Activity-Based Relationships for Aquatic Ecotoxicology Data: Use of the Activity Approach to Strengthen MoA Predictions

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EUROPEAN CENTRE FOR ECOTOXICOLOGY AND TOXICOLOGY OF CHEMICALS

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CONTENTS

SUMMARY

The relationship between chemical activity (as defined by phase equilibrium thermodynamics) and toxicity of narcotic chemicals was originally hypothesised at the end of the 1930s but has only recently been revisited by Mackay *et al* (2009). The work of this task force demonstrated that chemical activities can be used to determine toxicity for narcotics for any species (including mammals, fish, invertebrates) regardless of the exposure medium as the toxic effect is hypothesised to occur at a specific activity in the organisms (estimated by the above authors at around 0.01). Thus, toxicity can be substituted for another form of activity such as a physico-chemical parameter (e.g. solubility) and the regression slope of this parameter versus toxicity is expected to be 1. Nevertheless, the authors found that in practice the slope for this relationship is actually closer to 0.8. ECETOC set out to explore this relationship further using a high quality dataset and consider its potential for use as a QSAR to estimate acute and chronic toxicity for non-polar narcotics.

The following conclusions can be made based on this exercise:

- The results of this report are in line with those of previous work (Mackay *et al*, 2009);
- For MoA 1 substances the task force found strong similarities in slopes for both acute and chronic data between the trophic levels examined suggesting that for baseline narcosis, specific species characteristics (behaviour and biology) may play a minor role in determining toxicity at equilibrium;
- For MoA 1 substances, the intercepts for chronic activities were systematically lower (approximately half a log unit) than those for acute activities, in general agreement with the basic understanding of chemical activity;
- For MoA 1 substances, equilibrium of high log K_{OW} substances does not always appear to be reached within the timeframe of the standard acute toxicity test (from approximately log K_{OW} 4-5);
- This work, which separated MoAs and their relative activities, is in line with data from Verhaar and Russom (Verhaar *et al*, 1992; Russom *et al,* 1997) considering differences in activity for each MoA. From the relative activities for each MoA it does not appear possible to systematically determine the MoA from acute toxicity data alone (i.e. some MoA 3 or 4 values may be higher (closer to a slope of 1) than expected based on acute values). Nevertheless, no evidence was found in this study that substances behave as narcotics at acute level and specific MoA in chronic studies. The only cases found were of substances considered to be MoA 4 (e.g. chlorobutadiene) which showed no evidence of specific MoA in either acute or chronic studies;
- From this work there are various cases which have been reclassified based on Enoch *et al* (2008) (for certain MoA 2 substances). Other instances were also determined, indicating that care should be taken when identifying MoA (e.g. hexachlorobutadiene and hexachlorobenzene);
- MoA 2 data appeared to be completely different (trend lines, intercepts) from the MoA 1 data when plotted, and the dataset should be considered with care due to differences between ionised or unionised states at physiological pH and other confounding factors;

- The task force recommends that a high quality database should be developed based on appropriate technical protocols and incorporating techniques such as passive dosing which would improve the predictions and understanding of activity relationships within and between MoAs;
- The activity concept has not yet been applied in risk assessment. This task force is of the opinion that this work demonstrates proof of concept for application in the development of QSARs to predict acute and chronic toxicity. Ultimately these QSARs could reduce both acute and chronic experimental studies in a regulatory context.

1. INTRODUCTION

Environmental risk assessments (ERA) comprise two elements: exposure assessment and effects (or hazard) assessment. In ERA the likelihood of adverse effects of organic chemicals on aquatic organisms is evaluated by comparing exposure estimates with defined effect or no effect endpoints. The effects assessments are generally based on data obtained from a range of standardised toxicity tests of varying duration and employing a range of relevant species. The growing demand for data to support effects assessment underscores the importance of finding efficient approaches to experimental design and data interpretation. It is also important that ecotoxicologists continue to actively pursue the principles of the 3R's (replacement, reduction and refinement) (Russell and Burch, 1959) of animals used in regulatory studies.

Exposure to aquatic organisms can occur both from the water phase and the diet; however, current guidelines (OECD 203, 202, 201) (OECD, 1992, 2004, 2011) largely derive effects endpoints solely from water-born exposure The concentration in the test medium (water) is generally used to quantify the effect (toxicity) endpoint (e.g. Mackay *et al*, 1992); however, this exposure medium is only a surrogate for the amount of toxicant that actually reaches the site of toxic action in the organism resulting in the toxic effect at the assessment endpoint. It is generally accepted that the toxic effect is directly attributable to the delivered dose of chemical to a target within the organism and only indirectly to the external exposure (e.g. Escher and Hermens, 2002).

Alternative approaches to the use of these tests have, and are, being explored to establish whether there are more appropriate ways of assessing environmental hazards and whether alternative dose metrics could be more suitable. One approach is the use of critical body burden (CBB) or critical body residue (CBR). McCarty and Mackay (1993) proposed the use of CBRs for use in ecological risk assessment, where exceedance of an effect threshold leads to an observed biological response that is largely proportional to the amount of the chemical at the sites of toxic action. Considerable work has carried on CBRs over the last 20 years (e.g. Meador *et al*, 2011) and a number of reviews have been made of this concept e.g. Barron *et al* (1997, 2002), Sijm and Hermens (2000) and Thompson and Stewart (2003). Despite strategies such as lipid normalisation (Di Toro *et al*, 2000), CBRs tend to be noisy / variable. ECETOC (2005) proposed a multi-tiered approach to using CBB in risk assessment and a number of research projects addressing the value of CBB have been funded by the Cefic Long-range Research Initiative (Cefic LRI). The usefulness of CBB is highlighted by the recognition of a number of toxic modes of action (MoA). Mode of action can be defined as a common set of physiological and behavioural signs that characterise a type of adverse biological response (Escher and Hermens, 2002), where the major (but not all) biochemical steps are understood.

