1	0.039	1.02333E-07	250000		250000	0	250000	0.65597859
83164-33-4	83164334	951	Diflufenican	394.3	2_Pest	1180		1180	0	1180	0.002992645	15		15	0	15	3.80421E-05				1	0.039	9.89095E-08	0.1		0.1	0	0.1	2.5361E-07
834-12-8	834128	953	ametryn	227.34	2_Pest	100		100	0	100	0.00043987	700		700	0	700	0.003079089	5900		5900	0	5900	0.025952318	0.1		0.1	0	0.1	4.3987E-07
83657-24-3	83657243	955	Diniconazole	326.23	2_Pest	526.6666667		526.6666667	0	526.6666667	0.001614403				1	0.039	1.19548E-07				1	0.039	1.19548E-07				1	1	3.0653E-06
84087-01-4	84087014	958	Quinclorac	242.06	2_Pest	9100		9100	0	9100	0.037593985	102		102	0	102	0.000421383				1	0.039	1.61117E-07	500		500	0	500	0.0020656
841-06-5	841065	959	Methoprotryne	271.39	2_Pest	2666.666667		2666.666667	0	2666.666667	0.009825958				1	0.039	1.43705E-07				1	0.039	1.43705E-07				1	1	3.6847E-06
85509-19-9	85509199	967	Flusilazole	315.4	2_Pest				1	0.39	1.23653E-06				1	0.039	1.23653E-07				1	0.039	1.23653E-07	170		170	0	170	0.000539
86479-06-3	86479063	971	Hexaflumuron	461.15	2_Pest	123.5		123.5	0	123.5	0.000267809				1	0.039	8.45712E-08				1	0.039	8.45712E-08				1	1	2.1685E-06
86-50-0	86500	972	Azinphos-methyl	317.33	2_Pest	0.703		0.703	0	0.703	2.21536E-06	0.024		0.024	0	0.024	7.5631E-08	0.14		0.14	0	0.14	4.41181E-07	1800		1800	0	1800	0.00567233
87392-12-9	87392129	1115	S-Metolachlor	283.8	2_Pest	1500		1500	0	1500	0.005285412	30		30	0	30	0.000105708				1	0.039	1.37421E-07	1.5		1.5	0	1.5	5.2854E-06
87674-68-8	87674688	1109	Dimethenamid	275.8	2_Pest	1700		1700	0	1700	0.006163887	120		120	0	120	0.000435098				1	0.039	1.41407E-07	0.61		0.61	0	0.61	2.2117E-06
87820-88-0	87820880	981	Tralkoxydim	329.44	2_Pest	6100		6100	0	6100	0.01851627				1	0.039	1.18383E-07				1	0.039	1.18383E-07	5100		5100	0	5100	0.01548082
886-50-0	886500	104	Terbutryn	241.37	2_Pest	540		540	0	540	0.002237229	1000		1000	0	1000	0.004143017				1	0.039	1.61578E-07	0.015	0.019	0.019	0	0.019	7.8717E-08
88671-89-0	88671890	984	Myclobutanil	288.79	2_Pest	490		490	0	490	0.001696735	2200		2200	0	2200	0.007617992				1	0.039	1.35046E-07	560		560	0	560	0.00193913
90717-03-6	90717036	1003	Quinmerac	221.64	2_Pest	46000		46000	0	46000	0.207543765				1	0.039	1.75961E-07				1	0.039	1.75961E-07	16166.66667		16166.66667	0	16166.6667	0.07294111
91465-08-6	91465086	5001	Lambda-Cyhalothrin	449.86	2_Pest	0.0001		0.0001	0	0.0001	2.22291E-10	0.025		0.025	0	0.025	5.55728E-08				1	0.039	8.66936E-08	310		310	0	310	0.0006891
919-86-8	919868	1010	Demeton-S-methyl	230.29	2_Pest				1	0.39	1.69352E-06				1	0.039	1.69352E-07				1	0.039	1.69352E-07				1	1	4.3424E-06
93-65-2	93652	108	Mecoprop	214.65	2_Pest	3333.333333		3333.333333	0	3333.333333	0.015529156				1	0.039	1.81691E-07				1	0.039	1.81691E-07	34220		34220	0	34220	0.15942232
94125-34-5	94125345	1021	Prosulfuron	419.39	2_Pest	155000		155000	0	155000	0.369584396	146000		146000	0	146000	0.348124657				1	0.039	9.29922E-08	3		3	0	3	7.1532E-06
94361-06-5	94361065	1022	Cyproconazole	291.79	2_Pest	1000		1000	0	1000	0.003427122	650		650	0	650	0.002227629				1	0.039	1.33658E-07	6		6	0	6	2.0563E-05
944-22-9	944229	1023	Fonofos	246.33	2_Pest	3		3	0	3	1.21788E-05	2.33		2.33	0	2.33	9.45886E-06	19		19	0	19	7.71323E-05				1	1	4.0596E-06
94-74-6	94746	110	MCPA	200.62	2_Pest	176.6666667		176.6666667	0	176.6666667	0.000880603				1	0.039	1.94397E-07				1	0.039	1.94397E-07	2130		2130	0	2130	0.01061709
94-75-7	94757	111	2,4-D	221.04	2_Pest	652		652	0	652	0.002949692	160		160	0	160	0.000723851				1	0.039	1.76439E-07	4.28		4.28	0	4.28	1.9363E-05
94-81-5	94815	5015	MCPB	228.68	2_Pest	23.33333333		23.33333333	0	23.33333333	0.000102035				1	0.039	1.70544E-07				1	0.039	1.70544E-07				1	1	4.3729E-06
94-82-6	94826	4327	2,4-DB	249.09	2_Pest	666.6666667		666.6666667	0	666.6666667	0.002676409				1	0.039	1.5657E-07				1	0.039	1.5657E-07				1	1	4.0146E-06
950-37-8	950378	1025	Methidathion	302.33	2_Pest	1.87		1.87	0	1.87	6.18529E-06	6.1		6.1	0	6.1	2.01766E-05				1	0.039	1.28998E-07	3666.666667		3666.666667	0	3666.66667	0.01212803
95266-40-3	95266403	1026	Trinexapac-Ethyl	252.27	2_Pest	20000		20000	0	20000	0.079280136	410		410	0	410	0.001625243	12000		12000	0	12000	0.047568082	110		110	0	110	0.00043604
95465-99-9	95465999	1027	Cadusafos	270.39	2_Pest	89		89	0	89	0.000329154	5.22		5.22	0	5.22	1.93054E-05				1	0.039	1.44236E-07	1000		1000	0	1000	0.00369836
95617-09-7	95617097	4947	Fenoxaprop	333.73	2_Pest	105.4092553		105.4092553	0	105.4092553	0.000315852				1	0.039	1.16861E-07				1	0.039	1.16861E-07	296.9333333		296.9333333	0	296.933333	0.00088974
96489-71-3	96489713	1055	Pyridaben	364.94	2_Pest	0.29		0.29	0	0.29	7.94651E-07	0.255		0.255	0	0.255	6.98745E-07				1	0.039	1.06867E-07	13.4		13.4	0	13.4	3.6718E-05
99105-77-8	99105778	1083	Sulcotrione	328.77	2_Pest	75666.66667		75666.66667	0	75666.66667	0.230150764	3200		3200	0	3200	0.009733248				1	0.039	1.18624E-07	190		190	0	190	0.00057791
99129-21-2	99129212	1084	Clethodim	359.92	2_Pest	18000		18000	0	18000	0.050011114	10		10	0	10	2.7784E-05				1	0.039	1.08357E-07	8000		8000	0	8000	0.02222716
99-30-9	99309	1085	Dicloran	207.02	2_Pest	180		180	0	180	0.000869481				1	0.039	1.88388E-07				1	0.039	1.88388E-07	433.3333333		433.3333333	0	433.333333	0.0020932
2458-08-4	2458084	1246	12-Ketochenodeoxycholic acid	406.56	3_REACH	70290		70290	0	70290	0.17288961				1	0.039	9.59268E-08				1	0.039	9.59268E-08	30640		30640	0	30640	0.07536403
2478-10-6	2478106	1247	4-hydroxybutyl acrylate	144.17	3_REACH	10000		10000	0	10000	0.069362558				1	0.039	2.70514E-07				1	0.039	2.70514E-07	4000		4000	0	4000	0.02774502
2536-05-2	2536052	1249	2,2'-methylenediphenyl diisocyanate	250.26	3_REACH	500000		500000	0	500000	1.997922161				1	0.039	1.55838E-07				1	0.039	1.55838E-07	1640000		1640000	0	1640000	6.55318469
2550-02-9	2550029	1250	triethoxypropylsilane	206.36	3_REACH	58000		58000	0	58000	0.281062221				1	0.039	1.8899E-07				1	0.039	1.8899E-07	237000		237000	0	237000	1.14847839
2550-06-3	2550063	1251	trichloro(3-chloropropyl)silane	211.98	3_REACH	100000		100000	0	100000	0.471742617				1	0.039	1.8398E-07				1	0.039	1.8398E-07	167000		167000	0	167000	0.78781017

2554-06-5	2554065	1252	2,4,6,8-tetramethyl-2,4,6,8-	344.66	3_REACH	16		16	0	16	4.64226E-05	4.4	4.4	0	4.4	1.27662E-05			1	0.039	1.13155E-07	12	12	0	12	3.4817E-05
2643-07-4	2643074	1253	p-[(2-	211.69	3_REACH	1000		1000	0	1000	0.004723889			1	0.039	1.84232E-07			1	0.039	1.84232E-07	2420	2420	0	2420	0.01143181
2680-03-7	2680037	1254	N,N-dimethylacrylamide	99.134	3_REACH	120000		120000	0	120000	1.210482781			1	0.039	3.93407E-07			1	0.039	3.93407E-07	50000	50000	0	50000	0.50436783
3081-01-4	3081014	1257	N-(1,4-dimethylpentyl)-N'-	282.43	3_REACH	9.333333333	32.3333333	32.33333333	0	32.33333333	0.000114483	3.7	3.7	0	3.7	1.31006E-05			1	0.039	1.38087E-07	95.8	95.8	0	95.8	0.0003392
3302-10-1	3302101	1259	3,5,5-trimethylhexanoic	158.24	3_REACH	5000		5000	0	5000	0.031597573	9205	9205	0	9205	0.058171132			1	0.039	2.46461E-07	10000	10000	0	10000	0.06319515
3452-07-1	3452071	1261	icos-1-ene	280.54	3_REACH	1000000		1000000	0	1000000	3.564554074			1	0.039	1.39018E-07			1	0.039	1.39018E-07	1000000	1000000	0	1000000	3.56455407
3913-02-8	3913028	1263	2-butyloctan-1-ol	186.34	3_REACH	320		320	0	320	0.001717291			1	0.039	2.09295E-07			1	0.039	2.09295E-07	5.15	5.15	0	5.15	2.7638E-05
4130-08-9	4130089	1265	triacetoxyvinylsilane	232.26	3_REACH	27792.88478		27792.88478	0	27792.88478	0.119662812			1	0.039	1.67915E-07			1	0.039	1.67915E-07	16840	16840	0	16840	0.07250495
4223-03-4	4223034	1266	N-(1,1,3,3-	183.3	3_REACH	25000		25000	0	25000	0.136388434			1	0.039	2.12766E-07			1	0.039	2.12766E-07	4270	4270	0	4270	0.02329514
4292-10-8	4292108	1267	(carboxymethyl)dimethyl-3-	342.53	3_REACH	540		540	0	540	0.001576504	135	135	0	135	0.000394126			1	0.039	1.13859E-07	300	300	0	300	0.00087584
4719-04-4	4719044	117	2,2',2''-(hexahydro-1,3,5-	219.29	3_REACH	5000		5000	0	5000	0.022800857			1	0.039	1.77847E-07			1	0.039	1.77847E-07	1560	1560	0	1560	0.00711387
5117-12-4	5117124	4397	4-(1-oxo-2-propenyl)-	141.17	3_REACH	102000		102000	0	102000	0.722533116			1	0.039	2.76263E-07			1	0.039	2.76263E-07	120000	120000	0	120000	0.85003896
6318-09-8	6318098	1282	2,4,6-Tri(propan-2-	234.39	3_REACH	6300		6300	0	6300	0.02687828			1	0.039	1.66389E-07			1	0.039	1.66389E-07	2850	2850	0	2850	0.01215922
6992-11-6	6992116	1287	4-[(2,5-dichlorophenyl)azo]-	492.33	3_REACH	1000		1000	0	1000	0.002031158			1	0.039	7.92152E-08			1	0.039	7.92152E-08	1000	1000	0	1000	0.00203116
7027-11-4	7027114	4392	3-cyano-3,5,5-	165.24	3_REACH	4944.132325		4944.132325	0	4944.132325	0.029920917			1	0.039	2.3602E-07			1	0.039	2.3602E-07	78000	78000	0	78000	0.47204067
7651-02-7	7651027	1289	N-[3-	368.65	3_REACH	100		100	0	100	0.00027126	100	100	0	100	0.00027126			1	0.039	1.05791E-07	71	71	0	71	0.00019259
100-00-5	100005	119	1-chloro-4-nitrobenzene	157.56	3_REACH	1000		1000	0	1000	0.006346789	100	100	0	100	0.000634679			1	0.039	2.47525E-07	2200	2200	0	2200	0.01396293
100-01-6	100016	120	4-nitroaniline	138.13	3_REACH	11666.66667		11666.66667	0	11666.66667	0.084461498			1	0.039	2.82343E-07			1	0.039	2.82343E-07	22666.66667	22666.66667	0	22666.6667	0.16409662
100-02-7	100027	1	4-nitrophenol	139.11	3_REACH	14.93584142	29.8021275	29.80212754	0	29.80212754	0.000214234	1160	1160	0	1160	0.008338725			1	0.039	2.80354E-07	1396.666667	1396.666667	0	1396.66667	0.01004002
1001354-72-8	1001354728	4779	3-Aminooctan-4-ol	145.25	3_REACH	22666.66667		22666.66667	0	22666.66667	0.156052783	103000	103000	0	103000	0.709122203			1	0.039	2.68503E-07	810	810	0	810	0.00557659
10016-20-3	10016203	1295	cyclohexapentylose	972.85	3_REACH	100000		100000	0	100000	0.102790769			1	0.039	4.00884E-08			1	0.039	4.00884E-08	150000	150000	0	150000	0.15418615
100-18-5	100185	1296	1,4-diisopropylbenzene	162.28	3_REACH	250		250	0	250	0.001540547			1	0.039	2.40325E-07			1	0.039	2.40325E-07	310	310	0	310	0.00191028
100-20-9	100209	1297	terephthaloyl dichloride	203.02	3_REACH	250000		250000	0	250000	1.231405773			1	0.039	1.92099E-07			1	0.039	1.92099E-07	668000	668000	0	668000	3.29031623
100-21-0	100210	122	terephthalic acid	166.13	3_REACH	18600		18600	0	18600	0.111960513			1	0.039	2.34756E-07			1	0.039	2.34756E-07	19000	19000	0	19000	0.11436827
1003-52-7	1003527	1302	4-methyloxazole-5-	108.1	3_REACH				1	0.39	3.60777E-06	28600	28600	0	28600	0.264569843			1	0.039	3.60777E-07	76000	76000	0	76000	0.70305273
100-37-8	100378	123	2-diethylaminoethanol	117.19	3_REACH	80000		80000	0	80000	0.682652103			1	0.039	3.32793E-07			1	0.039	3.32793E-07	5000	5000	0	5000	0.04266576
10042-59-8	10042598	1306	2-propylheptan-1-ol	158.29	3_REACH	1100		1100	0	1100	0.00694927			1	0.039	2.46383E-07			1	0.039	2.46383E-07	780	780	0	780	0.00492766
100-46-9	100469	127	benzylamine	107.16	3_REACH	20000		20000	0	20000	0.186636805			1	0.039	3.63942E-07			1	0.039	3.63942E-07	6000	6000	0	6000	0.05599104
100-47-0	100470	128	benzonitrile	103.13	3_REACH	5000		5000	0	5000	0.048482498			1	0.039	3.78163E-07			1	0.039	3.78163E-07			1	1	9.6965E-06
100-51-6	100516	129	benzyl alcohol	108.14	3_REACH	3333.333333		3333.333333	0	3333.333333	0.03082424	5100	5100	0	5100	0.047161087			1	0.039	3.60644E-07	16000	16000	0	16000	0.14795635
100-52-7	100527	130	benzaldehyde	106.12	3_REACH	120		120	0	120	0.001130795	220	220	0	220	0.002073125			1	0.039	3.67508E-07	20000	20000	0	20000	0.18846589
100-54-9	100549	131	nicotinonitrile	104.11	3_REACH				1	0.39	3.74604E-06			1	0.039	3.74604E-07			1	0.039	3.74604E-07	77384.33333	77384.33333	0	77384.3333	0.74329395
100-61-8	100618	133	N-methylaniline	107.16	3_REACH	25.37066667		25.37066667	0	25.37066667	0.000236755	3566.666667	3566.666667	0	3566.666667	0.033283564			1	0.039	3.63942E-07	211.6601049	211.6601049	0	211.660105	0.00197518
100-63-0	100630	134	phenylhydrazine	108.15	3_REACH	383.3333333		383.3333333	0	383.3333333	0.00354446			1	0.039	3.6061E-07			1	0.039	3.6061E-07			1	1	9.2464E-06
100-64-1	100641	135	cyclohexanone oxime	113.16	3_REACH	5000		5000	0	5000	0.044185224			1	0.039	3.44645E-07			1	0.039	3.44645E-07	500	500	0	500	0.00441852
100-69-6	100696	1309	2-vinylpyridine	105.14	3_REACH	938		938	0	938	0.008921438			1	0.039	3.70934E-07			1	0.039	3.70934E-07	30900	30900	0	30900	0.29389386
10081-67-1	10081671	1310	4-(1-methyl-1-phenylethyl)-	405.59	3_REACH	33333.33333		33333.33333	0	33333.33333	0.082184801			1	0.039	9.61562E-08			1	0.039	9.61562E-08	23000	23000	0	23000	0.05670751
100-83-4	100834	138	3-hydroxybenzaldehyde	122.12	3_REACH				1	0.39	3.19358E-06			1	0.039	3.19358E-07			1	0.039	3.19358E-07	33333.33333	33333.33333	0	33333.3333	0.27295556
100-97-0	100970	2	methenamine	140.19	3_REACH	3333333.333		3333333.333	0	3333333.333	23.77725468			1	0.039	2.78194E-07			1	0.039	2.78194E-07	1500000	1500000	0	1500000	10.6997646
10097-02-6	10097026	4315	2,2-	148.16	3_REACH	100000		100000	0	100000	0.674946004			1	0.039	2.63229E-07			1	0.039	2.63229E-07	10000	10000	0	10000	0.0674946
101-02-0	101020	140	triphenyl phosphite	310.29	3_REACH	233.3333333		233.3333333	0	233.3333333	0.000751985			1	0.039	1.25689E-07			1	0.039	1.25689E-07			1	1	3.2228E-06
101-14-4	101144	1315	4,4'-methylenebis[2-	267.16	3_REACH	300		300	0	300	0.001122923			1	0.039	1.4598E-07			1	0.039	1.4598E-07	736	736	0	736	0.0027549
101-20-2	101202	143	triclocarban	315.59	3_REACH	1.4		1.4	0	1.4	4.43614E-06	1.6	1.6	0	1.6	5.06987E-06			1	0.039	1.23578E-07	10	10	0	10	3.1687E-05
101238-01-1	101238011	1317	2,2,6,6-	339.57	3_REACH	4		4	0	4	1.17796E-05			1	0.039	1.14851E-07			1	0.039	1.14851E-07	36	36	0	36	0.00010602
101-37-1	101371	1318	2,4,6-triallyloxy-1,3,5-	249.27	3_REACH	3900		3900	0	3900	0.015645685			1	0.039	1.56457E-07			1	0.039	1.56457E-07	2500	2500	0	2500	0.01002929
1013-88-3	1013883	4621	diphenylmethanimine	181.24	3_REACH	974.6794345		974.6794345	0	974.6794345	0.005377838			1	0.039	2.15184E-07			1	0.039	2.15184E-07	1000	1000	0	1000	0.00551755
101-39-3	101393	1320	alpha-	146.19	3_REACH	930		930	0	930	0.006361584			1	0.039	2.66776E-07			1	0.039	2.66776E-07	6100	6100	0	6100	0.04172652
101-41-7	101417	1321	methyl phenylacetate	150.18	3_REACH	5000		5000	0	5000	0.033293381			1	0.039	2.59688E-07			1	0.039	2.59688E-07	25704.33333	25704.33333	0	25704.3333	0.17115683
101-43-9	101439	1322	cyclohexyl methacrylate	168.24	3_REACH	196666.6667		196666.6667	0	196666.6667	1.168964971	9400	9400	0	9400	0.055872563			1	0.039	2.31812E-07	2200	2200	0	2200	0.01307656
101-54-2	101542	1323	N-(4-aminophenyl)aniline	184.24	3_REACH	680		680	0	680	0.003690838			1	0.039	2.1168E-07			1	0.039	2.1168E-07	1410	1410	0	1410	0.00765306
101-68-8	101688	1325	4,4'-methylenediphenyl	250.26	3_REACH	500000		500000	0	500000	1.997922161			1	0.039	1.55838E-07			1	0.039	1.55838E-07	1640000	1640000	0	1640000	6.55318469
1017183-70-8	1017183708	4503	3-(4-fluorophenyl)-2-	200.64	3_REACH	45500		45500	0	45500	0.226774322			1	0.039	1.94378E-07			1	0.039	1.94378E-07	8000	8000	0	8000	0.03987241
101-72-4	101724	1326	N-isopropyl-N'-phenyl-p-	226.32	3_REACH	113.3333333		113.3333333	0	113.3333333	0.000500766	3.7	3.7	0	3.7	1.63485E-05			1	0.039	1.72322E-07	230	230	0	230	0.00101626
101-77-9	101779	1328	4,4'-methylenedianiline	198.27	3_REACH	18000		18000	0	18000	0.090785293			1	0.039	1.96701E-07			1	0.039	1.96701E-07	930	930	0	930	0.00469057
101-80-4	101804	1329	4,4'-oxydianiline	200.24	3_REACH	5000		5000	0	5000	0.024970036			1	0.039	1.94766E-07			1	0.039	1.94766E-07	2600	2600	0	2600	0.01298442
101-84-8	101848	150	diphenyl ether	170.21	3_REACH	800		800	0	800	0.004700076			1	0.039	2.29129E-07			1	0.039	2.29129E-07	320	320	0	320	0.00188003
101-96-2	101962	1331	N,N'-di-sec-butyl-p-	220.36	3_REACH	56		56	0	56	0.00025413	3.7	3.7	0	3.7	1.67907E-05			1	0.039	1.76983E-07	95.8	95.8	0	95.8	0.00043474
102-01-2	102012	1334	acetoacetanilide	177.2	3_REACH	242000		242000	0	242000	1.365688488			1	0.039	2.2009E-07			1	0.039	2.2009E-07	180000	180000	0	180000	1.01580135
102-06-7	102067	1335	1,3-diphenylguanidine	211.27	3_REACH	1000		1000	0	1000	0.00473328	1300	1300	0	1300	0.006153264			1	0.039	1.84598E-07	13	13	0	13	6.1533E-05
102-08-9	102089	151	1,3-diphenyl-2-thiourea	228.32	3_REACH	6300		6300	0	6300	0.027592852			1	0.039	1.70813E-07			1	0.039	1.70813E-07	2600	2600	0	2600	0.01138753
102-09-0	102090	1336	diphenyl carbonate	214.22	3_REACH	910		910	0	910	0.004247969			1	0.039	1.82056E-07			1	0.039	1.82056E-07	110	110	0	110	0.00051349
10233-13-3	10233133	1339	isopropyl laurate	242.4	3_REACH	62500		62500	0	62500	0.257838284			1	0.039	1.60891E-07			1	0.039	1.60891E-07	54	54	0	54	0.00022277
102-36-3	102363	1341	3,4-dichlorophenyl	188.01	3_REACH	35400		35400	0	35400	0.188287857			1	0.039	2.07436E-07			1	0.039	2.07436E-07	1000	1000	0	1000	0.00531887
10254-57-6	10254576	1344	4,4'-methylene	422.79	3_REACH	60		60	0	60	0.000141914			1	0.039	9.22444E-08			1	0.039	9.22444E-08	32.5	32.5	0	32.5	7.687E-05
102-60-3	102603	1347	1,1',1'',1'''-	292.42	3_REACH	2000000		2000000	0	2000000	6.839477464			1	0.039	1.3337E-07			1	0.039	1.3337E-07	4250	4250	0	4250	0.01453389
102-69-2	102692	154	tripropylamine	143.28	3_REACH	21500		21500	0	21500	0.150055835	1500	1500	0	1500	0.010469012			1	0.039	2.72194E-07	2940	2940	0	2940	0.02051926
102-71-6	102716	155	2,2',2''-nitrilotriethanol	149.19	3_REACH	1666666.667		1666666.667	0	1666666.667	11.17143687			1	0.039	2.61412E-07			1	0.039	2.61412E-07	1800	1800	0	1800	0.01206515
102-76-1	102761	1352	triacetin	218.21	3_REACH	100000		100000	0	100000	0.45827414	100000	100000	0	100000	0.45827414			1	0.039	1.78727E-07	468000	468000	0	468000	2.14472297
102-77-2	102772	1353	2-	252.36	3_REACH	103.3333333		103.3333333	0	103.3333333	0.000409468	41	41	0	41	0.000162466			1	0.039	1.54541E-07	66	66	0	66	0.00026153
102-81-8	102818	1354	2-dibutylaminoethanol	173.3	3_REACH	17000		17000	0	17000	0.098095788			1	0.039	2.25043E-07			1	0.039	2.25043E-07	1650	1650	0	1650	0.00952106
102-82-9	102829	156	tributylamine	185.36	3_REACH	5433.333333		5433.333333	0	5433.333333	0.029312329	1000	1000	0	1000	0.005394907			1	0.039	2.10401E-07	1177	1177	0	1177	0.00634981
102985-93-3	102985933	4723	2,2-dimethyl-3-oxopropyl	284.44	3_REACH	1000		1000	0	1000	0.00351568			1	0.039	1.37112E-07			1	0.039	1.37112E-07	180	180	0	180	0.00063282
103-09-3	103093	1359	2-ethylhexyl acetate	172.27	3_REACH	2510		2510	0	2510	0.014570152			1	0.039	2.26389E-07			1	0.039	2.26389E-07	10300	10300	0	10300	0.05978986
103-11-7	103117	159	2-ethylhexyl acrylate	184.28	3_REACH	381		381	0	381	0.002067506			1	0.039	2.11634E-07			1	0.039	2.11634E-07	55	55	0	55	0.00029846
103-23-1	103231	160	bis(2-ethylhexyl) adipate	370.57	3_REACH	260		260	0	260	0.000701622			1	0.039	1.05243E-07			1	0.039	1.05243E-07	260	260	0	260	0.00070162
103-26-4	103264	1362	methyl cinnamate	162.19	3_REACH	980		980	0	980	0.006042296			1	0.039	2.40459E-07			1	0.039	2.40459E-07	2100	2100	0	2100	0.01294778
10326-41-7	10326417	161	(R)-lactic acid	90.078	3_REACH	43333.33333		43333.33333	0	43333.33333	0.481064559	2180	2180	0	2180	0.024201248			1	0.039	4.32958E-07	1900000	1900000	0	1900000	21.0928307
103-45-7	103457	1367	phenethyl acetate	164.2	3_REACH	3500		3500	0	3500	0.021315469			1	0.039	2.37515E-07			1	0.039	2.37515E-07	4400	4400	0	4400	0.02679659
103-49-1	103491	1368	dibenzylamine	197.28	3_REACH	10800		10800	0	10800	0.054744526			1	0.039	1.97689E-07			1	0.039	1.97689E-07	100	100	0	100	0.00050689
103-50-4	103504	1369	dibenzyl ether	198.26	3_REACH	2266.666667		2266.666667	0	2266.666667	0.011432799	480	480	0	480	0.002421063			1	0.039	1.96711E-07	320	320	0	320	0.00161404
103-60-6	103606	1374	2-phenoxyethyl isobutyrate	208.26	3_REACH	11000		11000	0	11000	0.052818592			1	0.039	1.87266E-07			1	0.039	1.87266E-07	1600	1600	0	1600	0.0076827
103694-68-4	103694684	4367	Trimethylbenzenepropanol	178.28	3_REACH	8500		8500	0	8500	0.04767781			1	0.039	2.18757E-07			1	0.039	2.18757E-07	7200	7200	0	7200	0.04038591
103-69-5	103695	162	N-ethylaniline	121.18	3_REACH	3333.333333		3333.333333	0	3333.333333	0.027507289	43500	43500	0	43500	0.358970127			1	0.039	3.21835E-07	17000	17000	0	17000	0.14028718
103-71-9	103719	1378	phenyl isocyanate	119.12	3_REACH	50000		50000	0	50000	0.419744795	390	390	0	390	0.003274009			1	0.039	3.27401E-07	73000	73000	0	73000	0.6128274
103-74-2	103742	163	2-(2-pyridyl)ethanol	123.16	3_REACH	965077		965077	0	965077	7.835961351			1	0.039	3.16661E-07			1	0.039	3.16661E-07	189196.3333	189196.3333	0	189196.333	1.53618328
103-83-3	103833	164	benzyldimethylamine	135.21	3_REACH	10000		10000	0	10000	0.073959027			1	0.039	2.8844E-07			1	0.039	2.8844E-07	240	240	0	240	0.00177502
103-95-7	103957	1382	3-p-cumenyl-2-	190.29	3_REACH	364		364	0	364	0.00191287			1	0.039	2.0495E-07			1	0.039	2.0495E-07	200	200	0	200	0.00105103
10411-92-4	10411924	1383	cis-4-tert-butylcyclohexyl	198.31	3_REACH	2866.666667		2866.666667	0	2866.666667	0.014455482			1	0.039	1.96662E-07			1	0.039	1.96662E-07	6800	6800	0	6800	0.03428975
10420-33-4	10420334	1387	dimethyl acetylsuccinate	188.18	3_REACH	47838.66667		47838.66667	0	47838.66667	0.254217593			1	0.039	2.07248E-07			1	0.039	2.07248E-07	4030	4030	0	4030	0.02141567
104-23-4	104234	1388	4'-aminoazobenzene-4-	277.31	3_REACH	19977.76667		19977.76667	0	19977.76667	0.072041278			1	0.039	1.40637E-07			1	0.039	1.40637E-07	4373.666667	4373.666667	0	4373.66667	0.01577176
104-38-1	104381	1393	2,2'-p-	198.22	3_REACH	1044000		1044000	0	1044000	5.266875189			1	0.039	1.96751E-07			1	0.039	1.96751E-07	250000	250000	0	250000	1.2612249
104468-21-5	104468215	4316	2,2-dimethyl 3-methyl-3-	170.25	3_REACH	300000		300000	0	300000	1.762114537			1	0.039	2.29075E-07			1	0.039	2.29075E-07	10000	10000	0	10000	0.05873715
104-55-2	104552	168	cinnamaldehyde	132.16	3_REACH	700		700	0	700	0.00529661			1	0.039	2.95097E-07			1	0.039	2.95097E-07	37231.37	37231.37	0	37231.37	0.28171436
104-61-0	104610	1395	nonan-4-olide	156.22	3_REACH	1833.333333		1833.333333	0	1833.333333	0.011735587			1	0.039	2.49648E-07			1	0.039	2.49648E-07	779	779	0	779	0.00498656
104-66-5	104665	1397	1,2-diphenoxyethane	214.26	3_REACH	360		360	0	360	0.001680202			1	0.039	1.82022E-07			1	0.039	1.82022E-07	106	106	0	106	0.00049473
104-67-6	104676	1398	undecan-4-olide	184.28	3_REACH	1833.333333		1833.333333	0	1833.333333	0.009948629			1	0.039	2.11634E-07			1	0.039	2.11634E-07	779	779	0	779	0.00422726
104-68-7	104687	1399	2-(2-	182.22	3_REACH	305000		305000	0	305000	1.6738009			1	0.039	2.14027E-07			1	0.039	2.14027E-07	84666.66667	84666.66667	0	84666.6667	0.46463981
1047-16-1	1047161	1400	5,12-dihydroquino[2,3-	312.33	3_REACH	100000		100000	0	100000	0.320174175	10000	10000	0	10000	0.032017417			1	0.039	1.24868E-07	1000	1000	0	1000	0.00320174
104-75-6	104756	169	2-ethylhexylamine	129.25	3_REACH	8000		8000	0	8000	0.061895551			1	0.039	3.01741E-07			1	0.039	3.01741E-07	30	30	0	30	0.00023211
104-76-7	104767	170	2-ethylhexan-1-ol	144.26	3_REACH	14000		14000	0	14000	0.097046998			1	0.039	2.70345E-07			1	0.039	2.70345E-07	1300	1300	0	1300	0.00901151
104-88-1	104881	171	4-chlorobenzaldehyde	140.57	3_REACH	733.3333333		733.3333333	0	733.3333333	0.005216855			1	0.039	2.77442E-07			1	0.039	2.77442E-07	2823.333333	2823.333333	0	2823.33333	0.02008489
104-90-5	104905	172	5-ethyl-2-methylpyridine	121.18	3_REACH	9500		9500	0	9500	0.078395775			1	0.039	3.21835E-07			1	0.039	3.21835E-07	689	689	0	689	0.00568576
104-93-8	104938	1403	4-methylanisole	122.17	3_REACH	21500		21500	0	21500	0.175984284			1	0.039	3.19227E-07			1	0.039	3.19227E-07	279030	279030	0	279030	2.2839486
105-05-5	105055	1405	1,4-diethylbenzene	134.22	3_REACH	600		600	0	600	0.004470273			1	0.039	2.90568E-07			1	0.039	2.90568E-07	600	600	0	600	0.00447027
10543-57-4	10543574	175	N,N'-ethylenebis[N-	228.25	3_REACH	140000		140000	0	140000	0.613362541			1	0.039	1.70865E-07			1	0.039	1.70865E-07	655000	655000	0	655000	2.86966046
105-53-3	105533	177	diethyl malonate	160.17	3_REACH	3600		3600	0	3600	0.022476119			1	0.039	2.43491E-07			1	0.039	2.43491E-07	30100	30100	0	30100	0.18792533
105-55-5	105555	178	1,3-diethyl-2-thiourea	132.23	3_REACH	100000		100000	0	100000	0.756258035	1000	1000	0	1000	0.00756258			1	0.039	2.94941E-07	73000	73000	0	73000	0.55206837
105-56-6	105566	1415	ethyl cyanoacetate	113.12	3_REACH	19666.66667		19666.66667	0	19666.66667	0.173856671			1	0.039	3.44767E-07			1	0.039	3.44767E-07	17000	17000	0	17000	0.15028289
105-59-9	105599	1416	2,2'-methyliminodiethanol	119.17	3_REACH	464000		464000	0	464000	3.893597382			1	0.039	3.27264E-07			1	0.039	3.27264E-07	6250	6250	0	6250	0.05244609
105-60-2	105602	180	Caprolactam	113.16	3_REACH	100000		100000	0	100000	0.883704489			1	0.039	3.44645E-07			1	0.039	3.44645E-07	1000000	1000000	0	1000000	8.83704489
10563-26-5	10563265	1417	N,N'-bis(3-	174.3	3_REACH	100000		100000	0	100000	0.573723465			1	0.039	2.23752E-07			1	0.039	2.23752E-07	50000	50000	0	50000	0.28686173
10563-29-8	10563298	1418	N'-(3-aminopropyl)-N,N-	159.28	3_REACH	100000		100000	0	100000	0.627825213			1	0.039	2.44852E-07			1	0.039	2.44852E-07	1900	1900	0	1900	0.01192868
105-67-9	105679	181	2,4-xylenol	122.17	3_REACH	1233.333333		1233.333333	0	1233.333333	0.010095223	2475.217162	2475.217162	0	2475.217162	0.020260434			1	0.039	3.19227E-07			1	1	8.1853E-06
105-75-9	105759	182	dibutyl fumarate	228.29	3_REACH	32		32	0	32	0.000140173			1	0.039	1.70835E-07			1	0.039	1.70835E-07	200	200	0	200	0.00087608
105-76-0	105760	183	dibutyl maleate	228.29	3_REACH	140	179.333333	179.3333333	0	179.3333333	0.000785551			1	0.039	1.70835E-07			1	0.039	1.70835E-07	4200	4200	0	4200	0.01839765
105812-81-5	105812815	4223	(-)-trans-4-(4'-fluorophenyl)-	223.29	3_REACH	10000		10000	0	10000	0.044784809			1	0.039	1.74661E-07			1	0.039	1.74661E-07	2500	2500	0	2500	0.0111962
105827-91-6	105827916	4348	2-chloro-5-	168.05	3_REACH	1200		1200	0	1200	0.007140732			1	0.039	2.32074E-07			1	0.039	2.32074E-07	130	130	0	130	0.00077358
105-83-9	105839	1420	N,N-bis(3-	145.25	3_REACH	48876.261		48876.261	0	48876.261	0.336497494			1	0.039	2.68503E-07			1	0.039	2.68503E-07	3200	3200	0	3200	0.02203098
105-95-3	105953	1422	1,4-dioxacycloheptadecane	270.37	3_REACH	410		410	0	410	0.00151644			1	0.039	1.44247E-07			1	0.039	1.44247E-07	262.6666667	262.6666667	0	262.666667	0.00097151
105-99-7	105997	184	dibutyl adipate	258.36	3_REACH	1213.333333		1213.333333	0	1213.333333	0.004696289			1	0.039	1.50952E-07			1	0.039	1.50952E-07	2000	2000	0	2000	0.00774114
106-02-5	106025	1425	pentadecan-15-olide	240.39	3_REACH	110		110	0	110	0.00045759	27	27	0	27	0.000112317			1	0.039	1.62236E-07	260	260	0	260	0.00108158
106-20-7	106207	1430	bis(2-ethylhexyl)amine	241.46	3_REACH	460		460	0	460	0.001905077			1	0.039	1.61517E-07			1	0.039	1.61517E-07	34	34	0	34	0.00014081
106-21-8	106218	1431	3,7-dimethyloctan-1-ol	158.29	3_REACH	10000		10000	0	10000	0.063175185			1	0.039	2.46383E-07			1	0.039	2.46383E-07	9500	9500	0	9500	0.06001643
106-22-9	106229	185	citronellol	156.27	3_REACH	4600		4600	0	4600	0.029436232			1	0.039	2.49568E-07			1	0.039	2.49568E-07	1100	1100	0	1100	0.0070391
106-23-0	106230	1432	citronellal	154.25	3_REACH	10000		10000	0	10000	0.064829822			1	0.039	2.52836E-07			1	0.039	2.52836E-07	1260	1260	0	1260	0.00816856
106-24-1	106241	186	geraniol	154.25	3_REACH	10000		10000	0	10000	0.064829822			1	0.039	2.52836E-07			1	0.039	2.52836E-07	1000	1000	0	1000	0.00648298
106-25-2	106252	187	nerol	154.25	3_REACH	10000		10000	0	10000	0.064829822			1	0.039	2.52836E-07			1	0.039	2.52836E-07	1000	1000	0	1000	0.00648298
106-26-3	106263	1433	(Z)-3,7-dimethylocta-2,6-	152.24	3_REACH	4600		4600	0	4600	0.030215449			1	0.039	2.56174E-07			1	0.039	2.56174E-07	3000	3000	0	3000	0.01970573
106-43-4	106434	190	4-chlorotoluene	126.59	3_REACH	1733.333333		1733.333333	0	1733.333333	0.013692498	1900	1900	0	1900	0.015009084	3400	3400	0	3400	0.026858362	430	430	0	430	0.00339679
106-44-5	106445	191	p-cresol	108.14	3_REACH	300		300	0	300	0.002774182	1350	1350	0	1350	0.012483817			1	0.039	3.60644E-07	2300	2300	0	2300	0.02126873
106461-41-0	106461410	4581	2,4-dihydro-4-(4-(4-(4-	393.5	3_REACH	230		230	0	230	0.000584498			1	0.039	9.91105E-08			1	0.039	9.91105E-08	360	360	0	360	0.00091487
106-46-7	106467	192	1,4-dichlorobenzene	147	3_REACH	440		440	0	440	0.002993197	100	100	0	100	0.000680272	2100	2100	0	2100	0.014285714	570	570	0	570	0.00387755
106-47-8	106478	193	4-chloroaniline	127.58	3_REACH	800	800	800	0	800	0.006270575	200	200	0	200	0.001567644			1	0.039	3.05691E-07	3	3	0	3	2.3515E-05
106-48-9	106489	194	4-chlorophenol	128.56	3_REACH	386.6666667	633.333333	633.3333333	0	633.3333333	0.004926364			1	0.039	3.0336E-07			1	0.039	3.0336E-07	390	390	0	390	0.0030336
106-49-0	106490	195	p-toluidine	107.16	3_REACH	14000		14000	0	14000	0.130645763	13000	13000	0	13000	0.121313923			1	0.039	3.63942E-07	67	67	0	67	0.00062523
106-50-3	106503	196	p-phenylenediamine	108.15	3_REACH	9.333333333		9.333333333	0	9.333333333	8.62999E-05			1	0.039	3.6061E-07			1	0.039	3.6061E-07	8	8	0	8	7.3971E-05
106-51-4	106514	197	p-benzoquinone	108.1	3_REACH	15		15	0	15	0.00013876			1	0.039	3.60777E-07			1	0.039	3.60777E-07			1	1	9.2507E-06
1067-33-0	1067330	199	dibutyltin di(acetate)	351.01	3_REACH	279.6666667		279.6666667	0	279.6666667	0.000796748			1	0.039	1.11108E-07			1	0.039	1.11108E-07	11.66666667	11.66666667	0	11.6666667	3.3237E-05
106-79-6	106796	1446	dimethyl sebacate	230.3	3_REACH	5800		5800	0	5800	0.025184542			1	0.039	1.69344E-07			1	0.039	1.69344E-07	490	490	0	490	0.00212766
106797-53-9	106797539	4354	2-hydroxy-4'-hydroxyethoxy	224.26	3_REACH	46000		46000	0	46000	0.205119058			1	0.039	1.73905E-07			1	0.039	1.73905E-07	1000	1000	0	1000	0.00445911
106-91-2	106912	1449	2,3-epoxypropyl	142.15	3_REACH	933.3333333		933.3333333	0	933.3333333	0.006565834	1200	1200	0	1200	0.008441787			1	0.039	2.74358E-07	2400	2400	0	2400	0.01688357
1071-22-3	1071223	1455	3-	188.52	3_REACH	110000		110000	0	110000	0.583492468			1	0.039	2.06875E-07			1	0.039	2.06875E-07	1800	1800	0	1800	0.00954806
1072-63-5	1072635	1457	1-vinylimidazole	94.119	3_REACH	460000		460000	0	460000	4.887429743			1	0.039	4.14369E-07			1	0.039	4.14369E-07	138500	138500	0	138500	1.47154135
1073-69-4	1073694	1461	(4-chlorophenyl)hydrazine	142.59	3_REACH	100		100	0	100	0.000701311			1	0.039	2.73511E-07			1	0.039	2.73511E-07	1023.333333	1023.333333	0	1023.33333	0.00717675
107-41-5	107415	219	2-methylpentane-2,4-diol	118.18	3_REACH	2666666.667	2666666.67	2666666.667	0	2666666.667	22.56444971			1	0.039	3.30005E-07			1	0.039	3.30005E-07	429000	429000	0	429000	3.63005585
107-56-2	107562	1465	O,O-diisopropyl hydrogen	214.29	3_REACH	33132.72971		33132.72971	0	33132.72971	0.154616313			1	0.039	1.81996E-07			1	0.039	1.81996E-07	2000	2000	0	2000	0.00933315
107-58-4	107584	1466	N-tert-butylacrylamide	127.19	3_REACH	62993.1		62993.1	0	62993.1	0.49526771			1	0.039	3.06628E-07			1	0.039	3.06628E-07	11410.11	11410.11	0	11410.11	0.08970918
107-66-4	107664	1467	dibutyl hydrogen	210.21	3_REACH	100000		100000	0	100000	0.475714761			1	0.039	1.85529E-07			1	0.039	1.85529E-07	50000	50000	0	50000	0.23785738

107737-97-3	107737973	4619	2,2-Dimethyl-3-(3-	176.26	3_REACH	4500		4500	0	4500	0.025530466				1	0.039	2.21264E-07				1	0.039	2.21264E-07	3500		3500	0	3500	0.01985703
107-75-5	107755	1468	7-hydroxycitronellal	172.27	3_REACH	10533.33333		10533.33333	0	10533.33333	0.061144328				1	0.039	2.26389E-07				1	0.039	2.26389E-07	42360		42360	0	42360	0.24589307
107-88-0	107880	1470	butane-1,3-diol	90.122	3_REACH	1000000		1000000	0	1000000	11.09606977	846000		846000	0	846000	9.387275027				1	0.039	4.32747E-07	1070000		1070000	0	1070000	11.8727947
107898-54-4	107898544	4225	Supersantol	222.37	3_REACH	270		270	0	270	0.001214193				1	0.039	1.75383E-07				1	0.039	1.75383E-07	450		450	0	450	0.00202365
107-92-6	107926	224	butyric acid	88.106	3_REACH	25666.66667		25666.66667	0	25666.66667	0.291315764				1	0.039	4.42649E-07				1	0.039	4.42649E-07	29400		29400	0	29400	0.33368897
107-93-7	107937	225	trans-crotonic acid	86.09	3_REACH	22000		22000	0	22000	0.255546521				1	0.039	4.53014E-07				1	0.039	4.53014E-07				1	1	1.1616E-05
107-96-0	107960	1473	3-mercaptopropionic acid	106.14	3_REACH	15000		15000	0	15000	0.141322781				1	0.039	3.67439E-07				1	0.039	3.67439E-07	4100		4100	0	4100	0.03862823
108-39-4	108394	237	m-cresol	108.14	3_REACH	2000	2533.33333	2533.333333	0	2533.333333	0.023426423	1350		1350	0	1350	0.012483817				1	0.039	3.60644E-07	13000		13000	0	13000	0.12021454
108-42-9	108429	238	3-chloroaniline	127.58	3_REACH	49		49	0	49	0.000384073	5600		5600	0	5600	0.043894027	5600		5600	0	5600	0.043894027	7000		7000	0	7000	0.05486753
108-44-1	108441	239	m-toluidine	107.16	3_REACH	11333.33333		11333.33333	0	11333.33333	0.105760856	12100		12100	0	12100	0.112915267				1	0.039	3.63942E-07	6100		6100	0	6100	0.05692423
108-45-2	108452	1484	m-phenylenediamine	108.15	3_REACH	170666.6667		170666.6667	0	170666.6667	1.57805517				1	0.039	3.6061E-07				1	0.039	3.6061E-07	915		915	0	915	0.00846047
108-46-3	108463	240	resorcinol	110.11	3_REACH	25000		25000	0	25000	0.227045682	32000		32000	0	32000	0.290618472				1	0.039	3.54191E-07	47000		47000	0	47000	0.42684588
108-67-8	108678	242	mesitylene	120.19	3_REACH	1738.666667		1738.666667	0	1738.666667	0.014465984				1	0.039	3.24486E-07				1	0.039	3.24486E-07	1063.666667		1063.666667	0	1063.66667	0.00884988
108-68-9	108689	243	3,5-xylenol	122.17	3_REACH	7333.333333		7333.333333	0	7333.333333	0.060025647				1	0.039	3.19227E-07				1	0.039	3.19227E-07	1700		1700	0	1700	0.01391504
108-69-0	108690	244	3,5-xylidine	121.18	3_REACH	5666.666667		5666.666667	0	5666.666667	0.046762392	810		810	0	810	0.006684271				1	0.039	3.21835E-07	5800		5800	0	5800	0.04786268
108-78-1	108781	4	melamine	126.13	3_REACH	3000000		3000000	0	3000000	23.78498375	125000		125000	0	125000	0.991040989				1	0.039	3.09205E-07	98000		98000	0	98000	0.77697614
108-80-5	108805	245	cyanuric acid	129.08	3_REACH	420		420	0	420	0.003253796	1000000		1000000	0	1000000	7.747133561				1	0.039	3.02138E-07	100000		100000	0	100000	0.77471336
108-83-8	108838	1490	2,6-dimethylheptan-4-one	142.24	3_REACH	23100		23100	0	23100	0.162401575				1	0.039	2.74184E-07				1	0.039	2.74184E-07	3550		3550	0	3550	0.02495782
108-93-0	108930	250	cyclohexanol	100.16	3_REACH	13333.33333		13333.33333	0	13333.33333	0.133120341				1	0.039	3.89377E-07				1	0.039	3.89377E-07	30		30	0	30	0.00029952
108-95-2	108952	252	phenol	94.113	3_REACH	12.347232	826.666667	826.6666667	0	826.6666667	0.008783767	1.7	77	77	0	77	0.000818165				1	0.039	4.14395E-07	495		495	0	495	0.00525963
108-98-5	108985	1491	benzenethiol	110.18	3_REACH	3		3	0	3	2.72282E-05				1	0.039	3.53966E-07				1	0.039	3.53966E-07	30		30	0	30	0.00027228
109-13-7	109137	1494	tert-butyl peroxyisobutyrate	160.21	3_REACH	2900		2900	0	2900	0.018101242				1	0.039	2.4343E-07				1	0.039	2.4343E-07	280		280	0	280	0.00174771
109-16-0	109160	1495	2,2'-ethylenedioxydiethyl	286.32	3_REACH	5466.666667		5466.666667	0	5466.666667	0.019092856				1	0.039	1.36211E-07				1	0.039	1.36211E-07	18600		18600	0	18600	0.06496228
109-52-4	109524	256	valeric acid	102.13	3_REACH	13000		13000	0	13000	0.12728875				1	0.039	3.81866E-07				1	0.039	3.81866E-07	3566.666667		3566.666667	0	3566.66667	0.03492281
109-77-3	109773	266	malononitrile	66.065	3_REACH	186.6666667		186.6666667	0	186.6666667	0.0028255				1	0.039	5.90328E-07				1	0.039	5.90328E-07				1	1	1.5137E-05
110-15-6	110156	274	succinic acid	118.09	3_REACH	100000		100000	0	100000	0.846811754				1	0.039	3.30257E-07				1	0.039	3.30257E-07	25000		25000	0	25000	0.21170294
110-16-7	110167	275	maleic acid	116.07	3_REACH	1666.666667		1666.666667	0	1666.666667	0.014359151				1	0.039	3.36004E-07				1	0.039	3.36004E-07	4150		4150	0	4150	0.03575429
110-25-8	110258	1515	(Z)-N-methyl-N-(1-oxo-9-	353.55	3_REACH	6810		6810	0	6810	0.019261773				1	0.039	1.1031E-07				1	0.039	1.1031E-07	910		910	0	910	0.00257389
110-41-8	110418	1519	2-methylundecanal	184.32	3_REACH	110		110	0	110	0.000596788				1	0.039	2.11589E-07				1	0.039	2.11589E-07	57		57	0	57	0.00030924
110-42-9	110429	1520	methyl decanoate	186.29	3_REACH	30000		30000	0	30000	0.16103924				1	0.039	2.09351E-07				1	0.039	2.09351E-07	42		42	0	42	0.00022545
110-44-1	110441	1521	hexa-2,4-dienoic acid	112.13	3_REACH	56000		56000	0	56000	0.499420316				1	0.039	3.47811E-07				1	0.039	3.47811E-07	6470		6470	0	6470	0.05770088
110-63-4	110634	1526	butane-1,4-diol	90.122	3_REACH	5000		5000	0	5000	0.055480349				1	0.039	4.32747E-07				1	0.039	4.32747E-07	76000		76000	0	76000	0.8433013
110-64-5	110645	1527	but-2-ene-1,4-diol	88.106	3_REACH	142333.3333		142333.3333	0	142333.3333	1.615478325				1	0.039	4.42649E-07				1	0.039	4.42649E-07	48000		48000	0	48000	0.54479831
110-65-6	110656	281	but-2-yne-1,4-diol	86.09	3_REACH	21500		21500	0	21500	0.249738646				1	0.039	4.53014E-07				1	0.039	4.53014E-07	125000		125000	0	125000	1.45196887
110-77-0	110770	283	2-(ethylthio)ethanol	106.19	3_REACH				1	0.39	3.67266E-06				1	0.039	3.67266E-07				1	0.039	3.67266E-07	100000		100000	0	100000	0.94170826
110-93-0	110930	291	6-methylhept-5-en-2-one	126.2	3_REACH	16666.66667		16666.66667	0	16666.66667	0.132065504				1	0.039	3.09033E-07				1	0.039	3.09033E-07	10000		10000	0	10000	0.0792393
110964-79-9	110964799	1534	4-(methylsulfonyl)-2-	245.21	3_REACH	120000		120000	0	120000	0.489376453	100000		100000	0	100000	0.407813711				1	0.039	1.59047E-07	100000		100000	0	100000	0.40781371
110-97-4	110974	292	1,1'-iminodipropan-2-ol	133.19	3_REACH	460000		460000	0	460000	3.453712741				1	0.039	2.92815E-07				1	0.039	2.92815E-07	24666.66667		24666.66667	0	24666.6667	0.18519909
111-11-5	111115	1538	methyl octanoate	158.24	3_REACH	30000		30000	0	30000	0.18958544				1	0.039	2.46461E-07				1	0.039	2.46461E-07	1586.666667		1586.666667	0	1586.66667	0.01002696
111-14-8	111148	293	heptanoic acid	130.19	3_REACH				1	0.39	2.99562E-06				1	0.039	2.99562E-07				1	0.039	2.99562E-07	40900		40900	0	40900	0.31415623
111-18-2	111182	1540	N,N,N',N'-	172.32	3_REACH	21500		21500	0	21500	0.124767874				1	0.039	2.26323E-07				1	0.039	2.26323E-07	8820		8820	0	8820	0.05118384
111-21-7	111217	1542	2,2'-[ethane-1,2-	234.25	3_REACH	61666.66667		61666.66667	0	61666.66667	0.263251512				1	0.039	1.66489E-07				1	0.039	1.66489E-07	28000		28000	0	28000	0.11953042
111-27-3	111273	294	hexan-1-ol	102.18	3_REACH	30000		30000	0	30000	0.29359953	11601		11601	0	11601	0.113534938				1	0.039	3.81679E-07	4720		4720	0	4720	0.04619299
111-30-8	111308	296	glutaral	100.12	3_REACH	1700		1700	0	1700	0.016979624	1600		1600	0	1600	0.015980823				1	0.039	3.89533E-07	42		42	0	42	0.0004195
111-40-0	111400	299	2,2'-iminodi(ethylamine)	103.17	3_REACH	100000		100000	0	100000	0.969274014				1	0.039	3.78017E-07				1	0.039	3.78017E-07	10000		10000	0	10000	0.0969274
111-41-1	111411	1547	2-(2-	104.16	3_REACH	490000		490000	0	490000	4.704301075				1	0.039	3.74424E-07				1	0.039	3.74424E-07	100000		100000	0	100000	0.96006144
111-42-2	111422	300	2,2'-iminodiethanol	105.14	3_REACH	33333.33333		33333.33333	0	33333.33333	0.317037601				1	0.039	3.70934E-07				1	0.039	3.70934E-07	733.3333333		733.3333333	0	733.333333	0.00697483
111-44-4	111444	301	bis(2-chloroethyl) ether	143.01	3_REACH	200000		200000	0	200000	1.398503601				1	0.039	2.72708E-07				1	0.039	2.72708E-07				1	1	6.9925E-06
111-46-6	111466	302	2,2'-oxydiethanol	106.12	3_REACH	1666666.667		1666666.667	0	1666666.667	15.70549064	7694000		7694000	0	7694000	72.50282699				1	0.039	3.67508E-07	2700000		2700000	0	2700000	25.4428948
111-64-8	111648	1551	octanoyl chloride	162.66	3_REACH	1640		1640	0	1640	0.01008238				1	0.039	2.39764E-07				1	0.039	2.39764E-07	97		97	0	97	0.00059634
111-69-3	111693	307	adiponitrile	108.15	3_REACH	128000		128000	0	128000	1.183541378				1	0.039	3.6061E-07				1	0.039	3.6061E-07				1	1	9.2464E-06
111-70-6	111706	308	heptan-1-ol	116.2	3_REACH	1512.17283		1512.17283	0	1512.17283	0.013013536				1	0.039	3.35628E-07				1	0.039	3.35628E-07	1100		1100	0	1100	0.00946644
1117-31-3	1117313	1555	1,3-butylene diacetate	174.2	3_REACH	18000		18000	0	18000	0.103329506				1	0.039	2.23881E-07				1	0.039	2.23881E-07	60000		60000	0	60000	0.34443169
111-75-1	111751	1556	2-butylaminoethanol	117.19	3_REACH	46400		46400	0	46400	0.39593822	231610		231610	0	231610	1.976363171				1	0.039	3.32793E-07	320		320	0	320	0.00273061
111-76-2	111762	309	2-butoxyethanol	118.18	3_REACH	730000		730000	0	730000	6.177018108				1	0.039	3.30005E-07				1	0.039	3.30005E-07	35000		35000	0	35000	0.2961584
111-77-3	111773	310	2-(2-	120.15	3_REACH	960000		960000	0	960000	7.990012484				1	0.039	3.24594E-07				1	0.039	3.24594E-07	1000000		1000000	0	1000000	8.32292967
1117-86-8	1117868	1557	octane-1,2-diol	146.23	3_REACH	2200		2200	0	2200	0.015044792				1	0.039	2.66703E-07				1	0.039	2.66703E-07	15000		15000	0	15000	0.10257813
111-81-9	111819	1558	methyl undec-10-enoate	198.31	3_REACH	220		220	0	220	0.001109374				1	0.039	1.96662E-07				1	0.039	1.96662E-07	280		280	0	280	0.00141193
111-82-0	111820	1559	methyl laurate	214.35	3_REACH	980000		980000	0	980000	4.571961745				1	0.039	1.81945E-07				1	0.039	1.81945E-07	39.6		39.6	0	39.6	0.00018474
111-85-3	111853	1561	1-chlorooctane	148.68	3_REACH	8000		8000	0	8000	0.053806833				1	0.039	2.62308E-07				1	0.039	2.62308E-07	320		320	0	320	0.00215227
111-86-4	111864	313	octylamine	129.25	3_REACH	1000		1000	0	1000	0.007736944				1	0.039	3.01741E-07				1	0.039	3.01741E-07	10		10	0	10	7.7369E-05
111-87-5	111875	314	octan-1-ol	130.23	3_REACH	1500		1500	0	1500	0.011518083	750		750	0	750	0.005759042				1	0.039	2.9947E-07	1900		1900	0	1900	0.01458957
111-88-6	111886	1563	octane-1-thiol	146.3	3_REACH	114		114	0	114	0.000779221				1	0.039	2.66576E-07				1	0.039	2.66576E-07	3.763		3.763	0	3.763	2.5721E-05
111-90-0	111900	315	2-(2-ethoxyethoxy)ethanol	134.18	3_REACH	100000		100000	0	100000	0.745267551				1	0.039	2.90654E-07				1	0.039	2.90654E-07	100000		100000	0	100000	0.74526755
111-91-1	111911	316	bis(2-	173.04	3_REACH	16733.33333		16733.33333	0	16733.33333	0.096702111	2400		2400	0	2400	0.013869626				1	0.039	2.25381E-07	10000		10000	0	10000	0.05779011
111-92-2	111922	317	dibutylamine	129.25	3_REACH	1833.333333		1833.333333	0	1833.333333	0.014184397				1	0.039	3.01741E-07				1	0.039	3.01741E-07	70		70	0	70	0.00054159
1120-21-4	1120214	1567	undecane	156.31	3_REACH	1000		1000	0	1000	0.006397543	116		116	0	116	0.000742115				1	0.039	2.49504E-07	3000	3000	3000	0	3000	0.01919263
1120-24-7	1120247	1568	decyldimethylamine	185.36	3_REACH	10	100	100	0	100	0.000539491				1	0.039	2.10401E-07				1	0.039	2.10401E-07	0.5	1	1	0	1	5.3949E-06
112-02-7	112027	7	cetrimonium chloride	320.01	3_REACH	33.33333333		33.33333333	0	33.33333333	0.000104163	32.2		32.2	0	32.2	0.000100622				1	0.039	1.21871E-07	40		40	0	40	0.000125
1120-36-1	1120361	1569	tetradec-1-ene	196.38	3_REACH	3.4	3.4	3.4	0	3.4	1.73134E-05				1	0.039	1.98595E-07				1	0.039	1.98595E-07	0.93	0.93	0.93	0	0.93	4.7357E-06
112-05-0	112050	320	nonanoic acid	158.24	3_REACH	2333.333333		2333.333333	0	2333.333333	0.014745534				1	0.039	2.46461E-07				1	0.039	2.46461E-07	29000		29000	0	29000	0.18326593
1120-71-4	1120714	1572	1,3-propanesultone	122.14	3_REACH	32000		32000	0	32000	0.261994433	51870		51870	0	51870	0.424676601				1	0.039	3.19306E-07	60200		60200	0	60200	0.49287703
112-07-2	112072	1573	2-butoxyethyl acetate	160.21	3_REACH	13000		13000	0	13000	0.081143499				1	0.039	2.4343E-07				1	0.039	2.4343E-07	300000		300000	0	300000	1.87254229
112-15-2	112152	1577	2-(2-ethoxyethoxy)ethyl	176.21	3_REACH	36666.66667		36666.66667	0	36666.66667	0.20808505				1	0.039	2.21327E-07				1	0.039	2.21327E-07	22000		22000	0	22000	0.12485103
112-16-3	112163	1578	lauroyl chloride	218.77	3_REACH	1640		1640	0	1640	0.007496457	2000		2000	0	2000	0.009142021				1	0.039	1.78269E-07	97		97	0	97	0.00044339
112-18-5	112185	321	dodecyldimethylamine	213.41	3_REACH	100		100	0	100	0.000468582				1	0.039	1.82747E-07				1	0.039	1.82747E-07	2.6		2.6	0	2.6	1.2183E-05
112-25-4	112254	1580	2-hexyloxyethanol	146.23	3_REACH	40000		40000	0	40000	0.273541681				1	0.039	2.66703E-07				1	0.039	2.66703E-07	11080		11080	0	11080	0.07577105
112-27-6	112276	322	2,2'-	150.17	3_REACH	40496.91346	1666666.67	1666666.667	0	1666666.667	11.09853277	31749.01573		31749.01573	0	31749.01573	0.211420495				1	0.039	2.59706E-07				1	1	6.6591E-06
112-29-8	112298	324	1-bromodecane	221.19	3_REACH	6233.333333		6233.333333	0	6233.333333	0.0281809				1	0.039	1.76319E-07				1	0.039	1.76319E-07				1	1	4.521E-06
112-30-1	112301	325	decan-1-ol	158.29	3_REACH	632.455532		632.455532	0	632.455532	0.00399555				1	0.039	2.46383E-07				1	0.039	2.46383E-07	1054.092553		1054.092553	0	1054.09255	0.00665925
112-31-2	112312	1581	decanal	156.27	3_REACH	1320		1320	0	1320	0.008446919				1	0.039	2.49568E-07				1	0.039	2.49568E-07	759		759	0	759	0.00485698
112-33-4	112334	1583	2-[2-(3-	163.22	3_REACH	227060		227060	0	227060	1.391128538				1	0.039	2.38941E-07				1	0.039	2.38941E-07	100000		100000	0	100000	0.61267002
112-34-5	112345	326	2-(2-butoxyethoxy)ethanol	162.23	3_REACH	1080000		1080000	0	1080000	6.657215065				1	0.039	2.40399E-07				1	0.039	2.40399E-07	53000		53000	0	53000	0.32669667
112-35-6	112356	1584	2-(2-(2-	164.2	3_REACH	10000000		10000000	0	10000000	60.90133983	133000000		133000000	0	133000000	809.9878197				1	0.039	2.37515E-07	1000000		1000000	0	1000000	6.09013398
112-36-7	112367	327	bis(2-ethoxyethyl) ether	162.23	3_REACH	869782.3333		869782.3333	0	869782.3333	5.361414864				1	0.039	2.40399E-07				1	0.039	2.40399E-07	97255		97255	0	97255	0.59948838
112-38-9	112389	1585	undec-10-enoic acid	184.28	3_REACH	15800		15800	0	15800	0.085739093				1	0.039	2.11634E-07				1	0.039	2.11634E-07	210		210	0	210	0.00113957
112-40-3	112403	1587	dodecane	170.34	3_REACH	1000		1000	0	1000	0.005870612				1	0.039	2.28954E-07				1	0.039	2.28954E-07	3000		3000	0	3000	0.01761184
112-41-4	112414	1588	dodec-1-ene	168.32	3_REACH	3.4		3.4	0	3.4	2.01996E-05				1	0.039	2.31702E-07				1	0.039	2.31702E-07	0.93		0.93	0	0.93	5.5252E-06
112-42-5	112425	329	undecan-1-ol	172.31	3_REACH	346.6666667		346.6666667	0	346.6666667	0.002011878				1	0.039	2.26336E-07				1	0.039	2.26336E-07				1	1	5.8035E-06
112-44-7	112447	1589	undecanal	170.3	3_REACH	3500		3500	0	3500	0.020551967				1	0.039	2.29008E-07				1	0.039	2.29008E-07	970		970	0	970	0.00569583
112-45-8	112458	1590	undec-10-enal	168.28	3_REACH	1320		1320	0	1320	0.007844069				1	0.039	2.31757E-07				1	0.039	2.31757E-07	41		41	0	41	0.00024364
112-49-2	112492	330	1,2-bis(2-	178.23	3_REACH	5000000		5000000	0	5000000	28.05363856				1	0.039	2.18818E-07				1	0.039	2.18818E-07	3000000		3000000	0	3000000	16.8321831
112-50-5	112505	331	2-(2-(2-	178.23	3_REACH	1666666.667		1666666.667	0	1666666.667	9.351212852	4762000		4762000	0	4762000	26.71828536				1	0.039	2.18818E-07	62500		62500	0	62500	0.35067048
112-53-8	112538	332	dodecan-1-ol	186.34	3_REACH	1000		1000	0	1000	0.005366534	66		66	0	66	0.000354191				1	0.039	2.09295E-07	85		85	0	85	0.00045616
112-54-9	112549	333	dodecanal	184.32	3_REACH	866.6619647		866.6619647	0	866.6619647	0.004701942				1	0.039	2.11589E-07				1	0.039	2.11589E-07	14		14	0	14	7.5955E-05
112-55-0	112550	1592	dodecane-1-thiol	202.4	3_REACH	100000		100000	0	100000	0.494071146				1	0.039	1.92688E-07				1	0.039	1.92688E-07	14.5		14.5	0	14.5	7.164E-05
112-59-4	112594	1593	2-(2-	190.28	3_REACH	95000		95000	0	95000	0.499264242				1	0.039	2.04961E-07				1	0.039	2.04961E-07	11080		11080	0	11080	0.05822998
112-67-4	112674	1597	palmitoyl chloride	274.88	3_REACH	1640		1640	0	1640	0.00596624				1	0.039	1.4188E-07				1	0.039	1.4188E-07	97		97	0	97	0.00035288
112-69-6	112696	1598	hexadecyldimethylamine	269.52	3_REACH	10	100	100	0	100	0.00037103				1	0.039	1.44702E-07				1	0.039	1.44702E-07	0.5	1	1	0	1	3.7103E-06
112-72-1	112721	1599	tetradecanol	214.39	3_REACH	93.33333333		93.33333333	0	93.33333333	0.000435344	11		11	0	11	5.13084E-05				1	0.039	1.81911E-07	100		100	0	100	0.00046644
112-73-2	112732	1600	bis(2-butoxyethyl) ether	218.34	3_REACH	139000		139000	0	139000	0.636621783				1	0.039	1.78621E-07				1	0.039	1.78621E-07	16100		16100	0	16100	0.07373821
112-75-4	112754	1601	dimethyl(tetradecyl)amine	241.46	3_REACH	10	100	100	0	100	0.000414147				1	0.039	1.61517E-07				1	0.039	1.61517E-07	0.005333333	0.0183333	0.018333333	0	0.01833333	7.5927E-08
112-76-5	112765	1602	stearoyl chloride	302.93	3_REACH	1640		1640	0	1640	0.005413792				1	0.039	1.28743E-07				1	0.039	1.28743E-07	97		97	0	97	0.00032021
112-85-6	112856	1608	docosanoic acid	340.59	3_REACH	4000		4000	0	4000	0.011744326	2000		2000	0	2000	0.005872163				1	0.039	1.14507E-07	600		600	0	600	0.00176165
112-88-9	112889	1609	octadec-1-ene	252.49	3_REACH	3.4	3.4	3.4	0	3.4	1.34659E-05				1	0.039	1.54462E-07				1	0.039	1.54462E-07	0.93	0.93	0.93	0	0.93	3.6833E-06
112-92-5	112925	1611	octadecan-1-ol	270.5	3_REACH	400		400	0	400	0.001478743				1	0.039	1.44177E-07				1	0.039	1.44177E-07	100		100	0	100	0.00036969
1134-94-7	1134947	4363	2-Phenylsulfanylaniline	201.29	3_REACH	390		390	0	390	0.001937503	100		100	0	100	0.000496796				1	0.039	1.9375E-07	240		240	0	240	0.00119231
114772-54-2	114772542	1625	4'-(Bromomethyl)-2-	272.15	3_REACH	7		7	0	7	2.57211E-05				1	0.039	1.43303E-07				1	0.039	1.43303E-07	10		10	0	10	3.6744E-05
115-27-5	115275	1635	1,4,5,6,7,7-hexachloro-	370.83	3_REACH	140900		140900	0	140900	0.379958472				1	0.039	1.05169E-07				1	0.039	1.05169E-07	48400		48400	0	48400	0.13051803
1154308-86-7	1154308867	1636	N-(2-Hydroxyethyl)-3,5,5-	201.31	3_REACH	12100		12100	0	12100	0.060106304				1	0.039	1.93731E-07				1	0.039	1.93731E-07	3220		3220	0	3220	0.01599523
115-70-8	115708	1638	2-amino-2-ethylpropanediol	119.17	3_REACH	100000		100000	0	100000	0.839137367				1	0.039	3.27264E-07				1	0.039	3.27264E-07	26800		26800	0	26800	0.22488881
115-77-5	115775	341	pentaerythritol	136.15	3_REACH	56000		56000	0	56000	0.411311054				1	0.039	2.86449E-07				1	0.039	2.86449E-07				1	1	7.3448E-06
115-86-6	115866	9	triphenyl phosphate	326.29	3_REACH	200		200	0	200	0.000612952	1.4		1.4	0	1.4	4.29066E-06				1	0.039	1.19526E-07	10		10	0	10	3.0648E-05
115-95-7	115957	1640	linalyl acetate	196.29	3_REACH	10000		10000	0	10000	0.05094503				1	0.039	1.98686E-07				1	0.039	1.98686E-07	9600		9600	0	9600	0.04890723
115-96-8	115968	10	tris(2-chloroethyl)	285.49	3_REACH	5000		5000	0	5000	0.017513748				1	0.039	1.36607E-07				1	0.039	1.36607E-07	200		200	0	200	0.00070055
116-37-0	116370	1648	1,1'-isopropylidenebis(p-	344.45	3_REACH	2933.333333		2933.333333	0	2933.333333	0.008515992				1	0.039	1.13224E-07				1	0.039	1.13224E-07	2500		2500	0	2500	0.00725795
116539-55-0	116539550	1651	(1S)-3-(methylamino)-1-(2-	171.26	3_REACH	52914.33333		52914.33333	0	52914.33333	0.308970766				1	0.039	2.27724E-07				1	0.039	2.27724E-07	1210		1210	0	1210	0.00706528
116-75-6	116756	1653	1,4-	474.61	3_REACH	1000		1000	0	1000	0.002106993				1	0.039	8.21727E-08				1	0.039	8.21727E-08	9070.993		9070.993	0	9070.993	0.01911252
117-08-8	117088	1655	tetrachlorophthalic	285.9	3_REACH	500000		500000	0	500000	1.748863239				1	0.039	1.36411E-07				1	0.039	1.36411E-07	25000		25000	0	25000	0.08744316
117-21-5	117215	1657	3-chlorophthalic anhydride	182.56	3_REACH	1200000		1200000	0	1200000	6.57318142				1	0.039	2.13628E-07				1	0.039	2.13628E-07	290000		290000	0	290000	1.58851884
117-61-3	117613	1661	benzidine-2,2'-disulphonic	344.37	3_REACH	2083.333333		2083.333333	0	2083.333333	0.006049695				1	0.039	1.1325E-07				1	0.039	1.1325E-07	6746.168613		6746.168613	0	6746.16861	0.01958988
117-81-7	117817	346	bis(2-ethylhexyl) phthalate	390.56	3_REACH	170		170	0	170	0.000435272	0.1		0.1	0	0.1	2.56043E-07				1	0.039	9.98566E-08	5.6		5.6	0	5.6	1.4338E-05
118135-28-7	118135287	1666	8-tert-Butyl-2-	246.78	3_REACH	180		180	0	180	0.000729395				1	0.039	1.58035E-07				1	0.039	1.58035E-07	720		720	0	720	0.00291758
118-45-6	118456	1670	4-chlorophthalic anhydride	182.56	3_REACH	1070000		1070000	0	1070000	5.861086766				1	0.039	2.13628E-07				1	0.039	2.13628E-07	478000		478000	0	478000	2.61831727
118-48-9	118489	1671	4H-3,1-benzoxazine-	163.13	3_REACH	22000		22000	0	22000	0.134861767				1	0.039	2.39073E-07				1	0.039	2.39073E-07	2300		2300	0	2300	0.01409918
118-58-1	118581	1674	benzyl salicylate	228.25	3_REACH	800		800	0	800	0.003504929				1	0.039	1.70865E-07				1	0.039	1.70865E-07	502		502	0	502	0.00219934
118-60-5	118605	1675	2-ethylhexyl salicylate	250.34	3_REACH	220		220	0	220	0.000878805				1	0.039	1.55788E-07				1	0.039	1.55788E-07	11		11	0	11	4.394E-05
118-69-4	118694	1676	2,6-dichlorotoluene	161.03	3_REACH	2133.333333		2133.333333	0	2133.333333	0.013248049				1	0.039	2.42191E-07				1	0.039	2.42191E-07	5866.666667		5866.666667	0	5866.66667	0.03643213
118-75-2	118752	1677	tetrachloro-p-	245.88	3_REACH	1600		1600	0	1600	0.006507239				1	0.039	1.58614E-07				1	0.039	1.58614E-07	1230		1230	0	1230	0.00500244
118-79-6	118796	348	2,4,6-tribromophenol	330.82	3_REACH	80		80	0	80	0.000241823	1565.247584		1565.247584	0	1565.247584	0.004731418				1	0.039	1.17889E-07	100		100	0	100	0.00030228
118-82-1	118821	1679	2,2',6,6'-tetra-tert-butyl-4,4'-	424.67	3_REACH	273333.3333		273333.3333	0	273333.3333	0.64363702	0.038		0.038	0	0.038	8.94812E-08				1	0.039	9.1836E-08	0.0265		0.0265	0	0.0265	6.2401E-08
1189-08-8	1189088	1682	1-methyltrimethylene	226.27	3_REACH	25000		25000	0	25000	0.110487471				1	0.039	1.7236E-07				1	0.039	1.7236E-07	2110		2110	0	2110	0.00932514
118-92-3	118923	1683	anthranilic acid	137.14	3_REACH	100000		100000	0	100000	0.729181858				1	0.039	2.84381E-07				1	0.039	2.84381E-07	7033.333333		7033.333333	0	7033.33333	0.05128579
118-96-7	118967	349	2,4,6-trinitrotoluene	227.13	3_REACH	153.3333333		153.3333333	0	153.3333333	0.000675091	5		5	0	5	2.20138E-05				1	0.039	1.71708E-07	100		100	0	100	0.00044028
119-17-5	119175	1686	m-(4,5-dihydro-3-methyl-5-	254.27	3_REACH	215000		215000	0	215000	0.845557872				1	0.039	1.5338E-07				1	0.039	1.5338E-07	8800		8800	0	8800	0.03460888
119313-12-1	119313121	4343	2-benzyl-2-dimethylamino-	366.51	3_REACH	300		300	0	300	0.000818532	100		100	0	100	0.000272844				1	0.039	1.06409E-07	100		100	0	100	0.00027284
119462-56-5	119462565	4277	1,3-bis(3-methyl-2,5-dioxo-	324.34	3_REACH	65.9		65.9	0	65.9	0.000203182				1	0.039	1.20244E-07				1	0.039	1.20244E-07	83.33333333		83.33333333	0	83.3333333	0.00025693
119-53-9	119539	1694	benzoin	212.25	3_REACH	2561		2561	0	2561	0.01206596				1	0.039	1.83746E-07				1	0.039	1.83746E-07	11009		11009	0	11009	0.05186808
119-61-9	119619	354	benzophenone	182.22	3_REACH	2100		2100	0	2100	0.011524531	554.7972603		554.7972603	0	554.7972603	0.003044656				1	0.039	2.14027E-07	460		460	0	460	0.00252442
119-64-2	119642	355	1,2,3,4-	132.21	3_REACH	2400		2400	0	2400	0.018152939				1	0.039	2.94985E-07				1	0.039	2.94985E-07	3600		3600	0	3600	0.02722941
119-65-3	119653	356	isoquinoline	129.16	3_REACH	4666.666667		4666.666667	0	4666.666667	0.036130897				1	0.039	3.01951E-07				1	0.039	3.01951E-07	2923.333333		2923.333333	0	2923.33333	0.02263343
119-80-2	119802	357	2,2'-dithiodi(benzoic acid)	306.36	3_REACH	28000		28000	0	28000	0.091395744				1	0.039	1.27301E-07				1	0.039	1.27301E-07	12000		12000	0	12000	0.0391696
119851-28-4	119851284	1700	1-[2-Chloro-4-(4-	281.14	3_REACH	500		500	0	500	0.001778473				1	0.039	1.38721E-07				1	0.039	1.38721E-07	50		50	0	50	0.00017785
120068-79-3	120068793	4457	PYRAZOLE MB 45897	321.09	3_REACH	1000		1000	0	1000	0.003114392				1	0.039	1.21461E-07				1	0.039	1.21461E-07	1333.333333		1333.333333	0	1333.33333	0.00415252
120100-77-8	120100778	1704	2-Chloro-4-(methylsulfonyl)	346.71	3_REACH	100000		100000	0	100000	0.288425485				1	0.039	1.12486E-07				1	0.039	1.12486E-07	100000		100000	0	100000	0.28842549
120-12-7	120127	358	anthracene	178.23	3_REACH	0.423333333		0.423333333	0	0.423333333	2.37521E-06	6		6	0	6	3.36644E-05				1	0.039	2.18818E-07	1.596871942		1.596871942	0	1.59687194	8.9596E-06
120-18-3	120183	12	naphthalene-2-sulphonic	208.24	3_REACH	33333.33333		33333.33333	0	33333.33333	0.160071712				1	0.039	1.87284E-07				1	0.039	1.87284E-07	25000		25000	0	25000	0.12005378
120298-38-6	120298386	4257	(S,S)-trans-4-(acetylamino)-	338.43	3_REACH	155000		155000	0	155000	0.457997222				1	0.039	1.15238E-07				1	0.039	1.15238E-07	210		210	0	210	0.00062051

120-40-1	120401	13	N,N-bis(2-	287.44	3_REACH	1000		1000	0	1000	0.003478987	320		320	0	320	0.001113276				1	0.039	1.3568E-07	300		300	0	300	0.0010437
120-46-7	120467	1712	1,3-diphenylpropane-1,3-	224.26	3_REACH	3770.666667		3770.666667	0	3770.666667	0.016813817	552		552	0	552	0.002461429				1	0.039	1.73905E-07	814		814	0	814	0.00362972
120-47-8	120478	14	ethyl 4-hydroxybenzoate	166.18	3_REACH	8700		8700	0	8700	0.05235287				1	0.039	2.34685E-07				1	0.039	2.34685E-07	2100		2100	0	2100	0.0126369
120-55-8	120558	1714	oxydiethylene dibenzoate	314.34	3_REACH	60		60	0	60	0.000190876				1	0.039	1.24069E-07				1	0.039	1.24069E-07	1000		1000	0	1000	0.00318127
120-57-0	120570	1715	piperonal	150.13	3_REACH	1600		1600	0	1600	0.01065743				1	0.039	2.59775E-07				1	0.039	2.59775E-07	380		380	0	380	0.00253114
120570-77-6	120570776	1716	2-(2-Formyloxyethoxy)ethyl	162.14	3_REACH	33100		33100	0	33100	0.204144566				1	0.039	2.40533E-07				1	0.039	2.40533E-07	90600		90600	0	90600	0.55877637
120578-03-2	120578032	4461	3-(2-(7-Chloroquinolin-2-	293.75	3_REACH	610		610	0	610	0.002076596				1	0.039	1.32766E-07				1	0.039	1.32766E-07	350		350	0	350	0.00119149
120-61-6	120616	1717	dimethyl terephthalate	194.19	3_REACH	5370		5370	0	5370	0.027653329				1	0.039	2.00834E-07				1	0.039	2.00834E-07	6500		6500	0	6500	0.03347237
120-78-5	120785	360	di(benzothiazol-2-yl)	332.49	3_REACH	6333.333333		6333.333333	0	6333.333333	0.019048192				1	0.039	1.17297E-07				1	0.039	1.17297E-07	233.3333333		233.3333333	0	233.333333	0.00070178
120-80-9	120809	361	pyrocatechol	110.11	3_REACH	2800		2800	0	2800	0.025429116				1	0.039	3.54191E-07				1	0.039	3.54191E-07	6000		6000	0	6000	0.05449096
120-82-1	120821	362	1,2,4-trichlorobenzene	181.45	3_REACH	600		600	0	600	0.003306696	40		40	0	40	0.000220446				1	0.039	2.14935E-07	300		300	0	300	0.00165335
120-83-2	120832	363	2,4-dichlorophenol	163	3_REACH	86.66666667	356.666667	356.6666667	0	356.6666667	0.002188139	99		99	0	99	0.000607362				1	0.039	2.39264E-07	350		350	0	350	0.00214724
120-93-4	120934	367	2-imidazolidone	86.096	3_REACH	122000		122000	0	122000	1.417022858	3333333.333		3333333.333	0	3333333.333	38.71647154				1	0.039	4.52983E-07	5333.333333		5333.333333	0	5333.33333	0.06194635
121219-07-6	121219076	4298	1-Ethoxy-2,3-	158.15	3_REACH	10000		10000	0	10000	0.06323111				1	0.039	2.46601E-07				1	0.039	2.46601E-07	2700		2700	0	2700	0.0170724
121-32-4	121324	368	3-ethoxy-4-	166.18	3_REACH	28100		28100	0	28100	0.169093754				1	0.039	2.34685E-07				1	0.039	2.34685E-07	47000		47000	0	47000	0.28282585
121-33-5	121335	369	vanillin	152.15	3_REACH	19000		19000	0	19000	0.124876766				1	0.039	2.56326E-07				1	0.039	2.56326E-07	40000		40000	0	40000	0.26289846
121-57-3	121573	372	sulphanilic acid	173.19	3_REACH	100000		100000	0	100000	0.577400543				1	0.039	2.25186E-07				1	0.039	2.25186E-07	4600		4600	0	4600	0.02656042
121-60-8	121608	1730	N-acetylsulphanilyl chloride	233.67	3_REACH	56663.66667		56663.66667	0	56663.66667	0.242494401				1	0.039	1.66902E-07				1	0.039	1.66902E-07	63645.46667		63645.46667	0	63645.4667	0.27237329
121-69-7	121697	373	N,N-dimethylaniline	121.18	3_REACH	10999.85476		10999.85476	0	10999.85476	0.090772857				1	0.039	3.21835E-07				1	0.039	3.21835E-07	14000		14000	0	14000	0.11553062
121-82-4	121824	375	perhydro-1,3,5-trinitro-	222.12	3_REACH	9.75		9.75	0	9.75	4.38952E-05	625		625	0	625	0.002813794	3200		3200	0	3200	0.014406627	500		500	0	500	0.00225104
121-86-8	121868	376	2-chloro-4-nitrotoluene	171.58	3_REACH	5500		5500	0	5500	0.032055018				1	0.039	2.27299E-07				1	0.039	2.27299E-07	3000		3000	0	3000	0.01748456
121-91-5	121915	1739	isophthalic acid	166.13	3_REACH	18600		18600	0	18600	0.111960513				1	0.039	2.34756E-07				1	0.039	2.34756E-07	19000		19000	0	19000	0.11436827
122-00-9	122009	1740	4'-methylacetophenone	134.18	3_REACH	5247.666667		5247.666667	0	5247.666667	0.039109157	8247		8247	0	8247	0.061462215				1	0.039	2.90654E-07	2700		2700	0	2700	0.02012222
122-01-0	122010	1741	4-chlorobenzoyl chloride	175.01	3_REACH	10000		10000	0	10000	0.057139592				1	0.039	2.22844E-07				1	0.039	2.22844E-07	38000		38000	0	38000	0.21713045
122-03-2	122032	377	4-isopropylbenzaldehyde	148.21	3_REACH	2206.666667		2206.666667	0	2206.666667	0.014888784				1	0.039	2.6314E-07				1	0.039	2.6314E-07				1	1	6.7472E-06
122-20-3	122203	1743	1,1',1''-nitrilotripropan-2-ol	191.27	3_REACH	1000000		1000000	0	1000000	5.228211429				1	0.039	2.039E-07				1	0.039	2.039E-07	640		640	0	640	0.00334606
12225-08-0	12225080	1744	N-(2,3-dihydro-2-oxo-1H-	576.59	3_REACH	1000		1000	0	1000	0.001734335				1	0.039	6.76391E-08				1	0.039	6.76391E-08	1000		1000	0	1000	0.00173433
12225-18-2	12225182	1745	N-(4-chloro-2,5-	591.04	3_REACH	1000		1000	0	1000	0.001691933				1	0.039	6.59854E-08				1	0.039	6.59854E-08	1000		1000	0	1000	0.00169193
12236-62-3	12236623	1747	2-[(4-chloro-2-	416.79	3_REACH	1000		1000	0	1000	0.00239929				1	0.039	9.35723E-08				1	0.039	9.35723E-08	1000		1000	0	1000	0.00239929
12236-64-5	12236645	1748	N-[4-(acetylamino)phenyl]-	501.94	3_REACH	100000		100000	0	100000	0.199226999				1	0.039	7.76985E-08				1	0.039	7.76985E-08	1000		1000	0	1000	0.00199227
122-39-4	122394	379	diphenylamine	169.23	3_REACH	710		710	0	710	0.004195474	710		710	0	710	0.004195474				1	0.039	2.30456E-07	20		20	0	20	0.00011818
122-52-1	122521	1751	triethyl phosphite	166.16	3_REACH	543600.6667		543600.6667	0	543600.6667	3.271549511	538628.6667		538628.6667	0	538628.6667	3.241626545				1	0.039	2.34714E-07	70051		70051	0	70051	0.42158763