In a series of papers, Verhaar *et al* (1992, 2000) proposed a framework for the identification of four classes of compounds with different MoA, including two for narcosis with non-polar narcosis defined as baseline toxicity (inert substances) and polar narcosis (less inert chemicals, more toxic than predicted by baseline toxicity estimations), which are commonly identified as possessing a hydrogen bond donor (see Table 1). Another MoA scheme is that described by Russom *et al* (1997) which classifies substances into one of seven groups. Other studies (Veith *et al*, 1983) have demonstrated a relationship between the octanol-water partition coefficient (K_{ow}) and non-polar narcosis. The concept has been further developed using approaches that use the Abraham (1994) polyparameter Linear Free Energy Relationships (ppLFERs) to identify non-polar

and polar narcotics (Kipka and Di Toro, 2009) instead of K_{ow}. The K_{ow} and ppLFER approaches seek to characterise the same underlying behaviour of chemical partitioning from the aqueous exposure medium to hypothesised target sites in the body, i.e. toxicokinetics.

A second approach considers the link between activity and toxicity, first proposed by Ferguson (1939) for baseline narcotics, has been explored more recently by Mackay *et al* (1992), Kipka and Di Toro (2009), Mayer and Reichenberg (2006), Reichenberg and Mayer (2006) and Schmidt *et al* (2013). Precise laboratory exposures can be achieved by passive dosing techniques using solid sorbents as the vehicle for chemical delivery as demonstrated by Schmidt *et al* (2013). These authors also showed that the toxicity of mixtures can be assessed by addition of activities, as lethality from exposures to individual chemicals and mixtures occurred to springtails at a total activity over a very narrow range from 0.015 to 0.050 with 50% lethality at an activity of approximately 0.03. The chemical 'activity additivity' approach is similar in principle to adding toxic units (Escher and Hermens, 2002). Potential additional advantages of expressing toxicity using the activity framework are that it can be applied to air-breathing and water-respiring animals, it avoids the variability in CBR attributable to lipid content differences and it enables measured activities causing baseline toxicity in laboratory studies to be compared with activities that are measured or predicted in the environment (Mackay and Arnot, 2011; Mackay *et al*, 2011).

1.1 Activity, aqueous concentration and toxicity

Ferguson (1939) demonstrated that chemical activity could be used as a metric of toxicity, the inherent assumption being that at equilibrium the activity in the organism will approach the activity in the exposure medium. Fundamentally, equilibrium partitioning of a substance between two phases occurs when the criterion of equilibrium chemical potential of the substance is equal in both phases, Schwarzenbach *et al,* (2003). More convenient criteria of equilibrium are the related quantities of chemical activity and fugacity that are linearly related to concentrations, at least at low concentrations, and can also be applied to air, water, soils, sediments and biota. Fugacity is essentially the chemical's partial pressure and can range from zero to a maximum of the substance's liquid state vapour pressure. Activity is the dimensionless ratio of fugacity to that vapour pressure and can thus range from zero to 1.0. Activity is essentially the fraction of saturation. The activity concept is also used for ions but with a different definition from that used here.

Activity thus serves as a direct link between external exposure and delivered dose. Further, for a series of chemicals, if it is hypothesised that narcotic toxicity occurs at relatively similar concentrations (and hence activities) in membrane lipids and in whole organisms, then activities in the exposure medium of water will also be similar, however, the corresponding lethal concentrations in the exposure medium (LCs) can be widely different. The test of the hypothesis is that the highly variable LCs for a diverse set of chemical substances will correspond to a relatively narrow range of activities. Rather than calculate the activities corresponding to the LCs and ECs, it is more convenient to plot these metrics of toxicity against solubility of the liquid state chemical. Since activity is the ratio of concentration and solubility, points corresponding to equal activity will fall on a 45 degree diagonal on a log-log plot and a cluster of points will fall around a 45 degree diagonal with a slope of 1.0. In reality, the slope observed by Mackay *et al* (2009) was lower and about 0.8.

When the chemical is a solid, i.e. the melting point (T_M; units K) exceeds ambient temperature, it is necessary to use the sub-cooled liquid state properties to estimate chemical activity. In a solution at low concentration the chemical behaves as if its saturation condition or reference state is that of the sub-cooled liquid state vapour pressure or solubility, not the solid state that is additionally influenced by crystalline interactions in the solid. The vapour pressure and solubility of the solid substance are thus lower than that of the hypothetical sub-cooled liquid by a factor termed the fugacity ratio (F). The fugacity ratio can be estimated at the ambient temperature (T; units K) from the substance's T_M (also units K) and the entropy of fusion at the melting point (ΔS; units J/mol K). A value of 56.5 J/mol K can be assumed in some cases to estimate ΔS and thus F can be calculated as exp (-6.79(T_M/T-1)), where 6.79 = 56.5/8.314, i.e. the estimate for ΔS divided by the gas constant (R; units 8.314 J/mol K).

An example is solid naphthalene with a molar mass of 128 g/mol, melting point of 80^{O}C (353K) a solid vapour pressure of 10.9 Pa and solubility of 33 mg/L. At 25^{O}C, F is 0.286, thus the corresponding liquid state values are 38.1 Pa and 115.4 mg/L or 0.90 mol/m^3 and 0.00090 mol/L. At a low concentration in air and water the effective reference or saturation state is that of the liquid, thus at 1% of saturation the fugacity or partial pressure of naphthalene is 0.381 Pa, the concentration in water is 1.154 mg/L and the activity is 0.01. The activity corresponding to the solid state vapour pressure and solubility is 0.286, the fugacity ratio. An implication is that naphthalene cannot exist in solution in air or water at conditions exceeding an activity of 0.286 because at higher activities solid naphthalene will phase separate or 'precipitate' from solution. High melting point solids such as hexachlorobenzene may be unable to achieve concentrations and activities necessary to cause toxic effects (Di Toro *et al*, 1991). This constraint does not necessarily apply to liquid mixtures of high melting point solids such as commercial polychlorinated biphenyls (PCBs), crude oils and petroleum products (Kipka and Di Toro, 2009).

It is apparent from the work of Mackay *et al* (2009, 2011) that Ferguson's hypothesis appears to be valid and that the use of chemical activity provides an estimate of toxic potency for narcotic chemicals within an order of magnitude. As such, chemical activity is a preferred metric over the use of chemical concentrations, which can span several orders of magnitude in environmental and toxicity testing media. It should be noted that the relatively simplistic chemical activity / toxicity concept cannot be applied to non-narcotics because the toxicity of chemicals with specific mode(s) of action do not have a simple relationship between toxicity and hydrophobicity. The potency of such chemicals is greater than baseline (narcotic toxicity) because these chemicals have a tendency and/or ability to interact with biological processes in organisms through non-hydrophobic and more specific modes of action / binding mechanisms (e.g. hydrogen bonding, ionic interactions or covalent bonding). Thus, screening out chemicals with toxicity exceeding baseline toxicity is seen as one of the advantages of using the chemical activity approach (Mackay *et al*, 2009). More recently, the Target Lipid Model (TLM) has been successful in expressing the toxicity of narcotic chemicals to aquatic organisms (Kipka and Di Toro, 2009; McGrath and Di Toro, 2009). The TLM is consistent with these concepts of narcosis in that chemical toxicity is induced by a relatively constant concentration of the chemical (e.g. hydrocarbons) in lipid membranes causing loss of essential function. For structurally similar substances, the lipid concentration is proportional to the chemical activity because their activity coefficients in octanol and probably in lipids, are similar (Xiao and Wania, 2003). Mayer *et al* (2009) also observed similar activities for a range of PAHs in several lipid types. The TLM has been successfully applied within the CONCAWE PETROTOX model, which has been used to predict the aquatic toxicity of

various petroleum distillate substances as part of EU REACH registration requirements (McGrath *et al*, 2005; Redman *et al,* 2007; 2012).

An ECETOC Task Force was set up to consider the value of CBB related strategies such as activities as defined by phase equilibrium thermodynamics. The aim was to evaluate the potential for the activity framework to contribute to more effective risk assessment by integrating information on chemical structure and properties, MoA, acute and chronic effects for a range of aquatic organisms. In doing so the observed variability in activity levels corresponding to toxicity and time to steady state and equilibrium, and how activity may assist in the assignment of toxic MoAs was addressed. If successful, the activity concept or hypothesis could be applied in the regulatory process as a 'weight of evidence' component for toxicity evaluation and eventually applied predictively to reduce the number and cost of acute and chronic toxicity studies and animal usage in a regulatory context.

2. METHODOLOGY

The relationships between chemical activity and adverse effects and no effect level estimates on aquatic organisms were explored by analysing only high quality toxicity data for various aquatic taxa and MoA. It was thus hoped to understand whether the observed variability of data in Mackay *et al* (2009) was due to data quality issues or the current capacity of the activity concept to quantifiably describe toxicity. In the first step, a database of critically reviewed data in the form of lethal, effect and no-effect concentrations (LCs, ECs or NOECs) in water corresponding to acute and chronic effect test endpoints was compiled. The chemicals were then assigned into four groups according to MoA (the Task Force choose to follow the Verhaar system). In the third step the aqueous solubility data was converted into a format suitable for establishing chemical activities. The resulting relationships between LCs, ECs, NOECs, solubilities and activities were then analysed and discussed.

The first critical step of this assessment was to obtain high quality data for a large number of substances. Various sources were used, including the newly disseminated European Chemicals Agency (ECHA) database (http://www.echa.europa.eu, retrieved June-December 2011) and the Ecetoc Aquatic Toxicity 3 database (ECETOC 2003).

The recent REACH regulation (EC, 2006) in Europe required the submission by industry of large amounts of toxicology data to ECHA. Data for large volume chemicals were submitted in December 2010, and disseminated in a reduced format to the public in 2011. As a part of this evaluation and registration, industry was required to perform a literature review and assess each study available for each of the substances registered. This provided a large resource of reviewed and validated toxicological and ecotoxicological data. The studies submitted for these registration dossiers had been classified according to the Klimisch rating (Klimisch *et al,* 1997).

The collection of these data for a large number of chemicals provides an opportunity to extract information from this ECHA database. Given that the REACH dossiers must also report the solubility of the substance in water, this allows the calculation of activity through the liquid solubility in water and direct comparison with validated toxicity results for a wide variety of substances. These dossiers were accessed through the ECHA online dissemination tool (European Chemical Agency retrieved June - December 2011 from http://www.echa.europa.eu).

For the purposes of the present study the REACH registration dossiers of a series of selected organic substances were examined. The submitted data on acute and chronic toxicity to fish, invertebrates and algae, as well as solubility, were reviewed. As an initial screening exercise, only data rated Klimisch 1 (reliable without restrictions) or Klimisch 2 (reliable with restrictions) were used. It must be noted that this screening depended on the Klimisch rating assigned by the REACH registrants. QSAR data were not used. Where a REACH registration dossier was not available for a particular substance, then other dossiers were used. In the case of some chlorinated substances that are no longer produced, Euro Chlor (Euro Chlor (1999-2006), retrieved October 2011 from http://www.eurochlor.org/download-centre/marine-risk-assessments.aspx) has published risk assessments under the framework of the OSPAR convention, including the Klimisch rating of studies. Additionally, since pesticides and plant protection products were not registered under REACH, data for these substances were mostly obtained from the US EPA Ecotox Database (Environment Protection

Agency, retrieved October 2011 from http://cfpub.epa.gov/ecotox/). Other data were taken directly from peer-reviewed publications (McGrath *et al*, 2005; Thomas *et al*,) and other sources such as AQUIRE database. These were used after validation.