122-57-6	122576	1752	4-phenylbutenone	146.19	3_REACH	5100		5100	0	5100	0.034886107	9930		9930	0	9930	0.067925303				1	0.039	2.66776E-07	9680		9680	0	9680	0.0662152
122-62-3	122623	1755	bis(2-ethylhexyl) sebacate	426.68	3_REACH	32333.33333		32333.33333	0	32333.33333	0.075778882				1	0.039	9.14034E-08				1	0.039	9.14034E-08	0.037666667		0.037666667	0	0.03766667	8.8278E-08
122-99-6	122996	384	2-phenoxyethanol	138.17	3_REACH	5000		5000	0	5000	0.036187305	23000		23000	0	23000	0.166461605				1	0.039	2.82261E-07	70000		70000	0	70000	0.50662228
123-04-6	123046	1760	3-(chloromethyl)heptane	148.68	3_REACH	15400		15400	0	15400	0.103578154				1	0.039	2.62308E-07				1	0.039	2.62308E-07	191		191	0	191	0.00128464
123-05-7	123057	1761	2-ethylhexanal	128.22	3_REACH	1800		1800	0	1800	0.014038372				1	0.039	3.04165E-07				1	0.039	3.04165E-07	2200		2200	0	2200	0.01715801
123-11-5	123115	1763	anisaldehyde	136.15	3_REACH	100000		100000	0	100000	0.734484025				1	0.039	2.86449E-07				1	0.039	2.86449E-07	24450		24450	0	24450	0.17958134
123-17-1	123171	1764	2,6,8-trimethylnonan-4-ol	186.34	3_REACH	239		239	0	239	0.001282602				1	0.039	2.09295E-07				1	0.039	2.09295E-07	252		252	0	252	0.00135237
123-30-8	123308	386	4-aminophenol	109.13	3_REACH	156.6666667		156.6666667	0	156.6666667	0.001435597	280		280	0	280	0.002565747				1	0.039	3.57372E-07	36		36	0	36	0.00032988
123-31-9	123319	388	hydroquinone	110.11	3_REACH	14.66666667		14.66666667	0	14.66666667	0.0001332				1	0.039	3.54191E-07				1	0.039	3.54191E-07	1.5		1.5	0	1.5	1.3623E-05
123-39-7	123397	392	N-methylformamide	59.069	3_REACH	10000000		10000000	0	10000000	169.2935381				1	0.039	6.60245E-07				1	0.039	6.60245E-07				1	1	1.6929E-05
123-42-2	123422	393	4-hydroxy-4-methylpentan-	116.16	3_REACH	140000		140000	0	140000	1.20523416				1	0.039	3.35744E-07				1	0.039	3.35744E-07	530000		530000	0	530000	4.56267218
123-68-2	123682	1773	allyl hexanoate	156.22	3_REACH	62.2		62.2	0	62.2	0.000398156				1	0.039	2.49648E-07				1	0.039	2.49648E-07	2		2	0	2	1.2802E-05
123-77-3	123773	1775	C,C'-azodi(formamide)	116.08	3_REACH	50000		50000	0	50000	0.430737422				1	0.039	3.35975E-07				1	0.039	3.35975E-07	6700		6700	0	6700	0.05771881
1238449-42-7	1238449427	1776	bis(2-propylheptyl)	342.56	3_REACH	100000		100000	0	100000	0.291919664				1	0.039	1.13849E-07				1	0.039	1.13849E-07	100000		100000	0	100000	0.29191966
123-96-6	123966	399	octan-2-ol	130.23	3_REACH	25000		25000	0	25000	0.191968057				1	0.039	2.9947E-07				1	0.039	2.9947E-07	8700		8700	0	8700	0.06680488
124-04-9	124049	400	adipic acid	146.14	3_REACH	32333.33333		32333.33333	0	32333.33333	0.221249031	50000		50000	0	50000	0.342137676				1	0.039	2.66867E-07	13960		13960	0	13960	0.09552484
124-07-2	124072	401	octanoic acid	144.21	3_REACH	7333.333333		7333.333333	0	7333.333333	0.050851767	2000		2000	0	2000	0.013868664				1	0.039	2.70439E-07	70		70	0	70	0.0004854
124-09-4	124094	1783	hexamethylenediamine	116.21	3_REACH	46000		46000	0	46000	0.395835126				1	0.039	3.35599E-07				1	0.039	3.35599E-07	3200		3200	0	3200	0.02753636
124-13-0	124130	1786	octanal	128.22	3_REACH				1	0.39	3.04165E-06	2633.333333		2633.333333	0	2633.333333	0.020537618				1	0.039	3.04165E-07	140		140	0	140	0.00109187
124-17-4	124174	1787	2-(2-butoxyethoxy)ethyl	204.27	3_REACH	50000		50000	0	50000	0.244774074				1	0.039	1.90924E-07				1	0.039	1.90924E-07	300000		300000	0	300000	1.46864444
124-18-5	124185	402	decane	142.29	3_REACH	1000		1000	0	1000	0.007027901	111		111	0	111	0.000780097				1	0.039	2.74088E-07	5.333333333		5.333333333	0	5.33333333	3.7482E-05
1241-94-7	1241947	403	2-ethylhexyl diphenyl	362.41	3_REACH	410		410	0	410	0.001131315	21.1		21.1	0	21.1	5.82214E-05				1	0.039	1.07613E-07	30		30	0	30	8.2779E-05
124-19-6	124196	1788	nonanal	142.24	3_REACH	1320		1320	0	1320	0.00928009				1	0.039	2.74184E-07				1	0.039	2.74184E-07	759		759	0	759	0.00533605
124-26-5	124265	1789	stearamide	283.5	3_REACH	55		55	0	55	0.000194004				1	0.039	1.37566E-07				1	0.039	1.37566E-07	170		170	0	170	0.00059965
124-28-7	124287	1790	dimantine	297.57	3_REACH	10	100	100	0	100	0.000336055				1	0.039	1.31062E-07				1	0.039	1.31062E-07	0.5	1	1	0	1	3.3606E-06
124-30-1	124301	1791	octadecylamine	269.52	3_REACH	20		20	0	20	7.4206E-05				1	0.039	1.44702E-07				1	0.039	1.44702E-07	0.266666667	0.3666667	0.366666667	0	0.36666667	1.3604E-06
124655-09-0	124655090	4568	tert-butyl2-[(4R,6S)-6-	260.33	3_REACH	56000		56000	0	56000	0.215111589				1	0.039	1.4981E-07				1	0.039	1.4981E-07	83000		83000	0	83000	0.31882611
125-12-2	125122	1796	exo-1,7,7-	196.29	3_REACH	10000		10000	0	10000	0.05094503				1	0.039	1.98686E-07				1	0.039	1.98686E-07	436		436	0	436	0.0022212
12542-30-2	12542302	1797	hexahydro-4,7-methano-1H	204.27	3_REACH	686.6666667		686.6666667	0	686.6666667	0.003361564				1	0.039	1.90924E-07				1	0.039	1.90924E-07	1580		1580	0	1580	0.00773486
125971-57-5	125971575	1800	(2Z)-2-Benzylidene-4-	293.37	3_REACH	100		100	0	100	0.000340866	710		710	0	710	0.002420152				1	0.039	1.32938E-07	410		410	0	410	0.00139755
125971-96-2	125971962	4497	4-(4-F-PHENYL)-4-OXO-3-	417.48	3_REACH	280		280	0	280	0.000670691				1	0.039	9.34176E-08				1	0.039	9.34176E-08	58		58	0	58	0.00013893
126-33-0	126330	406	tetrahydrothiophene 1,1-	120.17	3_REACH	46666.66667		46666.66667	0	46666.66667	0.388338742				1	0.039	3.2454E-07				1	0.039	3.2454E-07	171000		171000	0	171000	1.42298411
126586-91-2	126586912	4597	N2-[1-(S)-ethoxycarbonyl-3-	414.43	3_REACH	67000		67000	0	67000	0.161667833				1	0.039	9.41052E-08				1	0.039	9.41052E-08	100000		100000	0	100000	0.24129527
126-71-6	126716	18	triisobutyl phosphate	266.32	3_REACH	9400		9400	0	9400	0.035295885				1	0.039	1.4644E-07				1	0.039	1.4644E-07	13000		13000	0	13000	0.04881346
126-73-8	126738	19	tributyl phosphate	266.32	3_REACH	433.3333333	433.333333	433.3333333	0	433.3333333	0.001627115	820		820	0	820	0.003079003				1	0.039	1.4644E-07	370		370	0	370	0.00138931
127-47-9	127479	1812	retinyl acetate	328.5	3_REACH	875		875	0	875	0.002663623				1	0.039	1.18721E-07				1	0.039	1.18721E-07	50		50	0	50	0.00015221
128-37-0	128370	413	2,6-di-tert-butyl-p-cresol	220.36	3_REACH	66.33333333		66.33333333	0	66.33333333	0.000301023				1	0.039	1.76983E-07				1	0.039	1.76983E-07	400		400	0	400	0.00181521
128-39-2	128392	1820	2,6-di-tert-butylphenol	206.33	3_REACH	296.6666667		296.6666667	0	296.6666667	0.001437826	210		210	0	210	0.001017787				1	0.039	1.89018E-07	160		160	0	160	0.00077546
128-69-8	128698	1822	perylene-3,4:9,10-	392.32	3_REACH	7600		7600	0	7600	0.019371941				1	0.039	9.94086E-08				1	0.039	9.94086E-08	100000		100000	0	100000	0.25489396
129-00-0	129000	21	pyrene	202.26	3_REACH	666.6666667		666.6666667	0	666.6666667	0.003296088				1	0.039	1.92821E-07				1	0.039	1.92821E-07	1.2		1.2	0	1.2	5.933E-06
129909-90-6	129909906	415	Amicarbazone	241.3	3_REACH	118000		118000	0	118000	0.48901782	2300		2300	0	2300	0.009531703				1	0.039	1.61625E-07	5.67		5.67	0	5.67	2.3498E-05
13048-33-4	13048334	1837	hexamethylene diacrylate	226.27	3_REACH	2260.776661		2260.776661	0	2260.776661	0.0099915				1	0.039	1.7236E-07				1	0.039	1.7236E-07	500		500	0	500	0.00220975
130755-46-3	130755463	1842	4,4'-dithiobis[5-amino-3-	704.3	3_REACH	8		8	0	8	1.13588E-05				1	0.039	5.53741E-08				1	0.039	5.53741E-08	1500		1500	0	1500	0.00212977
13076-17-0	13076170	1843	Lactide, D-	144.13	3_REACH	43333.33333		43333.33333	0	43333.33333	0.300654502	2180		2180	0	2180	0.015125234				1	0.039	2.70589E-07	1900000		1900000	0	1900000	13.1825435
130841-23-5	130841235	1844	Benzene,1,4-dichloro-2-	358.02	3_REACH	27		27	0	27	7.54148E-05	50		50	0	50	0.000139657				1	0.039	1.08932E-07	10		10	0	10	2.7931E-05
131-11-3	131113	417	dimethyl phthalate	194.19	3_REACH	9666.666667		9666.666667	0	9666.666667	0.049779426	11000		11000	0	11000	0.056645553				1	0.039	2.00834E-07	10000		10000	0	10000	0.05149596
131-17-9	131179	418	diallyl phthalate	246.26	3_REACH	180		180	0	180	0.000730935				1	0.039	1.58369E-07				1	0.039	1.58369E-07	1600		1600	0	1600	0.0064972
13122-18-4	13122184	1847	tert-butyl 3,5,5-	230.35	3_REACH	3000		3000	0	3000	0.01302366				1	0.039	1.69308E-07				1	0.039	1.69308E-07	40		40	0	40	0.00017365
13127-18-9	13127189	1848	Erythromycin oxime	748.95	3_REACH	100000		100000	0	100000	0.133520262				1	0.039	5.20729E-08				1	0.039	5.20729E-08	6000		6000	0	6000	0.00801122
1315251-11-6	1315251116	1849	7,7,8,9,9-pentamethyl-	242.37	3_REACH	183.3333333		183.3333333	0	183.3333333	0.000756419				1	0.039	1.60911E-07				1	0.039	1.60911E-07	57		57	0	57	0.00023518
131538-00-6	131538006	4321	2,3-bis((2-	260.52	3_REACH	10		10	0	10	3.83848E-05				1	0.039	1.49701E-07				1	0.039	1.49701E-07	9.47		9.47	0	9.47	3.635E-05
131-56-6	131566	1850	2,4-	214.22	3_REACH	1600		1600	0	1600	0.007468957	1454		1454	0	1454	0.006787415				1	0.039	1.82056E-07	706.6666667		706.6666667	0	706.666667	0.00329879
131-57-7	131577	22	oxybenzone	228.25	3_REACH	720		720	0	720	0.003154436				1	0.039	1.70865E-07				1	0.039	1.70865E-07	80		80	0	80	0.00035049
13170-23-5	13170235	1851	diacetoxydi-tert-	292.4	3_REACH	27792.88478		27792.88478	0	27792.88478	0.095050906				1	0.039	1.33379E-07				1	0.039	1.33379E-07	18000		18000	0	18000	0.06155951
132694-65-6	132694656	4685	4-[4-[(1-Oxo-2-	602.64	3_REACH	100000		100000	0	100000	0.165936546				1	0.039	6.47153E-08				1	0.039	6.47153E-08	950		950	0	950	0.0015764
1333-07-9	1333079	1866	toluenesulphonamide	171.22	3_REACH	56000		56000	0	56000	0.327064595				1	0.039	2.27777E-07				1	0.039	2.27777E-07	7700		7700	0	7700	0.04497138
133467-41-1	133467411	4415	4-[4-(2-	339.5	3_REACH	120		120	0	120	0.000353461				1	0.039	1.14875E-07				1	0.039	1.14875E-07	270		270	0	270	0.00079529
13361-34-7	13361347	1870	2-ethylhexyl cyanoacetate	197.28	3_REACH	14000		14000	0	14000	0.070965126				1	0.039	1.97689E-07				1	0.039	1.97689E-07	380		380	0	380	0.0019262
133636-82-5	133636825	4540	Spiro[bicyclo[3.1.1]heptane-	218.34	3_REACH	640		640	0	640	0.002931208				1	0.039	1.78621E-07				1	0.039	1.78621E-07	2000		2000	0	2000	0.00916003
133-91-5	133915	1872	3,5-diiodosalicylic acid	389.91	3_REACH	1098.810991		1098.810991	0	1098.810991	0.002818114				1	0.039	1.00023E-07				1	0.039	1.00023E-07	1318.286419		1318.286419	0	1318.28642	0.003381
13393-93-6	13393936	1873	tetradecahydro-7-isopropyl-	292.51	3_REACH	100000		100000	0	100000	0.341868654				1	0.039	1.33329E-07				1	0.039	1.33329E-07	100000		100000	0	100000	0.34186865
13402-02-3	13402023	1875	hexadecyl acrylate	296.5	3_REACH	100000		100000	0	100000	0.337268128				1	0.039	1.31535E-07				1	0.039	1.31535E-07	100000		100000	0	100000	0.33726813
134605-64-4	134605644	433	1-(allyloxy)-2-methyl-1-	474.82	3_REACH	2500		2500	0	2500	0.005265153	11		11	0	11	2.31667E-05	22		22	0	22	4.63333E-05	0.066		0.066	0	0.066	1.39E-07
134701-20-5	134701205	4329	2,4-dimethyl-6-(1-methyl-	346.6	3_REACH	7190		7190	0	7190	0.020744374				1	0.039	1.12522E-07				1	0.039	1.12522E-07	6570		6570	0	6570	0.01895557
13472-08-7	13472087	1882	2,2'-azobis[2-	192.27	3_REACH	193333.3333		193333.3333	0	193333.3333	1.005530417	10000		10000	0	10000	0.052010194				1	0.039	2.0284E-07	12500		12500	0	12500	0.06501274
13501-76-3	13501763	1885	(3-	209.77	3_REACH	211000		211000	0	211000	1.005863565				1	0.039	1.85918E-07				1	0.039	1.85918E-07	57000		57000	0	57000	0.27172618
13515-40-7	13515407	1887	2-[(4-chloro-2-	390.79	3_REACH	1000		1000	0	1000	0.002558919				1	0.039	9.97978E-08				1	0.039	9.97978E-08	1000		1000	0	1000	0.00255892
135-19-3	135193	435	2-naphthol	144.17	3_REACH	1000		1000	0	1000	0.006936256	1		1	0	1	6.93626E-06				1	0.039	2.70514E-07	2100		2100	0	2100	0.01456614
135590-91-9	135590919	436	1-(2,4-Dichlorophenyl)-4,5-	373.24	3_REACH	1000		1000	0	1000	0.002679241	100		100	0	100	0.000267924				1	0.039	1.0449E-07	270		270	0	270	0.0007234
136210-30-5	136210305	4527	1,4-diethyl 2-{[4-({4-[(1,4-	554.73	3_REACH	24000		24000	0	24000	0.043264291				1	0.039	7.03045E-08				1	0.039	7.03045E-08	6250		6250	0	6250	0.01126674
136239-66-2	136239662	4294	1-butoxy-2,3-	186.2	3_REACH	1510		1510	0	1510	0.00810956				1	0.039	2.09452E-07				1	0.039	2.09452E-07	240		240	0	240	0.00128894
136465-81-1	136465811	4454	PHIQ	238.38	3_REACH	32000		32000	0	32000	0.13423945				1	0.039	1.63604E-07				1	0.039	1.63604E-07	4800		4800	0	4800	0.02013592
1364731-90-7	1364731907	1900	2,6-dimethylphenyl 4-	278.33	3_REACH	910		910	0	910	0.0032695				1	0.039	1.40121E-07				1	0.039	1.40121E-07	2183.333333		2183.333333	0	2183.33333	0.00784441
13674-84-5	13674845	24	tris(2-chloro-1-methylethyl)	327.57	3_REACH	6300		6300	0	6300	0.01923253				1	0.039	1.19059E-07				1	0.039	1.19059E-07	6000		6000	0	6000	0.0183167
13674-87-8	13674878	25	tris[2-chloro-1-	430.91	3_REACH	560		560	0	560	0.001299575				1	0.039	9.05061E-08				1	0.039	9.05061E-08	1200		1200	0	1200	0.0027848
13749-61-6	13749616	1909	N-isopropylmethacrylamide	127.19	3_REACH	100000		100000	0	100000	0.786225332				1	0.039	3.06628E-07				1	0.039	3.06628E-07	125000		125000	0	125000	0.98278167
13752-51-7	13752517	1911	4-	248.37	3_REACH	3033.333333		3033.333333	0	3033.333333	0.012212962				1	0.039	1.57024E-07				1	0.039	1.57024E-07	2480		2480	0	2480	0.0099851
137863-20-8	137863208	1913	Valsartan benzyl ester	525.66	3_REACH	8700		8700	0	8700	0.016550622				1	0.039	7.41924E-08				1	0.039	7.41924E-08	11500		11500	0	11500	0.02187726
138564-59-7	138564597	4458	5-methyl-2-[(2-	259.283	3_REACH	77		77	0	77	0.000296973				1	0.039	1.50415E-07				1	0.039	1.50415E-07	132		132	0	132	0.0005091
138-59-0	138590	445	(3R,4S,5R)-3,4,5-	174.15	3_REACH	33332.75913		33332.75913	0	33332.75913	0.191402579				1	0.039	2.23945E-07				1	0.039	2.23945E-07	48000		48000	0	48000	0.27562446
139007-06-0	139007060	1915	(E)-2-Ethoxy-N-(2-methyl-1	219.33	3_REACH	20333.33333		20333.33333	0	20333.33333	0.092706576				1	0.039	1.77814E-07				1	0.039	1.77814E-07	6000		6000	0	6000	0.02735604
139122-17-1	139122171	4737	2-(3-chloro-2-oxo-2,3-	315.76	3_REACH	120		120	0	120	0.000380035				1	0.039	1.23512E-07				1	0.039	1.23512E-07	23		23	0	23	7.284E-05
139-13-9	139139	27	nitrilotriacetic acid	191.14	3_REACH	28333.33333		28333.33333	0	28333.33333	0.148233407	40000		40000	0	40000	0.209270692				1	0.039	2.04039E-07	1560		1560	0	1560	0.00816156
139189-30-3	139189303	4566	Phosphoric acid, P,P'-1,3-	686.68	3_REACH	27		27	0	27	3.93196E-05				1	0.039	5.6795E-08				1	0.039	5.6795E-08	31		31	0	31	4.5145E-05
139504-68-0	139504680	4286	1-[(2-tert-	228.38	3_REACH	1800		1800	0	1800	0.007881601	220		220	0	220	0.000963307				1	0.039	1.70768E-07	1500		1500	0	1500	0.006568
140-11-4	140114	448	benzyl acetate	150.18	3_REACH	1333.333333		1333.333333	0	1333.333333	0.008878235	920		920	0	920	0.006125982				1	0.039	2.59688E-07	52000		52000	0	52000	0.34625117
140-29-4	140294	1926	phenylacetonitrile	117.15	3_REACH	5000		5000	0	5000	0.042680324				1	0.039	3.32907E-07				1	0.039	3.32907E-07	117000		117000	0	117000	0.99871959
140-31-8	140318	449	2-piperazin-1-ylethylamine	129.21	3_REACH	259000		259000	0	259000	2.004488817				1	0.039	3.01834E-07				1	0.039	3.01834E-07	31000		31000	0	31000	0.23991951
14064-10-9	14064109	450	diethyl chloromalonate	194.61	3_REACH	316.6666667		316.6666667	0	316.6666667	0.001627186				1	0.039	2.00401E-07				1	0.039	2.00401E-07				1	1	5.1385E-06
140-66-9	140669	451	4-(1,1,3,3-	206.33	3_REACH	210		210	0	210	0.001017787	6		6	0	6	2.90796E-05	12		12	0	12	5.81593E-05	30		30	0	30	0.0001454
14073-97-3	14073973	1929	L-menthan-3-one	154.25	3_REACH	28000		28000	0	28000	0.181523501				1	0.039	2.52836E-07				1	0.039	2.52836E-07	10000		10000	0	10000	0.06482982
14078-41-2	14078412	1930	3,3'-di-tert-butyl-5,5'-	358.48	3_REACH	100000		100000	0	100000	0.27895559				1	0.039	1.08793E-07				1	0.039	1.08793E-07	100000		100000	0	100000	0.27895559
141-05-9	141059	454	diethyl maleate	172.18	3_REACH	6000		6000	0	6000	0.034847253				1	0.039	2.26507E-07				1	0.039	2.26507E-07	5510		5510	0	5510	0.03200139
141-10-6	141106	1932	6,10-dimethylundeca-3,5,9-	192.3	3_REACH	4600		4600	0	4600	0.023920957				1	0.039	2.02808E-07				1	0.039	2.02808E-07	530		530	0	530	0.00275611
141-17-3	141173	1933	bis(2-(2-	434.57	3_REACH	13000		13000	0	13000	0.029914628				1	0.039	8.97439E-08				1	0.039	8.97439E-08	180		180	0	180	0.0004142
141-18-4	141184	1934	bis(2-butoxyethyl) adipate	346.46	3_REACH	1500		1500	0	1500	0.004329504				1	0.039	1.12567E-07				1	0.039	1.12567E-07	1440		1440	0	1440	0.00415632
141-27-5	141275	1935	(E)-3,7-dimethylocta-2,6-	152.24	3_REACH	4600		4600	0	4600	0.030215449				1	0.039	2.56174E-07				1	0.039	2.56174E-07	3000		3000	0	3000	0.01970573
141-62-8	141628	1939	decamethyltetrasiloxane	310.69	3_REACH	6.3		6.3	0	6.3	2.02774E-05	5.3		5.3	0	5.3	1.70588E-05				1	0.039	1.25527E-07	2.2		2.2	0	2.2	7.081E-06
141-63-9	141639	1940	dodecamethylpentasiloxan	384.85	3_REACH	0.075		0.075	0	0.075	1.94881E-07	0.039		0.039	0	0.039	1.01338E-07				1	0.039	1.01338E-07	2.2		2.2	0	2.2	5.7165E-06
141-97-9	141979	459	ethyl acetoacetate	130.14	3_REACH	100000		100000	0	100000	0.768403258				1	0.039	2.99677E-07				1	0.039	2.99677E-07	100000		100000	0	100000	0.76840326
141-98-0	141980	460	O-isopropyl	147.24	3_REACH	14142.13562		14142.13562	0	14142.13562	0.096048191				1	0.039	2.64874E-07				1	0.039	2.64874E-07	1000		1000	0	1000	0.00679163
142-16-5	142165	1948	bis(2-ethylhexyl) maleate	340.5	3_REACH	40000		40000	0	40000	0.117474302				1	0.039	1.14537E-07				1	0.039	1.14537E-07	52		52	0	52	0.00015272
142-19-8	142198	1950	allyl heptanoate	170.25	3_REACH	58		58	0	58	0.000340675				1	0.039	2.29075E-07				1	0.039	2.29075E-07	158		158	0	158	0.00092805
14246-53-8	14246538	1956	N-(1-oxooctyl)glycine	201.27	3_REACH	100000		100000	0	100000	0.496845034				1	0.039	1.9377E-07				1	0.039	1.9377E-07	2360		2360	0	2360	0.01172554
142-62-1	142621	462	hexanoic acid	116.16	3_REACH	26666.66667		26666.66667	0	26666.66667	0.229568411				1	0.039	3.35744E-07				1	0.039	3.35744E-07	32000		32000	0	32000	0.27548209
142-90-5	142905	465	dodecyl methacrylate	254.41	3_REACH	4333333.333		4333333.333	0	4333333.333	17.03287345				1	0.039	1.53296E-07				1	0.039	1.53296E-07	6.2		6.2	0	6.2	2.437E-05
142-91-6	142916	1957	isopropyl palmitate	298.51	3_REACH	10000000		10000000	0	10000000	33.49971525				1	0.039	1.30649E-07				1	0.039	1.30649E-07	54		54	0	54	0.0001809
142-92-7	142927	466	hexyl acetate	144.21	3_REACH	1333.333333		1333.333333	0	1333.333333	0.009245776				1	0.039	2.70439E-07				1	0.039	2.70439E-07	323.3333333		323.3333333	0	323.333333	0.0022421
143-07-7	143077	468	lauric acid	200.32	3_REACH	1200		1200	0	1200	0.005990415	2000		2000	0	2000	0.009984026				1	0.039	1.94688E-07	4400		4400	0	4400	0.02196486
143-08-8	143088	469	nonan-1-ol	144.26	3_REACH	1840		1840	0	1840	0.012754748				1	0.039	2.70345E-07				1	0.039	2.70345E-07	1054.092553		1054.092553	0	1054.09255	0.00730689
143-22-6	143226	1959	2-(2-(2-	206.28	3_REACH	65666.66667		65666.66667	0	65666.66667	0.318337535	411195		411195	0	411195	1.993382781				1	0.039	1.89063E-07	62500		62500	0	62500	0.30298623
143-24-8	143248	28	bis(2-(2-	222.28	3_REACH	5000000		5000000	0	5000000	22.49415152				1	0.039	1.75454E-07				1	0.039	1.75454E-07	625000		625000	0	625000	2.81176894
143-28-2	143282	1962	(Z)-octadec-9-enol	268.49	3_REACH	633333.3333		633333.3333	0	633333.3333	2.358871218				1	0.039	1.45257E-07				1	0.039	1.45257E-07	71.33333333		71.33333333	0	71.3333333	0.00026568
14338-82-0	14338820	1965	dibutyl	308.46	3_REACH	10400		10400	0	10400	0.033715879				1	0.039	1.26435E-07				1	0.039	1.26435E-07	1380		1380	0	1380	0.00447384
144-19-4	144194	1974	2,2,4-trimethylpentane-1,3-	146.23	3_REACH	420000		420000	0	420000	2.87218765				1	0.039	2.66703E-07				1	0.039	2.66703E-07	100000		100000	0	100000	0.6838542
14433-76-2	14433762	471	N,N-dimethyldecan-1-	199.34	3_REACH	5000		5000	0	5000	0.025082773	710		710	0	710	0.003561754				1	0.039	1.95646E-07	1800		1800	0	1800	0.0090298

144-62-7	144627	472	oxalic acid	90.034	3_REACH	100000	100000	0	100000	1.110691517			1	0.039	4.3317E-07			1	0.039	4.3317E-07	80000	80000	0	80000	0.88855321
144-83-2	144832	29	sulfapyridine	249.29	3_REACH			1	0.39	1.56444E-06			1	0.039	1.56444E-07			1	0.039	1.56444E-07	1760	1760	0	1760	0.00706005
1453-58-3	1453583	1985	3-methylpyrazole	82.108	3_REACH	100000	100000	0	100000	1.217908121			1	0.039	4.74984E-07			1	0.039	4.74984E-07	23210	23210	0	23210	0.28267647
145783-14-8	145783148	1988	4,6-dichloro-5-nitro-2-	268.13	3_REACH	9.5	9.5	0	9.5	3.54306E-05			1	0.039	1.45452E-07			1	0.039	1.45452E-07	18	18	0	18	6.7132E-05
1459-93-4	1459934	1990	dimethyl isophthalate	194.19	3_REACH	6300	6300	0	6300	0.032442453			1	0.039	2.00834E-07			1	0.039	2.00834E-07	2110	2110	0	2110	0.01086565
146421-65-0	146421650	4455	URACROSS P 3307	400.52	3_REACH	400	400	0	400	0.000998702			1	0.039	9.73734E-08			1	0.039	9.73734E-08	100000	100000	0	100000	0.24967542
14657-64-8	14657648	4379	3-	214.16	3_REACH	71500	71500	0	71500	0.333862533			1	0.039	1.82107E-07			1	0.039	1.82107E-07	32000	32000	0	32000	0.14942099
147315-50-2	147315502	4308	2-(4,6-diphenyl-1,3,5-	425.54	3_REACH	9200	9200	0	9200	0.021619589			1	0.039	9.16483E-08			1	0.039	9.16483E-08	74500	74500	0	74500	0.17507167
147504-92-5	147504925	4409	4,6-bis[2-(4-	378.47	3_REACH	473.3333333	473.3333333	0	473.3333333	0.00125065			1	0.039	1.03046E-07			1	0.039	1.03046E-07	509	509	0	509	0.00134489
1477-55-0	1477550	1997	m-	136.2	3_REACH	56000	56000	0	56000	0.411160059			1	0.039	2.86344E-07			1	0.039	2.86344E-07	6250	6250	0	6250	0.0458884
147-85-3	147853	1999	L-proline	115.13	3_REACH	3500000	3500000	0	3500000	30.40041692			1	0.039	3.38748E-07			1	0.039	3.38748E-07			1	1	8.6858E-06
14814-09-6	14814096	2001	3-	238.42	3_REACH	350000	350000	0	350000	1.467997651			1	0.039	1.63577E-07			1	0.039	1.63577E-07	36000	36000	0	36000	0.15099404
148528-05-6	148528056	2002	2-Methyloctane-1,8-	158.29	3_REACH	24533.33333	24533.33333	0	24533.33333	0.154989787			1	0.039	2.46383E-07			1	0.039	2.46383E-07	820	820	0	820	0.00518037
14858-73-2	14858732	2004	bis(2-ethylhexyl) carbonate	286.46	3_REACH	758	758	0	758	0.002646094			1	0.039	1.36145E-07			1	0.039	1.36145E-07	384	384	0	384	0.0013405
14901-07-6	14901076	477	4-(2,6,6-trimethylcyclohex-	192.3	3_REACH	487.254	487.254	0	487.254	0.002533822			1	0.039	2.02808E-07			1	0.039	2.02808E-07	656.195	656.195	0	656.195	0.00341235
149-30-4	149304	478	benzothiazole-2-thiol	167.25	3_REACH	243.3333333	243.3333333	0	243.3333333	0.001454908	41	41	0	41	0.000245142			1	0.039	2.33184E-07	8.333333333	8.333333333	0	8.33333333	4.9826E-05
1493-13-6	1493136	2005	trifluoromethanesulphonic	150.07	3_REACH	100000	100000	0	100000	0.666355701			1	0.039	2.59879E-07			1	0.039	2.59879E-07	5700	5700	0	5700	0.03798227
149-57-5	149575	479	2-ethylhexanoic acid	144.21	3_REACH	125000	125000	0	125000	0.866791485			1	0.039	2.70439E-07			1	0.039	2.70439E-07	32000	32000	0	32000	0.22189862
149-74-6	149746	2006	dichloro(methyl)(phenyl)sil	191.13	3_REACH	100000	100000	0	100000	0.523204102			1	0.039	2.0405E-07			1	0.039	2.0405E-07	57000	57000	0	57000	0.29822634
149850-30-6	149850306	5029	methyl N-[3-acetylamino)-4-	468.43	3_REACH	800	800	0	800	0.001707833			1	0.039	8.32568E-08			1	0.039	8.32568E-08	2300	2300	0	2300	0.00491002
150-76-5	150765	483	mequinol	124.14	3_REACH	10000	10000	0	10000	0.080554213			1	0.039	3.14161E-07			1	0.039	3.14161E-07	4400	4400	0	4400	0.03544385
150-78-7	150787	484	1,4-dimethoxybenzene	138.17	3_REACH	14366.66667	14366.66667	0	14366.66667	0.103978191	16600	16600	0	16600	0.120141854			1	0.039	2.82261E-07	6800	6800	0	6800	0.04921474
150-84-5	150845	2012	citronellyl acetate	198.31	3_REACH	2300	2300	0	2300	0.011598003			1	0.039	1.96662E-07			1	0.039	1.96662E-07	2220	2220	0	2220	0.01119459
15214-89-8	15214898	2021	2-acrylamido-2-	207.25	3_REACH	130000	130000	0	130000	0.627261761			1	0.039	1.88179E-07			1	0.039	1.88179E-07	2000000	2000000	0	2000000	9.65018094
152402-98-7	152402987	2023	2-[[(3-Methyl-4-nitro-pyridin-	300.34	3_REACH	810	810	0	810	0.002696943			1	0.039	1.29853E-07			1	0.039	1.29853E-07	1600	1600	0	1600	0.0053273
15267-95-5	15267955	2025	(chloromethyl)triethoxysilan	212.75	3_REACH	100000	100000	0	100000	0.470035253			1	0.039	1.83314E-07			1	0.039	1.83314E-07	50000	50000	0	50000	0.23501763
1530-32-1	1530321	2028	ethyltriphenylfosfonium	371.26	3_REACH	420.3333333	420.3333333	0	420.3333333	0.001132181	156	156	0	156	0.000420191			1	0.039	1.05048E-07	192.7026	192.7026	0	192.7026	0.00051905
15307-79-6	15307796	30	sodium [2-[(2,6-	318.14	3_REACH	473.3333333	473.3333333	0	473.3333333	0.001487815	1.6	1.6	0	1.6	5.02923E-06			1	0.039	1.22588E-07	160	160	0	160	0.00050292
15356-60-2	15356602	486	(+)-menthol	156.27	3_REACH	13200	13200	0	13200	0.084469188			1	0.039	2.49568E-07			1	0.039	2.49568E-07	9650	9650	0	9650	0.0617521
153719-38-1	153719381	4548	N-nitro-N-(3-methyl-3,6-	160.14	3_REACH	100000	100000	0	100000	0.624453603	115000	115000	0	115000	0.718121644			1	0.039	2.43537E-07	3200	3200	0	3200	0.01998252
15396-00-6	15396006	2033	3-(trimethoxysilyl)propyl	205.29	3_REACH	100000	100000	0	100000	0.487115787			1	0.039	1.89975E-07			1	0.039	1.89975E-07	1300	1300	0	1300	0.00633251
154279-60-4	154279604	2034	4,4'-methylenebis(N-sec-	322.58	3_REACH	5433.333333	5433.333333	0	5433.333333	0.016843367			1	0.039	1.209E-07			1	0.039	1.209E-07	0.89	0.89	0	0.89	2.759E-06
15471-17-7	15471177	2039	1-(3-	201.25	3_REACH			1	0.39	1.93789E-06	45820730	45820730	0	45820730	227.680646			1	0.039	1.93789E-07	6312990	6312990	0	6312990	31.3688944
15520-10-2	15520102	2040	2-methylpentane-1,5-	116.21	3_REACH	100000	100000	0	100000	0.860511144			1	0.039	3.35599E-07			1	0.039	3.35599E-07	3200	3200	0	3200	0.02753636
15625-89-5	15625895	2046	2-ethyl-2-[[(1-	296.32	3_REACH	490	490	0	490	0.001653618			1	0.039	1.31614E-07			1	0.039	1.31614E-07	1620	1620	0	1620	0.00546706
156-43-4	156434	2048	p-phenetidine	137.18	3_REACH	10080	10080	0	10080	0.073480099			1	0.039	2.84298E-07			1	0.039	2.84298E-07	2323.333333	2323.333333	0	2323.33333	0.01693639
1570-64-5	1570645	495	4-chloro-o-cresol	142.59	3_REACH	483.3333333	483.3333333	0	483.3333333	0.003389672			1	0.039	2.73511E-07			1	0.039	2.73511E-07	4936.666667	4936.666667	0	4936.66667	0.03462141
15721-78-5	15721785	2055	bis(4-(1,1,3,3-	393.66	3_REACH	3333.333333	3333.333333	0	3333.333333	0.008467544			1	0.039	9.90703E-08			1	0.039	9.90703E-08	5821.861903	5821.861903	0	5821.8619	0.01478906
15827-60-8	15827608	2059	[[(phosphonomethyl)imino]	573.2	3_REACH	180000	180000	0	180000	0.314026518	25600	25600	0	25600	0.044661549			1	0.039	6.80391E-08	150	150	0	150	0.00026169
15834-04-5	15834045	2060	2,2-bis[[(1-	472.62	3_REACH	4800	4800	0	4800	0.010156151			1	0.039	8.25187E-08			1	0.039	8.25187E-08	50700	50700	0	50700	0.10727434
15848-49-4	15848494	2062	Ethyl 2-(cyclopent-2-EN-1-	154.21	3_REACH	1640	1640	0	1640	0.010634849			1	0.039	2.52902E-07			1	0.039	2.52902E-07	4380	4380	0	4380	0.02840283
15894-70-9	15894709	2065	N,N'''-1,6-hexanediylbis[N'-	250.32	3_REACH	13000	13000	0	13000	0.051933525			1	0.039	1.55801E-07			1	0.039	1.55801E-07	2500	2500	0	2500	0.00998722
15993-42-7	15993427	2069	N-(5-chloro-2-	420.81	3_REACH	1000	1000	0	1000	0.002376369			1	0.039	9.26784E-08			1	0.039	9.26784E-08	1000	1000	0	1000	0.00237637
16111-62-9	16111629	2079	bis(2-ethylhexyl)	346.46	3_REACH	14000	14000	0	14000	0.040408705			1	0.039	1.12567E-07			1	0.039	1.12567E-07	7260	7260	0	7260	0.0209548
161462-35-7	161462357	4456	1-cyclopropyl-3-(2-	302.31	3_REACH	130	130	0	130	0.000430022			1	0.039	1.29007E-07			1	0.039	1.29007E-07	40	40	0	40	0.00013231
16219-75-3	16219753	2083	5-ethylidene-8,9,10-	120.19	3_REACH	1040	1040	0	1040	0.008652966	364	364	0	364	0.003028538			1	0.039	3.24486E-07	852	852	0	852	0.00708878
162208-27-7	162208277	4901	Diethyl thiophosphoril-(z)-	353.36	3_REACH	1800	1800	0	1800	0.005093955			1	0.039	1.10369E-07			1	0.039	1.10369E-07	11000	11000	0	11000	0.03112973
16298-38-7	16298387	4407	4,4'-methylenebis(2-	310.49	3_REACH	390	390	0	390	0.001256079			1	0.039	1.25608E-07			1	0.039	1.25608E-07	5900	5900	0	5900	0.01900222
16415-12-6	16415126	2092	hexadecyltrimethoxysilane	346.63	3_REACH	1000000	1000000	0	1000000	2.88492052			1	0.039	1.12512E-07			1	0.039	1.12512E-07	300	300	0	300	0.00086548
164578-11-4	164578114	4335	2,9-bis[N-[3-	696.9	3_REACH	33333.33333	33333.33333	0	33333.33333	0.04783087			1	0.039	5.59621E-08			1	0.039	5.59621E-08	9	9	0	9	1.2914E-05
165184-98-5	165184985	2096	alpha-	216.32	3_REACH	930	930	0	930	0.004299186			1	0.039	1.80288E-07			1	0.039	1.80288E-07	65	65	0	65	0.00030048
16634-82-5	16634825	4584	2-Chloro-N-(4-	183.64	3_REACH	720	720	0	720	0.003920714			1	0.039	2.12372E-07			1	0.039	2.12372E-07	10	10	0	10	5.4454E-05
166524-65-8	166524658	2105	2-ethoxy-4,6-	160.13	3_REACH	3000	3000	0	3000	0.018734778			1	0.039	2.43552E-07			1	0.039	2.43552E-07	15000	15000	0	15000	0.09367389
167004-78-6	167004786	2110	3-	261.26	3_REACH	3200	3200	0	3200	0.012248335			1	0.039	1.49277E-07			1	0.039	1.49277E-07	41	41	0	41	0.00015693
16712-64-4	16712644	2111	6-hydroxy-2-naphthoic acid	188.18	3_REACH	40800	40800	0	40800	0.216813689			1	0.039	2.07248E-07			1	0.039	2.07248E-07	7210	7210	0	7210	0.03831438
1696-20-4	1696204	2118	4-acetylmorpholine	129.16	3_REACH	4600000	4600000	0	4600000	35.61474141			1	0.039	3.01951E-07			1	0.039	3.01951E-07	35300	35300	0	35300	0.27330443
1704-62-7	1704627	2119	2-[2-	133.19	3_REACH	215000	215000	0	215000	1.614235303			1	0.039	2.92815E-07			1	0.039	2.92815E-07	23000	23000	0	23000	0.17268564
1709-70-2	1709702	2121	Tris-bht mesitylene	775.22	3_REACH	1200	1200	0	1200	0.001547948			1	0.039	5.03083E-08			1	0.039	5.03083E-08	100000	100000	0	100000	0.12899564
1724-39-6	1724396	2126	cyclododecanol	184.32	3_REACH	1300	1300	0	1300	0.007052951			1	0.039	2.11589E-07			1	0.039	2.11589E-07	1000	1000	0	1000	0.00542535
172529-93-0	172529930	2128	1,3-dimethyl 2-[2-(2-amino-	327.73	3_REACH	136000	136000	0	136000	0.414975742			1	0.039	1.19E-07			1	0.039	1.19E-07	8100	8100	0	8100	0.02471547
1738-25-6	1738256	2132	3-	98.151	3_REACH	215000	215000	0	215000	2.190502389			1	0.039	3.97347E-07			1	0.039	3.97347E-07	30300	30300	0	30300	0.30870801
173904-11-5	173904115	2133	N,N'-[cyclohexane-1,3-	250.43	3_REACH	6250	6250	0	6250	0.024957074			1	0.039	1.55732E-07			1	0.039	1.55732E-07	6130	6130	0	6130	0.0244779
1739-84-0	1739840	2135	1,2-dimethylimidazole	96.135	3_REACH	21500	21500	0	21500	0.223643834			1	0.039	4.0568E-07			1	0.039	4.0568E-07	8820	8820	0	8820	0.09174598
174489-43-1	174489431	2137	1-(allyloxy)-2-methyl-1-	297.74	3_REACH	180	180	0	180	0.000604554			1	0.039	1.30987E-07			1	0.039	1.30987E-07	9050	9050	0	9050	0.03039565
174489-76-0	174489760	2138	1-(allyloxy)-2-methyl-1-	327.72	3_REACH	220	220	0	220	0.000671305			1	0.039	1.19004E-07			1	0.039	1.19004E-07	715	715	0	715	0.00218174
1746-23-2	1746232	2139	p-tert-butylstyrene	160.26	3_REACH	660	660	0	660	0.004118308	108	108	0	108	0.000673905			1	0.039	2.43355E-07	1600	1600	0	1600	0.00998378