As discussed above, the concept fugacity has been used to describe the partitioning of substances into various environmental compartments. More recently, the related concept of activity has been compared to environmental concentrations in order to validate the approach and show the feasibility of using activity in environmental risk assessment. The recent availability of a large amount of high quality physico-chemical and ecotoxicity data from the REACH process had allowed the examination of these data through the prism of the fugacity approach.

After collection of the study details, the data were further reviewed for experimental errors and non-standard conditions, such as open systems for volatile substances, as well as studies with a reported NOEC or E/LC50 higher than the reported water solubility were excluded. For acute endpoints, only standard durations for each trophic level were deemed appropriate. Sub-chronic results were rejected as unsuitable for meeting the chronic toxicity endpoint. In addition, non-standard regulatory effects endpoints were not accepted. Studies that reported only nominal concentrations for volatile substances were also excluded. Data were preferentially obtained from the same dossier where multiple dossiers exist for a single substance. The studies from dossiers not submitted to ECHA were also reviewed for non-standard conditions.

Despite best efforts, the methodology applied is not sufficient to completely guarantee that all the included endpoints are free of scientific error or inadequate reporting. However, the authors believe that the methodology has provided a high quality dataset with reduced uncertainty.

Data on the solid or liquid solubility of the chemicals in water, melting point and molecular weight of each substance were collected at the test temperature. For liquids, the fugacity ratio F, as previously defined, is equal to 1.0 and the liquid solubility was used directly. For solids, F was calculated and the higher sub-cooled liquid solubility calculated as the solid solubility divided by F. The solubilities, typically reported in mg/L were converted into mol L^{-1}. For substances that are miscible with water, a hypothetical solubility of 55.5 mol L^{-1} was used as reported by Mackay (2001), i.e. the reciprocal of the molar volume of water. A more accurate conversion could be made using a reported activity coefficient or a vapour pressure and Henry's Law Constant but this applies to relatively polar chemicals.

The substances selected were also divided into four groups according to the Verhaar and modified Verhaar classifications (Verhaar *et al*, 1992; Verhaar *et al*, 2000; and Enoch *et al*, 2008). Mode of action was established using the Toxtree software (Patlewicz *et al*, 2008 and Joint Research Centre of the European Commission, 2011, retrieved August 2011 from http://ihcp.jrc.ec.europa.eu/our_labs/computational_toxicology/qsar_tools/toxtree). Class 1 substances are the non-polar narcotics, which are expected to show baseline toxicity only. Class 2 substances are polar narcotics which are expected to show slightly higher toxicity. Class 3 refers to those substances containing a reactive group, which can react in a non-specific manner with biomolecules, leading to higher toxicity. Class 4 substances are those that interact with specific receptors within an organism causing toxicity (see Table 1).

Table 1: Definitions of Modes of Action (Verhaar et al, 1992)

Mode of Action	Definition
Type 1 Non polar narcotic substances	Narcosis (or baseline) toxicity is believed to be the result of reversible and non-specific disturbance of membrane integrity and function resulting from the partitioning of the chemical into biological membranes (Escher and Hermens, 2002). Because the effects are not specific to particular chemical structures, this can be considered the minimum (or baseline) toxicity that any chemical will display, if it is not obscured by greater toxicity through other modes of action. This MOA is therefore displayed by chemicals that are 'inert' in terms of chemical or biological reactivity, and by interactions with specific biological receptors.
Type 2 Polar narcotic substances	This group consists of more polar but essentially non-reactive substances such as substituted phenols and anilines which ionise to some extent depending on pH and display slightly greater toxicity (external concentration) than would be predicted by 'baseline' toxicity QSARs. They are often characterised as possessing hydrogen bond donor acidity.
Type 3 Reactive substances	Reactive substances are considered as a group that includes diverse modes of action resulting from non-selective reactions with biomolecular structures and consequently displaying enhanced toxicity (lower CBBs) compared with baseline narcotics (Verhaar *et al,* 1992). This group also includes chemicals that are metabolically activated into reactive substances. Of particular importance are electrophilic substances that react with amino, hydroxyl and sulphydryl groups within proteins and DNA (Hermens, 1990), such as certain carbonyls, epoxides, nitriles, hydrazines, acid anhydrides and aldehydes.
Type 4 Specifically active receptor-active substances	Specifically acting chemicals can be classified by their interaction with one of four major protein targets i.e. (a) receptors; (b) ion channels; (c) enzymes and (d) transporters (Rang *et al*, 2003).

The data collected were compiled into a single dataset in Excel (available in the supporting Appendix B). The data for acute fish, acute invertebrate, acute algae, chronic fish, chronic invertebrate and chronic algae studies were separated into different data sheets, and the log E/LC50 plotted against the log liquid solubility in water.

Similar graphs to those presented by Mackay *et al* (2009) have been prepared using homogenous datasets when possible for a detailed examination of:

1. individual groups of substances (with structural similarities when possible, e.g. alcohols);
2. species or phylum, (fish, arthropods, mainly *Daphnia* and algae);
3. acute and chronic data.

The results of individual substances were reviewed, and if sufficient evidence was observed to justify a change of class, the MoA was reassigned.

To determine whether the slopes of the graphs may be reduced by failure to reach equilibrium within the test duration for low solubility substances, an existing method (Spacie and Hamelink (1982) included in an Annex of OECD 305) was used to obtain an approximate value for the equilibrium time at various log K_{OW} values and these were then related to the solubility data. This method uses the following equation to provide an approximation of time to reach equilibrium assuming that the water concentration is constant:

$$C_f = C_{f,s}.(1 - e^{-k_t t}) \quad \text{..... Equation 2}$$

Where C_f = concentration in the fish

$C_{f,s}$ = concentration in the fish at steady state

k_2 = depuration rate

and t = time of exposure

This can be reduced to:

$$t_{95} = \frac{3.0}{k_2} \quad \text{..... Equation 3}$$

Where t_{95} = 95 percent of steady state.

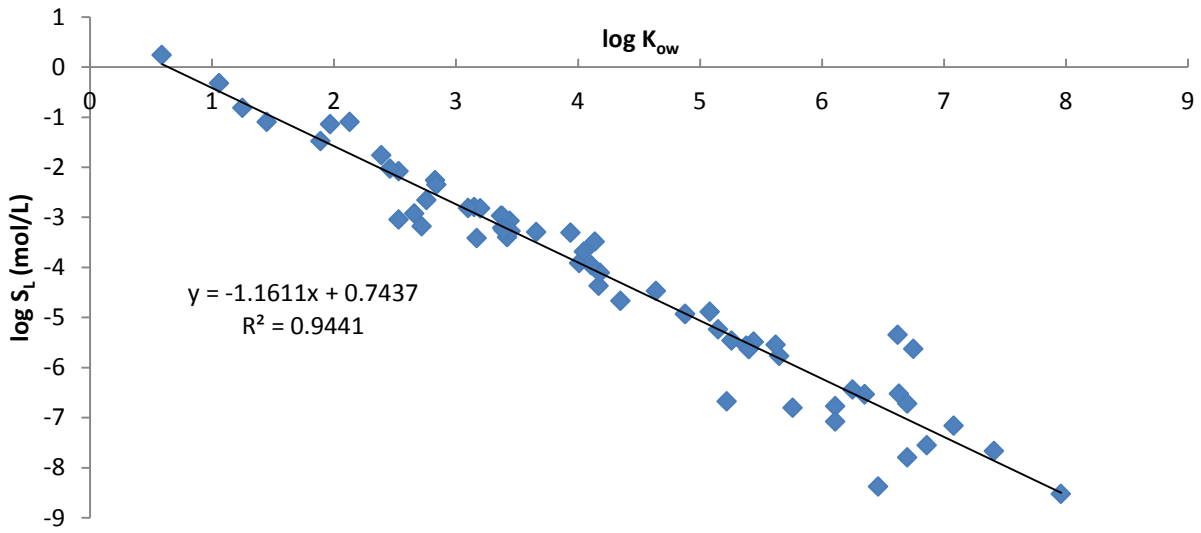
Then k_2 can be determined from the following empirical relationship (Spacie and Hamelink, 1982):

$$\log_{10} k_2 = -0.414 \log_{10}(K_{ow}) + 1.47 (R^2 = 0.95) \quad \text{..... Equation 4}$$

As time to reach steady state is related to k_1/k_2, k_2 can be used to describe a certain percentage of steady state and therefore the time necessary to achieve an appropriate percentage of uptake. For a (non-metabolising) substance with a log K_{OW} of 4, 95% of uptake (k_1) would be expected to take 4.6 days. Thus, for fish, substances with a log K_{OW} of 4 would not be expected to quite reach equilibrium at the end of the 96 h study period. For substances that metabolise rapidly, steady state would be expected to take longer.

The log K_{OW} at 95% equilibrium for a study duration of 96 h was correlated with the solubility to determine the corresponding cut-off value (see Figure 1). From the graph, at log K_{OW} 4 the equivalent solubility would be approximately 10^{-4} mol L^{-1}. This value was used to compare slopes of data at, and prior to, equilibrium for fish.

Figure 1: log K_{OW} v log sol (MoA 1)



3. RESULTS

Toxicity data were compiled and screened and are available as part of the supporting information. Over 2000 individual data points were available. After screening the data for quality as outlined in Chapter 2, the number of usable data points decreased to just over 660 for 123 substances, which include acute and chronic data for fish, aquatic invertebrates and algae. This highlights the narrow availability of data that may be useful for critical analyses, including chemicals risk assessment.

Plots similar to those presented by Mackay *et al* (2009) for non-polar narcotics are seen in Figures 2 to 7, for a detailed examination of:

1. individual groups of substances (with structural similarities when possible, e.g. alcohols);
2. species or phylum, (fish, Arthropods, mainly Daphnia and algae);
3. acute and chronic data;
4. known narcotics and non-narcotics.

The data plotted in each figure were regressed, and the slope, intercept and coefficient of determination (R^2) for MoA 1 and 2 substances are presented in Table 2. Values are not presented from plots on MoA 3 and 4 data as no direct relationship with hydrophobicity can be expected between reactive or specifically acting chemicals as the toxicity will be related to other mechanisms than hydrophobicity. However, the data have been plotted on the same graphical format such that the relative position of MoA 3 and 4 substances can be compared to those of MoA 1 and 2. MoA 2 regression slopes have also been included but due to lack of data and clear slopes and R^2 values, these should only be used qualitatively.