1760-24-3	1760243	2145	N-(3-	222.36	3_REACH	344000	344000	0	344000	1.547040835			1	0.039	1.75391E-07			1	0.039	1.75391E-07	1600	1600	0	1600	0.00719554
17689-77-9	17689779	2148	triacetoxyethylsilane	234.28	3_REACH	27792.88478	27792.88478	0	27792.88478	0.11863106			1	0.039	1.66467E-07			1	0.039	1.66467E-07	16980	16980	0	16980	0.07247738
176969-34-9	176969349	2150	3-(difluoromethyl)-1-methyl-	176.12	3_REACH	100000	100000	0	100000	0.567794685			1	0.039	2.2144E-07			1	0.039	2.2144E-07	19430	19430	0	19430	0.11032251
17796-82-6	17796826	2153	N-	261.34	3_REACH	390	390	0	390	0.001492309			1	0.039	1.49231E-07			1	0.039	1.49231E-07	93	93	0	93	0.00035586
17832-28-9	17832289	2154	4-(vinyloxy)butan-1-ol	116.16	3_REACH	19100	19100	0	19100	0.164428375			1	0.039	3.35744E-07			1	0.039	3.35744E-07	9820	9820	0	9820	0.08453857
17865-07-5	17865075	2155	propyltriacetoxysilane	248.31	3_REACH	27792.88478	27792.88478	0	27792.88478	0.111928174			1	0.039	1.57062E-07			1	0.039	1.57062E-07	18000	18000	0	18000	0.07249003
17928-28-8	17928288	2158	1,1,1,3,5,5,5-heptamethyl-	310.69	3_REACH	6.3	6.3	0	6.3	2.02774E-05	5.3	5.3	0	5.3	1.70588E-05			1	0.039	1.25527E-07	2.2	2.2	0	2.2	7.081E-06
18063-03-1	18063031	2163	2,6-difluorobenzamide	157.12	3_REACH	100000	100000	0	100000	0.636456212			1	0.039	2.48218E-07			1	0.039	2.48218E-07	77700	77700	0	77700	0.49452648
1809-19-4	1809194	2164	dibutyl phosphonate	194.21	3_REACH	37900	37900	0	37900	0.19514958			1	0.039	2.00814E-07			1	0.039	2.00814E-07	3000	3000	0	3000	0.0154472
18127-01-0	18127010	2166	3-(4-tert-	190.29	3_REACH	348.3333333	348.3333333	0	348.3333333	0.001830539			1	0.039	2.0495E-07			1	0.039	2.0495E-07	200	200	0	200	0.00105103
181587-01-9	181587019	4655	Ethiprole	397.21	3_REACH	50	50	0	50	0.000125878	10	10	0	10	2.51756E-05			1	0.039	9.81848E-08	470	470	0	470	0.00118325
18171-19-2	18171192	2172	(3-	182.72	3_REACH	107000	107000	0	107000	0.585595447			1	0.039	2.13441E-07			1	0.039	2.13441E-07	57000	57000	0	57000	0.31195271
18379-25-4	18379254	2187	trichloro(2,4,4-	247.67	3_REACH	100000	100000	0	100000	0.403763072			1	0.039	1.57468E-07			1	0.039	1.57468E-07	100000	100000	0	100000	0.40376307
1843-03-4	1843034	2190	4,4',4''-(1-methylpropanyl-3	544.82	3_REACH	100000	100000	0	100000	0.18354686			1	0.039	7.15833E-08			1	0.039	7.15833E-08	1000000	1000000	0	1000000	1.8354686
18479-58-8	18479588	2192	2,6-dimethyloct-7-en-2-ol	156.27	3_REACH	3500	3500	0	3500	0.022397133			1	0.039	2.49568E-07			1	0.039	2.49568E-07	25000	25000	0	25000	0.15997952
1852-17-1	1852171	2196	perhydropyrimidin-2-one	100.12	3_REACH	10000000	10000000	0	10000000	99.88014383			1	0.039	3.89533E-07			1	0.039	3.89533E-07	5333333.333	5333333.333	0	5333333.33	53.26941
18600-59-4	18600594	4312	2,2-(1,4-phenylene)bis((4H-	368.35	3_REACH	250	250	0	250	0.000678702			1	0.039	1.05878E-07			1	0.039	1.05878E-07	20	20	0	20	5.4296E-05
1860-26-0	1860260	2200	2-ethyl-N,N-bis(2-	353.68	3_REACH	68100	68100	0	68100	0.192546935			1	0.039	1.10269E-07			1	0.039	1.10269E-07	100000	100000	0	100000	0.28274146
186817-80-1	186817801	2203	Propanoic acid, 2-hydroxy-,	202.29	3_REACH	3333.333333	3333.333333	0	3333.333333	0.016477994	2180	2180	0	2180	0.010776608			1	0.039	1.92793E-07	3666.666667	3666.666667	0	3666.66667	0.01812579
1879-09-0	1879090	2209	6-tert-butyl-2,4-xylenol	178.28	3_REACH	833.3333333	833.3333333	0	833.3333333	0.004674295			1	0.039	2.18757E-07			1	0.039	2.18757E-07	380	380	0	380	0.00213148
18835-33-1	18835331	2210	hexacos-1-ene	364.7	3_REACH	1000000	1000000	0	1000000	2.741979709			1	0.039	1.06937E-07			1	0.039	1.06937E-07	1000000	1000000	0	1000000	2.74197971
18835-34-2	18835342	2211	octacos-1-ene	392.76	3_REACH	1000000	1000000	0	1000000	2.546084123			1	0.039	9.92973E-08			1	0.039	9.92973E-08	1000000	1000000	0	1000000	2.54608412
1889-67-4	1889674	2214	1,1'-(1,1,2,2-	238.37	3_REACH	316227.766	316227.766	0	316227.766	1.326625691			1	0.039	1.63611E-07			1	0.039	1.63611E-07	316227.766	316227.766	0	316227.766	1.32662569
19234-20-9	19234209	2228	2-(1-methylethoxy)ethyl	146.19	3_REACH	32000	32000	0	32000	0.218893221			1	0.039	2.66776E-07			1	0.039	2.66776E-07	100000	100000	0	100000	0.68404132
19444-21-4	19444214	2233	allyl 2-hydroxy-2-	144.17	3_REACH	990	990	0	990	0.006866893			1	0.039	2.70514E-07			1	0.039	2.70514E-07	2000	2000	0	2000	0.01387251
1948-33-0	1948330	523	2-tert-butylhydroquinone	166.22	3_REACH	19.66666667	19.66666667	0	19.66666667	0.000118317			1	0.039	2.34629E-07			1	0.039	2.34629E-07	137.6666667	137.6666667	0	137.666667	0.00082822
1955-46-0	1955460	2235	methyl 5-	225.16	3_REACH	10140.31667	10140.31667	0	10140.31667	0.045036048	57402	57402	0	57402	0.25493871			1	0.039	1.7321E-07	8284.88	8284.88	0	8284.88	0.03679552
1962-75-0	1962750	525	dibutyl terephthalate	278.35	3_REACH	100	100	0	100	0.00035926	24	24	0	24	8.62224E-05			1	0.039	1.40111E-07	13	13	0	13	4.6704E-05
1975-78-6	1975786	2239	decanenitrile	153.27	3_REACH	1062	1062	0	1062	0.006928949			1	0.039	2.54453E-07			1	0.039	2.54453E-07	802.6666667	802.6666667	0	802.666667	0.00523695
1999-85-5	1999855	2247	alpha,alpha'-Dihydroxy-1,3-	194.27	3_REACH	150000	150000	0	150000	0.772121275	150000	150000	0	150000	0.772121275			1	0.039	2.00752E-07	100000	100000	0	100000	0.51474752
20030-30-2	20030302	2248	2,5,6-trimethylcyclohex-2-	138.21	3_REACH	21500	21500	0	21500	0.155560379			1	0.039	2.82179E-07			1	0.039	2.82179E-07	59700	59700	0	59700	0.43195138
20120-33-6	20120336	2250	dimethyl [3-	211.16	3_REACH	978000	978000	0	978000	4.631559007			1	0.039	1.84694E-07			1	0.039	1.84694E-07	14000	14000	0	14000	0.06630044
20292-08-4	20292084	2257	2-ethylhexyl laurate	312.54	3_REACH	1000000	1000000	0	1000000	3.199590452			1	0.039	1.24784E-07			1	0.039	1.24784E-07	33333.33333	33333.33333	0	33333.3333	0.10665302
20298-69-5	20298695	2258	cis-2-tert-butylcyclohexyl	198.31	3_REACH	1866.666667	1866.666667	0	1866.666667	0.009412872			1	0.039	1.96662E-07			1	0.039	1.96662E-07	570	570	0	570	0.00287429
2031-67-6	2031676	2259	triethoxy(methyl)silane	178.3	3_REACH	133333.3333	133333.3333	0	133333.3333	0.747803328			1	0.039	2.18732E-07			1	0.039	2.18732E-07	500000	500000	0	500000	2.80426248
2040-90-6	2040906	4576	2-chloro-6-fluoro-phenol	146.55	3_REACH	18000	18000	0	18000	0.122824974			1	0.039	2.66121E-07			1	0.039	2.66121E-07	3900	3900	0	3900	0.02661208
2044-64-6	2044646	2265	N,N-dimethyl-3-	129.16	3_REACH	977740	977740	0	977740	7.569990709			1	0.039	3.01951E-07			1	0.039	3.01951E-07	122700	122700	0	122700	0.94998452
204918-22-9	204918229	2267	1-(allyloxy)-2-methyl-1-	323.73	3_REACH	466.6666667	466.6666667	0	466.6666667	0.00144153			1	0.039	1.20471E-07			1	0.039	1.20471E-07	3800	3800	0	3800	0.01173818
20592-85-2	20592852	2271	[nitrilotris(methylene)]trisph	299.05	3_REACH	53333.33333	53333.33333	0	53333.33333	0.178342529	23000	23000	0	23000	0.076910216			1	0.039	1.30413E-07	93000	93000	0	93000	0.31098479
20749-68-2	20749682	2272	8,9,10,11-tetrachloro-12H-	408.07	3_REACH	100000	100000	0	100000	0.245055995			1	0.039	9.55718E-08			1	0.039	9.55718E-08	100000	100000	0	100000	0.245056
2082-81-7	2082817	2277	tetramethylene	226.27	3_REACH	25000	25000	0	25000	0.110487471			1	0.039	1.7236E-07			1	0.039	1.7236E-07	2110	2110	0	2110	0.00932514
21282-97-3	21282973	2288	2-[(2-methyl-1-	214.22	3_REACH	38800	38800	0	38800	0.181122211			1	0.039	1.82056E-07			1	0.039	1.82056E-07	11100	11100	0	11100	0.05181589
2135-17-3	2135173	532	flumetasone	410.46	3_REACH	33333.57696	33333.57696	0	33333.57696	0.081210293			1	0.039	9.50153E-08			1	0.039	9.50153E-08	33333.57696	33333.57696	0	33333.577	0.08121029
2146-71-6	2146716	2295	vinyl laurate	226.36	3_REACH	100000	100000	0	100000	0.441774165			1	0.039	1.72292E-07			1	0.039	1.72292E-07	250	250	0	250	0.00110444
21542-96-1	21542961	2298	N,N-dimethyldocosylamine	353.68	3_REACH	22000	22000	0	22000	0.062203121			1	0.039	1.10269E-07			1	0.039	1.10269E-07	0.26	0.26	0	0.26	7.3513E-07
2156-97-0	2156970	533	dodecyl acrylate	240.39	3_REACH	4340	4340	0	4340	0.018053996			1	0.039	1.62236E-07			1	0.039	1.62236E-07	21300	21300	0	21300	0.08860602
2162-73-4	2162734	2299	2,4,6-triisopropyl-m-	286.38	3_REACH	54833.33333	54833.33333	0	54833.33333	0.19147054	0.365	0.365	0	0.365	1.27453E-06			1	0.039	1.36183E-07	21	21	0	21	7.3329E-05
2162-74-5	2162745	2300	bis(2,6-	362.56	3_REACH	100	100	0	100	0.000275816	0.0559	0.0559	0	0.0559	1.54181E-07			1	0.039	1.07568E-07	1000	1000	0	1000	0.00275816
2163-00-0	2163000	2301	1,6-dichlorohexane	155.07	3_REACH	7300	7300	0	7300	0.047075514			1	0.039	2.51499E-07			1	0.039	2.51499E-07	3240	3240	0	3240	0.02089379
2163-42-0	2163420	4357	2-methyl-1,3-propanediol	90.122	3_REACH	1000000	1000000	0	1000000	11.09606977			1	0.039	4.32747E-07			1	0.039	4.32747E-07	1000000	1000000	0	1000000	11.0960698
21643-42-5	21643425	2302	tetradecyl acrylate	268.44	3_REACH	4340	4340	0	4340	0.016167486			1	0.039	1.45284E-07			1	0.039	1.45284E-07	21300	21300	0	21300	0.07934734
21743-27-1	21743271	4770	4-	263.41	3_REACH	95700	95700	0	95700	0.363311947			1	0.039	1.48058E-07			1	0.039	1.48058E-07	800	800	0	800	0.00303709
2186-92-7	2186927	2308	p-(dimethoxymethyl)anisole	182.22	3_REACH	100000	100000	0	100000	0.54878718			1	0.039	2.14027E-07			1	0.039	2.14027E-07	95000	95000	0	95000	0.52134782
22047-49-0	22047490	2316	2-ethylhexyl stearate	396.7	3_REACH	10000000	10000000	0	10000000	25.20796572			1	0.039	9.83111E-08			1	0.039	9.83111E-08	30000	30000	0	30000	0.0756239
220727-26-4	220727264	4596	S-(3-	364.616	3_REACH	17	17	0	17	4.66244E-05			1	0.039	1.06962E-07			1	0.039	1.06962E-07	1.8	1.8	0	1.8	4.9367E-06
22094-93-5	22094935	2317	2,2'-[(2,2',5,5'-	754.51	3_REACH	100	100	0	100	0.000132536			1	0.039	5.16892E-08			1	0.039	5.16892E-08	100000	100000	0	100000	0.13253635
2210-79-9	2210799	2319	2,3-epoxypropyl o-tolyl	164.2	3_REACH	1259.629575	1259.629575	0	1259.629575	0.007671313			1	0.039	2.37515E-07			1	0.039	2.37515E-07	1700	1700	0	1700	0.01035323
2216-51-5	2216515	538	L-menthol	156.27	3_REACH	13200	13200	0	13200	0.084469188			1	0.039	2.49568E-07			1	0.039	2.49568E-07	9650	9650	0	9650	0.0617521
2224-33-1	2224331	2325	butan-2-one O,O',O''-	313.48	3_REACH	15000	15000	0	15000	0.047849943	50000	50000	0	50000	0.159499809			1	0.039	1.2441E-07	1000	1000	0	1000	0.00319
2226-96-2	2226962	2327	4-hydroxy-2,2,6,6-	173.26	3_REACH	200000	200000	0	200000	1.154334526			1	0.039	2.25095E-07			1	0.039	2.25095E-07	22000	22000	0	22000	0.1269768
2235-00-9	2235009	2331	1-vinylhexahydro-2H-	139.2	3_REACH	208000	208000	0	208000	1.494252874			1	0.039	2.80172E-07			1	0.039	2.80172E-07	25000	25000	0	25000	0.1795977
224049-04-1	224049041	2333	Isotianil	298.15	3_REACH	710	710	0	710	0.002381352			1	0.039	1.30807E-07			1	0.039	1.30807E-07	220	220	0	220	0.00073788
2243-62-1	2243621	542	1,5-naphthylenediamine	158.21	3_REACH	15000	15000	0	15000	0.094810695			1	0.039	2.46508E-07			1	0.039	2.46508E-07	32	32	0	32	0.00020226
2280-49-1	2280491	2338	N-phenyl-N-	382.72	3_REACH	400000	400000	0	400000	1.045150502			1	0.039	1.01902E-07			1	0.039	1.01902E-07	100000	100000	0	100000	0.26128763
22871-58-5	22871585	2340	3-Amino-5-((2-	601.89	3_REACH	100000	100000	0	100000	0.166143315			1	0.039	6.47959E-08			1	0.039	6.47959E-08	100000	100000	0	100000	0.16614332
22984-54-9	22984549	2341	butan-2-one O,O',O''-	301.47	3_REACH	15000	15000	0	15000	0.049756195	50000	50000	0	50000	0.165853982			1	0.039	1.29366E-07	1000	1000	0	1000	0.00331708
2312-35-8	2312358	548	propargite	350.48	3_REACH	14	14	0	14	3.99452E-05	5.7	5.7	0	5.7	1.62634E-05			1	0.039	1.11276E-07	1.27	1.27	0	1.27	3.6236E-06
232938-43-1	232938431	4564	3-(3-Tosylureido)phenyl p-	460.53	3_REACH			1	0.39	8.4685E-07	890	890	0	890	0.001932556			1	0.039	8.4685E-08	140	140	0	140	0.000304
23410-40-4	23410404	2351	N-[3-(dimethoxymethylsilyl)	220.39	3_REACH	344000	344000	0	344000	1.560869368			1	0.039	1.76959E-07			1	0.039	1.76959E-07	1600	1600	0	1600	0.00725986
2362-14-3	2362143	2353	4,4'-cyclohexylidenedi-o-	296.41	3_REACH	143	143	0	143	0.00048244			1	0.039	1.31575E-07			1	0.039	1.31575E-07	161	161	0	161	0.00054317
2370-88-9	2370889	2355	2,4,6,8-	236.48	3_REACH	213333333.3	213333333.3	0	213333333.3	902.119982			1	0.039	1.64919E-07			1	0.039	1.64919E-07	100000	100000	0	100000	0.42286874
2372-82-9	2372829	554	N-(3-aminopropyl)-N-	299.55	3_REACH	180	180	0	180	0.000600901			1	0.039	1.30195E-07			1	0.039	1.30195E-07	6.9	6.9	0	6.9	2.3035E-05
23779-32-0	23779320	2358	[3-	264.4	3_REACH	100000	100000	0	100000	0.378214826			1	0.039	1.47504E-07			1	0.039	1.47504E-07	10000	10000	0	10000	0.03782148
23783-42-8	23783428	2359	3,6,9,12-tetraoxotridecanol	208.25	3_REACH	10000000	10000000	0	10000000	48.01920768	11482000	11482000	0	11482000	55.13565426			1	0.039	1.87275E-07	1000000	1000000	0	1000000	4.80192077
2380-86-1	2380861	4816	6-hydroxyindole	133.15	3_REACH	7233.333333	7233.333333	0	7233.333333	0.054324696			1	0.039	2.92903E-07			1	0.039	2.92903E-07	640	640	0	640	0.00480661
23847-08-7	23847087	2360	1,1'-dithiobis[hexahydro-2H	288.43	3_REACH	5600	5600	0	5600	0.019415456	158070	158070	0	158070	0.548035919			1	0.039	1.35215E-07	70660	70660	0	70660	0.24498145
2385-77-5	2385775	2361	(R)-3,7-dimethyloct-6-enal	154.25	3_REACH	10000	10000	0	10000	0.064829822			1	0.039	2.52836E-07			1	0.039	2.52836E-07	1260	1260	0	1260	0.00816856
2386-87-0	2386870	2362	7-oxabicyclo[4.1.0]hept-3-	252.31	3_REACH	3200	3200	0	3200	0.012682811			1	0.039	1.54572E-07			1	0.039	1.54572E-07	22000	22000	0	22000	0.08719432
2402-79-1	2402791	2367	2,3,5,6-tetrachloropyridine	216.88	3_REACH	330	330	0	330	0.001521579			1	0.039	1.79823E-07			1	0.039	1.79823E-07	2300	2300	0	2300	0.01060494
2403-88-5	2403885	2368	2,2,6,6-tetramethylpiperidin	157.26	3_REACH	200000	200000	0	200000	1.271779219	25000	25000	0	25000	0.158972402			1	0.039	2.47997E-07	10000	10000	0	10000	0.06358896
2403-89-6	2403896	2369	1,2,2,6,6-	171.29	3_REACH	32400	32400	0	32400	0.189152899			1	0.039	2.27684E-07			1	0.039	2.27684E-07	866.6666667	866.6666667	0	866.666667	0.00505965
24085-06-1	24085061	2372	(5-Acetyl-2-	250.25	3_REACH	20	20	0	20	7.99201E-05			1	0.039	1.55844E-07			1	0.039	1.55844E-07	340	340	0	340	0.00135864

2409-55-4	2409554	2373	2-tert-butyl-p-cresol	164.25	3_REACH	1000	1000	0	1000	0.00608828			1	0.039	2.37443E-07			1	0.039	2.37443E-07	190	190	0	190	0.00115677
2416-94-6	2416946	558	2,3,6-trimethylphenol	136.19	3_REACH	3980	3980	0	3980	0.029223878			1	0.039	2.86365E-07			1	0.039	2.86365E-07	15000	15000	0	15000	0.11014025
24199-46-0	24199460	2376	6-methyloct-5-en-2-one	140.23	3_REACH	16666.66667	16666.66667	0	16666.66667	0.118852362			1	0.039	2.78115E-07			1	0.039	2.78115E-07	3400	3400	0	3400	0.02424588
2421-28-5	2421285	2378	benzophenone-3,3',4,4'-	322.23	3_REACH	1864000	1864000	0	1864000	5.784687956			1	0.039	1.21032E-07			1	0.039	1.21032E-07	25000	25000	0	25000	0.07758433
2425-77-6	2425776	2381	2-hexyldecan-1-ol	242.45	3_REACH	320	320	0	320	0.00131986			1	0.039	1.60858E-07			1	0.039	1.60858E-07	5.15	5.15	0	5.15	2.1241E-05
24279-39-8	24279398	4333	2,6-dichloro-4-	230.02	3_REACH	70	70	0	70	0.000304321			1	0.039	1.6955E-07			1	0.039	1.6955E-07	430	430	0	430	0.0018694
24293-43-4	24293434	2384	bis(2-ethylhexyl) 2,2'-	374.58	3_REACH	300	300	0	300	0.000800897			1	0.039	1.04117E-07			1	0.039	1.04117E-07	25	25	0	25	6.6741E-05
2439-35-2	2439352	2391	2-(dimethylamino)ethyl	143.19	3_REACH	4600	4600	0	4600	0.032125148	1000	1000	0	1000	0.006983728			1	0.039	2.72365E-07	10	10	0	10	6.9837E-05
24424-99-5	24424995	2393	di(tert-butyl) carbonate	218.25	3_REACH	73333.33333	73333.33333	0	73333.33333	0.336006109	23000	23000	0	23000	0.105383734			1	0.039	1.78694E-07	18000	18000	0	18000	0.08247423
24468-13-1	24468131	2395	2-ethylhexyl chloroformate	192.69	3_REACH	1000	1000	0	1000	0.005189683			1	0.039	2.02398E-07			1	0.039	2.02398E-07	97	97	0	97	0.0005034
24549-06-2	24549062	2397	6-ethyl-2-toluidine	135.21	3_REACH	32000	32000	0	32000	0.236668885			1	0.039	2.8844E-07			1	0.039	2.8844E-07	9400	9400	0	9400	0.06952149
2461-15-6	2461156	561	[[(2-	186.29	3_REACH	4666.666667	4666.666667	0	4666.666667	0.025050548			1	0.039	2.09351E-07			1	0.039	2.09351E-07	500000	500000	0	500000	2.68398733
24650-42-8	24650428	2400	2,2-dimethoxy-1,2-	256.3	3_REACH	9890	9890	0	9890	0.038587593	3215	3215	0	3215	0.012543894			1	0.039	1.52165E-07	6555.333333	6555.333333	0	6555.33333	0.0255768
24800-44-0	24800440	2404	[(methylethylene)bis(oxy)]di	192.26	3_REACH	6122666.667	6122666.667	0	6122666.667	31.84576442	1631000	1631000	0	1631000	8.483303859			1	0.039	2.0285E-07	1000000	1000000	0	1000000	5.20128992
24863-70-5	24863705	2405	1-Cyclopentene-1-acetic	224.3	3_REACH	5450	5450	0	5450	0.024297815			1	0.039	1.73874E-07			1	0.039	1.73874E-07	12500	12500	0	12500	0.05572893
2495-37-6	2495376	565	benzyl methacrylate	176.22	3_REACH	4480	4480	0	4480	0.025422767			1	0.039	2.21314E-07			1	0.039	2.21314E-07	899	899	0	899	0.00510158
2500-88-1	2500881	2411	dioctadecyl disulphide	571.12	3_REACH	100000	100000	0	100000	0.175094551			1	0.039	6.82869E-08			1	0.039	6.82869E-08	100000	100000	0	100000	0.17509455
25013-15-4	25013154	2412	vinyltoluene	118.18	3_REACH	866.6666667	866.6666667	0	866.6666667	0.007333446	563	563	0	563	0.004763919			1	0.039	3.30005E-07	866.6666667	866.6666667	0	866.666667	0.00733345
2512-29-0	2512290	2416	2-[(4-methyl-2-	340.34	3_REACH	1000	1000	0	1000	0.002938238			1	0.039	1.14591E-07			1	0.039	1.14591E-07	1000	1000	0	1000	0.00293824
25265-71-8	25265718	566	oxydipropanol	134.18	3_REACH	1666666.667	1666666.667	0	1666666.667	12.42112585	1340000	1340000	0	1340000	9.986585184			1	0.039	2.90654E-07	322666.6667	322666.6667	0	322666.667	2.40472996
25265-77-4	25265774	2426	isobutyric acid, monoester	216.32	3_REACH	4300	4300	0	4300	0.019877959			1	0.039	1.80288E-07			1	0.039	1.80288E-07	2000	2000	0	2000	0.00924556
2526-62-7	2526627	2427	3-	175.26	3_REACH	110000	110000	0	110000	0.627638936			1	0.039	2.22527E-07			1	0.039	2.22527E-07	1800	1800	0	1800	0.01027046
2528-61-2	2528612	2428	heptanoyl chloride	148.63	3_REACH	1640	1640	0	1640	0.011034112			1	0.039	2.62397E-07			1	0.039	2.62397E-07	97	97	0	97	0.00065263
25307-17-9	25307179	2429	2,2'-(octadec-9-	355.61	3_REACH	33.33333333	33.33333333	0	33.33333333	9.37356E-05			1	0.039	1.09671E-07			1	0.039	1.09671E-07	2.4	2.4	0	2.4	6.749E-06
2530-87-2	2530872	2430	3-	198.72	3_REACH	100000	100000	0	100000	0.503220612			1	0.039	1.96256E-07			1	0.039	1.96256E-07	167000	167000	0	167000	0.84037842
25322-69-4	25322694	568	Propane-1,2-diol,	134.175	3_REACH	216666.6667	216666.6667	0	216666.6667	1.614806534	1878000	1878000	0	1878000	13.99664617			1	0.039	2.90665E-07	100000	100000	0	100000	0.74529532
25498-49-1	25498491	2436	[2-(2-	206.28	3_REACH	5600000	5600000	0	5600000	27.14756641			1	0.039	1.89063E-07			1	0.039	1.89063E-07	3023000	3023000	0	3023000	14.6548381
2550-26-7	2550267	2437	4-phenylbutan-2-one	148.21	3_REACH	54000	54000	0	54000	0.364347885			1	0.039	2.6314E-07			1	0.039	2.6314E-07	24800	24800	0	24800	0.16733014
25601-41-6	25601416	2440	Methyl 9-decenoate	184.28	3_REACH	1600	1600	0	1600	0.00868244			1	0.039	2.11634E-07			1	0.039	2.11634E-07	120	120	0	120	0.00065118
256473-04-8	256473048	2441	2-Chloro-3-(2,2,2-	211.57	3_REACH	3666.666667	3666.666667	0	3666.666667	0.017330749			1	0.039	1.84336E-07			1	0.039	1.84336E-07	16500	16500	0	16500	0.07798837
256473-05-9	256473059	2442	2-(isopropylthio)-3-(2,2,2-	251.27	3_REACH	796.6666667	796.6666667	0	796.6666667	0.00317056			1	0.039	1.55212E-07			1	0.039	1.55212E-07	2060	2060	0	2060	0.00819835
2568-90-3	2568903	2443	1,1'-	160.26	3_REACH	9114.666667	9114.666667	0	9114.666667	0.056874246	2903	2903	0	2903	0.018114314			1	0.039	2.43355E-07	5077	5077	0	5077	0.03167977
2602-34-8	2602348	2449	[3-(2,3-	278.42	3_REACH	71000	71000	0	71000	0.255010416			1	0.039	1.40076E-07			1	0.039	1.40076E-07	53000	53000	0	53000	0.19035989
2605-79-0	2605790	2452	N,N-dimethyldecylamine N-	201.35	3_REACH	800	800	0	800	0.003973181	420	420	0	420	0.00208592			1	0.039	1.93693E-07	2	2	0	2	9.933E-06
2612-57-9	2612579	2455	2,4-dichlorophenyl	188.01	3_REACH	14000	14000	0	14000	0.074464124			1	0.039	2.07436E-07			1	0.039	2.07436E-07	2000	2000	0	2000	0.01063773
26159-31-9	26159319	572	(±)-2-(6-methoxy-2-	230.26	3_REACH	64333.33333	64333.33333	0	64333.33333	0.279394308	21300	21300	0	21300	0.092504126			1	0.039	1.69374E-07	46000	46000	0	46000	0.19977417
26218-04-2	26218042	4353	2-ethylhexyl 4-	249.35	3_REACH	170	170	0	170	0.000681773			1	0.039	1.56407E-07			1	0.039	1.56407E-07	160	160	0	160	0.00064167
26272-90-2	26272902	2460	hexadecyl chloroformate	304.9	3_REACH	400	400	0	400	0.001311906			1	0.039	1.27911E-07			1	0.039	1.27911E-07	97	97	0	97	0.00031814
2627-86-3	2627863	2461	L-1-Phenylethylamine	121.18	3_REACH	5666.666667	5666.666667	0	5666.666667	0.046762392			1	0.039	3.21835E-07			1	0.039	3.21835E-07	2400	2400	0	2400	0.01980525
26364-65-8	26364658	4511	2-	127.17	3_REACH	100000	100000	0	100000	0.786348982			1	0.039	3.06676E-07			1	0.039	3.06676E-07	56000	56000	0	56000	0.44035543
26399-02-0	26399020	2468	2-ethylhexyl oleate	394.68	3_REACH	10000000	10000000	0	10000000	25.33698186			1	0.039	9.88142E-08			1	0.039	9.88142E-08	33333.33333	33333.33333	0	33333.3333	0.08445661
26523-78-4	26523784	2474	tris(nonylphenyl) phosphite	689.02	3_REACH	5800	5800	0	5800	0.008417753			1	0.039	5.66021E-08			1	0.039	5.66021E-08	100000	100000	0	100000	0.14513367
26586-02-7	26586027	2480	(E)-3-formylbut-2-enyl	142.15	3_REACH	10000	10000	0	10000	0.070348224			1	0.039	2.74358E-07			1	0.039	2.74358E-07	1820	1820	0	1820	0.01280338
26741-53-7	26741537	2485	3,9-bis(2,4-di-tert-	604.71	3_REACH	50000	50000	0	50000	0.082684262			1	0.039	6.44937E-08			1	0.039	6.44937E-08	15400	15400	0	15400	0.02546675
26761-45-5	26761455	2487	2,3-epoxypropyl	228.33	3_REACH	1666.666667	1666.666667	0	1666.666667	0.007299377			1	0.039	1.70805E-07			1	0.039	1.70805E-07	400	400	0	400	0.00175185
2687-91-4	2687914	2489	1-ethylpyrrolidin-2-one	113.16	3_REACH	215000	215000	0	215000	1.899964652			1	0.039	3.44645E-07			1	0.039	3.44645E-07	101000	101000	0	101000	0.89254153
26896-20-8	26896208	2491	neodecanoic acid	172.27	3_REACH	57735.02692	57735.02692	0	57735.02692	0.335142665	1600	1600	0	1600	0.009287746			1	0.039	2.26389E-07	29666.66667	29666.66667	0	29666.6667	0.17221029
2691-41-0	2691410	575	octahydro-1,3,5,7-tetranitro-	296.16	3_REACH	15000	15000	0	15000	0.050648298			1	0.039	1.31686E-07			1	0.039	1.31686E-07	10666.66667	10666.66667	0	10666.6667	0.03601657
2705-87-5	2705875	2493	allyl 3-	196.29	3_REACH	58	58	0	58	0.000295481			1	0.039	1.98686E-07			1	0.039	1.98686E-07	280	280	0	280	0.00142646
27458-94-2	27458942	2507	isononyl alcohol	144.26	3_REACH	8600	8600	0	8600	0.059614585			1	0.039	2.70345E-07			1	0.039	2.70345E-07	2800	2800	0	2800	0.0194094
2752-17-2	2752172	2511	2,2'-oxydi(ethylamine)	104.16	3_REACH	46400	46400	0	46400	0.44546851			1	0.039	3.74424E-07			1	0.039	3.74424E-07	3200	3200	0	3200	0.03072197
2778-42-9	2778429	2517	1,3-bis(1-isocyanato-1-	244.3	3_REACH	320	320	0	320	0.001309865			1	0.039	1.5964E-07			1	0.039	1.5964E-07	1360	1360	0	1360	0.00556693
2786-76-7	2786767	2520	4-[[4-	454.49	3_REACH	100000	100000	0	100000	0.220026843			1	0.039	8.58105E-08			1	0.039	8.58105E-08	1000	1000	0	1000	0.00220027
27955-94-8	27955948	4403	4,4',4''-(ethan-1,1,1-	306.36	3_REACH	18500	18500	0	18500	0.060386473			1	0.039	1.27301E-07			1	0.039	1.27301E-07	190	190	0	190	0.00062019
2809-21-4	2809214	578	etidronic acid	206.03	3_REACH	104000	104000	0	104000	0.504780857	60000	60000	0	60000	0.291219725			1	0.039	1.89293E-07	3000	3000	0	3000	0.01456099
281-23-2	281232	579	tricyclo[3.3.1.13,7]decane	136.24	3_REACH	95	95	0	95	0.000697299			1	0.039	2.8626E-07			1	0.039	2.8626E-07			1	1	7.34E-06
28219-61-6	28219616	2525	2-ethyl-4-(2,2,3-trimethyl-3-	208.35	3_REACH	490	490	0	490	0.002351812			1	0.039	1.87185E-07			1	0.039	1.87185E-07	440	440	0	440	0.00211183
28479-22-3	28479223	2533	3-chloro-p-tolyl isocyanate	167.6	3_REACH	10000	10000	0	10000	0.059665871			1	0.039	2.32697E-07			1	0.039	2.32697E-07	400	400	0	400	0.00238663
28535-81-1	28535811	2535	Methyl 3alpha,7alpha-	504.66	3_REACH	70290	70290	0	70290	0.139281893			1	0.039	7.72798E-08			1	0.039	7.72798E-08	30640	30640	0	30640	0.06071414
2855-13-2	2855132	2536	3-aminomethyl-3,5,5-	170.3	3_REACH	70000	70000	0	70000	0.411039342			1	0.039	2.29008E-07			1	0.039	2.29008E-07	1500	1500	0	1500	0.00880799
28553-12-0	28553120	582	di-"isononyl" phthalate	418.62	3_REACH	100	100	0	100	0.00023888			1	0.039	9.31633E-08			1	0.039	9.31633E-08	1800	1800	0	1800	0.00429984
2867-47-2	2867472	583	2-dimethylaminoethyl	157.21	3_REACH	6366.666667	6366.666667	0	6366.666667	0.040497848	2960	2960	0	2960	0.018828319			1	0.039	2.48076E-07	10	10	0	10	6.3609E-05
28768-32-3	28768323	2543	4,4'-methylenebis[N,N-	422.53	3_REACH	2309.401077	2309.401077	0	2309.401077	0.00546565			1	0.039	9.23011E-08			1	0.039	9.23011E-08	190	190	0	190	0.00044967
288-13-1	288131	43	pyrazole	68.081	3_REACH	1000000	1000000	0	1000000	14.68838589			1	0.039	5.72847E-07			1	0.039	5.72847E-07	8833.333333	8833.333333	0	8833.33333	0.12974741
288-88-0	288880	584	1,2,4-triazole	69.07	3_REACH	378000	378000	0	378000	5.472708846			1	0.039	5.64645E-07			1	0.039	5.64645E-07	500	500	0	500	0.00723903
2896-70-0	2896700	2550	2,2,6,6-tetramethyl-4-	171.24	3_REACH	56000	56000	0	56000	0.327026396			1	0.039	2.27751E-07			1	0.039	2.27751E-07	100000	100000	0	100000	0.58397571
2915-57-3	2915573	2559	bis(2-ethylhexyl) succinate	342.52	3_REACH	100000	100000	0	100000	0.291953755			1	0.039	1.13862E-07			1	0.039	1.13862E-07	180000	180000	0	180000	0.52551676
29171-20-8	29171208	2560	3,7-dimethyloct-6-en-1-yn-	152.24	3_REACH	21500	21500	0	21500	0.141224383			1	0.039	2.56174E-07			1	0.039	2.56174E-07	30400	30400	0	30400	0.19968471
2920-38-9	2920389	2561	p-phenylbenzonitrile	179.22	3_REACH	3280	3280	0	3280	0.018301529			1	0.039	2.1761E-07			1	0.039	2.1761E-07	1876.666667	1876.666667	0	1876.66667	0.0104713
2935-90-2	2935902	2563	methyl 3-	120.17	3_REACH	400	400	0	400	0.003328618			1	0.039	3.2454E-07			1	0.039	3.2454E-07	8	8	0	8	6.6572E-05
2942-59-8	2942598	2566	2-chloronicotinic acid	157.56	3_REACH	8407.333333	8407.333333	0	8407.333333	0.053359567			1	0.039	2.47525E-07			1	0.039	2.47525E-07	140850	140850	0	140850	0.89394516
2943-75-1	2943751	2567	triethoxyoctylsilane	276.49	3_REACH	55	55	0	55	0.000198922			1	0.039	1.41054E-07			1	0.039	1.41054E-07	130	130	0	130	0.00047018
294-62-2	294622	587	cyclododecane	168.32	3_REACH	1000	1000	0	1000	0.005941065			1	0.039	2.31702E-07			1	0.039	2.31702E-07	2100	2100	0	2100	0.01247624
294-90-6	294906	4493	1,4,7,10-	172.28	3_REACH	100000	100000	0	100000	0.58045043			1	0.039	2.26376E-07			1	0.039	2.26376E-07	10	10	0	10	5.8045E-05
29761-21-5	29761215	588	isodecyl diphenyl	390.46	3_REACH	1000	1000	0	1000	0.002561082	57	57	0	57	0.000145982			1	0.039	9.98822E-08	23666.66667	23666.66667	0	23666.6667	0.06061227
298-06-6	298066	591	O,O-diethyl hydrogen	186.23	3_REACH			1	0.39	2.09418E-06			1	0.039	2.09418E-07			1	0.039	2.09418E-07	1000000	1000000	0	1000000	5.36970413
29806-73-3	29806733	2572	2-ethylhexyl palmitate	368.65	3_REACH	10000000	10000000	0	10000000	27.12600027			1	0.039	1.05791E-07			1	0.039	1.05791E-07	30000	30000	0	30000	0.081378
298-07-7	298077	592	bis(2-ethylhexyl) hydrogen	322.43	3_REACH	6666.666667	6666.666667	0	6666.666667	0.020676323	20600	20600	0	20600	0.063889837			1	0.039	1.20956E-07	50000	50000	0	50000	0.15507242
298-12-4	298124	2573	glyoxylic acid	74.035	3_REACH	48266.66667	48266.66667	0	48266.66667	0.6519439			1	0.039	5.26778E-07			1	0.039	5.26778E-07	37100	37100	0	37100	0.50111434
29911-28-2	29911282	2578	1-(2-butoxy-1-	190.28	3_REACH	180000	180000	0	180000	0.945974354			1	0.039	2.04961E-07			1	0.039	2.04961E-07	173000	173000	0	173000	0.90918646
29920-31-8	29920318	2579	dimethyl 5-[[1-[[(2,3-	453.42	3_REACH	1000	1000	0	1000	0.002205461			1	0.039	8.6013E-08			1	0.039	8.6013E-08	1000	1000	0	1000	0.00220546
29964-84-9	29964849	2581	isodecyl methacrylate	226.36	3_REACH	450000	450000	0	450000	1.987983743			1	0.039	1.72292E-07			1	0.039	1.72292E-07	9.2	9.2	0	9.2	4.0643E-05
2996-92-1	2996921	2582	trimethoxyphenylsilane	198.29	3_REACH	74	74	0	74	0.000373191			1	0.039	1.96682E-07			1	0.039	1.96682E-07	200	200	0	200	0.00100862
3030-47-5	3030475	2590	bis(2-	173.31	3_REACH	100000	100000	0	100000	0.57700075			1	0.039	2.2503E-07			1	0.039	2.2503E-07	35000	35000	0	35000	0.20195026
3031-66-1	3031661	2591	hex-3-yne-2,5-diol	114.14	3_REACH	100000	100000	0	100000	0.876117049			1	0.039	3.41686E-07			1	0.039	3.41686E-07	350	350	0	350	0.00306641
3033-62-3	3033623	2592	N,N,N',N'-tetramethyl-2,2'-	160.26	3_REACH	46400	46400	0	46400	0.289529515			1	0.039	2.43355E-07			1	0.039	2.43355E-07	260	260	0	260	0.00162236
3047-32-3	3047323	2598	3-ethyloxetane-3-methanol	116.16	3_REACH	5000000	5000000	0	5000000	43.04407713			1	0.039	3.35744E-07			1	0.039	3.35744E-07	1250000	1250000	0	1250000	10.7610193
3049-71-6	3049716	2600	2,9-bis[4-	750.78	3_REACH	7600	7600	0	7600	0.010122806			1	0.039	5.1946E-08			1	0.039	5.1946E-08	100000	100000	0	100000	0.13319481
3061-75-4	3061754	2604	docosanamide	339.61	3_REACH	55	55	0	55	0.00016195			1	0.039	1.14838E-07			1	0.039	1.14838E-07	170	170	0	170	0.00050057
30674-80-7	30674807	2606	2-isocyanatoethyl	155.15	3_REACH	54000	54000	0	54000	0.348050274			1	0.039	2.5137E-07			1	0.039	2.5137E-07	97400	97400	0	97400	0.62777957
3069-29-2	3069292	2608	N-[3-	206.36	3_REACH	344000	344000	0	344000	1.666989727			1	0.039	1.8899E-07			1	0.039	1.8899E-07	1600	1600	0	1600	0.00775344
3069-40-7	3069407	2609	trimethoxyoctylsilane	234.41	3_REACH	55	55	0	55	0.000234632			1	0.039	1.66375E-07			1	0.039	1.66375E-07	130	130	0	130	0.00055458
3081-14-9	3081149	2612	N,N'-bis(1,4-	304.52	3_REACH	9.333333333	9.333333333	0	9.333333333	3.06493E-05	3.7	3.7	0	3.7	1.21503E-05			1	0.039	1.2807E-07	95.8	95.8	0	95.8	0.00031459
3089-16-5	3089165	2614	4,11-dichloro-5,12-	381.22	3_REACH	100000	100000	0	100000	0.262315723	10000	10000	0	10000	0.026231572			1	0.039	1.02303E-07	1000	1000	0	1000	0.00262316
3089-17-6	3089176	2615	2,9-dichloro-5,12-	381.22	3_REACH	100000	100000	0	100000	0.262315723	10000	10000	0	10000	0.026231572			1	0.039	1.02303E-07	1000	1000	0	1000	0.00262316
31024-56-3	31024563	2617	N-[3-	235.4	3_REACH	50000	50000	0	50000	0.212404418			1	0.039	1.65675E-07			1	0.039	1.65675E-07	1000	1000	0	1000	0.00424809
31027-31-3	31027313	2618	p-isopropylphenyl	161.21	3_REACH	35000	35000	0	35000	0.21710812			1	0.039	2.4192E-07			1	0.039	2.4192E-07	1600	1600	0	1600	0.00992494
3115-49-9	3115499	2619	(4-nonylphenoxy)acetic	278.39	3_REACH	5800	5800	0	5800	0.020834082			1	0.039	1.40091E-07			1	0.039	1.40091E-07	11200	11200	0	11200	0.04023133
31335-74-7	31335747	2625	2,2-dimethyl-1,3-	356.55	3_REACH	86	86	0	86	0.0002412			1	0.039	1.09382E-07			1	0.039	1.09382E-07	6.5	6.5	0	6.5	1.823E-05