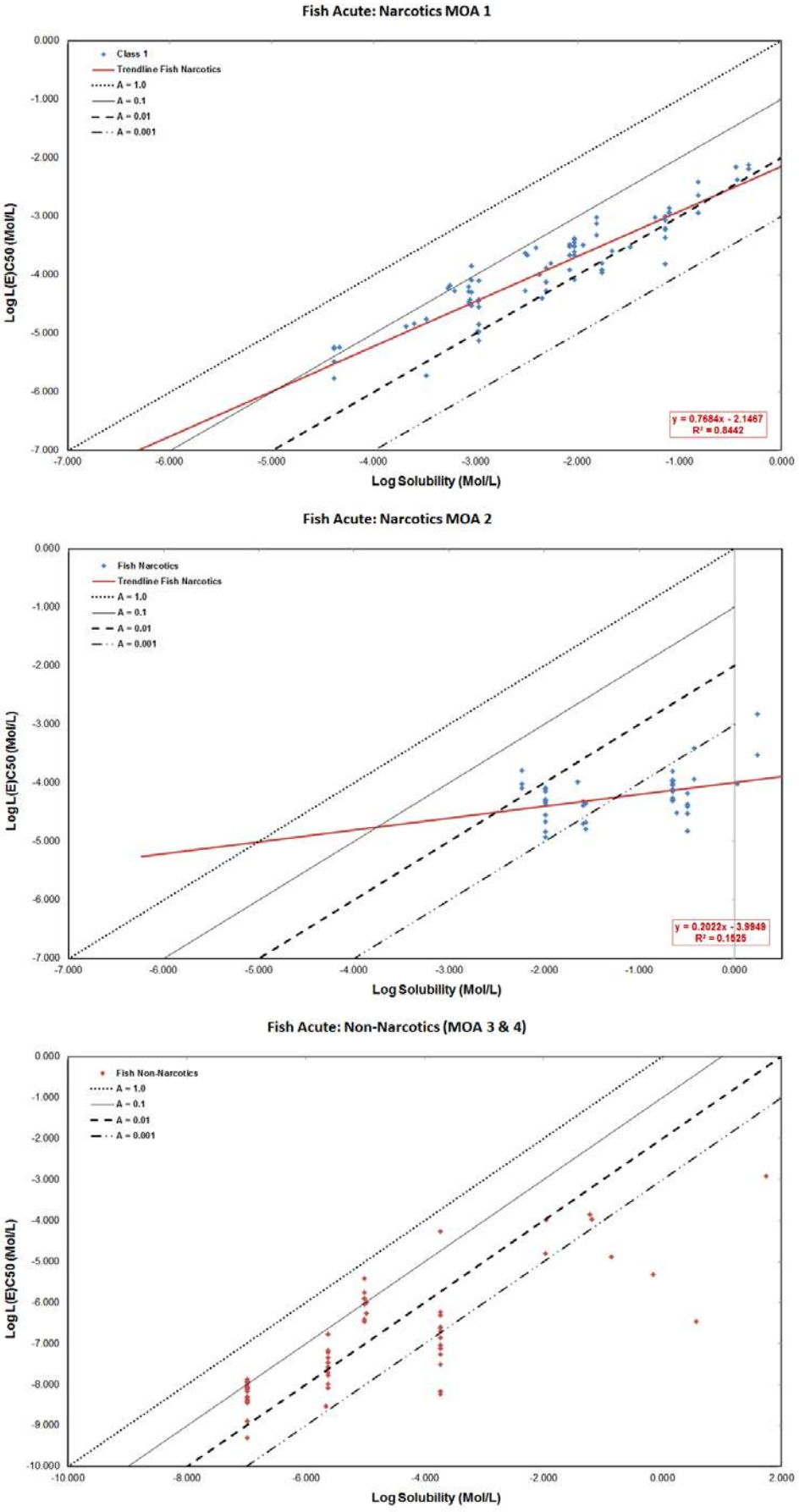
Table 2: Summary of regression data from plots in Figures 2-7

Data	MoA	Slope	Intercept	R^2
Fish Acute	1	0.729	-2.22	0.84
	2	0.202	-3.99	0.15
	3 and 4	N/A		
Invert Acute	1	0.594	-2.63	0.80
	2	0.078	-4.64	0.01
	3 and 4	N/A		
Algae Acute	1	0.729	-2.16	0.72
	2	0.756	-3.05	0.48
	3 and 4	N/A		
Fish Chronic	1	0.867	-2.65	0.91
	2	N/A		
	3 and 4	N/A		
Invert Chronic	1	0.742	-3.20	0.79
	2	N/A		
	3 and 4	N/A		
Algae Chronic	1	0.731	-2.74	0.83
	2	N/A		
	3 and 4	N/A		

3.1 Fish acute toxicity data

Fish acute toxicity data are presented in Figure 2 as three plots which include MoA 1, MoA 2 and a combination of MoA 3 and 4 chemicals. The dataset for MoA 1 substances is the most complete. Higher solubility substances classified as MoA 2 in the Verhaar scheme appear to deviate from activity-based predictions.

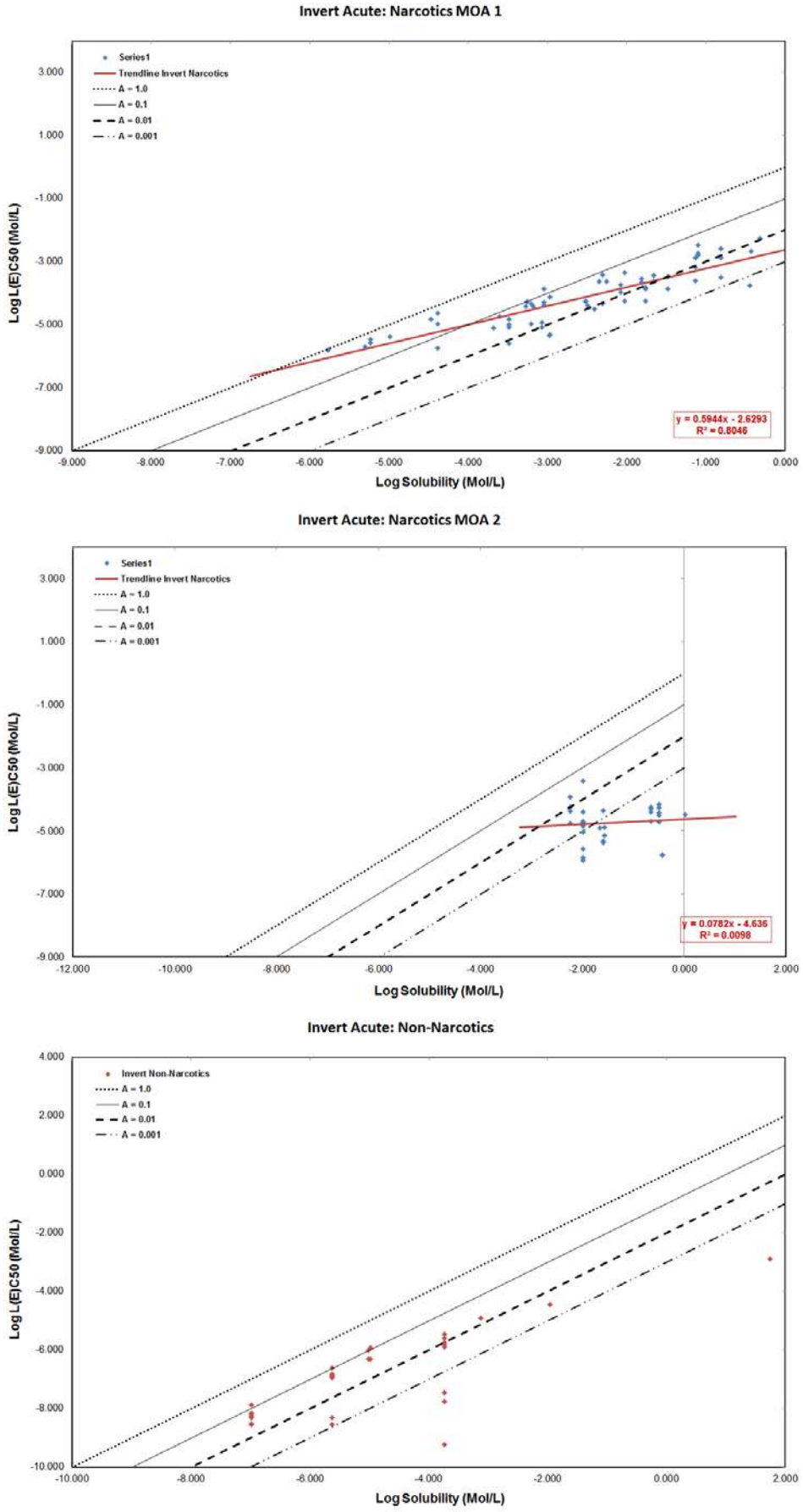
Figure 2: Fish acute toxicity data: MoA 1, MoA 2 and MoA 3 / 4



3.2 Invertebrate acute toxicity data

Invertebrate acute toxicity data are presented in Figure 3. Similar to fish acute toxicity data, the largest dataset is comprised of MoA 1 substances. A lack of test substance variety for MoA 2 substances rendered an analysis difficult.

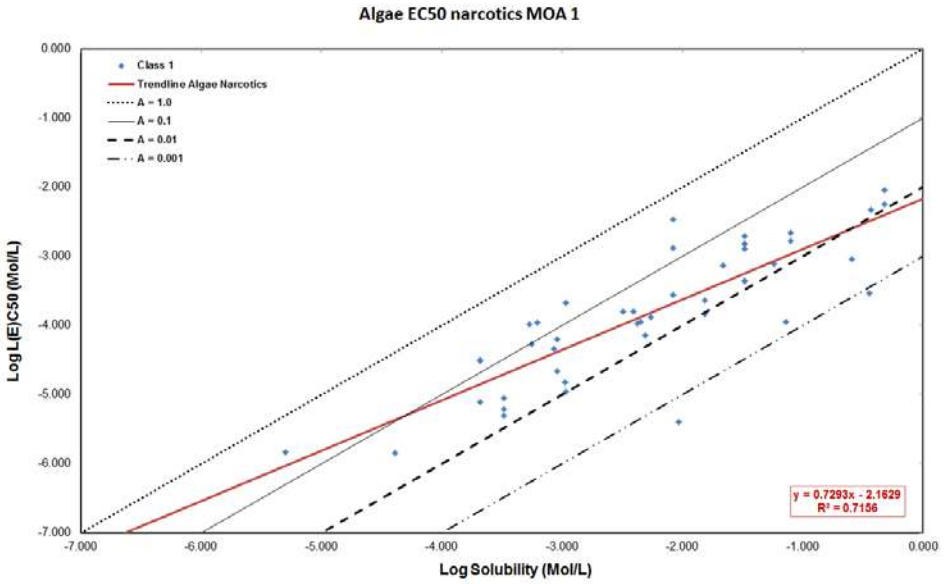
Figure 3: Invertebrate acute toxicity: MoA 1, MoA 2, MoA 3 / 4