3148-73-0	3148730	2627	N,N'-diacetylhydrazine	116.12	3_REACH			1	0.39	3.35859E-06			1	0.039	3.35859E-07			1	0.039	3.35859E-07	100000	100000	0	100000	0.86117809
3173-72-6	3173726	2631	1,5-naphthylene	210.19	3_REACH	50000	50000	0	50000	0.237880013			1	0.039	1.85546E-07			1	0.039	1.85546E-07	73	73	0	73	0.0003473
31775-20-9	31775209	2632	2,2'-[(3,3'-dichloro[1,1'-	717.62	3_REACH	100	100	0	100	0.00013935			1	0.039	5.43463E-08			1	0.039	5.43463E-08	100000	100000	0	100000	0.13934952
31775-89-0	31775890	2633	3-[(3-sulfanylbutanoyl)oxy]-	544.77	3_REACH	53.33333333	53.33333333	0	53.33333333	9.79006E-05			1	0.039	7.15898E-08			1	0.039	7.15898E-08	21	21	0	21	3.8548E-05
31778-10-6	31778106	2634	butyl 2-[[3-[[(2,3-dihydro-2-	523.55	3_REACH	1000	1000	0	1000	0.001910037			1	0.039	7.44915E-08			1	0.039	7.44915E-08	1000	1000	0	1000	0.00191004
3179-47-3	3179473	2635	decyl methacrylate	226.36	3_REACH	450000	450000	0	450000	1.987983743			1	0.039	1.72292E-07			1	0.039	1.72292E-07	9.2	9.2	0	9.2	4.0643E-05
3179-63-3	3179633	2636	3-dimethylaminopropan-1-	103.17	3_REACH	100000	100000	0	100000	0.969274014			1	0.039	3.78017E-07			1	0.039	3.78017E-07	14000	14000	0	14000	0.13569836
3179-76-8	3179768	2637	3-	191.35	3_REACH	934000	934000	0	934000	4.881107917			1	0.039	2.03815E-07			1	0.039	2.03815E-07	1300	1300	0	1300	0.00679383
31837-42-0	31837420	2639	2-[[1-[[(2,3-dihydro-2-oxo-	381.35	3_REACH	1000	1000	0	1000	0.002622263			1	0.039	1.02268E-07			1	0.039	1.02268E-07	1000	1000	0	1000	0.00262226
319002-92-1	319002921	4599	Propyl (2S)-2-(2-	202.29	3_REACH	10000	10000	0	10000	0.049433981			1	0.039	1.92793E-07			1	0.039	1.92793E-07	85000	85000	0	85000	0.42018884
3209-22-1	3209221	600	1,2-dichloro-3-	192	3_REACH	2600	2600	0	2600	0.013541667	330	330	0	330	0.00171875			1	0.039	2.03125E-07	966.6666667	966.6666667	0	966.666667	0.00503472
3234-85-3	3234853	2648	tetradecyl myristate	424.75	3_REACH	0.189	0.189	0	0.189	4.44968E-07			1	0.039	9.18187E-08			1	0.039	9.18187E-08	1.465	1.465	0	1.465	3.4491E-06
32388-55-9	32388559	2651	Acetyl cedrene	246.39	3_REACH	766.6666667	766.6666667	0	766.6666667	0.003111598			1	0.039	1.58286E-07			1	0.039	1.58286E-07	490	490	0	490	0.00198872
329-01-1	329011	2668	3-(Trifluoromethyl)phenyl	187.12	3_REACH	3500	3500	0	3500	0.018704575			1	0.039	2.08422E-07			1	0.039	2.08422E-07	3200	3200	0	3200	0.01710133
3290-92-4	3290924	2669	propylidynetrimethyl	338.4	3_REACH	1000	1000	0	1000	0.002955083	138	138	0	138	0.000407801			1	0.039	1.15248E-07	177	177	0	177	0.00052305
3296-90-0	3296900	2671	2,2-	261.95	3_REACH	100000	100000	0	100000	0.381752243			1	0.039	1.48883E-07			1	0.039	1.48883E-07	12500	12500	0	12500	0.04771903
3320-83-0	3320830	2677	2-chlorophenyl isocyanate	153.57	3_REACH	666.6666667	666.6666667	0	666.6666667	0.004341126			1	0.039	2.53956E-07			1	0.039	2.53956E-07	10666.66667	10666.66667	0	10666.6667	0.06945801
3332-27-2	3332272	2679	N,N-	257.46	3_REACH	800	800	0	800	0.003107279	420	420	0	420	0.001631321			1	0.039	1.5148E-07	2	2	0	2	7.7682E-06
33329-35-0	33329350	2680	N,N-bis[3-	272.49	3_REACH	20500	20500	0	20500	0.075232119			1	0.039	1.43125E-07			1	0.039	1.43125E-07	500	500	0	500	0.00183493
33704-61-9	33704619	2684	1,2,3,5,6,7-hexahydro-	206.33	3_REACH	706.6666667	706.6666667	0	706.6666667	0.003424934			1	0.039	1.89018E-07			1	0.039	1.89018E-07	1400	1400	0	1400	0.00678525
337906-36-2	337906362	2686	2-(methoxymethyl)benzene	152.2	3_REACH			1	0.39	2.56242E-06	325	325	0	325	0.002135348			1	0.039	2.56242E-07	680	680	0	680	0.00446781
3407-42-9	3407429	2689	3-(5,5,6-	236.4	3_REACH	3993.927002	3993.927002	0	3993.927002	0.016894784			1	0.039	1.64975E-07			1	0.039	1.64975E-07	3924.415906	3924.415906	0	3924.41591	0.01660074
34090-76-1	34090761	2690	tetrahydro-4-methylphthalic	166.18	3_REACH	100000	100000	0	100000	0.601757131	33333.33333	33333.33333	0	33333.33333	0.20058571			1	0.039	2.34685E-07	27500	27500	0	27500	0.16548321
34206-40-1	34206401	2694	butan-2-one O,O',O'',O'''-	372.55	3_REACH	300400	300400	0	300400	0.80633472	50000	50000	0	50000	0.134210173			1	0.039	1.04684E-07	1000	1000	0	1000	0.0026842
342-25-6	342256	2695	2,4'-difluorobenzophenone	218.2	3_REACH	2366.666667	2366.666667	0	2366.666667	0.010846318			1	0.039	1.78735E-07			1	0.039	1.78735E-07	310	310	0	310	0.00142071
34316-64-8	34316648	2700	hexyl laurate	284.48	3_REACH	1000000	1000000	0	1000000	3.515185602			1	0.039	1.37092E-07			1	0.039	1.37092E-07	33333.33333	33333.33333	0	33333.3333	0.11717285
3437-84-1	3437841	2701	bisisobutyryl peroxide	174.2	3_REACH	100000	100000	0	100000	0.574052813			1	0.039	2.23881E-07			1	0.039	2.23881E-07	15600	15600	0	15600	0.08955224
34396-03-7	34396037	2702	trimethoxy(2,4,4-	234.41	3_REACH	100000	100000	0	100000	0.426602961			1	0.039	1.66375E-07			1	0.039	1.66375E-07	100000	100000	0	100000	0.42660296
3452-97-9	3452979	609	3,5,5-trimethylhexan-1-ol	144.26	3_REACH	3226.666667	3226.666667	0	3226.666667	0.022367023	1280	1280	0	1280	0.008872868			1	0.039	2.70345E-07	4700	4700	0	4700	0.03258006
345-92-6	345926	2710	bis(4-fluorophenyl) ketone	218.2	3_REACH	6500	6500	0	6500	0.029789184			1	0.039	1.78735E-07			1	0.039	1.78735E-07	230	230	0	230	0.00105408
34690-00-1	34690001	2714	[[(phosphonomethyl)imino]	685.42	3_REACH	56666.66667	56666.66667	0	56666.66667	0.08267437	74000	74000	0	74000	0.107963001			1	0.039	5.68994E-08	54333.33333	54333.33333	0	54333.3333	0.07927013
34893-92-0	34893920	2717	1,3-dichloro-5-	188.01	3_REACH	4530	4530	0	4530	0.024094463			1	0.039	2.07436E-07			1	0.039	2.07436E-07	1000	1000	0	1000	0.00531887
350-46-9	350469	611	1-fluoro-4-nitrobenzene	141.1	3_REACH	9466.666667	9466.666667	0	9466.666667	0.067091897	11100	11100	0	11100	0.078667612			1	0.039	2.764E-07	16000	16000	0	16000	0.11339476
3508-98-3	3508983	4362	2-phenylhexanenitrile	173.26	3_REACH	733.3333333	733.3333333	0	733.3333333	0.00423256			1	0.039	2.25095E-07			1	0.039	2.25095E-07	260	260	0	260	0.00150063
35265-04-4	35265044	2726	2-[(1-	117.19	3_REACH	4500	4500	0	4500	0.038399181			1	0.039	3.32793E-07			1	0.039	3.32793E-07	1000	1000	0	1000	0.00853315
35435-21-3	35435213	2734	triethoxy(2,4,4-	276.49	3_REACH	10000	10000	0	10000	0.036167673			1	0.039	1.41054E-07			1	0.039	1.41054E-07	130	130	0	130	0.00047018
3547-33-9	3547339	613	2-(octylthio)ethanol	190.35	3_REACH	560	560	0	560	0.002941949			1	0.039	2.04886E-07			1	0.039	2.04886E-07			1	1	5.2535E-06
35636-63-6	35636636	2742	dimethyl 2-[[1-[[(2,3-	453.42	3_REACH	1000	1000	0	1000	0.002205461			1	0.039	8.6013E-08			1	0.039	8.6013E-08	1000	1000	0	1000	0.00220546
3576-88-3	3576883	2746	2,2'-iminobis[4,6-diamino-	235.23	3_REACH	14000	14000	0	14000	0.059516218			1	0.039	1.65795E-07			1	0.039	1.65795E-07	8390	8390	0	8390	0.03566722
35836-72-7	35836727	2750	2-Pinene-10-methyl	208.3	3_REACH	3813.333333	3813.333333	0	3813.333333	0.018306929			1	0.039	1.8723E-07			1	0.039	1.8723E-07	1010	1010	0	1010	0.00484878
35948-25-5	35948255	2754	6H-	216.18	3_REACH	100000	100000	0	100000	0.462577482			1	0.039	1.80405E-07			1	0.039	1.80405E-07	4600	4600	0	4600	0.02127856
36177-92-1	36177921	2761	N-butyl-2,2,6,6-	212.38	3_REACH	100000	100000	0	100000	0.470854129			1	0.039	1.83633E-07			1	0.039	1.83633E-07	2100	2100	0	2100	0.00988794
3622-84-2	3622842	2763	N-	213.3	3_REACH	12233.33333	12233.33333	0	12233.33333	0.057352711	78000	78000	0	78000	0.365682138			1	0.039	1.82841E-07	9100	9100	0	9100	0.04266292
3634-83-1	3634831	2766	1,3-	188.19	3_REACH	29200	29200	0	29200	0.155162336			1	0.039	2.07237E-07			1	0.039	2.07237E-07	21600	21600	0	21600	0.11477762
36443-68-2	36443682	2767	ethylenebis(oxyethylene)	586.77	3_REACH	11500	11500	0	11500	0.019598821			1	0.039	6.64656E-08			1	0.039	6.64656E-08	100000	100000	0	100000	0.17042453
36483-57-5	36483575	2768	2,2-dimethylpropan-1-ol,	324.86	3_REACH	18000	18000	0	18000	0.055408484	5600	5600	0	5600	0.017238195			1	0.039	1.20052E-07	2200	2200	0	2200	0.00677215
36635-56-0	36635560	2772	N-[[(4-	213.26	3_REACH	105409.2553	105409.2553	0	105409.2553	0.494275792			1	0.039	1.82875E-07			1	0.039	1.82875E-07	3000	3000	0	3000	0.01406734
36727-29-4	36727294	2775	3,5,5-trimethylhexanoyl	176.69	3_REACH	1640	1640	0	1640	0.009281793			1	0.039	2.20726E-07			1	0.039	2.20726E-07	1450	1450	0	1450	0.00820646
36768-62-4	36768624	2776	2,2,6,6-tetramethyl-4-	156.28	3_REACH	160000	160000	0	160000	1.02380343			1	0.039	2.49552E-07			1	0.039	2.49552E-07	25000	25000	0	25000	0.15996929

3681-71-8	3681718	2779	(Z)-hex-3-enyl acetate	142.2	3_REACH	10000		10000	0	10000	0.070323488			1	0.039	2.74262E-07			1	0.039	2.74262E-07	23000	23000	0	23000	0.16174402
3687-22-7	3687227	4777	2,4-Dinitro-6-(1-	296.32	3_REACH	1.01		1.01	0	1.01	3.40848E-06	42.5	42.5	0	42.5	0.000143426			1	0.039	1.31614E-07	29.4	29.4	0	29.4	9.9217E-05
369634-22-0	369634220	4583	Octalynol	140.18	3_REACH	2100		2100	0	2100	0.014980739			1	0.039	2.78214E-07			1	0.039	2.78214E-07	1500	1500	0	1500	0.01070053
3699-54-5	3699545	2788	1-(2-	130.15	3_REACH	1004000		1004000	0	1004000	7.714175951			1	0.039	2.99654E-07			1	0.039	2.99654E-07	1059000	1059000	0	1059000	8.13676527
37052-78-1	37052781	2789	1,3-dihydro-5-methoxy-2H-	180.23	3_REACH	3666.666667		3666.666667	0	3666.666667	0.020344375			1	0.039	2.1639E-07			1	0.039	2.1639E-07	12123.91535	12123.91535	0	12123.9154	0.06726913
3710-84-7	3710847	2791	N,N-diethylhydroxylamine	89.139	3_REACH	134000		134000	0	134000	1.503270174			1	0.039	4.37519E-07			1	0.039	4.37519E-07	26000	26000	0	26000	0.29167929
3717-40-6	3717406	2792	N,N-Dimethyladamantan-1-	179.31	3_REACH	8333.333333		8333.333333	0	8333.333333	0.046474448			1	0.039	2.175E-07			1	0.039	2.175E-07	33333.33333	33333.33333	0	33333.3333	0.18589779
372-09-8	372098	2794	cyanoacetic acid	85.063	3_REACH	46000		46000	0	46000	0.54077566			1	0.039	4.58484E-07			1	0.039	4.58484E-07	1230	1230	0	1230	0.01445987
373-44-4	373444	2796	octamethylenediamine	144.26	3_REACH	22607.76661		22607.76661	0	22607.76661	0.156715421			1	0.039	2.70345E-07			1	0.039	2.70345E-07	93900	93900	0	93900	0.65090808
3741-80-8	3741808	5041	N-(1,1-dimethylethyl)bis(2-	403.61	3_REACH	2700		2700	0	2700	0.006689626	41	41	0	41	0.000101583			1	0.039	9.66279E-08	870	870	0	870	0.00215555
3748-13-8	3748138	2798	m-bis(1-	158.24	3_REACH	2066.666667		2066.666667	0	2066.666667	0.01306033			1	0.039	2.46461E-07			1	0.039	2.46461E-07	1640	1640	0	1640	0.010364
3749-87-9	3749879	2800	Methyl 3,7-di-O-	506.68	3_REACH	76.66666667		76.66666667	0	76.66666667	0.000151312			1	0.039	7.69717E-08			1	0.039	7.69717E-08	30640	30640	0	30640	0.06047209
3779-63-3	3779633	2809	(2,4,6-trioxotriazine-	504.59	3_REACH	6300		6300	0	6300	0.012485384			1	0.039	7.72905E-08			1	0.039	7.72905E-08	100000	100000	0	100000	0.1981807
37971-36-1	37971361	2811	2-phosphonobutane-1,2,4-	270.13	3_REACH				1	0.39	1.44375E-06	1042000	1042000	0	1042000	3.857401992			1	0.039	1.44375E-07	8000	8000	0	8000	0.02961537
38051-10-4	38051104	2812	2,2-	582.99	3_REACH	5666.666667		5666.666667	0	5666.666667	0.009720007	7000	7000	0	7000	0.012007067			1	0.039	6.68965E-08	2100	2100	0	2100	0.00360212
38083-17-9	38083179	620	climbazole	292.77	3_REACH	3700		3700	0	3700	0.012637907			1	0.039	1.3321E-07			1	0.039	1.3321E-07	6.2	6.2	0	6.2	2.1177E-05
3845-76-9	3845769	2822	N-[3-	156.23	3_REACH	19000		19000	0	19000	0.121615567			1	0.039	2.49632E-07			1	0.039	2.49632E-07	55000	55000	0	55000	0.35204506
3851-87-4	3851874	2823	bis(3,5,5-	314.47	3_REACH	3440		3440	0	3440	0.01093904			1	0.039	1.24018E-07			1	0.039	1.24018E-07	10000	10000	0	10000	0.03179954
3855-32-1	3855321	2824	N-[3-	201.36	3_REACH	20500		20500	0	20500	0.101807708			1	0.039	1.93683E-07			1	0.039	1.93683E-07	500	500	0	500	0.00248311
38668-48-3	38668483	2825	1,1'-(p-tolylimino)dipropan-	223.32	3_REACH	5666.666667		5666.666667	0	5666.666667	0.025374649			1	0.039	1.74637E-07			1	0.039	1.74637E-07	57800	57800	0	57800	0.25882142
3886-69-9	3886699	2827	D-alpha-	121.18	3_REACH	9433.333333		9433.333333	0	9433.333333	0.077845629			1	0.039	3.21835E-07			1	0.039	3.21835E-07	320	320	0	320	0.0026407
38888-98-1	38888981	2828	(phenylethyl)benzene	182.27	3_REACH	35.33333333		35.33333333	0	35.33333333	0.000193852			1	0.039	2.13968E-07			1	0.039	2.13968E-07	36.66666667	36.66666667	0	36.6666667	0.00020117
393509-79-0	393509790	4634	methyl 2-chlorosulfonyl-4-	341.79	3_REACH	32000		32000	0	32000	0.09362474			1	0.039	1.14105E-07			1	0.039	1.14105E-07	560	560	0	560	0.00163843
39515-51-0	39515510	625	m-phenoxybenzaldehyde	198.22	3_REACH				1	0.39	1.96751E-06			1	0.039	1.96751E-07			1	0.039	1.96751E-07	666.6666667	666.6666667	0	666.666667	0.00336327
39670-09-2	39670092	2846	2-[2-(2-	246.3	3_REACH	300000		300000	0	300000	1.218026797			1	0.039	1.58343E-07			1	0.039	1.58343E-07	12500	12500	0	12500	0.05075112
40306-75-0	40306750	2857	3-acetamido-5-amino-4-	246.24	3_REACH	49276.43333		49276.43333	0	49276.43333	0.20011547			1	0.039	1.58382E-07			1	0.039	1.58382E-07	10000	10000	0	10000	0.04061079
40601-76-1	40601761	2859	1,3,5-tris[[4-tert-butyl-3-	699.94	3_REACH	100000		100000	0	100000	0.142869389			1	0.039	5.57191E-08			1	0.039	5.57191E-08	12	12	0	12	1.7144E-05
4065-45-6	4065456	52	sulisobenzone	308.31	3_REACH	73333.33333		73333.33333	0	73333.33333	0.237855838	1048	1048	0	1048	0.003399176			1	0.039	1.26496E-07	2440724.333	2440724.333	0	2440724.33	7.91646179
4073-98-7	4073987	2864	4,4'-methylenebis(2,6-	254.38	3_REACH	100000		100000	0	100000	0.393112666			1	0.039	1.53314E-07			1	0.039	1.53314E-07	20	20	0	20	7.8623E-05
40758-65-4	40758654	2865	4,6-Dichloro-2-	193.04	3_REACH	3300		3300	0	3300	0.017094903			1	0.039	2.02031E-07			1	0.039	2.02031E-07	310	310	0	310	0.00160588
4083-64-1	4083641	629	p-toluenesulphonyl	197.21	3_REACH	199001.8164		199001.8164	0	199001.8164	1.009085829			1	0.039	1.97759E-07			1	0.039	1.97759E-07	10000	10000	0	10000	0.05070737
4098-71-9	4098719	2867	3-isocyanatomethyl-3,5,5-	222.29	3_REACH	1000		1000	0	1000	0.004498628			1	0.039	1.75446E-07			1	0.039	1.75446E-07	4400	4400	0	4400	0.01979396
41198-08-7	41198087	631	Profenofos	373.64	3_REACH	0.5		0.5	0	0.5	1.33819E-06	2	2	0	2	5.35275E-06			1	0.039	1.04379E-07	187.5	187.5	0	187.5	0.00050182
41340-36-7	41340367	4309	2-(7-ethyl-1H-indol-3-	189.26	3_REACH	3000		3000	0	3000	0.01585121			1	0.039	2.06066E-07			1	0.039	2.06066E-07	1600	1600	0	1600	0.00845398
41620-33-1	41620331	4337	2-[[2-(acetyloxy)-3-(1,1-	382.54	3_REACH	210000		210000	0	210000	0.5489622	1.4	1.4	0	1.4	3.65975E-06			1	0.039	1.0195E-07	10000	10000	0	10000	0.02614106
4180-23-8	4180238	635	(E)-anethole	148.21	3_REACH	4800		4800	0	4800	0.032386479			1	0.039	2.6314E-07			1	0.039	2.6314E-07	3104.333333	3104.333333	0	3104.33333	0.02094551
42019-78-3	42019783	2886	4-chloro-4'-	232.67	3_REACH	6547.206667		6547.206667	0	6547.206667	0.028139454			1	0.039	1.67619E-07			1	0.039	1.67619E-07	10418.38667	10418.38667	0	10418.3867	0.04477752
42125-46-2	42125462	2889	4-tert-butylcyclohexyl	218.72	3_REACH	4600		4600	0	4600	0.021031456			1	0.039	1.7831E-07			1	0.039	1.7831E-07	97	97	0	97	0.00044349
4245-76-5	4245765	2892	610-029-6	118.1	3_REACH	100000		100000	0	100000	0.846740051			1	0.039	3.30229E-07			1	0.039	3.30229E-07	50000	50000	0	50000	0.42337003
4246-51-9	4246519	2893	3,3'-	220.32	3_REACH	100000		100000	0	100000	0.453885258			1	0.039	1.77015E-07			1	0.039	1.77015E-07	5400	5400	0	5400	0.0245098
4253-34-3	4253343	2896	methylsilanetriyl triacetate	220.25	3_REACH	27792.88478		27792.88478	0	27792.88478	0.126187899			1	0.039	1.77072E-07			1	0.039	1.77072E-07	3600	3600	0	3600	0.01634506
43057-68-7	43057687	4478	2-Ethyl-2-methyl-1,3-	212.3	3_REACH	4600		4600	0	4600	0.021667452			1	0.039	1.83702E-07			1	0.039	1.83702E-07	6.733333333	6.733333333	0	6.73333333	3.1716E-05
4378-61-4	4378614	2916	4,10-	464.12	3_REACH	1000		1000	0	1000	0.002154615			1	0.039	8.403E-08			1	0.039	8.403E-08	1000	1000	0	1000	0.00215462
4394-85-8	4394858	2918	4-morpholinecarbaldehyde	115.13	3_REACH	500000		500000	0	500000	4.342916703			1	0.039	3.38748E-07			1	0.039	3.38748E-07	10760000	10760000	0	10760000	93.4595674
4402-30-6	4402306	2919	1,1'-(methylimino)dipropan-	147.22	3_REACH	215000		215000	0	215000	1.460399402			1	0.039	2.6491E-07			1	0.039	2.6491E-07	640	640	0	640	0.00434724
4404-43-7	4404437	641	4,4'-bis[4-[bis(2-	917.01	3_REACH	3600	3600	3600	0	3600	0.003925802			1	0.039	4.25295E-08			1	0.039	4.25295E-08	3230	3230	0	3230	0.00352232
4431-83-8	4431838	2921	2,5,7,10-tetraoxaundecane	164.2	3_REACH				1	0.39	2.37515E-06	2562913	2562913	0	2562913	15.60848356			1	0.039	2.37515E-07	100000	100000	0	100000	0.6090134
4443-26-9	4443269	2925	1,3-dihydro-1,3-dioxo-2H-	261.28	3_REACH	500000		500000	0	500000	1.913655848			1	0.039	1.49265E-07			1	0.039	1.49265E-07	25000	25000	0	25000	0.09568279
4457-71-0	4457710	2927	3-methylpentane-1,5-diol	118.18	3_REACH	100000		100000	0	100000	0.846166864	100000	100000	0	100000	0.846166864			1	0.039	3.30005E-07	100000	100000	0	100000	0.84616686
4488-57-7	4488577	2933	3a,4,5,6,7,7a-hexahydro-	134.22	3_REACH	1433.333333		1433.333333	0	1433.333333	0.010678985	980	980	0	980	0.007301445			1	0.039	2.90568E-07	18000	18000	0	18000	0.13410818
4500-29-2	4500292	2936	2,2'-	187.28	3_REACH	100000		100000	0	100000	0.533959846	100000	100000	0	100000	0.533959846			1	0.039	2.08244E-07	8100	8100	0	8100	0.04325075
4511-42-6	4511426	2938	(3S-cis)-3,6-dimethyl-1,4-	144.13	3_REACH	43333.33333		43333.33333	0	43333.33333	0.300654502	2180	2180	0	2180	0.015125234			1	0.039	2.70589E-07	1900000	1900000	0	1900000	13.1825435
4531-49-1	4531491	2939	2,2'-[(3,3'-dichloro[1,1'-	689.56	3_REACH	100		100	0	100	0.00014502			1	0.039	5.65578E-08			1	0.039	5.65578E-08	100000	100000	0	100000	0.14502001
4559-86-8	4559868	2943	tetrabutylurea	284.49	3_REACH	365		365	0	365	0.001282998			1	0.039	1.37087E-07			1	0.039	1.37087E-07	140	140	0	140	0.00049211
461-58-5	461585	2948	cyanoguanidine	84.086	3_REACH	8000000		8000000	0	8000000	95.14068929	100000	100000	0	100000	1.189258616			1	0.039	4.63811E-07	560000	560000	0	560000	6.65984825
462-94-2	462942	2950	pentamethylenediamine	102.18	3_REACH	1000000		1000000	0	1000000	9.786651008			1	0.039	3.81679E-07			1	0.039	3.81679E-07	3200	3200	0	3200	0.03131728
4635-59-0	4635590	2951	4-chlorobutyryl chloride	141	3_REACH	1640		1640	0	1640	0.011631206			1	0.039	2.76596E-07			1	0.039	2.76596E-07	97	97	0	97	0.00068794
4651-67-6	4651676	2954	Nutriacholic acid	390.56	3_REACH	70290		70290	0	70290	0.179972347			1	0.039	9.98566E-08			1	0.039	9.98566E-08	30640	30640	0	30640	0.07845145
4672-38-2	4672382	2957	propylphosphonic acid	124.08	3_REACH	100000		100000	0	100000	0.805931657			1	0.039	3.14313E-07			1	0.039	3.14313E-07	33333.33333	33333.33333	0	33333.3333	0.26864389
470-82-6	470826	645	cineole	154.25	3_REACH	32000		32000	0	32000	0.207455429			1	0.039	2.52836E-07			1	0.039	2.52836E-07	9100	9100	0	9100	0.05899514
4724-48-5	4724485	2964	octylphosphonic acid	194.21	3_REACH	40000		40000	0	40000	0.205962618			1	0.039	2.00814E-07			1	0.039	2.00814E-07	12000	12000	0	12000	0.06178879
474-25-9	474259	2966	chenodeoxycholic acid	392.58	3_REACH	70290		70290	0	70290	0.179046309			1	0.039	9.93428E-08			1	0.039	9.93428E-08	30640	30640	0	30640	0.07804779
479-27-6	479276	646	1,8-naphthylenediamine	158.21	3_REACH	1000		1000	0	1000	0.006320713			1	0.039	2.46508E-07			1	0.039	2.46508E-07	100	100	0	100	0.00063207
4813-57-4	4813574	2971	octadecyl acrylate	324.55	3_REACH	100000		100000	0	100000	0.308118934			1	0.039	1.20166E-07			1	0.039	1.20166E-07	100000	100000	0	100000	0.30811893
48145-04-6	48145046	2972	2-phenoxyethyl acrylate	192.21	3_REACH	3333.333333		3333.333333	0	3333.333333	0.017342143			1	0.039	2.02903E-07			1	0.039	2.02903E-07	110	110	0	110	0.00057229
482-89-3	482893	647	2-(1,3-dihydro-3-oxo-2H-	262.27	3_REACH	14000		14000	0	14000	0.053380104			1	0.039	1.48702E-07			1	0.039	1.48702E-07	211630	211630	0	211630	0.80691654
4904-61-4	4904614	648	cyclododeca-1,5,9-triene	162.28	3_REACH	33.33333333		33.33333333	0	33.33333333	0.000205406			1	0.039	2.40325E-07			1	0.039	2.40325E-07	120	120	0	120	0.00073946
4948-15-6	4948156	2983	2,9-bis(3,5-	598.66	3_REACH	7600		7600	0	7600	0.012695019			1	0.039	6.51455E-08			1	0.039	6.51455E-08	100000	100000	0	100000	0.16703972
497-18-7	497187	2989	carbonohydrazide	90.09	3_REACH	4130		4130	0	4130	0.045843046			1	0.039	4.329E-07			1	0.039	4.329E-07	74	74	0	74	0.0008214
4979-32-2	4979322	2990	N,N-	346.56	3_REACH	243.3333333		243.3333333	0	243.3333333	0.000702139	41	41	0	41	0.000118306			1	0.039	1.12535E-07	12	12	0	12	3.4626E-05
50-21-5	50215	654	lactic acid	90.078	3_REACH	43333.33333		43333.33333	0	43333.33333	0.481064559	2180	2180	0	2180	0.024201248			1	0.039	4.32958E-07	1900000	1900000	0	1900000	21.0928307
502-44-3	502443	2999	hexan-6-olide	114.14	3_REACH	250000		250000	0	250000	2.190292623			1	0.039	3.41686E-07			1	0.039	3.41686E-07	256000	256000	0	256000	2.24285965
5026-74-4	5026744	3000	p-(2,3-epoxypropoxy)-N,N-	277.32	3_REACH	3200		3200	0	3200	0.011539016			1	0.039	1.40632E-07			1	0.039	1.40632E-07	2400	2400	0	2400	0.00865426
5036-48-6	5036486	3003	1H-imidazole-1-	125.18	3_REACH	127888.8406		127888.8406	0	127888.8406	1.021639564			1	0.039	3.11551E-07			1	0.039	3.11551E-07	6270	6270	0	6270	0.05008787
503-74-2	503742	657	isovaleric acid	102.13	3_REACH	700		700	0	700	0.00685401			1	0.039	3.81866E-07			1	0.039	3.81866E-07	6380	6380	0	6380	0.0624694
504-29-0	504290	658	2-pyridylamine	94.119	3_REACH	2000		2000	0	2000	0.021249695			1	0.039	4.14369E-07			1	0.039	4.14369E-07	2033.333333	2033.333333	0	2033.33333	0.02160386
504-63-2	504632	660	propane-1,3-diol	76.095	3_REACH	1666666.667		1666666.667	0	1666666.667	21.9024465			1	0.039	5.12517E-07			1	0.039	5.12517E-07	500000	500000	0	500000	6.57073395
506-30-9	506309	3012	icosanoic acid	312.54	3_REACH	1556.666667		1556.666667	0	1556.666667	0.004980696			1	0.039	1.24784E-07			1	0.039	1.24784E-07	1268.666667	1268.666667	0	1268.66667	0.00405921
507448-65-9	507448659	3018	ethyl (2Z)-4,4,4-trifluoro-3-	197.16	3_REACH	6000		6000	0	6000	0.030432136			1	0.039	1.97809E-07			1	0.039	1.97809E-07	100000	100000	0	100000	0.50720227
5089-70-3	5089703	3022	(3-	240.8	3_REACH	58000		58000	0	58000	0.240863787			1	0.039	1.6196E-07			1	0.039	1.6196E-07	237000	237000	0	237000	0.98421927
5102-83-0	5102830	3025	2,2'-[(3,3'-dichloro[1,1'-	685.62	3_REACH	100		100	0	100	0.000145853			1	0.039	5.68828E-08			1	0.039	5.68828E-08	100000	100000	0	100000	0.14585339
51-03-6	51036	667	2-(2-butoxyethoxy)ethyl 6-	338.44	3_REACH	625		625	0	625	0.001846708	180	180	0	180	0.000531852			1	0.039	1.15235E-07	56.66666667	56.66666667	0	56.6666667	0.00016743
51167-18-1	51167181	3028	2'-[2,4-dichloro-5-(1-	319.23	3_REACH	10000		10000	0	10000	0.031325377			1	0.039	1.22169E-07			1	0.039	1.22169E-07	1000	1000	0	1000	0.00313254
5124-30-1	5124301	3030	4,4'-methylenedicyclohexyl	262.36	3_REACH	690		690	0	690	0.002629974			1	0.039	1.48651E-07			1	0.039	1.48651E-07	310	310	0	310	0.00118158
51-28-5	51285	57	2,4-dinitrophenol	184.11	3_REACH	20	130	130	0	130	0.0007061	30.29851482	30.29851482	0	30.29851482	0.000164567			1	0.039	2.1183E-07	1000	1000	0	1000	0.00543154
5131-66-8	5131668	3032	1-butoxypropan-2-ol	132.2	3_REACH	353333.3333		353333.3333	0	353333.3333	2.672718104			1	0.039	2.95008E-07			1	0.039	2.95008E-07	175000	175000	0	175000	1.32375189
51920-12-8	51920128	3049	N-(2,3-dihydro-2-oxo-1H-	560.6	3_REACH	1000		1000	0	1000	0.001783803			1	0.039	6.95683E-08			1	0.039	6.95683E-08	1000	1000	0	1000	0.0017838
5208-93-5	5208935	3052	3-methyl-1-(2,6,6-	220.36	3_REACH	1000		1000	0	1000	0.004538029			1	0.039	1.76983E-07			1	0.039	1.76983E-07	2500	2500	0	2500	0.01134507
521-18-6	521186	672	androstanolone	290.45	3_REACH	6.5		6.5	0	6.5	2.23791E-05	0.95	0.95	0	0.95	3.27079E-06			1	0.039	1.34274E-07			1	1	3.4429E-06
52449-76-0	52449760	3059	Methyl 4-cyano-2-	206.16	3_REACH	6250		6250	0	6250	0.030316259			1	0.039	1.89173E-07			1	0.039	1.89173E-07	500	500	0	500	0.0024253
52-51-7	52517	674	bronopol	200	3_REACH	2900		2900	0	2900	0.0145	1940	1940	0	1940	0.0097			1	0.039	0.000000195	12	12	0	12	0.00006
52722-86-8	52722868	3072	4-hydroxy-2,2,6,6-	201.31	3_REACH	100000		100000	0	100000	0.496746312			1	0.039	1.93731E-07			1	0.039	1.93731E-07	100000	100000	0	100000	0.49674631
5280-68-2	5280682	3074	N-(4-chloro-2,5-	611.06	3_REACH	100000		100000	0	100000	0.163650051			1	0.039	6.38235E-08			1	0.039	6.38235E-08	1000	1000	0	1000	0.0016365
5280-80-8	5280808	3076	3,3'-[(2,5-dimethyl-p-	916.66	3_REACH	100000		100000	0	100000	0.109091702			1	0.039	4.25458E-08			1	0.039	4.25458E-08	40000	40000	0	40000	0.04363668
52829-07-9	52829079	3077	bis(2,2,6,6-tetramethyl-4-	480.74	3_REACH	2800		2800	0	2800	0.005824354			1	0.039	8.11249E-08			1	0.039	8.11249E-08	50	50	0	50	0.00010401
5283-66-9	5283669	678	octyltrichlorosilane	247.67	3_REACH	100000		100000	0	100000	0.403763072			1	0.039	1.57468E-07			1	0.039	1.57468E-07	100000	100000	0	100000	0.40376307
52846-56-7	52846567	3078	N-(2,3-dihydro-2-oxo-1H-	382.34	3_REACH	1000		1000	0	1000	0.002615473			1	0.039	1.02003E-07			1	0.039	1.02003E-07	1000	1000	0	1000	0.00261547
5292-45-5	5292455	680	dimethyl 2-	239.18	3_REACH	1700		1700	0	1700	0.007107618			1	0.039	1.63057E-07			1	0.039	1.63057E-07			1	1	4.181E-06
5308-25-8	5308258	3087	1-ethylpiperazine	114.19	3_REACH	100000		100000	0	100000	0.875733427			1	0.039	3.41536E-07			1	0.039	3.41536E-07	32000	32000	0	32000	0.2802347
53-16-7	53167	61	estrone	270.37	3_REACH				1	0.39	1.44247E-06	0.034	0.034	0	0.034	1.25754E-07	0.307	0.307	0	0.307	1.13548E-06			1	1	3.6986E-06
53306-54-0	53306540	3094	bis(2-propylheptyl)	446.67	3_REACH	10000000		10000000	0	10000000	22.38789263			1	0.039	8.73128E-08			1	0.039	8.73128E-08	25000	25000	0	25000	0.05596973
5333-42-6	5333426	3096	2-octyldodecan-1-ol	298.56	3_REACH	320		320	0	320	0.001071811			1	0.039	1.30627E-07			1	0.039	1.30627E-07	5.15	5.15	0	5.15	1.7249E-05
5333-84-6	5333846	3097	1,2,3,6-tetrahydro-3-	166.18	3_REACH	100000		100000	0	100000	0.601757131	33333.33333	33333.33333	0	33333.33333	0.20058571			1	0.039	2.34685E-07	27500	27500	0	27500	0.16548321
534-03-2	534032	3100	2-aminopropane-1,3-diol	91.111	3_REACH	2200000		2200000	0	2200000	24.14637091			1	0.039	4.28049E-07			1	0.039	4.28049E-07	16000	16000	0	16000	0.17560997
5343-92-0	5343920	3102	pentane-1,2-diol	104.15	3_REACH	1096000		1096000	0	1096000	10.52328373			1	0.039	3.7446E-07			1	0.039	3.7446E-07	5477330	5477330	0	5477330	52.5907825
53445-37-7	53445377	3103	2,2,4(or 2,4,4)-	188.22	3_REACH	400000		400000	0	400000	2.12517267			1	0.039	2.07204E-07			1	0.039	2.07204E-07	10000	10000	0	10000	0.05312932
534-52-1	534521	682	2-methyl-4,6-dinitro-phenol	198.14	3_REACH	22	76.6666667	76.66666667	0	76.66666667	0.000386932	100	100	0	100	0.000504694			1	0.039	1.96831E-07	150	150	0	150	0.00075704
53651-69-7	53651697	3107	Propanoic acid	132.16	3_REACH	43333.33333		43333.33333	0	43333.33333	0.327885391	2180	2180	0	2180	0.016495157			1	0.039	2.95097E-07	800000	800000	0	800000	6.05326877
5372-81-6	5372816	683	dimethyl 2-	209.2	3_REACH	5100		5100	0	5100	0.024378585			1	0.039	1.86424E-07			1	0.039	1.86424E-07	3153.333333	3153.333333	0	3153.33333	0.0150733
540-97-6	540976	3124	dodecamethylcyclohexasilo	444.93	3_REACH				1	0.39	8.76542E-07	4.4	4.4	0	4.4	9.8892E-06			1	0.039	8.76542E-08	2	2	0	2	4.4951E-06
541-02-6	541026	3125	decamethylcyclopentasilox	370.77	3_REACH	15		15	0	15	4.04563E-05	5.8	5.8	0	5.8	1.56431E-05			1	0.039	1.05187E-07	12	12	0	12	3.2365E-05
5413-60-5	5413605	3128	3a,4,5,6,7,7a-hexahydro-	192.26	3_REACH	5029.953333		5029.953333	0	5029.953333	0.026162246	115554.3333	115554.3333	0	115554.3333	0.601031589			1	0.039	2.0285E-07	1705.702	1705.702	0	1705.702	0.00887185
541-73-1	541731	685	1,3-dichlorobenzene	147	3_REACH	1000		1000	0	1000	0.006802721	759.7367965	759.7367965	0	759.7367965	0.005168278			1	0.039	2.65306E-07	2200	2200	0	2200	0.01496599
542-05-2	542052	3134	3-oxoglutaric acid	146.1	3_REACH	73333.33333		73333.33333	0	73333.33333	0.501939311	548000000	548000000	0	548000000	3750.855578			1	0.039	2.6694E-07	51000000	51000000	0	51000000	349.075975
5435-64-3	5435643	3140	3,5,5-trimethylhexanal	142.24	3_REACH	15000		15000	0	15000	0.105455568			1	0.039	2.74184E-07			1	0.039	2.74184E-07	11000	11000	0	11000	0.07733408
544-01-4	544014	3141	diisopentyl ether	158.29	3_REACH	1566.666667		1566.666667	0	1566.666667	0.009897446			1	0.039	2.46383E-07			1	0.039	2.46383E-07	1150	1150	0	1150	0.00726515
54423-67-5	54423675	3143	vinyl neononanoate	184.28	3_REACH	1600		1600	0	1600	0.00868244			1	0.039	2.11634E-07			1	0.039	2.11634E-07	12000	12000	0	12000	0.0651183
5466-77-3	5466773	3151	2-ethylhexyl 4-	290.4	3_REACH	271300		271300	0	271300	0.93422865			1	0.039	1.34298E-07			1	0.039	1.34298E-07	32000	32000	0	32000	0.11019284
5468-75-7	5468757	3152	2,2'-[(3,3'-dichloro[1,1'-	657.56	3_REACH	100		100	0	100	0.000152077			1	0.039	5.93102E-08			1	0.039	5.93102E-08	100000	100000	0	100000	0.15207738
54839-24-6	54839246	3154	2-ethoxy-1-methylethyl	146.19	3_REACH	100000		100000	0	100000	0.684041316			1	0.039	2.66776E-07			1	0.039	2.66776E-07	100000	100000	0	100000	0.68404132
54914-37-3	54914373	3156	1,3,3-trimethyl-N-(2-	278.49	3_REACH	53700		53700	0	53700	0.192825595			1	0.039	1.40041E-07			1	0.039	1.40041E-07	9600	9600	0	9600	0.03447161
5521-31-3	5521313	3163	2,9-dimethylanthra[2,1,9-	418.41	3_REACH	7600		7600	0	7600	0.018164002			1	0.039	9.321E-08			1	0.039	9.321E-08	100000	100000	0	100000	0.23900002
55314-16-4	55314164	3166	611-255-8	176.22	3_REACH	100000		100000	0	100000	0.567472478			1	0.039	2.21314E-07			1	0.039	2.21314E-07	30000	30000	0	30000	0.17024174
553-86-6	553866	3169	(3H)-benzofuran-2-one	134.13	3_REACH	4000		4000	0	4000	0.029821815			1	0.039	2.90763E-07			1	0.039	2.90763E-07	390	390	0	390	0.00290763
554-00-7	554007	700	2,4-dichloroaniline	162.02	3_REACH	733.3333333		733.3333333	0	733.3333333	0.00452619	330	330	0	330	0.002036786			1	0.039	2.40711E-07	123.3333333	123.3333333	0	123.333333	0.00076122
556-67-2	556672	705	octamethylcyclotetrasiloxan	296.62	3_REACH	6.3		6.3	0	6.3	2.12393E-05	4.4	4.4	0	4.4	1.48338E-05			1	0.039	1.31481E-07	22	22	0	22	7.4169E-05
5567-15-7	5567157	706	2,2'-[(3,3'-dichloro[1,1'-	818.5	3_REACH	100		100	0	100	0.000122175			1	0.039	4.76481E-08			1	0.039	4.76481E-08	100000	100000	0	100000	0.12217471
556-88-7	556887	707	1-nitroguanidine	104.07	3_REACH	11500		11500	0	11500	0.110502546	1050000	1050000	0	1050000	10.08936293			1	0.039	3.74748E-07	20000	20000	0	20000	0.19217834
5578-42-7	5578427	3177	dichlorocyclohexylmethylsil	197.18	3_REACH	6100		6100	0	6100	0.0309362			1	0.039	1.97789E-07			1	0.039	1.97789E-07	12500	12500	0	12500	0.06339385
5580-57-4	5580574	3178	3,3'-[(2-chloro-5-methyl-p-	937.08	3_REACH	100000		100000	0	100000	0.106714475			1	0.039	4.16186E-08			1	0.039	4.16186E-08	40000	40000	0	40000	0.04268579
5580-58-5	5580585	3179	3,3'-[(2,5-dichloro-p-	957.49	3_REACH	100000		100000	0	100000	0.104439733			1	0.039	4.07315E-08			1	0.039	4.07315E-08	40000	40000	0	40000	0.04177589
55934-93-5	55934935	3182	[(butoxymethylethoxy)meth	248.36	3_REACH	180000		180000	0	180000	0.724754389			1	0.039	1.5703E-07			1	0.039	1.5703E-07	15900	15900	0	15900	0.06401997
561-41-1	561411	3187	4,4'-bis(dimethylamino)-4''-	375.52	3_REACH	5800		5800	0	5800	0.015445249			1	0.039	1.03856E-07			1	0.039	1.03856E-07	1309.113	1309.113	0	1309.113	0.00348613
56-18-8	56188	3188	3,3'-iminodi(propylamine)	131.23	3_REACH	147000		147000	0	147000	1.120170693			1	0.039	2.97188E-07			1	0.039	2.97188E-07	62500	62500	0	62500	0.47626305
56309-94-5	56309945	4472	4-(1,4-dioxa-spiro[4.5]dec-	238.33	3_REACH	56000		56000	0	56000	0.234968321			1	0.039	1.63639E-07			1	0.039	1.63639E-07	32000	32000	0	32000	0.13426761
56358-17-9	56358179	3192	N-(2-ethylhexyl)naphthalen-	255.41	3_REACH	100000		100000	0	100000	0.391527348			1	0.039	1.52696E-07			1	0.039	1.52696E-07	80	80	0	80	0.00031322
56-41-7	56417	3198	L-alanine	89.095	3_REACH	3200000		3200000	0	3200000	35.91671811			1	0.039	4.37735E-07			1	0.039	4.37735E-07			1	1	1.1224E-05
56519-71-2	56519712	3200	Propane-1,3-diyl	328.49	3_REACH	18000		18000	0	18000	0.054796189			1	0.039	1.18725E-07			1	0.039	1.18725E-07			1	1	3.0442E-06
56539-66-3	56539663	3201	3-methoxy-3-methylbutan-1	118.18	3_REACH	100000		100000	0	100000	0.846166864			1	0.039	3.30005E-07			1	0.039	3.30005E-07	1000000	1000000	0	1000000	8.46166864
56677-60-2	56677602	3208	tetradecyl chloroformate	276.85	3_REACH	1000		1000	0	1000	0.003612064			1	0.039	1.40871E-07			1	0.039	1.40871E-07	97	97	0	97	0.00035037
56706-10-6	56706106	3209	4,4,13,13-tetraethoxy-3,14-	474.83	3_REACH	1000000		1000000	0	1000000	2.10601689			1	0.039	8.21347E-08			1	0.039	8.21347E-08	32000	32000	0	32000	0.06739254
56718-71-9	56718719	3211	p-(2-methoxyethyl)phenol	152.19	3_REACH	78333.33333		78333.33333	0	78333.33333	0.514707493			1	0.039	2.56259E-07			1	0.039	2.56259E-07	100000	100000	0	100000	0.6570734
56-84-8	56848	3212	aspartic acid	133.1	3_REACH	100000		100000	0	100000	0.751314801			1	0.039	2.93013E-07			1	0.039	2.93013E-07	3810	3810	0	3810	0.02862509
56962-04-0	56962040	3217	3-Bromo-5-chlorophenol	207.46	3_REACH	600		600	0	600	0.002892124			1	0.039	1.87988E-07			1	0.039	1.87988E-07	2380	2380	0	2380	0.01147209
56973-87-6	56973876	4267	1-(3,3-	194.32	3_REACH	880		880	0	880	0.004528613			1	0.039	2.007E-07			1	0.039	2.007E-07	9000	9000	0	9000	0.04631536
57090-45-6	57090456	4249	(R)-3-chloropropane-1,2-	110.54	3_REACH	100000		100000	0	100000	0.9046499			1	0.039	3.52813E-07			1	0.039	3.52813E-07	75000	75000	0	75000	0.67848743
5726-19-2	5726192	3228	2-methylcyclohexyl acetate	156.22	3_REACH	7400		7400	0	7400	0.047369095			1	0.039	2.49648E-07			1	0.039	2.49648E-07	4200	4200	0	4200	0.02688516
57374-49-9	57374499	4553	methyl 3-acetoxy-2-pentyl-	268.35	3_REACH	1390		1390	0	1390	0.005179802			1	0.039	1.45333E-07			1	0.039	1.45333E-07	16000	16000	0	16000	0.05962363

576-26-1	576261	723	2,6-xylenol	122.17	3_REACH	1333.333333		1333.333333	0	1333.333333	0.010913754	7666.666667	7666.666667	0	7666.666667	0.062754086			1	0.039	3.19227E-07	2000		2000	0	2000	0.01637063
5766-67-6	5766676	3236	ethylenediaminetetraaceto	216.25	3_REACH	100000		100000	0	100000	0.462427746			1	0.039	1.80347E-07			1	0.039	1.80347E-07	18000		18000	0	18000	0.08323699
57843-53-5	57843535	3238	N,N,N',N'-tetrakis(2-	376.5	3_REACH	124000		124000	0	124000	0.32934927			1	0.039	1.03586E-07			1	0.039	1.03586E-07	98300		98300	0	98300	0.26108898
58190-57-1	58190571	3242	2-Propanone, 2,2',2''-	273.41	3_REACH	99333.33333		99333.33333	0	99333.33333	0.363312729			1	0.039	1.42643E-07			1	0.039	1.42643E-07	50000		50000	0	50000	0.18287553
583-39-1	583391	3244	benzimidazole-2-thiol	150.21	3_REACH	5559.736667		5559.736667	0	5559.736667	0.037013093			1	0.039	2.59637E-07			1	0.039	2.59637E-07	170.2477		170.2477	0	170.2477	0.0011334
583-78-8	583788	728	2,5-dichlorophenol	163	3_REACH	596.6666667		596.6666667	0	596.6666667	0.003660532			1	0.039	2.39264E-07			1	0.039	2.39264E-07				1	1	6.135E-06
58430-94-7	58430947	3247	3,5,5-trimethylhexyl acetate	186.29	3_REACH	4000		4000	0	4000	0.021471899			1	0.039	2.09351E-07			1	0.039	2.09351E-07	510		510	0	510	0.00273767
584-84-9	584849	729	4-methyl-m-phenylene	174.16	3_REACH	44333.33333		44333.33333	0	44333.33333	0.254555198			1	0.039	2.23932E-07			1	0.039	2.23932E-07	1076666.667		1076666.667	0	1076666.67	6.18205482
58567-11-6	58567116	3249	(ethoxymethoxy)cyclodode	242.4	3_REACH	1300		1300	0	1300	0.005363036			1	0.039	1.60891E-07			1	0.039	1.60891E-07	10000		10000	0	10000	0.04125413
586-62-9	586629	731	p-mentha-1,4(8)-diene	136.24	3_REACH	268.3333333		268.3333333	0	268.3333333	0.001969564			1	0.039	2.8626E-07			1	0.039	2.8626E-07	54		54	0	54	0.00039636
58670-89-6	58670896	3252	2-decyltetradecanol	354.66	3_REACH	1825741.858		1825741.858	0	1825741.858	5.147865162			1	0.039	1.09964E-07			1	0.039	1.09964E-07	5.15		5.15	0	5.15	1.4521E-05
5888-33-5	5888335	3257	exo-1,7,7-	208.3	3_REACH	431		431	0	431	0.002069131			1	0.039	1.8723E-07			1	0.039	1.8723E-07	153		153	0	153	0.00073452
5888-87-9	5888879	3258	N,N'-hexane-1,6-	394.52	3_REACH	22500		22500	0	22500	0.057031329			1	0.039	9.88543E-08			1	0.039	9.88543E-08	6500		6500	0	6500	0.01647572
591-27-5	591275	734	3-aminophenol	109.13	3_REACH	7433.034374		7433.034374	0	7433.034374	0.068111742	965232.3333	965232.3333	0	965232.3333	8.844793671			1	0.039	3.57372E-07	20000		20000	0	20000	0.18326766
59227-88-2	59227882	4300	1-octylazepin-2-one	225.38	3_REACH	1800		1800	0	1800	0.007986512			1	0.039	1.73041E-07			1	0.039	1.73041E-07	600		600	0	600	0.00266217
59447-55-1	59447551	3278	(pentabromophenyl)methyl	556.7	3_REACH	1000		1000	0	1000	0.0017963			1	0.039	7.00557E-08			1	0.039	7.00557E-08	4		4	0	4	7.1852E-06
59487-23-9	59487239	3279	4-[[5-[[[4-	654.08	3_REACH	100000		100000	0	100000	0.152886497			1	0.039	5.96257E-08			1	0.039	5.96257E-08	1000		1000	0	1000	0.00152886
59-50-7	59507	737	chlorocresol	142.59	3_REACH	366		366	0	366	0.0025668			1	0.039	2.73511E-07			1	0.039	2.73511E-07	1900		1900	0	1900	0.01332492
59719-67-4	59719674	3284	bis[2-[2-(1-methylethyl)-3-	486.66	3_REACH	70700		70700	0	70700	0.145275963			1	0.039	8.01381E-08			1	0.039	8.01381E-08	25.9		25.9	0	25.9	5.322E-05
5989-27-5	5989275	743	(R)-p-mentha-1,8-diene	136.24	3_REACH	268.5		268.5	0	268.5	0.001970787			1	0.039	2.8626E-07			1	0.039	2.8626E-07	775		775	0	775	0.00568849
5989-54-8	5989548	744	(S)-p-mentha-1,8-diene	136.24	3_REACH	229.3333333		229.3333333	0	229.3333333	0.001683304			1	0.039	2.8626E-07			1	0.039	2.8626E-07	301.3333333		301.3333333	0	301.333333	0.00221178
599-04-2	599042	3296	2,4-dihydroxy-3,3-	130.14	3_REACH	464000		464000	0	464000	3.565391117			1	0.039	2.99677E-07			1	0.039	2.99677E-07	22000		22000	0	22000	0.16904872
599-61-1	599611	3298	3,3'-sulphonyldianiline	248.31	3_REACH	100000		100000	0	100000	0.402722403			1	0.039	1.57062E-07			1	0.039	1.57062E-07	173.3333333		173.3333333	0	173.333333	0.00069805
599-64-4	599644	3299	P-Cumylphenol	212.29	3_REACH	300		300	0	300	0.001413161			1	0.039	1.83711E-07			1	0.039	1.83711E-07	500		500	0	500	0.00235527
60-00-4	60004	71	edetic acid	292.25	3_REACH	24000		24000	0	24000	0.082121471	25700	25700	0	25700	0.087938409			1	0.039	1.33447E-07	390		390	0	390	0.00133447
60-09-3	60093	746	4-aminoazobenzene	197.24	3_REACH	233.3333333		233.3333333	0	233.3333333	0.001182992			1	0.039	1.97729E-07			1	0.039	1.97729E-07	140		140	0	140	0.0007098
60111-54-8	60111548	3304	3,3-	432.89	3_REACH	0.0142		0.0142	0	0.0142	3.28028E-08			1	0.039	9.00922E-08			1	0.039	9.00922E-08	0.015		0.015	0	0.015	3.4651E-08
60-12-8	60128	3306	2-phenylethanol	122.17	3_REACH	100000		100000	0	100000	0.818531554			1	0.039	3.19227E-07			1	0.039	3.19227E-07	280000		280000	0	280000	2.29188835
603-35-0	603350	751	triphenylphosphine	262.29	3_REACH	333333.0029		333333.0029	0	333333.0029	1.270856696			1	0.039	1.4869E-07			1	0.039	1.4869E-07	1666.665015		1666.665015	0	1666.66501	0.00635428
6041-94-7	6041947	3310	4-[(2,5-dichlorophenyl)azo]-	436.3	3_REACH	500000		500000	0	500000	1.146000458			1	0.039	8.9388E-08			1	0.039	8.9388E-08	1000		1000	0	1000	0.002292
60658-04-0	60658040	4438	Ethyl 2-(3-	282.34	3_REACH	500		500	0	500	0.001770915			1	0.039	1.38131E-07			1	0.039	1.38131E-07	700		700	0	700	0.00247928
608-25-3	608253	3317	2-methylresorcinol	124.14	3_REACH	3943.333333		3943.333333	0	3943.333333	0.031765211	6941	6941	0	6941	0.055912679			1	0.039	3.14161E-07	1202.333333		1202.333333	0	1202.33333	0.0096853
611-06-3	611063	755	1,3-dichloro-4-	192	3_REACH	58.33333333		58.33333333	0	58.33333333	0.000303819	2200	2200	0	2200	0.011458333			1	0.039	2.03125E-07	193.3333333		193.3333333	0	193.333333	0.00100694
611-19-8	611198	3326	2-Chlorobenzyl chloride	161.03	3_REACH	90		90	0	90	0.000558902			1	0.039	2.42191E-07			1	0.039	2.42191E-07	45		45	0	45	0.00027945
611-70-1	611701	3328	isobutyrophenone	148.21	3_REACH	30000		30000	0	30000	0.202415492			1	0.039	2.6314E-07			1	0.039	2.6314E-07	7880		7880	0	7880	0.0531678
61260-55-7	61260557	3330	N,N'-bis(2,2,6,6-	394.7	3_REACH	100000		100000	0	100000	0.25335698			1	0.039	9.88092E-08			1	0.039	9.88092E-08	600		600	0	600	0.00152014
613-62-7	613627	4310	2-	234.3	3_REACH				1	0.39	1.66453E-06	1.6	1.6	0	1.6	6.82885E-06			1	0.039	1.66453E-07	16	16	16	0	16	6.8289E-05
614-45-9	614459	3334	tert-butyl perbenzoate	194.23	3_REACH	720		720	0	720	0.003706945			1	0.039	2.00793E-07			1	0.039	2.00793E-07	32		32	0	32	0.00016475
615-20-3	615203	3338	2-chlorobenzothiazole	169.63	3_REACH	3900		3900	0	3900	0.022991216			1	0.039	2.29912E-07			1	0.039	2.29912E-07	2290		2290	0	2290	0.01349997
615-60-1	615601	3339	4-chloro-o-xylene	140.61	3_REACH	958		958	0	958	0.006813171			1	0.039	2.77363E-07			1	0.039	2.77363E-07	590		590	0	590	0.004196
61597-98-6	61597986	3340	L-Menthyl lactate	228.33	3_REACH	13200		13200	0	13200	0.057811063			1	0.039	1.70805E-07			1	0.039	1.70805E-07	160		160	0	160	0.00070074
616-45-5	616455	757	2-pyrrolidone	85.107	3_REACH	4640000		4640000	0	4640000	54.51960473	598900	598900	0	598900	7.037023982			1	0.039	4.58247E-07	22200		22200	0	22200	0.26084811
616-47-7	616477	3346	1-methylimidazole	82.108	3_REACH	100000		100000	0	100000	1.217908121			1	0.039	4.74984E-07			1	0.039	4.74984E-07	121700		121700	0	121700	1.48219418
6166-86-5	6166865	3347	2,4,6,8,10-	295.6	3_REACH	213333333.3		213333333.3	0	213333333.3	721.6959856			1	0.039	1.31935E-07			1	0.039	1.31935E-07	29189.03904		29189.03904	0	29189.039	0.09874506
61826-76-4	61826764	4625	(S)-2-Hydroxy-2-(3-	225.25	3_REACH	900		900	0	900	0.00399556			1	0.039	1.73141E-07			1	0.039	1.73141E-07	130		130	0	130	0.00057714
61847-48-1	61847481	3356	methyl 4-[[(2,5-	643.49	3_REACH	100000		100000	0	100000	0.15540257			1	0.039	6.0607E-08			1	0.039	6.0607E-08	1000		1000	0	1000	0.00155403
618-62-2	618622	759	3,5-dichloronitrobenzene	192	3_REACH				1	0.39	2.03125E-06	2200	2200	0	2200	0.011458333			1	0.039	2.03125E-07	200		200	0	200	0.00104167
618-88-2	618882	3358	5-nitroisophthalic acid	211.13	3_REACH	1287093		1287093	0	1287093	6.096210865	1292481.667	1292481.667	0	1292481.667	6.121733845			1	0.039	1.8472E-07	268776		268776	0	268776	1.27303557
6197-30-4	6197304	3360	octocrilene	361.49	3_REACH	500		500	0	500	0.001383164			1	0.039	1.07887E-07			1	0.039	1.07887E-07	100000		100000	0	100000	0.27663283
621-29-4	621294	3362	m-tolyl isocyanate	133.15	3_REACH	19500		19500	0	19500	0.146451371	12100	12100	0	12100	0.090874953			1	0.039	2.92903E-07	10000		10000	0	10000	0.07510327
62-23-7	62237	761	4-nitrobenzoic acid	167.12	3_REACH	9966.666667		9966.666667	0	9966.666667	0.059637785			1	0.039	2.33365E-07			1	0.039	2.33365E-07	537796		537796	0	537796	3.21802298
622-40-2	622402	762	2-morpholinoethanol	131.18	3_REACH	5000		5000	0	5000	0.038115566			1	0.039	2.97301E-07			1	0.039	2.97301E-07	35300		35300	0	35300	0.2690959
622-58-2	622582	3365	p-tolyl isocyanate	133.15	3_REACH	13166.66667		13166.66667	0	13166.66667	0.098885968	600	600	0	600	0.004506196			1	0.039	2.92903E-07	3100		3100	0	3100	0.02328201
623-03-0	623030	763	4-chlorobenzonitrile	137.57	3_REACH	10000		10000	0	10000	0.072690267			1	0.039	2.83492E-07			1	0.039	2.83492E-07	22333.33333		22333.33333	0	22333.3333	0.1623416
623-40-5	623405	4785	2-Pentanone oxime	101.15	3_REACH	100000		100000	0	100000	0.988630746			1	0.039	3.85566E-07			1	0.039	3.85566E-07	32000		32000	0	32000	0.31636184
624-54-4	624544	3370	pentyl propionate	144.21	3_REACH	1300		1300	0	1300	0.009014631			1	0.039	2.70439E-07			1	0.039	2.70439E-07	4500		4500	0	4500	0.03120449
62-53-3	62533	765	aniline	93.13	3_REACH	360.2499133		360.2499133	0	360.2499133	0.003868248	390	390	0	390	0.004187695	5600	5600	0	5600	0.060131	2000	3000	3000	0	3000	0.03221304
62-56-6	62566	767	thiourea	76.123	3_REACH	600000		600000	0	600000	7.881980479	5000000	5000000	0	5000000	65.68317066			1	0.039	5.12329E-07	424.2640687		424.2640687	0	424.264069	0.0055734
6259-76-3	6259763	3375	hexyl salicylate	222.28	3_REACH	950		950	0	950	0.004273889			1	0.039	1.75454E-07			1	0.039	1.75454E-07	150		150	0	150	0.00067482
626-43-7	626437	768	3,5-dichloroaniline	162.02	3_REACH	2730		2730	0	2730	0.016849772	1000	1000	0	1000	0.006172078	1000	1000	0	1000	0.006172078	2500		2500	0	2500	0.01543019
6284-40-8	6284408	770	meglumine	195.22	3_REACH	50000		50000	0	50000	0.256121299			1	0.039	1.99775E-07			1	0.039	1.99775E-07	1000000		1000000	0	1000000	5.12242598
62889-66-1	62889661	3379	613-099-6	315.54	3_REACH	464		464	0	464	0.001470495			1	0.039	1.23598E-07			1	0.039	1.23598E-07	25		25	0	25	7.9229E-05
628-89-7	628897	3380	2-(2-chloroethoxy)ethanol	124.57	3_REACH	39766.6		39766.6	0	39766.6	0.319230954			1	0.039	3.13077E-07			1	0.039	3.13077E-07	150498.3		150498.3	0	150498.3	1.20814241
628-96-6	628966	3382	ethylene dinitrate	152.06	3_REACH	120		120	0	120	0.000789162	30	30	0	30	0.000197291			1	0.039	2.56478E-07	10000		10000	0	10000	0.06576351
629-11-8	629118	3385	hexane-1,6-diol	118.18	3_REACH	2200000		2200000	0	2200000	18.61567101			1	0.039	3.30005E-07			1	0.039	3.30005E-07	1180000		1180000	0	1180000	9.984769
6291-95-8	6291958	4276	1,3,5-tris(2-methyl-2-	291.35	3_REACH	12000		12000	0	12000	0.041187575			1	0.039	1.3386E-07			1	0.039	1.3386E-07	21600		21600	0	21600	0.07413764
629-40-3	629403	771	suberonitrile	136.2	3_REACH	176000		176000	0	176000	1.292217327			1	0.039	2.86344E-07			1	0.039	2.86344E-07	49900		49900	0	49900	0.36637298
629-50-5	629505	3389	tridecane	184.37	3_REACH	1000		1000	0	1000	0.005423876			1	0.039	2.11531E-07			1	0.039	2.11531E-07	3000	3000	3000	0	3000	0.01627163
629-59-4	629594	3390	tetradecane	198.39	3_REACH	1000		1000	0	1000	0.005040577			1	0.039	1.96582E-07			1	0.039	1.96582E-07	3000		3000	0	3000	0.01512173
629-62-9	629629	772	pentadecane	212.42	3_REACH				1	0.39	1.83599E-06			1	0.039	1.83599E-07			1	0.039	1.83599E-07				1	1	4.7077E-06
629-73-2	629732	3391	hexadec-1-ene	224.43	3_REACH	3.4	3.4	3.4	0	3.4	1.51495E-05			1	0.039	1.73774E-07			1	0.039	1.73774E-07	0.93	0.93	0.93	0	0.93	4.1438E-06
629-82-3	629823	3392	dioctyl ether	242.45	3_REACH	1000000		1000000	0	1000000	4.124561765			1	0.039	1.60858E-07			1	0.039	1.60858E-07	11430		11430	0	11430	0.04714374
63-05-8	63058	75	androst-4-ene-3,17-dione	286.42	3_REACH	2869.666667		2869.666667	0	2869.666667	0.010019086	0.7	0.7	0	0.7	2.44396E-06			1	0.039	1.36164E-07	2300		2300	0	2300	0.00803017
6309-51-9	6309519	3394	isopentyl laurate	270.46	3_REACH	10000000		10000000	0	10000000	36.97404422			1	0.039	1.44199E-07			1	0.039	1.44199E-07	33333.33333		33333.33333	0	33333.3333	0.12324681
6331-96-0	6331960	3399	2-amino-4,5-	242.08	3_REACH	100000		100000	0	100000	0.413086583			1	0.039	1.61104E-07			1	0.039	1.61104E-07	100000		100000	0	100000	0.41308658
63562-34-5	63562345	3405	bis(2-hydroxyethyl) (6H-	434.38	3_REACH	850		850	0	850	0.001956812			1	0.039	8.97831E-08			1	0.039	8.97831E-08	11000		11000	0	11000	0.02532345
6358-30-1	6358301	3406	8,18-dichloro-5,15-diethyl-	589.49	3_REACH	100000		100000	0	100000	0.169638162			1	0.039	6.61589E-08			1	0.039	6.61589E-08	100000		100000	0	100000	0.16963816
6358-37-8	6358378	3408	2,2'-[(3,3'-dichloro[1,1'-	657.56	3_REACH	100		100	0	100	0.000152077			1	0.039	5.93102E-08			1	0.039	5.93102E-08	100000		100000	0	100000	0.15207738
6358-64-1	6358641	3409	4-chloro-2,5-	187.63	3_REACH	35000		35000	0	35000	0.186537334			1	0.039	2.07856E-07			1	0.039	2.07856E-07	1816.666667		1816.666667	0	1816.66667	0.00968218
6358-85-6	6358856	3410	2,2'-[(3,3'-dichloro[1,1'-	629.51	3_REACH	100		100	0	100	0.000158854			1	0.039	6.19529E-08			1	0.039	6.19529E-08	100000		100000	0	100000	0.15885371
636-30-6	636306	774	2,4,5-trichloroaniline	196.47	3_REACH	1000		1000	0	1000	0.005089836	56	56	0	56	0.000285031	56	56	0	56	0.000285031	733.3333333		733.3333333	0	733.333333	0.00373255
6386-38-5	6386385	3420	methyl 3-(3,5-di-tert-butyl-4-	292.42	3_REACH	3200		3200	0	3200	0.010943164			1	0.039	1.3337E-07			1	0.039	1.3337E-07	500		500	0	500	0.00170987
6410-32-8	6410328	3424	3-hydroxy-4-[(2-methyl-4-	440.46	3_REACH	100000		100000	0	100000	0.227035372			1	0.039	8.85438E-08			1	0.039	8.85438E-08	1000		1000	0	1000	0.00227035
6410-41-9	6410419	3425	N-(5-chloro-2,4-	627.12	3_REACH	100000		100000	0	100000	0.159459115			1	0.039	6.21891E-08			1	0.039	6.21891E-08	1000		1000	0	1000	0.00159459
6419-19-8	6419198	3429	nitrilotrimethylenetris(phos	299.05	3_REACH	150000		150000	0	150000	0.501588363	23000	23000	0	23000	0.076910216			1	0.039	1.30413E-07	7400		7400	0	7400	0.02474503
6422-86-2	6422862	3430	bis(2-ethylhexyl)	390.56	3_REACH	250		250	0	250	0.000640107	280	280	0	280	0.000716919			1	0.039	9.98566E-08	860		860	0	860	0.00220197
6425-39-4	6425394	3432	2,2'-dimorpholinyldiethyl	244.34	3_REACH	215000		215000	0	215000	0.879921421			1	0.039	1.59614E-07			1	0.039	1.59614E-07	100000		100000	0	100000	0.40926578
64354-92-3	64354923	3434	3-	211.35	3_REACH	2200		2200	0	2200	0.010409274			1	0.039	1.84528E-07			1	0.039	1.84528E-07	829		829	0	829	0.0039224
6440-58-0	6440580	779	1,3-bis(hydroxymethyl)-5,5-	188.19	3_REACH	100000		100000	0	100000	0.531377863	14000	14000	0	14000	0.074392901			1	0.039	2.07237E-07	3800		3800	0	3800	0.02019236
6448-95-9	6448959	3436	3-hydroxy-4-[(2-methyl-5-	426.44	3_REACH	100000		100000	0	100000	0.234499578			1	0.039	9.14548E-08			1	0.039	9.14548E-08	1000		1000	0	1000	0.002345
645-62-5	645625	3438	2-ethylhex-2-enal	126.2	3_REACH	4600		4600	0	4600	0.036450079			1	0.039	3.09033E-07			1	0.039	3.09033E-07	9250		9250	0	9250	0.07329635
646-24-2	646242	3439	nonamethylenediamine	158.29	3_REACH	13500		13500	0	13500	0.085286499			1	0.039	2.46383E-07			1	0.039	2.46383E-07	31166.66667		31166.66667	0	31166.6667	0.19689599
6485-40-1	6485401	781	l-p-mentha-1(6),8-dien-2-	150.22	3_REACH	4500		4500	0	4500	0.029956064			1	0.039	2.59619E-07			1	0.039	2.59619E-07	4300		4300	0	4300	0.02862468
6485-55-8	6485558	3445	cis-2,6-dimethylmorpholine	115.18	3_REACH	100000		100000	0	100000	0.868206286			1	0.039	3.386E-07			1	0.039	3.386E-07	12490		12490	0	12490	0.10843897
6485-67-2	6485672	4453	(2R)-2-amino-2-	150.18	3_REACH	100000		100000	0	100000	0.665867626			1	0.039	2.59688E-07			1	0.039	2.59688E-07	32000		32000	0	32000	0.21307764
6486-23-3	6486233	3446	2-[(4-chloro-2-	395.21	3_REACH	1000		1000	0	1000	0.0025303			1	0.039	9.86817E-08			1	0.039	9.86817E-08	1000		1000	0	1000	0.0025303
6528-34-3	6528343	3450	2-[(4-methoxy-2-	386.37	3_REACH	1000		1000	0	1000	0.002588193			1	0.039	1.0094E-07			1	0.039	1.0094E-07	1000		1000	0	1000	0.00258819
65405-77-8	65405778	3452	(Z)-3-hexenyl salicylate	220.27	3_REACH	1150.217371		1150.217371	0	1150.217371	0.005221852			1	0.039	1.77055E-07			1	0.039	1.77055E-07	190		190	0	190	0.00086258
65-45-2	65452	784	salicylamide	137.14	3_REACH	61100		61100	0	61100	0.445530115			1	0.039	2.84381E-07			1	0.039	2.84381E-07	71		71	0	71	0.00051772
65520-46-9	65520469	3455	bis[2-[2-(2-	522.68	3_REACH	32333.33333		32333.33333	0	32333.33333	0.061860667			1	0.039	7.46154E-08			1	0.039	7.46154E-08	6815		6815	0	6815	0.01303857
65-85-0	65850	785	benzoic acid	122.12	3_REACH	10000		10000	0	10000	0.081886669			1	0.039	3.19358E-07			1	0.039	3.19358E-07	110		110	0	110	0.00090075
65855-02-9	65855029	4291	1-benzyl-5-	234.26	3_REACH	64000		64000	0	64000	0.273200717			1	0.039	1.66482E-07			1	0.039	1.66482E-07	56000		56000	0	56000	0.23905063
6600-31-3	6600313	3458	3,9-dicyclohex-3-enyl-	320.43	3_REACH	70000		70000	0	70000	0.218456449			1	0.039	1.21711E-07			1	0.039	1.21711E-07	100000		100000	0	100000	0.31208064
66063-15-8	66063158	3459	4-chloro-N-	209.72	3_REACH	5910		5910	0	5910	0.028180431			1	0.039	1.85962E-07			1	0.039	1.85962E-07	1.75		1.75	0	1.75	8.3445E-06
66068-84-6	66068846	3460	4-(5,5,6-	236.4	3_REACH	1012.256861		1012.256861	0	1012.256861	0.004281966			1	0.039	1.64975E-07			1	0.039	1.64975E-07	9121.811549		9121.811549	0	9121.81155	0.03858634
6610-29-3	6610293	3462	4-methylthiosemicarbazide	105.17	3_REACH	6666.666667		6666.666667	0	6666.666667	0.063389433			1	0.039	3.70828E-07			1	0.039	3.70828E-07	15000		15000	0	15000	0.14262622
66423-13-0	66423130	3473	octyl (R)-2-(4-chloro-2-	326.86	3_REACH	1000		1000	0	1000	0.003059414	50000	50000	0	50000	0.152970691			1	0.039	1.19317E-07	1000		1000	0	1000	0.00305941
66492-51-1	66492511	3475	(5-ethyl-1,3-dioxan-5-	200.23	3_REACH	1303		1303	0	1303	0.006507516			1	0.039	1.94776E-07			1	0.039	1.94776E-07	676		676	0	676	0.00337612
6674-22-2	6674222	3481	1,8-	152.24	3_REACH	100000		100000	0	100000	0.656857593			1	0.039	2.56174E-07			1	0.039	2.56174E-07	92600		92600	0	92600	0.60825013
67075-37-0	67075370	3484	2,9-bis(2-	598.66	3_REACH	7600		7600	0	7600	0.012695019			1	0.039	6.51455E-08			1	0.039	6.51455E-08	100000		100000	0	100000	0.16703972
6711-48-4	6711484	3485	N'-[3-	187.33	3_REACH	21400		21400	0	21400	0.114236908			1	0.039	2.08189E-07			1	0.039	2.08189E-07	1200		1200	0	1200	0.00640581
6712-98-7	6712987	3486	1-(N,N-bis(2-	163.22	3_REACH	100000		100000	0	100000	0.612670016			1	0.039	2.38941E-07			1	0.039	2.38941E-07	50000		50000	0	50000	0.30633501
67151-63-7	67151637	3487	1-[bis[3-	245.41	3_REACH	49333.33333		49333.33333	0	49333.33333	0.201024136			1	0.039	1.58918E-07			1	0.039	1.58918E-07	12500		12500	0	12500	0.05093517
6731-36-8	6731368	3488	di-tert-butyl 3,3,5-	302.45	3_REACH	43		43	0	43	0.000142172			1	0.039	1.28947E-07			1	0.039	1.28947E-07	110		110	0	110	0.0003637
67-43-6	67436	82	N-	393.35	3_REACH	750000		750000	0	750000	1.906698869	100000	100000	0	100000	0.254226516			1	0.039	9.91483E-08	2100		2100	0	2100	0.00533876
674-82-8	674828	3493	but-3-en-3-olide	84.074	3_REACH	50000		50000	0	50000	0.59471418			1	0.039	4.63877E-07			1	0.039	4.63877E-07	73333.33333		73333.33333	0	73333.3333	0.87224746
67801-15-4	67801154	3500	3-methyl-5-(2,2,3-trimethyl-	206.33	3_REACH	960		960	0	960	0.004652741			1	0.039	1.89018E-07			1	0.039	1.89018E-07	3100		3100	0	3100	0.01502448
6786-83-0	6786830	3502	alpha,alpha-Bis[4-	487.65	3_REACH	10547.61		10547.61	0	10547.61	0.021629468			1	0.039	7.99754E-08			1	0.039	7.99754E-08	11871.47		11871.47	0	11871.47	0.02434424
67990-05-0	67990050	3504	N-(5-chloro-2-	581.03	3_REACH	100000		100000	0	100000	0.172108153			1	0.039	6.71222E-08			1	0.039	6.71222E-08	1000		1000	0	1000	0.00172108
68-11-1	68111	798	mercaptoacetic acid	92.116	3_REACH	10000		10000	0	10000	0.108558774			1	0.039	4.23379E-07			1	0.039	4.23379E-07	7600		7600	0	7600	0.08250467
68134-22-5	68134225	3507	N-(2,3-dihydro-2-oxo-1H-	405.34	3_REACH	1000		1000	0	1000	0.002467065			1	0.039	9.62155E-08			1	0.039	9.62155E-08	1000		1000	0	1000	0.00246706
682-01-9	682019	3509	tetrapropyl orthosilicate	264.44	3_REACH	201000		201000	0	201000	0.760096808			1	0.039	1.47481E-07			1	0.039	1.47481E-07	22000		22000	0	22000	0.08319468
682-09-7	682097	3510	2,2-	214.31	3_REACH	400000		400000	0	400000	1.866455135			1	0.039	1.81979E-07			1	0.039	1.81979E-07	125000		125000	0	125000	0.58326723
682-11-1	682111	3511	2-allyloxymethyl-2-	174.24	3_REACH	400000		400000	0	400000	2.295684114			1	0.039	2.23829E-07			1	0.039	2.23829E-07	125000		125000	0	125000	0.71740129
68227-78-1	68227781	3512	N-(5-chloro-2-	565.03	3_REACH	100000		100000	0	100000	0.176981753			1	0.039	6.90229E-08			1	0.039	6.90229E-08	1000		1000	0	1000	0.00176982
68-26-8	68268	3514	retinol	286.46	3_REACH	100000		100000	0	100000	0.349088878			1	0.039	1.36145E-07			1	0.039	1.36145E-07	2380		2380	0	2380	0.00830832
6842-62-2	6842622	3515	614-477-3	239.1	3_REACH	260		260	0	260	0.001087411			1	0.039	1.63112E-07			1	0.039	1.63112E-07	16.8		16.8	0	16.8	7.0263E-05
6843-66-9	6843669	3516	dimethoxydiphenylsilane	244.37	3_REACH	6100		6100	0	6100	0.024962148			1	0.039	1.59594E-07			1	0.039	1.59594E-07	550		550	0	550	0.00225069
6850-63-1	6850631	801	2,6-	127.23	3_REACH	21500		21500	0	21500	0.168985302			1	0.039	3.06531E-07			1	0.039	3.06531E-07	7810		7810	0	7810	0.06138489
68516-73-4	68516734	3518	tetramethyl 2,2'-[1,4-	716.67	3_REACH	100000		100000	0	100000	0.139534235			1	0.039	5.44184E-08			1	0.039	5.44184E-08	40000		40000	0	40000	0.05581369
68610-86-6	68610866	3522	Butanamide, 2,2'-[(3,3'-	687.59	3_REACH	100		100	0	100	0.000145436			1	0.039	5.67198E-08			1	0.039	5.67198E-08	100000		100000	0	100000	0.14543551
687-47-8	687478	3526	ethyl (S)-2-	118.13	3_REACH	180000		180000	0	180000	1.523745027			1	0.039	3.30145E-07			1	0.039	3.30145E-07	320000		320000	0	320000	2.70888005
68855-18-5	68855185	3527	(3-Hydroxy-2,2-	216.32	3_REACH	86		86	0	86	0.000397559			1	0.039	1.80288E-07			1	0.039	1.80288E-07	6.5		6.5	0	6.5	3.0048E-05
688-84-6	688846	3529	2-ethylhexyl methacrylate	198.31	3_REACH	593.3333333		593.3333333	0	593.3333333	0.002991949	754	754	0	754	0.003802128			1	0.039	1.96662E-07	280		280	0	280	0.00141193
69045-84-7	69045847	4322	2,3-dichloro-5-	215.99	3_REACH	1600		1600	0	1600	0.00740775			1	0.039	1.80564E-07			1	0.039	1.80564E-07	280		280	0	280	0.00129636
6925-69-5	6925695	3537	12H-phthaloperin-12-one	270.29	3_REACH	100000		100000	0	100000	0.369972992			1	0.039	1.44289E-07			1	0.039	1.44289E-07	10700		10700	0	10700	0.03958711
693-21-0	693210	804	oxydiethylene dinitrate	196.12	3_REACH	86000		86000	0	86000	0.438507037	30	30	0	30	0.000152968			1	0.039	1.98858E-07	13033.33333		13033.33333	0	13033.3333	0.06645591
693-23-2	693232	3538	dodecanedioic acid	230.3	3_REACH	800000		800000	0	800000	3.473729917			1	0.039	1.69344E-07			1	0.039	1.69344E-07	5800		5800	0	5800	0.02518454
693-36-7	693367	3539	dioctadecyl 3,3'-	683.18	3_REACH	100000		100000	0	100000	0.146374308			1	0.039	5.7086E-08			1	0.039	5.7086E-08	3700		3700	0	3700	0.00541585
693-57-2	693572	3540	12-aminododecanoic acid	215.34	3_REACH	100000		100000	0	100000	0.464381908			1	0.039	1.81109E-07			1	0.039	1.81109E-07	3050		3050	0	3050	0.01416365
6938-94-9	6938949	3541	diisopropyl adipate	230.3	3_REACH	1213.333333		1213.333333	0	1213.333333	0.00526849			1	0.039	1.69344E-07			1	0.039	1.69344E-07	2000		2000	0	2000	0.00868432
693-98-1	693981	806	2-methylimidazole	82.108	3_REACH	100000		100000	0	100000	1.217908121			1	0.039	4.74984E-07			1	0.039	4.74984E-07	4390		4390	0	4390	0.05346617
6940-53-0	6940530	3543	1-chloro-2,5-dimethoxy-4-	217.61	3_REACH	7700		7700	0	7700	0.035384403			1	0.039	1.7922E-07			1	0.039	1.7922E-07	3260		3260	0	3260	0.01498093
694-83-7	694837	807	cyclohex-1,2-ylenediamine	114.19	3_REACH	100000		100000	0	100000	0.875733427			1	0.039	3.41536E-07			1	0.039	3.41536E-07	3200		3200	0	3200	0.02802347
700-13-0	700130	3554	2,3,5-	152.19	3_REACH	1000		1000	0	1000	0.006570734			1	0.039	2.56259E-07			1	0.039	2.56259E-07	8000		8000	0	8000	0.05256587
70356-09-1	70356091	3560	1-[4-(1,1-	310.39	3_REACH	3		3	0	3	9.66526E-06			1	0.039	1.25648E-07			1	0.039	1.25648E-07	3		3	0	3	9.6653E-06
70445-33-9	70445339	4370	3-(2-ethylhexyloxy)propane	204.31	3_REACH	7200		7200	0	7200	0.035240566	1500	1500	0	1500	0.007341785			1	0.039	1.90886E-07	22170		22170	0	22170	0.10851158
70516-41-5	70516415	3563	2'-anilino-6'-[ethyl(3-	518.66	3_REACH	3200		3200	0	3200	0.006169745			1	0.039	7.51938E-08			1	0.039	7.51938E-08	250000		250000	0	250000	0.48201134

70-55-3	**70553**	85	toluene-4-sulphonamide	171.22	3_REACH	18000		18000	**0**	**18000**	**0.105127906**				**1**	**0.039**	**2.27777E-07**	**1**	**0.039**	**2.27777E-07**	7700		7700	**0**	**7700**	**0.04497138**
706-14-9	**706149**	813	decan-4-olide	170.25	3_REACH	1833.333333		1833.333333	**0**	**1833.333333**	**0.010768478**				**1**	**0.039**	**2.29075E-07**	**1**	**0.039**	**2.29075E-07**	779		779	**0**	**779**	**0.00457562**
7069-42-3	**7069423**	3567	retinyl propionate	342.52	3_REACH	10000000		10000000	**0**	**10000000**	**29.19537545**				**1**	**0.039**	**1.13862E-07**	**1**	**0.039**	**1.13862E-07**	2380		2380	**0**	**2380**	**0.0069485**
70969-58-3	**70969583**	815	diisobutyl	284.4	3_REACH	500		500	**0**	**500**	**0.001758087**	42		42	**0**	**42**	**0.000147679**	**1**	**0.039**	**1.37131E-07**	139.3333333		139.3333333	**0**	**139.333333**	**0.00048992**
71048-82-3	**71048823**	3577	(2E)-1-[(1R,2S)-2,6,6-	192.3	3_REACH	323.3333333		323.3333333	**0**	**323.3333333**	**0.001681401**				**1**	**0.039**	**2.02808E-07**	**1**	**0.039**	**2.02808E-07**	380		380	**0**	**380**	**0.00197608**
712-50-5	**712505**	818	cyclohexyl phenyl ketone	188.27	3_REACH	3666.666667		3666.666667	**0**	**3666.666667**	**0.019475576**				**1**	**0.039**	**2.07149E-07**	**1**	**0.039**	**2.07149E-07**	1690		1690	**0**	**1690**	**0.00897647**
713-95-1	**713951**	3581	dodecan-5-olide	198.31	3_REACH	4061.086655		4061.086655	**0**	**4061.086655**	**0.020478476**				**1**	**0.039**	**1.96662E-07**	**1**	**0.039**	**1.96662E-07**	7138.599873		7138.599873	**0**	**7138.59987**	**0.03599718**
71604-74-5	**71604745**	3586	m-(2,3-epoxypropoxy)-N,N-	277.32	3_REACH	5600		5600	**0**	**5600**	**0.020193279**				**1**	**0.039**	**1.40632E-07**	**1**	**0.039**	**1.40632E-07**	2400		2400	**0**	**2400**	**0.00865426**
71617-10-2	**71617102**	3587	isopentyl p-	248.32	3_REACH	271300		271300	**0**	**271300**	**1.092541881**				**1**	**0.039**	**1.57055E-07**	**1**	**0.039**	**1.57055E-07**	60		60	**0**	**60**	**0.00024162**
71735-74-5	**71735745**	3588	ethyl 3-[[bis(1-	314.4	3_REACH	3200		3200	**0**	**3200**	**0.010178117**				**1**	**0.039**	**1.24046E-07**	**1**	**0.039**	**1.24046E-07**	5000		5000	**0**	**5000**	**0.01590331**
7173-62-8	**7173628**	3589	(Z)-N-9-	324.6	3_REACH	26.66666667		26.66666667	**0**	**26.66666667**	**8.21524E-05**				**1**	**0.039**	**1.20148E-07**	**1**	**0.039**	**1.20148E-07**	188		188	**0**	**188**	**0.00057917**
71902-23-3	**71902233**	3594	6-[(1-	271.4	3_REACH	500000		500000	**0**	**500000**	**1.842299189**				**1**	**0.039**	**1.43699E-07**	**1**	**0.039**	**1.43699E-07**	78100		78100	**0**	**78100**	**0.28776713**
7195-44-0	**7195440**	3595	bis(2,3-epoxypropyl)	278.26	3_REACH	638		638	**0**	**638**	**0.00229282**				**1**	**0.039**	**1.40157E-07**	**1**	**0.039**	**1.40157E-07**	327		327	**0**	**327**	**0.00117516**
72361-35-4	**72361354**	3603	triisotridecyl benzene-1,2,4-	757.19	3_REACH	4100		4100	**0**	**4100**	**0.005414757**				**1**	**0.039**	**5.15062E-08**	**1**	**0.039**	**5.15062E-08**	3500		3500	**0**	**3500**	**0.00462235**
7300-34-7	**7300347**	3612	3,3'-[butane-1,4-	204.32	3_REACH	100000		100000	**0**	**100000**	**0.489428348**				**1**	**0.039**	**1.90877E-07**	**1**	**0.039**	**1.90877E-07**	5400		5400	**0**	**5400**	**0.02642913**
7305-71-7	**7305717**	4342	2-amino-5-methylthiazole	114.17	3_REACH	50000		50000	**0**	**50000**	**0.437943418**				**1**	**0.039**	**3.41596E-07**	**1**	**0.039**	**3.41596E-07**	1000		1000	**0**	**1000**	**0.00875887**
732-26-3	**732263**	829	2,4,6-tri-tert-butylphenol	262.44	3_REACH	20.3		20.3	**0**	**20.3**	**7.7351E-05**				**1**	**0.039**	**1.48605E-07**	**1**	**0.039**	**1.48605E-07**				**1**	**1**	**3.8104E-06**
7328-22-5	**7328225**	3618	2-(2-butoxyethoxy)ethyl	230.3	3_REACH	7453.333333		7453.333333	**0**	**7453.333333**	**0.032363584**				**1**	**0.039**	**1.69344E-07**	**1**	**0.039**	**1.69344E-07**	16000		16000	**0**	**16000**	**0.0694746**
7381-13-7	**7381137**	3627	1,1'-(1,3-	356.42	3_REACH	36900		36900	**0**	**36900**	**0.103529544**				**1**	**0.039**	**1.09421E-07**	**1**	**0.039**	**1.09421E-07**	6300		6300	**0**	**6300**	**0.01767578**
7396-58-9	**7396589**	3629	N-methyldidecylamine	311.6	3_REACH	100		100	**0**	**100**	**0.000320924**				**1**	**0.039**	**1.2516E-07**	**1**	**0.039**	**1.2516E-07**	2		2	**0**	**2**	**6.4185E-06**
7397-62-8	**7397628**	3630	butyl glycollate	132.16	3_REACH	50000		50000	**0**	**50000**	**0.378329298**				**1**	**0.039**	**2.95097E-07**	**1**	**0.039**	**2.95097E-07**				**1**	**1**	**7.5666E-06**
74338-72-0	**74338720**	4323	2,4,4,7-tetramethyl-6-octen-	182.31	3_REACH	2900		2900	**0**	**2900**	**0.015906972**				**1**	**0.039**	**2.13921E-07**	**1**	**0.039**	**2.13921E-07**	1700		1700	**0**	**1700**	**0.00932478**
74441-05-7	**74441057**	3635	N-[4-	499.49	3_REACH	1000		1000	**0**	**1000**	**0.002002042**				**1**	**0.039**	**7.80796E-08**	**1**	**0.039**	**7.80796E-08**	1000		1000	**0**	**1000**	**0.00200204**
7473-98-5	**7473985**	3642	2-hydroxy-2-	164.2	3_REACH	100000		100000	**0**	**100000**	**0.609013398**				**1**	**0.039**	**2.37515E-07**	**1**	**0.039**	**2.37515E-07**	60.6		60.6	**0**	**60.6**	**0.00036906**
75-12-7	**75127**	851	formamide	45.042	3_REACH	166666.6667		166666.6667	**0**	**166666.6667**	**3.700250137**				**1**	**0.039**	**8.65859E-07**	**1**	**0.039**	**8.65859E-07**	77600		77600	**0**	**77600**	**1.72283646**
7526-26-3	**7526263**	3659	diphenyl	248.22	3_REACH	10000		10000	**0**	**10000**	**0.040286842**				**1**	**0.039**	**1.57119E-07**	**1**	**0.039**	**1.57119E-07**	3100		3100	**0**	**3100**	**0.01248892**
7534-94-3	**7534943**	3668	exo-1,7,7-	222.33	3_REACH	970		970	**0**	**970**	**0.004362884**				**1**	**0.039**	**1.75415E-07**	**1**	**0.039**	**1.75415E-07**	251		251	**0**	**251**	**0.00112895**
75490-39-0	**75490390**	4313	2,2,4-trimethyl-4-phenyl-	187.29	3_REACH	860		860	**0**	**860**	**0.004591809**				**1**	**0.039**	**2.08233E-07**	**1**	**0.039**	**2.08233E-07**	4500		4500	**0**	**4500**	**0.02402691**
756-80-9	**756809**	864	O,O-dimethyl hydrogen	158.18	3_REACH	5666.666667		5666.666667	**0**	**5666.666667**	**0.035824167**				**1**	**0.039**	**2.46555E-07**	**1**	**0.039**	**2.46555E-07**				**1**	**1**	**6.3219E-06**
75-75-2	**75752**	3683	methanesulphonic acid	96.104	3_REACH	56000		56000	**0**	**56000**	**0.582702073**				**1**	**0.039**	**4.0581E-07**	**1**	**0.039**	**4.0581E-07**	5800		5800	**0**	**5800**	**0.06035129**
7575-23-7	**7575237**	3684	pentaerythritol tetrakis(3-	488.66	3_REACH	17		17	**0**	**17**	**3.4789E-05**				**1**	**0.039**	**7.98101E-08**	**1**	**0.039**	**7.98101E-08**	120		120	**0**	**120**	**0.00024557**
75980-60-8	**75980608**	3692	diphenyl(2,4,6-	348.38	3_REACH	1000		1000	**0**	**1000**	**0.002870429**				**1**	**0.039**	**1.11947E-07**	**1**	**0.039**	**1.11947E-07**	1560		1560	**0**	**1560**	**0.00447787**
75-98-9	**75989**	868	pivalic acid	102.13	3_REACH	300000		300000	**0**	**300000**	**2.937432684**				**1**	**0.039**	**3.81866E-07**	**1**	**0.039**	**3.81866E-07**	25000		25000	**0**	**25000**	**0.24478606**
76-03-9	**76039**	90	trichloroacetic acid	163.39	3_REACH	92333.33333		92333.33333	**0**	**92333.33333**	**0.565110064**	7370000		7370000	**0**	**7370000**	**45.10679968**	**1**	**0.039**	**2.38693E-07**	10		10	**0**	**10**	**6.1203E-05**
7605-52-9	**7605529**	3696	methyl cis-3-	156.22	3_REACH	3210		3210	**0**	**3210**	**0.020547945**				**1**	**0.039**	**2.49648E-07**	**1**	**0.039**	**2.49648E-07**	1190		1190	**0**	**1190**	**0.00761746**
760-67-8	**760678**	3697	2-ethylhexanoyl chloride	162.66	3_REACH	1640		1640	**0**	**1640**	**0.01008238**				**1**	**0.039**	**2.39764E-07**	**1**	**0.039**	**2.39764E-07**	97		97	**0**	**97**	**0.00059634**
76114-73-3	**76114733**	3699	2-Propynyl butylcarbamate	155.2	3_REACH	97600		97600	**0**	**97600**	**0.628865979**				**1**	**0.039**	**2.51289E-07**	**1**	**0.039**	**2.51289E-07**	12500		12500	**0**	**12500**	**0.08054124**
76201-56-4	**76201564**	3704	3-[dimethyl(3-	650.47	3_REACH				**1**	**0.39**	**5.99566E-07**	5860		5860	**0**	**5860**	**0.009008871**	**1**	**0.039**	**5.99566E-08**	3430		3430	**0**	**3430**	**0.00527311**
762-04-9	**762049**	3705	diethyl phosphonate	138.1	3_REACH	99800		99800	**0**	**99800**	**0.722664736**				**1**	**0.039**	**2.82404E-07**	**1**	**0.039**	**2.82404E-07**	92800		92800	**0**	**92800**	**0.67197683**
76-22-2	**76222**	872	bornan-2-one	152.24	3_REACH	11666.66667		11666.66667	**0**	**11666.66667**	**0.076633386**				**1**	**0.039**	**2.56174E-07**	**1**	**0.039**	**2.56174E-07**	2317		2317	**0**	**2317**	**0.01521939**
763-69-9	**763699**	3710	ethyl 3-ethoxypropionate	146.19	3_REACH	23800		23800	**0**	**23800**	**0.162801833**				**1**	**0.039**	**2.66776E-07**	**1**	**0.039**	**2.66776E-07**	114860		114860	**0**	**114860**	**0.78568986**
764-99-8	**764998**	3714	1,1'-	158.2	3_REACH	220227.1555		220227.1555	**0**	**220227.1555**	**1.392080629**				**1**	**0.039**	**2.46523E-07**	**1**	**0.039**	**2.46523E-07**	50000		50000	**0**	**50000**	**0.31605563**
76524-94-2	**76524942**	3715	N-[3-	249.38	3_REACH	119000		119000	**0**	**119000**	**0.477183415**				**1**	**0.039**	**1.56388E-07**	**1**	**0.039**	**1.56388E-07**	560		560	**0**	**560**	**0.00224557**
7659-86-1	**7659861**	3721	2-ethylhexyl	204.33	3_REACH	130		130	**0**	**130**	**0.000636226**				**1**	**0.039**	**1.90868E-07**	**1**	**0.039**	**1.90868E-07**	136.6666667		136.6666667	**0**	**136.666667**	**0.00066885**
76855-69-1	**76855691**	4234	Azetidon	287.43	3_REACH	1800		1800	**0**	**1800**	**0.006262394**				**1**	**0.039**	**1.35685E-07**	**1**	**0.039**	**1.35685E-07**	1800		1800	**0**	**1800**	**0.00626239**
768-94-5	**768945**	878	amantadine	151.25	3_REACH	8333.333333		8333.333333	**0**	**8333.333333**	**0.055096419**				**1**	**0.039**	**2.57851E-07**	**1**	**0.039**	**2.57851E-07**	30800		30800	**0**	**30800**	**0.20363636**
7695-91-2	**7695912**	3727	3,4-dihydro-2,5,7,8-	472.75	3_REACH	11000		11000	**0**	**11000**	**0.023268112**				**1**	**0.039**	**8.2496E-08**	**1**	**0.039**	**8.2496E-08**	27800		27800	**0**	**27800**	**0.05880487**
770-35-4	**770354**	3730	1-phenoxypropan-2-ol	152.19	3_REACH	215000		215000	**0**	**215000**	**1.412707799**				**1**	**0.039**	**2.56259E-07**	**1**	**0.039**	**2.56259E-07**	12500		12500	**0**	**12500**	**0.08213417**
77-09-8	**77098**	879	phenolphthalein	318.33	3_REACH	12040		12040	**0**	**12040**	**0.037822386**				**1**	**0.039**	**1.22514E-07**	**1**	**0.039**	**1.22514E-07**	320		320	**0**	**320**	**0.00100525**
7747-35-5	**7747355**	880	7a-ethyldihydro-1H,3H,5H-	143.19	3_REACH	49500		49500	**0**	**49500**	**0.345694532**				**1**	**0.039**	**2.72365E-07**	**1**	**0.039**	**2.72365E-07**	513		513	**0**	**513**	**0.00358265**
77501-63-4	**77501634**	882	Lactofen	461.78	3_REACH	32		32	**0**	**32**	**6.92971E-05**	1.4		1.4	**0**	**1.4**	**3.03175E-06**	**1**	**0.039**	**8.44558E-08**	1.83		1.83	**0**	**1.83**	**3.9629E-06**
77-71-4	**77714**	883	5,5-dimethylhydantoin	128.13	3_REACH	972200		972200	**0**	**972200**	**7.587606337**	14000		14000	**0**	**14000**	**0.109264029**	**1**	**0.039**	**3.04378E-07**	1000000		1000000	**0**	**1000000**	**7.80457348**
77-73-6	**77736**	884	3a,4,7,7a-tetrahydro-4,7-	132.21	3_REACH	466.6666667		466.6666667	**0**	**466.6666667**	**0.003529738**	980		980	**0**	**980**	**0.00741245**	**1**	**0.039**	**2.94985E-07**	2400		2400	**0**	**2400**	**0.01815294**
77-78-1	**77781**	886	dimethyl sulphate	126.13	3_REACH	7500		7500	**0**	**7500**	**0.059462459**				**1**	**0.039**	**3.09205E-07**	**1**	**0.039**	**3.09205E-07**	10000		10000	**0**	**10000**	**0.07928328**
77804-81-0	**77804810**	3736	2,2'-[ethylenebis(oxyphenyl	732.72	3_REACH	1000		1000	**0**	**1000**	**0.001364778**				**1**	**0.039**	**5.32263E-08**	**1**	**0.039**	**5.32263E-08**	1000		1000	**0**	**1000**	**0.00136478**
77-83-8	**77838**	3738	ethyl 2,3-epoxy-3-	206.24	3_REACH	3200		3200	**0**	**3200**	**0.015515904**				**1**	**0.039**	**1.891E-07**	**1**	**0.039**	**1.891E-07**	9300		9300	**0**	**9300**	**0.0450931**
7785-26-4	**7785264**	887	(-)-pin-2(3)-ene	136.24	3_REACH	120		120	**0**	**120**	**0.000880799**				**1**	**0.039**	**2.8626E-07**	**1**	**0.039**	**2.8626E-07**	247		247	**0**	**247**	**0.00181298**
7785-70-8	**7785708**	888	(+)-pin-2(3)-ene	136.24	3_REACH	120		120	**0**	**120**	**0.000880799**				**1**	**0.039**	**2.8626E-07**	**1**	**0.039**	**2.8626E-07**	232.5		232.5	**0**	**232.5**	**0.00170655**
77-86-1	**77861**	3739	trometamol	121.14	3_REACH	4000000		4000000	**0**	**4000000**	**33.01964669**				**1**	**0.039**	**3.21942E-07**	**1**	**0.039**	**3.21942E-07**	100000		100000	**0**	**100000**	**0.82549117**
7787-93-1	**7787931**	3741	dichloro(3-	191.56	3_REACH	107000		107000	**0**	**107000**	**0.558571727**				**1**	**0.039**	**2.03592E-07**	**1**	**0.039**	**2.03592E-07**	2900		2900	**0**	**2900**	**0.01513886**
778-94-9	**778949**	3743	2-nitro-4-	216.12	3_REACH	1000		1000	**0**	**1000**	**0.004627059**				**1**	**0.039**	**1.80455E-07**	**1**	**0.039**	**1.80455E-07**	100		100	**0**	**100**	**0.00046271**
77-90-7	**77907**	3744	tributyl O-acetylcitrate	402.48	3_REACH	1280		1280	**0**	**1280**	**0.003180282**				**1**	**0.039**	**9.68992E-08**	**1**	**0.039**	**9.68992E-08**	1000		1000	**0**	**1000**	**0.0024846**
77-92-9	**77929**	889	citric acid	192.12	3_REACH	200000		200000	**0**	**200000**	**1.041016032**				**1**	**0.039**	**2.02998E-07**	**1**	**0.039**	**2.02998E-07**	80000		80000	**0**	**80000**	**0.41640641**
77-93-0	**77930**	92	triethyl citrate	276.29	3_REACH	40000		40000	**0**	**40000**	**0.144775417**				**1**	**0.039**	**1.41156E-07**	**1**	**0.039**	**1.41156E-07**	8166.666667		8166.666667	**0**	**8166.66667**	**0.02955831**
77-94-1	**77941**	3745	tributyl citrate	360.45	3_REACH	2266.666667		2266.666667	**0**	**2266.666667**	**0.006288436**				**1**	**0.039**	**1.08198E-07**	**1**	**0.039**	**1.08198E-07**	6000		6000	**0**	**6000**	**0.01664586**
77-99-6	**77996**	890	propylidynetrimethanol	134.18	3_REACH	100000		100000	**0**	**100000**	**0.745267551**				**1**	**0.039**	**2.90654E-07**	**1**	**0.039**	**2.90654E-07**				**1**	**1**	**7.4527E-06**
780-69-8	**780698**	891	triethoxy(phenyl)silane	240.38	3_REACH	1420		1420	**0**	**1420**	**0.005907313**				**1**	**0.039**	**1.62243E-07**	**1**	**0.039**	**1.62243E-07**	100000		100000	**0**	**100000**	**0.41600799**
78-08-0	**78080**	3746	triethoxy(vinyl)silane	190.32	3_REACH	92200		92200	**0**	**92200**	**0.484447247**				**1**	**0.039**	**2.04918E-07**	**1**	**0.039**	**2.04918E-07**	25000		25000	**0**	**25000**	**0.13135771**
78-11-5	**78115**	892	pentaerithrityl tetranitrate	316.14	3_REACH	308666.6667		308666.6667	**0**	**308666.6667**	**0.976360684**				**1**	**0.039**	**1.23363E-07**	**1**	**0.039**	**1.23363E-07**				**1**	**1**	**3.1632E-06**
78-27-3	**78273**	893	1-ethynylcyclohexanol	124.18	3_REACH	100000		100000	**0**	**100000**	**0.805282654**				**1**	**0.039**	**3.1406E-07**	**1**	**0.039**	**3.1406E-07**	141800		141800	**0**	**141800**	**1.1418908**
78-40-0	**78400**	894	triethyl phosphate	182.16	3_REACH	100000		100000	**0**	**100000**	**0.54896794**				**1**	**0.039**	**2.14097E-07**	**1**	**0.039**	**2.14097E-07**	73000		73000	**0**	**73000**	**0.4007466**
78-42-2	**78422**	895	tris(2-ethylhexyl)	434.64	3_REACH	100000		100000	**0**	**100000**	**0.230075465**				**1**	**0.039**	**8.97294E-08**	**1**	**0.039**	**8.97294E-08**	876		876	**0**	**876**	**0.00201546**
78-51-3	**78513**	93	tris(2-butoxyethyl)	398.48	3_REACH	2266.666667		2266.666667	**0**	**2266.666667**	**0.005688282**				**1**	**0.039**	**9.78719E-08**	**1**	**0.039**	**9.78719E-08**	7600		7600	**0**	**7600**	**0.01907248**
78521-39-8	**78521398**	3751	6-[[(4-	285.36	3_REACH	750000		750000	**0**	**750000**	**2.628259041**				**1**	**0.039**	**1.36669E-07**	**1**	**0.039**	**1.36669E-07**	120000		120000	**0**	**120000**	**0.42052145**
78531-61-0	**78531610**	4400	4-(trans-4-	244.38	3_REACH	10000		10000	**0**	**10000**	**0.040919879**				**1**	**0.039**	**1.59588E-07**	**1**	**0.039**	**1.59588E-07**	100000		100000	**0**	**100000**	**0.40919879**
78-59-1	**78591**	897	3,5,5-trimethylcyclohex-2-	138.21	3_REACH	46666.66667		46666.66667	**0**	**46666.66667**	**0.337650435**	8094.442538		8094.442538	**0**	**8094.442538**	**0.058566258**	**1**	**0.039**	**2.82179E-07**	29900		29900	**0**	**29900**	**0.21633746**
78605-96-6	**78605966**	3752	alpha-Amylcinnamaldehyde	202.3	3_REACH	2100		2100	**0**	**2100**	**0.010380623**				**1**	**0.039**	**1.92783E-07**	**1**	**0.039**	**1.92783E-07**	154		154	**0**	**154**	**0.00076125**
78-63-7	**78637**	3753	di-tert-butyl 1,1,4,4-	290.44	3_REACH	1500		1500	**0**	**1500**	**0.005164578**				**1**	**0.039**	**1.34279E-07**	**1**	**0.039**	**1.34279E-07**	78.66666667		78.66666667	**0**	**78.6666667**	**0.00027085**
78-67-1	**78671**	3754	2,2'-dimethyl-2,2'-	164.22	3_REACH				**1**	**0.39**	**2.37486E-06**	10000		10000	**0**	**10000**	**0.060893923**	**1**	**0.039**	**2.37486E-07**	1480		1480	**0**	**1480**	**0.0090123**
78-69-3	**78693**	3755	3,7-dimethyloctan-3-ol	158.29	3_REACH	5000		5000	**0**	**5000**	**0.031587592**				**1**	**0.039**	**2.46383E-07**	**1**	**0.039**	**2.46383E-07**	8500		8500	**0**	**8500**	**0.05369891**
78-70-6	**78706**	899	linalool	154.25	3_REACH	3500		3500	**0**	**3500**	**0.022690438**				**1**	**0.039**	**2.52836E-07**	**1**	**0.039**	**2.52836E-07**	38400		38400	**0**	**38400**	**0.24894652**
78850-37-0	**78850370**	5023	methyl (3aR,4R,7aR)-2-	413.38	3_REACH	89000		89000	**0**	**89000**	**0.215298273**				**1**	**0.039**	**9.43442E-08**	**1**	**0.039**	**9.43442E-08**	32000		32000	**0**	**32000**	**0.07741061**
78-97-7	**78977**	3762	lactonitrile	71.08	3_REACH	220		220	**0**	**220**	**0.003095104**				**1**	**0.039**	**5.48678E-07**	**1**	**0.039**	**5.48678E-07**	48		48	**0**	**48**	**0.0006753**
79-06-1	**79061**	911	acrylamide	71.08	3_REACH	28333.33333		28333.33333	**0**	**28333.33333**	**0.398611893**	5000		5000	**0**	**5000**	**0.070343275**	**1**	**0.039**	**5.48678E-07**	32000		32000	**0**	**32000**	**0.45019696**
79-07-2	**79072**	3765	2-chloroacetamide	93.514	3_REACH	12100		12100	**0**	**12100**	**0.12939239**				**1**	**0.039**	**4.1705E-07**	**1**	**0.039**	**4.1705E-07**	1670		1670	**0**	**1670**	**0.01785829**
79-08-3	**79083**	912	bromoacetic acid	138.95	3_REACH	100000		100000	**0**	**100000**	**0.719683339**	100000		100000	**0**	**100000**	**0.719683339**	**1**	**0.039**	**2.80677E-07**	20		20	**0**	**20**	**0.00014394**
79-11-8	**79118**	915	chloroacetic acid	94.497	3_REACH	43500		43500	**0**	**43500**	**0.460332074**	25000		25000	**0**	**25000**	**0.264558663**	**1**	**0.039**	**4.12712E-07**	5	5	5	**0**	**5**	**5.2912E-05**
791-28-6	**791286**	95	triphenylphosphine oxide	278.29	3_REACH	21500		21500	**0**	**21500**	**0.077257537**				**1**	**0.039**	**1.40142E-07**	**1**	**0.039**	**1.40142E-07**	3900		3900	**0**	**3900**	**0.01401416**
79-14-1	**79141**	3766	glycollic acid	76.051	3_REACH	130000		130000	**0**	**130000**	**1.709379232**				**1**	**0.039**	**5.12814E-07**	**1**	**0.039**	**5.12814E-07**	10000		10000	**0**	**10000**	**0.13149071**
79-16-3	**79163**	3767	N-methylacetamide	73.096	3_REACH	1000000		1000000	**0**	**1000000**	**13.68063916**				**1**	**0.039**	**5.33545E-07**	**1**	**0.039**	**5.33545E-07**	299000		299000	**0**	**299000**	**4.09051111**
793-24-8	**793248**	3771	N-1,3-dimethylbutyl-N'-	268.41	3_REACH	9.333333333		9.333333333	**0**	**9.333333333**	**3.47727E-05**	3.7		3.7	**0**	**3.7**	**1.37849E-05**	**1**	**0.039**	**1.453E-07**	33.33333333		33.33333333	**0**	**33.3333333**	**0.00012419**
79-33-4	**79334**	920	l-(+)-lactic acid	90.078	3_REACH	56000		56000	**0**	**56000**	**0.62168343**	2180		2180	**0**	**2180**	**0.024201248**	**1**	**0.039**	**4.32958E-07**	1900000		1900000	**0**	**1900000**	**21.0928307**
79-41-4	**79414**	3776	methacrylic acid	86.09	3_REACH	10000		10000	**0**	**10000**	**0.11615751**	10000		10000	**0**	**10000**	**0.11615751**	**1**	**0.039**	**4.53014E-07**	380		380	**0**	**380**	**0.00441399**
79456-26-1	**79456261**	4391	3-chloro-5-trifluoromethyl-2-	196.56	3_REACH	10000		10000	**0**	**10000**	**0.050875051**	13000		13000	**0**	**13000**	**0.066137566**	**1**	**0.039**	**1.98413E-07**	10000		10000	**0**	**10000**	**0.05087505**
79-74-3	**79743**	3781	2,5-di-tert-	250.38	3_REACH	10		10	**0**	**10**	**3.99393E-05**				**1**	**0.039**	**1.55763E-07**	**1**	**0.039**	**1.55763E-07**	566.6666667		566.6666667	**0**	**566.666667**	**0.00226323**
79-77-6	**79776**	926	(E)-4-(2,6,6-trimethyl-1-	192.3	3_REACH	2150		2150	**0**	**2150**	**0.011180447**				**1**	**0.039**	**2.02808E-07**	**1**	**0.039**	**2.02808E-07**	6160		6160	**0**	**6160**	**0.03203328**
79815-20-6	**79815206**	4252	(S)-2,3-dihydro-1H-indole-	163.18	3_REACH	100000		100000	**0**	**100000**	**0.612820199**				**1**	**0.039**	**2.39E-07**	**1**	**0.039**	**2.39E-07**	10000		10000	**0**	**10000**	**0.06128202**
79-94-7	**79947**	929	2,2',6,6'-tetrabromo-4,4'-	543.9	3_REACH	10		10	**0**	**10**	**1.83857E-05**	160		160	**0**	**160**	**0.000294172**	**1**	**0.039**	**7.17044E-08**	26.66666667		26.66666667	**0**	**26.6666667**	**4.9029E-05**
80-04-6	**80046**	931	4,4'-	240.39	3_REACH	12400		12400	**0**	**12400**	**0.051582845**				**1**	**0.039**	**1.62236E-07**	**1**	**0.039**	**1.62236E-07**	8500		8500	**0**	**8500**	**0.03535921**
80-05-7	**80057**	96	4,4'-isopropylidenediphenol	228.29	3_REACH	0.1		0.1	**0**	**0.1**	**4.38039E-07**	9.12	10	10	**0**	**10**	**4.38039E-05**	**1**	**0.039**	**1.70835E-07**	400		400	**0**	**400**	**0.00175216**
80-07-9	**80079**	3786	bis(4-chlorophenyl)	287.16	3_REACH	980		980	**0**	**980**	**0.003412732**				**1**	**0.039**	**1.35813E-07**	**1**	**0.039**	**1.35813E-07**	280		280	**0**	**280**	**0.00097507**
80-10-4	**80104**	3788	dichloro(diphenyl)silane	253.2	3_REACH	16000		16000	**0**	**16000**	**0.063191153**				**1**	**0.039**	**1.54028E-07**	**1**	**0.039**	**1.54028E-07**	550		550	**0**	**550**	**0.0021722**
80-15-9	**80159**	932	Cumene hydroperoxide	152.19	3_REACH	1500		1500	**0**	**1500**	**0.009856101**				**1**	**0.039**	**2.56259E-07**	**1**	**0.039**	**2.56259E-07**	1200		1200	**0**	**1200**	**0.00788488**
80-26-2	**80262**	934	p-menth-1-en-8-yl acetate	196.29	3_REACH				**1**	**0.39**	**1.98686E-06**				**1**	**0.039**	**1.98686E-07**	**1**	**0.039**	**1.98686E-07**	2700		2700	**0**	**2700**	**0.01375516**
80-43-3	**80433**	3791	Dicumyl peroxide	270.37	3_REACH	386		386	**0**	**386**	**0.001427673**				**1**	**0.039**	**1.44247E-07**	**1**	**0.039**	**1.44247E-07**	3200		3200	**0**	**3200**	**0.01183563**
80-46-6	**80466**	936	p-(1,1-	164.25	3_REACH	180		180	**0**	**180**	**0.00109589**	36		36	**0**	**36**	**0.000219178**	**1**	**0.039**	**2.37443E-07**	900		900	**0**	**900**	**0.00547945**
80-51-3	**80513**	3792	4,4'-	358.4	3_REACH	430		430	**0**	**430**	**0.001199777**				**1**	**0.039**	**1.08817E-07**	**1**	**0.039**	**1.08817E-07**	700		700	**0**	**700**	**0.00195313**
80-54-6	**80546**	3794	2-(4-tert-	204.31	3_REACH	1280		1280	**0**	**1280**	**0.006264989**				**1**	**0.039**	**1.90886E-07**	**1**	**0.039**	**1.90886E-07**	1696		1696	**0**	**1696**	**0.00830111**
80-56-8	**80568**	937	pin-2(3)-ene	136.24	3_REACH	59.66666667		59.66666667	**0**	**59.66666667**	**0.000437953**				**1**	**0.039**	**2.8626E-07**	**1**	**0.039**	**2.8626E-07**				**1**	**1**	**7.34E-06**
80-73-9	**80739**	3797	1,3-dimethylimidazolidin-2-	114.15	3_REACH	100000		100000	**0**	**100000**	**0.876040298**				**1**	**0.039**	**3.41656E-07**	**1**	**0.039**	**3.41656E-07**	100000		100000	**0**	**100000**	**0.8760403**
81-07-2	**81072**	98	1,2-benzisothiazol-3(2H)-	183.19	3_REACH	97803.66667		97803.66667	**0**	**97803.66667**	**0.533891952**				**1**	**0.039**	**2.12894E-07**	**1**	**0.039**	**2.12894E-07**	16266		16266	**0**	**16266**	**0.08879306**
81-19-6	**81196**	939	1,3-Dichloro-2-	229.92	3_REACH	316.6666667		316.6666667	**0**	**316.6666667**	**0.001377291**				**1**	**0.039**	**1.69624E-07**	**1**	**0.039**	**1.69624E-07**				**1**	**1**	**4.3493E-06**
81-25-4	**81254**	100	cholic acid	408.58	3_REACH	70290		70290	**0**	**70290**	**0.172034852**				**1**	**0.039**	**9.54525E-08**	**1**	**0.039**	**9.54525E-08**	30640		30640	**0**	**30640**	**0.07499143**
81-33-4	**81334**	3804	perylene-3,4:9,10-	390.36	3_REACH	7600		7600	**0**	**7600**	**0.019469208**				**1**	**0.039**	**9.99078E-08**	**1**	**0.039**	**9.99078E-08**	100000		100000	**0**	**100000**	**0.25617379**
81782-77-6	**81782776**	3814	4-methyl-3-decen-5-ol	170.3	3_REACH	1000		1000	**0**	**1000**	**0.005871991**				**1**	**0.039**	**2.29008E-07**	**1**	**0.039**	**2.29008E-07**	460		460	**0**	**460**	**0.00270112**
818-61-1	**818611**	943	2-hydroxyethyl acrylate	116.12	3_REACH	1203.333333		1203.333333	**0**	**1203.333333**	**0.010362843**				**1**	**0.039**	**3.35859E-07**	**1**	**0.039**	**3.35859E-07**	625		625	**0**	**625**	**0.00538236**
82199-12-0	**82199120**	3820	N-(2,3-dihydro-2-oxo-1H-	367.37	3_REACH	1000		1000	**0**	**1000**	**0.002722051**				**1**	**0.039**	**1.0616E-07**	**1**	**0.039**	**1.0616E-07**	1000		1000	**0**	**1000**	**0.00272205**
822-06-0	**822060**	3822	hexamethylene	168.2	3_REACH	22000		22000	**0**	**22000**	**0.130796671**				**1**	**0.039**	**2.31867E-07**	**1**	**0.039**	**2.31867E-07**	11700		11700	**0**	**11700**	**0.06956005**
826-36-8	**826368**	3834	2,2,6,6-tetramethyl-4-	155.24	3_REACH	18000		18000	**0**	**18000**	**0.115949498**				**1**	**0.039**	**2.51224E-07**	**1**	**0.039**	**2.51224E-07**	100000		100000	**0**	**100000**	**0.64416388**
82985-35-1	**82985351**	3839	bis(trimethoxysilylpropyl)a	341.55	3_REACH	100000		100000	**0**	**100000**	**0.292782901**				**1**	**0.039**	**1.14185E-07**	**1**	**0.039**	**1.14185E-07**	22000		22000	**0**	**22000**	**0.06441224**
830-13-7	**830137**	3840	cyclododecanone	182.31	3_REACH	8300		8300	**0**	**8300**	**0.04552685**				**1**	**0.039**	**2.13921E-07**	**1**	**0.039**	**2.13921E-07**	2000		2000	**0**	**2000**	**0.01097033**
83066-88-0	**83066880**	950	(2R)-2-[4-[[5-	327.26	3_REACH	96000		96000	**0**	**96000**	**0.293344741**	1460		1460	**0**	**1460**	**0.004461285**	**1**	**0.039**	**1.19171E-07**	349.6		349.6	**0**	**349.6**	**0.00106826**
83261-15-8	**83261158**	3844	isobutyl (S)-2-	164.63	3_REACH	10000		10000	**0**	**10000**	**0.060742271**				**1**	**0.039**	**2.36895E-07**	**1**	**0.039**	**2.36895E-07**	7500		7500	**0**	**7500**	**0.0455567**
83-32-9	**83329**	952	acenaphthene	154.21	3_REACH	193.3333333		193.3333333	**0**	**193.3333333**	**0.001253702**	710.2112362		710.2112362	**0**	**710.2112362**	**0.004605481**	**1**	**0.039**	**2.52902E-07**	107.3333333		107.3333333	**0**	**107.333333**	**0.00069602**
83-42-1	**83421**	954	2-chloro-6-nitrotoluene	171.58	3_REACH	4000		4000	**0**	**4000**	**0.02331274**	1733.333333		1733.333333	**0**	**1733.333333**	**0.010102188**	**1**	**0.039**	**2.27299E-07**	3400		3400	**0**	**3400**	**0.01981583**
83524-75-8	**83524758**	3848	2,9-bis(p-	630.66	3_REACH	7600		7600	**0**	**7600**	**0.012050867**				**1**	**0.039**	**6.184E-08**	**1**	**0.039**	**6.184E-08**	100000		100000	**0**	**100000**	**0.15856404**
83-73-8	**83738**	3850	diiodohydroxyquinoline	396.95	3_REACH	3801.933333		3801.933333	**0**	**3801.933333**	**0.009577865**	11		11	**0**	**11**	**2.77113E-05**	**1**	**0.039**	**9.82491E-08**	1437.055		1437.055	**0**	**1437.055**	**0.00362024**
83926-73-2	**83926732**	4796	4-cyclohexyl-2-methyl-2-	170.3	3_REACH	3200		3200	**0**	**3200**	**0.01879037**				**1**	**0.039**	**2.29008E-07**	**1**	**0.039**	**2.29008E-07**	12500		12500	**0**	**12500**	**0.07339988**
84170-74-1	**84170741**	3857	(2,2-Dimethyl-1,3-	328.4	3_REACH	900		900	**0**	**900**	**0.00274056**				**1**	**0.039**	**1.18758E-07**	**1**	**0.039**	**1.18758E-07**	710		710	**0**	**710**	**0.002162**
84281-74-3	**84281743**	3859	1,3-Benzenediamine,	346.41	3_REACH	560		560	**0**	**560**	**0.001616582**				**1**	**0.039**	**1.12583E-07**	**1**	**0.039**	**1.12583E-07**	13000		13000	**0**	**13000**	**0.03752778**
84418-63-3	**84418633**	3863	Isononanoic acid, mixed	328.4	3_REACH	1000000		1000000	**0**	**1000000**	**3.045066991**				**1**	**0.039**	**1.18758E-07**	**1**	**0.039**	**1.18758E-07**	100000		100000	**0**	**100000**	**0.3045067**
84434-11-7	**84434117**	3864	ethyl phenyl(2,4,6-	316.34	3_REACH	1000		1000	**0**	**1000**	**0.003161156**				**1**	**0.039**	**1.23285E-07**	**1**	**0.039**	**1.23285E-07**	33		33	**0**	**33**	**0.00010432**
84583-68-6	**84583686**	3868	2-Butenoic acid, 4-oxo-4-	297.44	3_REACH	4700		4700	**0**	**4700**	**0.015801506**				**1**	**0.039**	**1.31119E-07**	**1**	**0.039**	**1.31119E-07**	1800		1800	**0**	**1800**	**0.00605164**
84-65-1	**84651**	960	anthraquinone	208.22	3_REACH	45		45	**0**	**45**	**0.000216118**	45		45	**0**	**45**	**0.000216118**	**1**	**0.039**	**1.87302E-07**	35		35	**0**	**35**	**0.00016809**
84-66-2	**84662**	961	diethyl phthalate	222.24	3_REACH	1900		1900	**0**	**1900**	**0.008549316**	5000		5000	**0**	**5000**	**0.0224982**	**1**	**0.039**	**1.75486E-07**	1003.333333		1003.333333	**0**	**1003.33333**	**0.00451464**
84-69-5	**84695**	962	diisobutyl phthalate	278.35	3_REACH	243.3333333		243.3333333	**0**	**243.3333333**	**0.000874199**	100		100	**0**	**100**	**0.00035926**	**1**	**0.039**	**1.40111E-07**	280		280	**0**	**280**	**0.00100593**
84713-17-7	**84713177**	3874	2,2,4(or 2,4,4)-	150.23	3_REACH	25666.66667		25666.66667	**0**	**25666.66667**	**0.170849142**				**1**	**0.039**	**2.59602E-07**	**1**	**0.039**	**2.59602E-07**	15500		15500	**0**	**15500**	**0.10317513**
84-74-2	**84742**	963	dibutyl phthalate	278.35	3_REACH	320		320	**0**	**320**	**0.001149632**	100		100	**0**	**100**	**0.00035926**	**1**	**0.039**	**1.40111E-07**	130		130	**0**	**130**	**0.00046704**
84852-15-3	**84852153**	964	Phenol, 4-nonyl-, branched	220.36	3_REACH	2.3		2.3	**0**	**2.3**	**1.04375E-05**	6		6	**0**	**6**	**2.72282E-05**	**1**	**0.039**	**1.76983E-07**	9		9	**0**	**9**	**4.0842E-05**
84852-53-9	**84852539**	3878	1,1'-(ethane-1,2-	971.29	3_REACH	110000		110000	**0**	**110000**	**0.113251449**				**1**	**0.039**	**4.01528E-08**	**1**	**0.039**	**4.01528E-08**	110000		110000	**0**	**110000**	**0.11325145**
85-41-6	**85416**	965	phthalimide	147.13	3_REACH	1666.666667		1666.666667	**0**	**1666.666667**	**0.011327851**				**1**	**0.039**	**2.65072E-07**	**1**	**0.039**	**2.65072E-07**	600		600	**0**	**600**	**0.00407803**
85-42-7	**85427**	3889	cyclohexane-1,2-	154.16	3_REACH	1000000		1000000	**0**	**1000000**	**6.486766995**				**1**	**0.039**	**2.52984E-07**	**1**	**0.039**	**2.52984E-07**	46900		46900	**0**	**46900**	**0.30422937**
85-68-7	**85687**	968	benzyl butyl phthalate	312.37	3_REACH	170	170	170	**0**	**170**	**0.000544226**	18.1		18.1	**0**	**18.1**	**5.79441E-05**	**1**	**0.039**	**1.24852E-07**	60		60	**0**	**60**	**0.00019208**
85702-79-0	**85702790**	3896	6-	271.4	3_REACH	500000		500000	**0**	**500000**	**1.842299189**				**1**	**0.039**	**1.43699E-07**	**1**	**0.039**	**1.43699E-07**	78100		78100	**0**	**78100**	**0.28776713**
85-73-4	**85734**	3897	phthalylsulfathiazole	403.44	3_REACH	8957.333333		8957.333333	**0**	**8957.333333**	**0.022202393**				**1**	**0.039**	**9.66686E-08**	**1**	**0.039**	**9.66686E-08**	6444.666667		6444.666667	**0**	**6444.66667**	**0.01597429**
86261-90-7	**86261907**	3902	2-(2-oxoimidazolidin-1-	198.22	3_REACH	100000		100000	**0**	**100000**	**0.504489961**				**1**	**0.039**	**1.96751E-07**	**1**	**0.039**	**1.96751E-07**	97000		97000	**0**	**97000**	**0.48935526**
867-13-0	**867130**	3910	triethyl phosphonoacetate	224.19	3_REACH	100000		100000	**0**	**100000**	**0.446050225**				**1**	**0.039**	**1.7396E-07**	**1**	**0.039**	**1.7396E-07**	100000		100000	**0**	**100000**	**0.44605023**
86-73-7	**86737**	973	fluorene	166.22	3_REACH	273.3333333		273.3333333	**0**	**273.3333333**	**0.001644407**	57.6020833		57.6020833	**0**	**57.6020833**	**0.000346541**	**1**	**0.039**	**2.34629E-07**	1133.333333		1133.333333	**0**	**1133.33333**	**0.00681827**

86-74-8	86748	974	carbazole	167.21	3_REACH	600		600	0	600	0.003588302				1	0.039	2.3324E-07				1	0.039	2.3324E-07	400		400	0	400	0.0023922
868-77-9	868779	975	2-hydroxyethyl	130.14	3_REACH	10000		10000	0	10000	0.076840326	25000		25000	0	25000	0.192100815				1	0.039	2.99677E-07	160000		160000	0	160000	1.22944521
86960-46-5	86960465	3914	4-(decanoyloxy)benzoic	292.38	3_REACH	1000		1000	0	1000	0.003420207				1	0.039	1.33388E-07				1	0.039	1.33388E-07	2400		2400	0	2400	0.0082085
872-05-9	872059	3921	dec-1-ene	140.27	3_REACH	3.4		3.4	0	3.4	2.4239E-05				1	0.039	2.78035E-07				1	0.039	2.78035E-07	0.93		0.93	0	0.93	6.6301E-06
872-36-6	872366	3923	vinylene carbonate	86.046	3_REACH	800		800	0	800	0.009297353				1	0.039	4.53246E-07				1	0.039	4.53246E-07	390		390	0	390	0.00453246
872-50-4	872504	977	1-methyl-2-pyrrolidone	99.134	3_REACH	500000		500000	0	500000	5.043678254				1	0.039	3.93407E-07				1	0.039	3.93407E-07	125000		125000	0	125000	1.26091956
87305-03-1	87305031	3924	(1R,4R,5S)-6,6-Dimethyl-4-	376.89	3_REACH	1800		1800	0	1800	0.004775929				1	0.039	1.03478E-07				1	0.039	1.03478E-07	5000		5000	0	5000	0.01326647
873-32-5	873325	3927	2-chlorobenzonitrile	137.57	3_REACH	10000		10000	0	10000	0.072690267				1	0.039	2.83492E-07				1	0.039	2.83492E-07	14333.33333		14333.33333	0	14333.3333	0.10418938
87333-22-0	87333220	4632	methyl 2-(acetylamino)-3-	195.599	3_REACH	22000		22000	0	22000	0.112475013				1	0.039	1.99388E-07				1	0.039	1.99388E-07	60		60	0	60	0.00030675
87-59-2	87592	978	2,3-xylidine	121.18	3_REACH				1	0.39	3.21835E-06				1	0.039	3.21835E-07				1	0.039	3.21835E-07	14666.66667		14666.66667	0	14666.6667	0.12103207
87-61-6	87616	979	1,2,3-trichlorobenzene	181.45	3_REACH	116.6666667		116.6666667	0	116.6666667	0.000642969	250		250	0	250	0.00137779	450		450	0	450	0.002480022	220		220	0	220	0.00121246
87-62-7	87627	980	2,6-xylidine	121.18	3_REACH	22000		22000	0	22000	0.18154811				1	0.039	3.21835E-07				1	0.039	3.21835E-07	32000		32000	0	32000	0.26406998
87-99-0	87990	3944	xylitol	152.15	3_REACH	17333333.33		17333333.33	0	17333333.33	113.922664				1	0.039	2.56326E-07				1	0.039	2.56326E-07	25182223.33		25182223.33	0	25182223.3	165.50919
88-12-0	88120	3948	1-vinyl-2-pyrrolidone	111.15	3_REACH	464000		464000	0	464000	4.174538911				1	0.039	3.50877E-07				1	0.039	3.50877E-07	530000		530000	0	530000	4.76833108
88150-62-3	88150623	4393	3-ethyl 5-methyl 4-(2-	538.99	3_REACH	6900		6900	0	6900	0.012801722				1	0.039	7.23576E-08				1	0.039	7.23576E-08	6800		6800	0	6800	0.01261619
88-18-6	88186	983	2-tert-butylphenol	150.22	3_REACH	894		894	0	894	0.005951271	327		327	0	327	0.002176807				1	0.039	2.59619E-07	1200		1200	0	1200	0.00798828
88-27-7	88277	3954	2,6-DI-Tert-butyl-4-	263.43	3_REACH	302.3333333		302.3333333	0	302.3333333	0.00114768				1	0.039	1.48047E-07				1	0.039	1.48047E-07	99		99	0	99	0.00037581
88374-05-4	88374054	3955	2-(2-Fluorophenyl)-2-(4-	232.23	3_REACH	3330		3330	0	3330	0.014339233				1	0.039	1.67937E-07				1	0.039	1.67937E-07	100		100	0	100	0.00043061
88-44-8	88448	3956	4-aminotoluene-3-	187.22	3_REACH	180000		180000	0	180000	0.961435744				1	0.039	2.08311E-07				1	0.039	2.08311E-07	10000		10000	0	10000	0.0534131
88-45-9	88459	3957	2,5-	188.21	3_REACH	62962.4		62962.4	0	62962.4	0.334532703				1	0.039	2.07215E-07				1	0.039	2.07215E-07	6756.645		6756.645	0	6756.645	0.0358995
88-51-7	88517	3959	4-amino-6-chlorotoluene-3-	221.66	3_REACH	1000000		1000000	0	1000000	4.511413877				1	0.039	1.75945E-07				1	0.039	1.75945E-07	500000		500000	0	500000	2.25570694
88-60-8	88608	3961	6-tert-butyl-m-cresol	164.25	3_REACH	900		900	0	900	0.005479452				1	0.039	2.37443E-07				1	0.039	2.37443E-07	260		260	0	260	0.00158295
88-72-2	88722	985	2-nitrotoluene	137.14	3_REACH	9333.333333		9333.333333	0	9333.333333	0.068056973	1900		1900	0	1900	0.013854455				1	0.039	2.84381E-07	3100		3100	0	3100	0.02260464
88-73-3	88733	986	1-chloro-2-nitrobenzene	157.56	3_REACH	600		600	0	600	0.003808073	264		264	0	264	0.001675552				1	0.039	2.47525E-07	2293.333333		2293.333333	0	2293.33333	0.0145553
88-74-4	88744	987	2-nitroaniline	138.13	3_REACH	5666.666667		5666.666667	0	5666.666667	0.041024156				1	0.039	2.82343E-07				1	0.039	2.82343E-07	21533.33333		21533.33333	0	21533.3333	0.15589179
88-75-5	88755	988	2-nitrophenol	139.11	3_REACH	533.3333333		533.3333333	0	533.3333333	0.003833896	12649.11064		12649.11064	0	12649.11064	0.090928838				1	0.039	2.80354E-07				1	1	7.1886E-06
88-85-7	88857	989	dinoseb	240.22	3_REACH	9.333333333	10.6666667	10.66666667	0	10.66666667	4.44037E-05	0.25		0.25	0	0.25	1.04071E-06				1	0.039	1.62351E-07	30		30	0	30	0.00012489
88-99-3	88993	990	phthalic acid	166.13	3_REACH	200000		200000	0	200000	1.203876482	10000		10000	0	10000	0.060193824				1	0.039	2.34756E-07	100000		100000	0	100000	0.60193824
89182-60-5	89182605	3969	D-Glucitol, 1-deoxy-1-	209.2	3_REACH	99500		99500	0	99500	0.475621415				1	0.039	1.86424E-07				1	0.039	1.86424E-07	4400		4400	0	4400	0.0210325
89-48-5	89485	3976	menthyl acetate	198.31	3_REACH	14700		14700	0	14700	0.074126368				1	0.039	1.96662E-07				1	0.039	1.96662E-07	160		160	0	160	0.00080682
89604-91-1	89604911	4680	3-[2-(1,3-benzothiazol-2-	351.43	3_REACH	130		130	0	130	0.000369917				1	0.039	1.10975E-07				1	0.039	1.10975E-07	7.5		7.5	0	7.5	2.1341E-05
89-62-3	89623	991	2-nitro-p-toluidine	152.16	3_REACH	1666.666667		1666.666667	0	1666.666667	0.010953382	1329.666667		1329.666667	0	1329.666667	0.008738608				1	0.039	2.56309E-07	2108.666667		2108.666667	0	2108.66667	0.01385822
89-63-4	89634	992	4-chloro-2-nitroaniline	172.57	3_REACH	10540.92553		10540.92553	0	10540.92553	0.061082028				1	0.039	2.25995E-07				1	0.039	2.25995E-07	150		150	0	150	0.00086921
89-72-5	89725	993	2-sec-butylphenol	150.22	3_REACH				1	0.39	2.59619E-06				1	0.039	2.59619E-07				1	0.039	2.59619E-07	820		820	0	820	0.00545866
89-83-8	89838	996	thymol	150.22	3_REACH	1066.666667		1066.666667	0	1066.666667	0.007100697				1	0.039	2.59619E-07				1	0.039	2.59619E-07	1900		1900	0	1900	0.01264812
89-98-5	89985	997	2-chlorobenzaldehyde	140.57	3_REACH	816.6666667		816.6666667	0	816.6666667	0.00580968				1	0.039	2.77442E-07				1	0.039	2.77442E-07	2250		2250	0	2250	0.01600626
90-02-8	90028	998	salicylaldehyde	122.12	3_REACH	450		450	0	450	0.0036849				1	0.039	3.19358E-07				1	0.039	3.19358E-07	550		550	0	550	0.00450377
90-04-0	90040	999	o-anisidine	123.16	3_REACH	65333.33333		65333.33333	0	65333.33333	0.530475263	6000		6000	0	6000	0.048717116				1	0.039	3.16661E-07	3200		3200	0	3200	0.02598246
90-05-1	90051	3990	guaiacol	124.14	3_REACH	14666.66667		14666.66667	0	14666.66667	0.118146179				1	0.039	3.14161E-07				1	0.039	3.14161E-07	10000		10000	0	10000	0.08055421
90-12-0	90120	1000	1-methylnaphthalene	142.2	3_REACH	1133.333333		1133.333333	0	1133.333333	0.007969995				1	0.039	2.74262E-07				1	0.039	2.74262E-07				1	1	7.0323E-06
901-44-0	901440	3991	2,2'-isopropylidenebis(p-	316.4	3_REACH	7000		7000	0	7000	0.022123894				1	0.039	1.23262E-07				1	0.039	1.23262E-07	950		950	0	950	0.00300253
9016-45-9	9016459	1001	Nonylphenol, ethoxylated	308.462	3_REACH	433.3333333		433.3333333	0	433.3333333	0.001404819				1	0.039	1.26434E-07				1	0.039	1.26434E-07	6666.666667		6666.666667	0	6666.66667	0.0216126
90-17-5	90175	3992	2,2,2-trichloro-1-	267.54	3_REACH	4503.57755		4503.57755	0	4503.57755	0.016833287				1	0.039	1.45773E-07				1	0.039	1.45773E-07	6463.440577		6463.440577	0	6463.44058	0.02415878
90268-23-8	90268238	3995	Butanamide, 2,2'-[(3,3'-	659.54	3_REACH	100		100	0	100	0.000151621				1	0.039	5.91321E-08				1	0.039	5.91321E-08	100000		100000	0	100000	0.15162083
90268-24-9	90268249	3996	Butanamide, 2,2'-[(3,3'-	752.06	3_REACH	100		100	0	100	0.000132968				1	0.039	5.18576E-08				1	0.039	5.18576E-08	100000		100000	0	100000	0.13296811
90-30-2	90302	1002	N-1-naphthylaniline	219.29	3_REACH	146.6666667		146.6666667	0	146.6666667	0.000668825				1	0.039	1.77847E-07				1	0.039	1.77847E-07	83.33333333		83.33333333	0	83.3333333	0.00038001
90-43-7	90437	106	biphenyl-2-ol	170.21	3_REACH	1000		1000	0	1000	0.005875095	36		36	0	36	0.000211503				1	0.039	2.29129E-07	350		350	0	350	0.00205628
90474-13-8	90474138	4000	diethyl 1,2-	214.26	3_REACH	10000		10000	0	10000	0.046672267				1	0.039	1.82022E-07				1	0.039	1.82022E-07	10000		10000	0	10000	0.04667227
90498-90-1	90498901	4387	3,9-bis(2-(3-(3-tert-butyl-4-	740.98	3_REACH	1000000		1000000	0	1000000	1.349564091				1	0.039	5.2633E-08				1	0.039	5.2633E-08	330		330	0	330	0.00044536
90-51-7	90517	4001	6-amino-4-	239.25	3_REACH	5000		5000	0	5000	0.020898642				1	0.039	1.63009E-07				1	0.039	1.63009E-07	7477.415562		7477.415562	0	7477.41556	0.03125357
90-72-2	90722	4003	2,4,6-	265.4	3_REACH	58333.33333		58333.33333	0	58333.33333	0.219794022				1	0.039	1.46948E-07				1	0.039	1.46948E-07	28000		28000	0	28000	0.10550113
90-80-2	90802	4006	D-glucono-1,5-lactone	178.14	3_REACH	100000		100000	0	100000	0.561356237				1	0.039	2.18929E-07				1	0.039	2.18929E-07	100000		100000	0	100000	0.56135624
91-15-6	91156	1004	phthalonitrile	128.14	3_REACH	7533.333333		7533.333333	0	7533.333333	0.058789865				1	0.039	3.04355E-07				1	0.039	3.04355E-07	32000		32000	0	32000	0.24972686
91-17-8	91178	1005	decahydronaphthalene	138.25	3_REACH	80		80	0	80	0.000578662				1	0.039	2.82098E-07				1	0.039	2.82098E-07	336.6666667		336.6666667	0	336.666667	0.0024352
91-20-3	91203	107	naphthalene	128.17	3_REACH	400		400	0	400	0.003120855	36.66666667		36.66666667	0	36.66666667	0.000286078				1	0.039	3.04283E-07	149.0711985		149.0711985	0	149.071198	0.00116307
91-22-5	91225	1006	quinoline	129.16	3_REACH	146.6666667		146.6666667	0	146.6666667	0.001135542	4400		4400	0	4400	0.034066274				1	0.039	3.01951E-07	4800		4800	0	4800	0.03716321
91273-04-0	91273040	4271	1-(N,N-bis(2-	322.55	3_REACH	580		580	0	580	0.001798171				1	0.039	1.20911E-07				1	0.039	1.20911E-07	250		250	0	250	0.00077507
91-57-6	91576	1007	2-methylnaphthalene	142.2	3_REACH	485.3333333		485.3333333	0	485.3333333	0.003413033				1	0.039	2.74262E-07				1	0.039	2.74262E-07				1	1	7.0323E-06
91-64-5	91645	1008	coumarin	146.15	3_REACH	441.3333333		441.3333333	0	441.3333333	0.003019729	119		119	0	119	0.000814232				1	0.039	2.66849E-07	431		431	0	431	0.00294902
91-66-7	91667	1009	N,N-diethylaniline	149.24	3_REACH	2046.732496		2046.732496	0	2046.732496	0.013714369				1	0.039	2.61324E-07				1	0.039	2.61324E-07	933.3633531		933.3633531	0	933.363353	0.00625411
91-68-9	91689	4019	3-diethylaminophenol	165.24	3_REACH	3200		3200	0	3200	0.019365771				1	0.039	2.3602E-07				1	0.039	2.3602E-07	5080		5080	0	5080	0.03074316
91-76-9	91769	4021	6-phenyl-1,3,5-triazine-2,4-	187.21	3_REACH	32000		32000	0	32000	0.17093104				1	0.039	2.08322E-07				1	0.039	2.08322E-07	13000		13000	0	13000	0.06944074
919-30-2	919302	4023	3-	221.37	3_REACH	934000		934000	0	934000	4.219180557				1	0.039	1.76176E-07				1	0.039	1.76176E-07	1300		1300	0	1300	0.00587252
91-97-4	91974	4025	3,3'-dimethylbiphenyl-4,4'-	264.29	3_REACH	184.9324201		184.9324201	0	184.9324201	0.000699733				1	0.039	1.47565E-07				1	0.039	1.47565E-07	1500		1500	0	1500	0.00567558
923-02-4	923024	4030	N-	115.13	3_REACH	494413.2325		494413.2325	0	494413.2325	4.294390971				1	0.039	3.38748E-07				1	0.039	3.38748E-07	31600		31600	0	31600	0.27447234
925-21-3	925213	4038	butyl hydrogen maleate	172.18	3_REACH	3200		3200	0	3200	0.018585202				1	0.039	2.26507E-07				1	0.039	2.26507E-07	6250		6250	0	6250	0.03629922
92-52-4	92524	1012	biphenyl	154.21	3_REACH	483.3333333		483.3333333	0	483.3333333	0.003134254	229		229	0	229	0.001484988				1	0.039	2.52902E-07	587		587	0	587	0.0038065
92-69-3	92693	1013	biphenyl-4-ol	170.21	3_REACH				1	0.39	2.29129E-06				1	0.039	2.29129E-07				1	0.039	2.29129E-07	320		320	0	320	0.00188003
92-70-6	92706	4045	3-hydroxy-2-naphthoic acid	188.18	3_REACH	40800		40800	0	40800	0.216813689				1	0.039	2.07248E-07				1	0.039	2.07248E-07	6800		6800	0	6800	0.03613561
927-07-1	927071	4046	tert-butyl peroxypivalate	174.24	3_REACH	8650		8650	0	8650	0.049644169				1	0.039	2.23829E-07				1	0.039	2.23829E-07	96		96	0	96	0.00055096
92-84-2	92842	4051	phenothiazine	199.28	3_REACH	25000		25000	0	25000	0.125451626				1	0.039	1.95705E-07				1	0.039	1.95705E-07	100000		100000	0	100000	0.5018065
92-88-6	92886	1015	biphenyl-4,4'-diol	186.21	3_REACH				1	0.39	2.09441E-06				1	0.039	2.09441E-07				1	0.039	2.09441E-07	530		530	0	530	0.00284625
928-96-1	928961	1016	cis-hex-3-en-1-ol	100.16	3_REACH	103333.3333		103333.3333	0	103333.3333	1.031682641				1	0.039	3.89377E-07				1	0.039	3.89377E-07	76000		76000	0	76000	0.75878594
929-06-6	929066	4053	2-(2-aminoethoxy)ethanol	105.14	3_REACH	250000		250000	0	250000	2.377782005				1	0.039	3.70934E-07				1	0.039	3.70934E-07	62500		62500	0	62500	0.5944455
92952-81-3	92952813	4412	4-[(3-hydroxypropyl)amino]-	212.21	3_REACH	32000		32000	0	32000	0.150794025				1	0.039	1.8378E-07				1	0.039	1.8378E-07	10500		10500	0	10500	0.04947929
93-04-9	93049	1017	methyl 2-naphthyl ether	158.2	3_REACH	1846.666667		1846.666667	0	1846.666667	0.011672988	3332.333333		3332.333333	0	3332.333333	0.021064054				1	0.039	2.46523E-07	1789.666667		1789.666667	0	1789.66667	0.01131268
931-36-2	931362	4059	2-ethyl-4-methylimidazole	110.16	3_REACH	46000		46000	0	46000	0.417574437				1	0.039	3.54031E-07				1	0.039	3.54031E-07	3900		3900	0	3900	0.03540305
93-17-4	93174	4063	3,4-	177.2	3_REACH	46000		46000	0	46000	0.259593679				1	0.039	2.2009E-07				1	0.039	2.2009E-07	25000		25000	0	25000	0.14108352
93-20-9	93209	4065	2-(2-naphthyloxy)ethanol	188.23	3_REACH	9000		9000	0	9000	0.047813845				1	0.039	2.07193E-07				1	0.039	2.07193E-07	1000		1000	0	1000	0.00531265
932-64-9	932649	4066	1,2-dihydro-5-nitro-3H-	130.07	3_REACH	586690.6667		586690.6667	0	586690.6667	4.510576356				1	0.039	2.99839E-07				1	0.039	2.99839E-07	50000		50000	0	50000	0.3844084
93413-62-8	93413628	4069	4-[2-(Dimethylamino)-1-(1-	263.38	3_REACH	3133.333333		3133.333333	0	3133.333333	0.011896626	2100		2100	0	2100	0.007973271				1	0.039	1.48075E-07	2672.90936		2672.90936	0	2672.90936	0.01014849
93-58-3	93583	4073	methyl benzoate	136.15	3_REACH	13300		13300	0	13300	0.097686375	9533.333333		9533.333333	0	9533.333333	0.07002081				1	0.039	2.86449E-07	62400		62400	0	62400	0.45831803
936-49-2	936492	4076	2-phenyl-2-imidazoline	146.19	3_REACH	33000		33000	0	33000	0.225733634				1	0.039	2.66776E-07				1	0.039	2.66776E-07	70		70	0	70	0.00047883
93-69-6	93696	4079	1-o-tolylbiguanide	191.24	3_REACH	50000		50000	0	50000	0.261451579				1	0.039	2.03932E-07				1	0.039	2.03932E-07	10000		10000	0	10000	0.05229032
93-70-9	93709	4080	2'-chloroacetoacetanilide	211.65	3_REACH	50000		50000	0	50000	0.236239074				1	0.039	1.84266E-07				1	0.039	1.84266E-07	71100		71100	0	71100	0.33593196
93-92-5	93925	4093	1-phenylethyl acetate	164.2	3_REACH	1333.333333		1333.333333	0	1333.333333	0.008120179	1330		1330	0	1330	0.008099878				1	0.039	2.37515E-07	52000		52000	0	52000	0.31668697
93957-50-7	93957507	4490	3-[3-(4-fluorophenyl)-1-(1-	307.37	3_REACH	7		7	0	7	2.27739E-05				1	0.039	1.26883E-07				1	0.039	1.26883E-07	7		7	0	7	2.2774E-05
939-97-9	939979	4095	4-tert-butylbenzaldehyde	162.23	3_REACH	2150		2150	0	2150	0.013252789				1	0.039	2.40399E-07				1	0.039	2.40399E-07	5810		5810	0	5810	0.03581335
94-04-2	94042	4096	vinyl 2-ethylhexanoate	170.25	3_REACH	590		590	0	590	0.003465492				1	0.039	2.29075E-07				1	0.039	2.29075E-07	2500		2500	0	2500	0.01468429
94050-90-5	94050905	4248	(R)-2-(4-	182.18	3_REACH	100000		100000	0	100000	0.548907674				1	0.039	2.14074E-07				1	0.039	2.14074E-07	32000		32000	0	32000	0.17565046
94-13-3	94133	109	propyl 4-hydroxybenzoate	180.2	3_REACH	3400		3400	0	3400	0.018867925				1	0.039	2.16426E-07				1	0.039	2.16426E-07	2100		2100	0	2100	0.01165372
941-69-5	941695	4098	N-phenylmaleimide	173.17	3_REACH	275		275	0	275	0.001588035				1	0.039	2.25212E-07				1	0.039	2.25212E-07	490		490	0	490	0.00282959
947-04-6	947046	4110	dodecane-12-lactam	197.32	3_REACH	48000		48000	0	48000	0.24325968				1	0.039	1.97648E-07				1	0.039	1.97648E-07	135000		135000	0	135000	0.68416785
947-19-3	947193	4112	hydroxycyclohexyl phenyl	204.27	3_REACH	18000		18000	0	18000	0.088118666				1	0.039	1.90924E-07				1	0.039	1.90924E-07	700		700	0	700	0.00342684
94723-86-1	94723861	4485	2-butanoyl-3-hydroxy-5-	282.4	3_REACH	4640		4640	0	4640	0.016430595				1	0.039	1.38102E-07				1	0.039	1.38102E-07	6250		6250	0	6250	0.02213173
947753-66-4	947753664	4115	2-Ethylhexyl-2-cyano-3-(4-	391.51	3_REACH	0.564		0.564	0	0.564	1.44058E-06				1	0.039	9.96143E-08				1	0.039	9.96143E-08	11		11	0	11	2.8096E-05
94-91-7	94917	4116	N,N'-Bis(salicylidene)-1,2-	282.35	3_REACH	21500		21500	0	21500	0.076146627				1	0.039	1.38126E-07				1	0.039	1.38126E-07	116		116	0	116	0.00041084
94-96-2	94962	1024	2-ethylhexane-1,3-diol	146.23	3_REACH	489000		489000	0	489000	3.344047049				1	0.039	2.66703E-07				1	0.039	2.66703E-07	100000		100000	0	100000	0.6838542
95-14-7	95147	112	benzotriazole	119.13	3_REACH	5000		5000	0	5000	0.041970956				1	0.039	3.27373E-07				1	0.039	3.27373E-07	1180		1180	0	1180	0.00990515
95-16-9	95169	113	benzothiazole	135.19	3_REACH	13000		13000	0	13000	0.096160959	7200		7200	0	7200	0.053258377				1	0.039	2.88483E-07	5100		5100	0	5100	0.03772468
95235-30-6	95235306	4398	4-(4-	292.35	3_REACH	10000		10000	0	10000	0.034205576				1	0.039	1.33402E-07				1	0.039	1.33402E-07	460		460	0	460	0.00157346
95-31-8	95318	4124	N-tert-butylbenzothiazole-2	238.38	3_REACH	518		518	0	518	0.002173001	41		41	0	41	0.000171994				1	0.039	1.63604E-07	23		23	0	23	9.6485E-05
95-33-0	95330	4125	N-cyclohexylbenzothiazole-	264.42	3_REACH	700		700	0	700	0.002647304	41		41	0	41	0.000155056				1	0.039	1.47493E-07	8.4		8.4	0	8.4	3.1768E-05
95-38-5	95385	4126	2-(2-heptadec-8-enyl-2-	350.59	3_REACH	180		180	0	180	0.00051342				1	0.039	1.11241E-07				1	0.039	1.11241E-07	11		11	0	11	3.1376E-05
95-48-7	95487	1029	o-cresol	108.14	3_REACH	3800		3800	0	3800	0.035139634	1350		1350	0	1350	0.012483817				1	0.039	3.60644E-07	2200		2200	0	2200	0.020344
95-49-8	95498	1030	2-chlorotoluene	126.59	3_REACH	766.6666667		766.6666667	0	766.6666667	0.006056297	2014.944168		2014.944168	0	2014.944168	0.015917088				1	0.039	3.08081E-07	2600		2600	0	2600	0.02053875
95-51-2	95512	1031	2-chloroaniline	127.58	3_REACH	333.3333333		333.3333333	0	333.3333333	0.00261274	6.7		6.7	0	6.7	5.25161E-05				1	0.039	3.05691E-07	3900		3900	0	3900	0.03056905
95-53-4	95534	1032	o-toluidine	107.16	3_REACH	30000		30000	0	30000	0.279955207	12500		12500	0	12500	0.116648003				1	0.039	3.63942E-07	310		310	0	310	0.00289287
95-54-5	95545	1033	o-phenylenediamine	108.15	3_REACH	18000		18000	0	18000	0.166435506				1	0.039	3.6061E-07				1	0.039	3.6061E-07	48.33333333		48.33333333	0	48.3333333	0.00044691
95-63-6	95636	1035	1,2,4-trimethylbenzene	120.19	3_REACH	1136.666667		1136.666667	0	1136.666667	0.009457248	396		396	0	396	0.003294783				1	0.039	3.24486E-07	785.3333333		785.3333333	0	785.333333	0.0065341
95-68-1	95681	1036	2,4-xylidine	121.18	3_REACH	50000		50000	0	50000	0.412609341				1	0.039	3.21835E-07				1	0.039	3.21835E-07	430		430	0	430	0.00354844
95-74-9	95749	1037	3-chloro-p-toluidine	141.6	3_REACH	17800		17800	0	17800	0.125706215				1	0.039	2.75424E-07				1	0.039	2.75424E-07	1800		1800	0	1800	0.01271186
95-80-7	95807	1039	4-methyl-m-	122.17	3_REACH	107		107	0	107	0.000875829	40300		40300	0	40300	0.329868216				1	0.039	3.19227E-07	10000		10000	0	10000	0.08185316
95-82-9	95829	1040	2,5-dichloroaniline	162.02	3_REACH				1	0.39	2.40711E-06				1	0.039	2.40711E-07				1	0.039	2.40711E-07	3333.333333		3333.333333	0	3333.33333	0.02057359
95962-14-4	95962144	4305	2-(2-(4-methyl-3-	220.36	3_REACH	2250		2250	0	2250	0.010210565	320		320	0	320	0.001452169				1	0.039	1.76983E-07	56		56	0	56	0.00025413
95-96-5	95965	4140	dilactide	144.13	3_REACH	43333.33333		43333.33333	0	43333.33333	0.300654502	2180		2180	0	2180	0.015125234				1	0.039	2.70589E-07	1900000		1900000	0	1900000	13.1825435
96-09-3	96093	1044	(epoxyethyl)benzene	120.15	3_REACH	1513.333333		1513.333333	0	1513.333333	0.012595367				1	0.039	3.24594E-07				1	0.039	3.24594E-07	12000		12000	0	12000	0.09987516
96-12-8	96128	1045	1,2-dibromo-3-	236.35	3_REACH				1	0.39	1.6501E-06				1	0.039	1.6501E-07				1	0.039	1.6501E-07				1	1	4.231E-06
96-18-4	96184	1047	1,2,3-trichloropropane	147.43	3_REACH	10000		10000	0	10000	0.0678288	4400		4400	0	4400	0.029844672				1	0.039	2.64532E-07	12800		12800	0	12800	0.08682086
96-23-1	96231	1049	1,3-dichloropropan-2-ol	128.99	3_REACH	226666.6667		226666.6667	0	226666.6667	1.757242163				1	0.039	3.02349E-07				1	0.039	3.02349E-07	76666.66667		76666.66667	0	76666.6667	0.59436132
96-24-2	96242	1050	3-chloropropane-1,2-diol	110.54	3_REACH	716666.6667		716666.6667	0	716666.6667	6.483324287				1	0.039	3.52813E-07				1	0.039	3.52813E-07	100000		100000	0	100000	0.9046499
96-29-7	96297	1051	butanone oxime	87.123	3_REACH	180000		180000	0	180000	2.066044558	50000		50000	0	50000	0.573901266				1	0.039	4.47643E-07	1020		1020	0	1020	0.01170759
96-31-1	96311	1052	1,3-dimethylurea	88.112	3_REACH	4600000		4600000	0	4600000	52.20628291				1	0.039	4.42618E-07				1	0.039	4.42618E-07	62500		62500	0	62500	0.7093245
96-45-7	96457	1054	imidazolidine-2-thione	102.16	3_REACH	219000		219000	0	219000	2.143696163	100000		100000	0	100000	0.978856695				1	0.039	3.81754E-07	2480		2480	0	2480	0.02427565
96-48-0	96480	4148	Butyrolactone	86.09	3_REACH	18000		18000	0	18000	0.209083517				1	0.039	4.53014E-07				1	0.039	4.53014E-07	7810		7810	0	7810	0.09071901
96-49-1	96491	4149	ethylene carbonate	88.062	3_REACH	16333333.33		16333333.33	0	16333333.33	185.4753848				1	0.039	4.4287E-07				1	0.039	4.4287E-07	2000000		2000000	0	2000000	22.7112716
96-67-3	96673	4151	3-amino-2-hydroxy-5-	234.19	3_REACH	35163.8		35163.8	0	35163.8	0.150150732				1	0.039	1.66531E-07				1	0.039	1.66531E-07	8136.299		8136.299	0	8136.299	0.0347423
96-69-5	96695	4152	6,6'-di-tert-butyl-4,4'-thiodi-	358.54	3_REACH	26.66666667		26.66666667	0	26.66666667	7.43757E-05	18		18	0	18	5.02036E-05				1	0.039	1.08774E-07	455		455	0	455	0.00126904
96-76-4	96764	4153	2,4-di-tert-butylphenol	206.33	3_REACH	296.6666667		296.6666667	0	296.6666667	0.001437826	210		210	0	210	0.001017787				1	0.039	1.89018E-07	30		30	0	30	0.0001454
96-93-5	96935	4156	3-amino-4-hydroxy-5-	234.19	3_REACH	1289206		1289206	0	1289206	5.504957513	8015323		8015323	0	8015323	34.22572697				1	0.039	1.66531E-07	91082		91082	0	91082	0.38892352
96-96-8	96968	4157	2-nitro-p-anisidine	168.15	3_REACH	12246.66667		12246.66667	0	12246.66667	0.072831797				1	0.039	2.31936E-07				1	0.039	2.31936E-07	2579.666667		2579.666667	0	2579.66667	0.01534146
96-97-9	96979	4158	5-nitrosalicylic acid	183.12	3_REACH	1120		1120	0	1120	0.006116208				1	0.039	2.12975E-07				1	0.039	2.12975E-07	5333.1		5333.1	0	5333.1	0.02912353
97-00-7	97007	1056	1-chloro-2,4-	202.56	3_REACH	500		500	0	500	0.002468404	16		16	0	16	7.89889E-05				1	0.039	1.92536E-07	67		67	0	67	0.00033077
97-39-2	97392	4164	1,3-di-o-tolylguanidine	239.32	3_REACH	7560		7560	0	7560	0.031589504				1	0.039	1.62962E-07				1	0.039	1.62962E-07	2270		2270	0	2270	0.00948521
97-52-9	97529	4165	4-nitro-o-anisidine	168.15	3_REACH	35000		35000	0	35000	0.208147487				1	0.039	2.31936E-07				1	0.039	2.31936E-07	12500		12500	0	12500	0.07433839
97-53-0	97530	1057	eugenol	164.2	3_REACH	10000		10000	0	10000	0.06090134				1	0.039	2.37515E-07				1	0.039	2.37515E-07	22000		22000	0	22000	0.13398295
97-65-4	97654	4168	itaconic acid	130.1	3_REACH	63333.33333		63333.33333	0	63333.33333	0.486805022				1	0.039	2.99769E-07				1	0.039	2.99769E-07	2073.333333		2073.333333	0	2073.33333	0.01593646
976-71-6	976716	4170	canrenone	340.46	3_REACH	3606.167556		3606.167556	0	3606.167556	0.010592045				1	0.039	1.14551E-07				1	0.039	1.14551E-07	600		600	0	600	0.00176232
97-74-5	97745	1059	tetramethylthiuram	208.37	3_REACH	9.666666667		9.666666667	0	9.666666667	4.63918E-05	10		10	0	10	4.79916E-05				1	0.039	1.87167E-07	333.3333333		333.3333333	0	333.333333	0.00159972
97-78-9	97789	4172	N-lauroylsarcosine	271.4	3_REACH	50000		50000	0	50000	0.184229919				1	0.039	1.43699E-07				1	0.039	1.43699E-07	9200		9200	0	9200	0.03389831
97-88-1	97881	1061	butyl methacrylate	142.2	3_REACH	2650		2650	0	2650	0.018635724	780		780	0	780	0.005485232				1	0.039	2.74262E-07	19000		19000	0	19000	0.13361463
97-90-5	97905	4175	ethylene dimethacrylate	198.22	3_REACH	6250		6250	0	6250	0.031530623				1	0.039	1.96751E-07				1	0.039	1.96751E-07	804		804	0	804	0.0040561
98-00-0	98000	1063	furfuryl alcohol	98.101	3_REACH	113000		113000	0	113000	1.151874089				1	0.039	3.97549E-07				1	0.039	3.97549E-07	25000		25000	0	25000	0.2548394
980-26-7	980267	4177	5,12-dihydro-2,9-	340.38	3_REACH	100000		100000	0	100000	0.293789294	10000		10000	0	10000	0.029378929				1	0.039	1.14578E-07	1000		1000	0	1000	0.00293789
98-07-7	98077	1065	Benzotrichloride	195.48	3_REACH	2480000		2480000	0	2480000	12.68671987				1	0.039	1.99509E-07				1	0.039	1.99509E-07	34000		34000	0	34000	0.17393084
98-09-9	98099	1066	benzenesulphonyl chloride	176.62	3_REACH	1000		1000	0	1000	0.005661873	11999.66667		11999.66667	0	11999.66667	0.067940588				1	0.039	2.20813E-07				1	1	5.6619E-06
98-13-5	98135	1067	trichloro(phenyl)silane	211.55	3_REACH	100000		100000	0	100000	0.472701489				1	0.039	1.84354E-07				1	0.039	1.84354E-07	100000		100000	0	100000	0.47270149
98-16-8	98168	1068	3-Trifluoromethylaniline	161.13	3_REACH				1	0.39	2.42041E-06				1	0.039	2.42041E-07				1	0.039	2.42041E-07	3200		3200	0	3200	0.01985974

98-17-9	00170	1069	3-(Trifluoromethyl)phenol	162.11	3_REACH	3611.666667	3611.666667	0	3611.666667	0.022279111			1	0.000	2.400776-07		1	0.000	2.400776-07	6670.666667	6670.666667	0	6670.66667	0.04114601
98-29-3	00325	4181	4-tert-butylpyrocatechol	166.22	3_REACH	65	65	0	65	0.000201045			1	0.000	2.340285-07		1	0.000	2.340285-07	200	200	0	200	0.00123022
98-37-3	00375	4183	3-amino-4-chlorobenzenesulfonic acid	189.19	3_REACH	44446.73333	44446.73333	0	44446.73333	0.294931725			1	0.000	2.001435-07		1	0.000	2.001435-07	43317.19	43317.19	0	43317.19	0.23980151
98377-35-6	00377000	4501	1-(2-chlorophenyl)-1,2-diphenylethanone	196.6	3_REACH	25000	25000	0	25000	0.12718176			1	0.000	1.660726-07		1	0.000	1.660726-07	56000	56000	0	56000	0.28404252
98-44-2	00442	4185	2-aminobenzene-1,4-disulfonic acid	253.25	3_REACH	5000	5000	0	5000	0.016743937			1	0.000	1.556985-07		1	0.000	1.556985-07	118879	118879	0	118879	0.40941382
98-51-1	00511	1071	4-tert-butyltoluene	148.25	3_REACH	1400	1400	0	1400	0.004845808			1	0.000	2.650385-07		1	0.000	2.650385-07	5600	5600	0	5600	0.02777403
98-52-2	00522	1072	4-tert-butylcyclohexanol	156.27	3_REACH	2273.666667	2273.666667	0	2273.666667	0.014540604			1	0.000	2.460385-07		1	0.000	2.460385-07	14000	14000	0	14000	0.06935853
98-53-3	00533	4186	4-tert-butylcyclohexanone	154.25	3_REACH	1850	1850	0	1850	0.012038947			1	0.000	2.828385-07		1	0.000	2.828385-07	12100	12100	0	12100	0.07044428
98-54-4	00544	1073	4-tert-butylphenol	150.22	3_REACH	576.6666667	576.6666667	0	576.6666667	0.003835814	10	10	0	10	6.65985-05		1	0.000	2.890185-07	230	230	0	230	0.00135108
98-55-5	00555	1074	p-menth-1-en-8-ol	154.25	3_REACH	23333.33333	23333.33333	0	23333.33333	0.151206904			1	0.000	2.828385-07		1	0.000	2.828385-07	3900	3900	0	3900	0.02292088
98-59-9	00589	4188	tosyl chloride	190.65	3_REACH	18333.33333	18333.33333	0	18333.33333	0.098165222			1	0.000	2.040385-07		1	0.000	2.040385-07	2600	2600	0	2600	0.01528708
98730-04-2	00730042	4191	2,2-Dichloro-1-(3-methyl-2,4-dihydro-2H-1,4-benzoxazin-4-yl)-1-ethanone	260.12	3_REACH	670	670	0	670	0.002876734	4	4	0	4	1.007785-05		1	0.000	1.499285-07	220	220	0	220	0.00084676
98-73-7	00737	1075	4-tert-butylbenzoic acid	178.23	3_REACH	1333.333333	1333.333333	0	1333.333333	0.007140607			1	0.000	2.180185-07		1	0.000	2.180185-07	21000	21000	0	21000	0.11763528
98-82-8	00828	1076	cumene	120.19	3_REACH	1900	1900	0	1900	0.010820604	380	380	0	380	0.000101901		1	0.000	3.340285-07	220	220	0	220	0.00123044
98-83-9	00839	4193	2-phenylpropene	118.18	3_REACH	2130	2130	0	2130	0.012223804	1040	1040	0	1040	0.000502155		1	0.000	3.300285-07	172	172	0	172	0.00145541
98-85-1	00851	4194	1-phenylethanol	122.17	3_REACH	34536.46667	34536.46667	0	34536.46667	0.202051677			1	0.000	9.102276-07		1	0.000	9.102276-07	44237.26667	44237.26667	0	44237.2667	0.24820669
98-86-2	00862	1077	acetophenone	120.15	3_REACH	5000	5000	0	5000	0.041814048			1	0.000	3.340285-07		1	0.000	3.340285-07	24800	24800	0	24800	0.20040668
98967-40-9	00967040	1081	N-(2,6-difluorophenyl)-5-methyl-5,6-dihydro-4H-1,4-oxazine-3-carboxamide	325.3	3_REACH	293000	293000	0	293000	0.20070704	197000	197000	0	197000	0.000694939		1	0.000	1.199285-07	0.36	0.36	0	0.36	1.10676-05
99-08-1	00081	1082	3-nitrotoluene	137.14	3_REACH	2466.666667	2466.666667	0	2466.666667	0.017808488	2000	2000	0	2000	0.014182637		1	0.000	2.642285-07	1000	1000	0	1000	0.00729152
99189-50-3	00189000	4198	2-[1-(2-Amino-2-methylbutylamino)-butylidene]-5,6-dihydro-2H-[1,2,4]-thiadiazine-3,5-dione	199.25	3_REACH	100000	100000	0	100000	0.001862009			1	0.000	1.667945-07		1	0.000	1.667945-07	10000	10000	0	10000	0.00016921
993-13-5	00313	4203	methylphosphonic acid	96.022	3_REACH	3539	3539	0	3539	0.000099137			1	0.000	4.001876-07		1	0.000	4.001876-07	3200	3200	0	3200	0.00002257
99-34-3	00343	4204	3,5-dinitrobenzoic acid	212.12	3_REACH	14110	14110	0	14110	0.000316002			1	0.000	1.600285-07		1	0.000	1.600285-07	3257.333333	3257.333333	0	3257.33333	0.01539603
99-54-7	00547	1087	1,2-dichloro-4-nitrobenzene	192	3_REACH	2000	2000	0	2000	0.010419007			1	0.000	2.091285-07		1	0.000	2.091285-07	150	150	0	150	0.00278125
99-55-8	00558	1088	5-nitro-o-toluidine	152.15	3_REACH	6133.333333	6133.333333	0	6133.333333	0.040206447			1	0.000	2.600285-07		1	0.000	2.600285-07			1	1	6.6725-05
99-57-0	00570	4206	2-amino-4-nitrophenol	154.13	3_REACH	35895	35895	0	35895	0.235387922			1	0.000	2.850285-07		1	0.000	2.850285-07	13871.74416	13871.74416	0	13871.7442	0.08020628
99591-74-9	00591740	4207	1,5,2,4-dioxadithiane 2,5,4,4-tetraoxide	188.18	3_REACH	22333.33333	22333.33333	0	22333.33333	0.118000000			1	0.000	2.072485-07		1	0.000	2.072485-07	31000	31000	0	31000	0.19479699
99607-70-2	00607702	1089	Heptan-2-yl [(5-chloro-pyridin-8-yloxy)-acetoximino]-acetate	335.83	3_REACH	970	970	0	970	0.002888889	1260	1260	0	1260	0.000751899		1	0.000	1.19185-07	90	90	0	90	0.00028798
99-62-7	00627	4210	1,3-diisopropylbenzene	162.28	3_REACH	250	250	0	250	0.001540647			1	0.000	2.460285-07		1	0.000	2.460285-07	310	310	0	310	0.00101428
99-63-8	00638	4214	isophthaloyl dichloride	203.02	3_REACH	44566.66667	44566.66667	0	44566.66667	0.218196002			1	0.000	1.820285-07		1	0.000	1.820285-07	996000	996000	0	996000	4.8082206
99-75-2	00752	4215	methyl p-toluate	150.18	3_REACH	12500	12500	0	12500	0.080223405			1	0.000	2.890285-07		1	0.000	2.890285-07	260	260	0	260	0.00179125
99-76-3	00763	4216	methyl 4-hydroxybenzoate	152.15	3_REACH	50000	50000	0	50000	0.328523609			1	0.000	2.890285-07		1	0.000	2.890285-07	17000	17000	0	17000	0.11779184
99817-36-4	00817304	4328	2,4-dichloro-3-ethyl-6-methylphenol	236.06	3_REACH	286	286	0	286	0.001211936			1	0.000	1.662185-07		1	0.000	1.662185-07	138	138	0	138	0.00095849
99-87-6	00876	1092	p-cymene	134.22	3_REACH	16000	16000	0	16000	0.110027272			1	0.000	2.660285-07		1	0.000	2.660285-07	7333.333333	7333.333333	0	7333.33333	0.05485667
99-88-7	00887	4221	4-isopropylaniline	135.21	3_REACH	15333.33333	15333.33333	0	15333.33333	0.111403841			1	0.000	2.86445-07		1	0.000	2.86445-07	680	680	0	680	0.00003821
99-93-4	00934	4222	4'-hydroxyacetophenone	136.15	3_REACH	14000	14000	0	14000	0.102527703			1	0.000	2.004485-07		1	0.000	2.004485-07	2800	2800	0	2800	0.00200655
99-96-7	00967	1093	4-hydroxybenzoic acid	138.12	3_REACH	23300	23300	0	23300	0.169555889	22166.66667	22166.66667	0	22166.66667	0.109458404		1	0.000	2.629285-07	10133.33333	10133.33333	0	10133.3333	0.07355015
99-97-8	00978	1094	N,N-dimethyl-p-toluidine	135.21	3_REACH	5116.31	5116.31	0	5116.31	0.037539731	8297.333333	8297.333333	0	8297.333333	0.041334027		1	0.000	2.85445-07	5160.333333	5160.333333	0	5160.33333	0.03816052
99-99-0	00990	1095	4-nitrotoluene	137.14	3_REACH	3500	3500	0	3500	0.025251505	800	800	0	800	0.005803455		1	0.000	2.540285-07	3300	3300	0	3300	0.024048