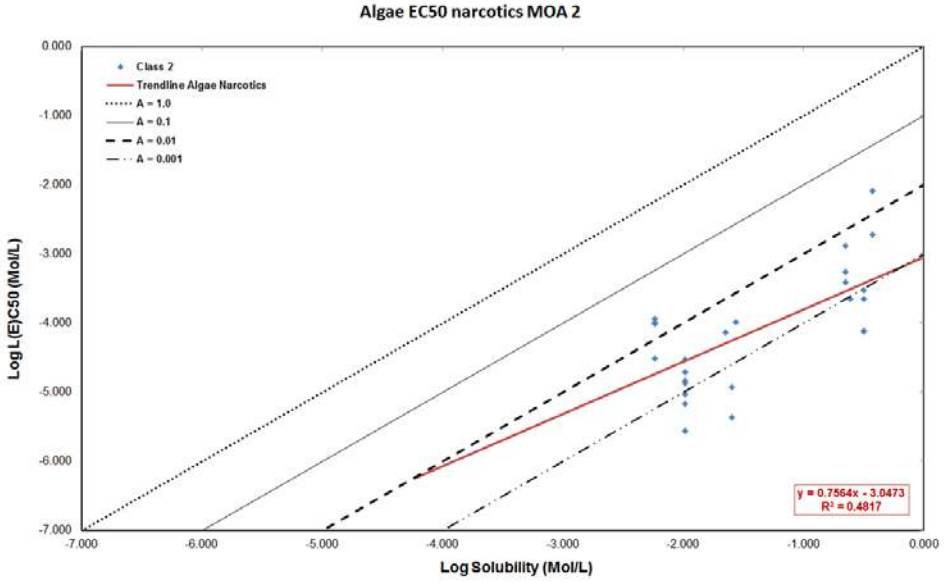


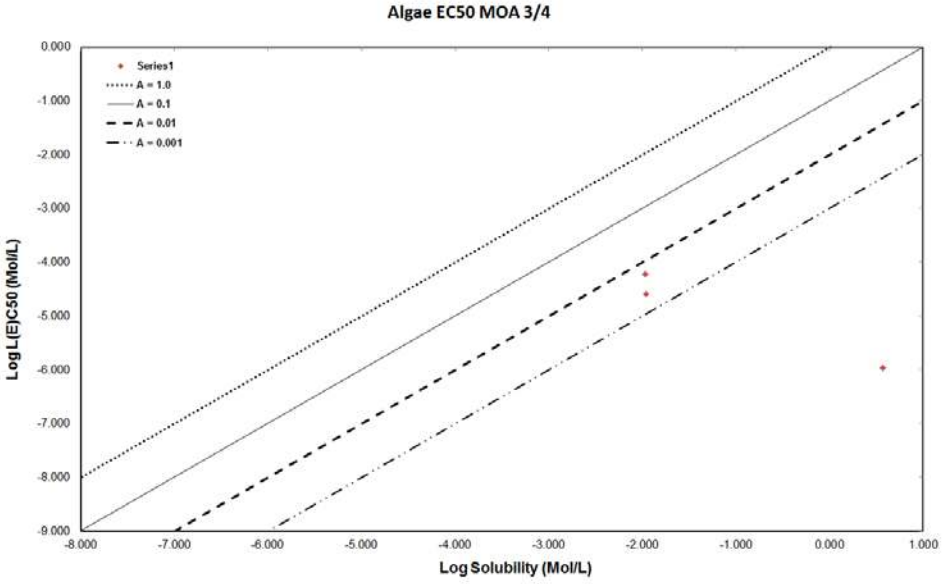
3.3 Algal EC50 toxicity data

EC50 data calculated for the specific growth of algae are presented in Figure 4. The slope and intercept of the MoA 1 plot are similar to the fish acute toxicity data, although there is a greater spread to the data, potentially due to the difficulty in measuring truly dissolved concentrations of test substance in the algal system. Unlike both the fish and the invertebrate MoA 2 data, some inference may be possible from this plot with algae, indicating that for MoA 2 substances, algae may be slightly more predictive although no reason can be provided why algae should behave differently from daphnids or fish to polar narcotics.

Figure 4: Algal EC50 toxicity: MoA 1, MoA 2, MoA 3



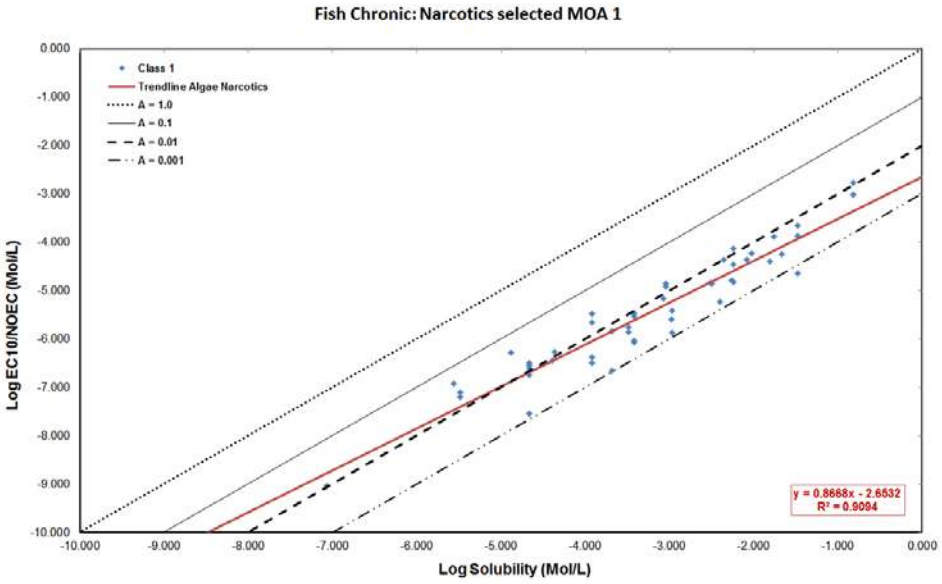


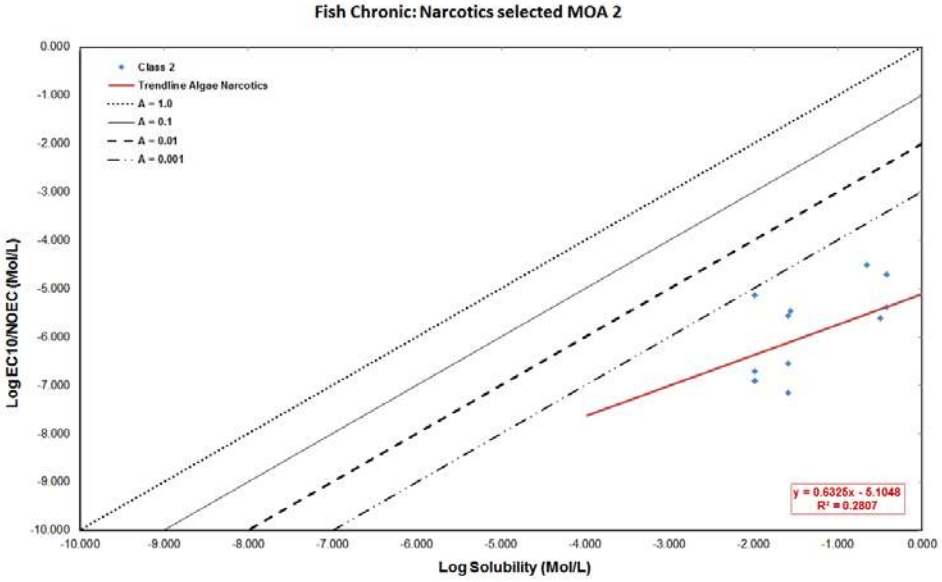


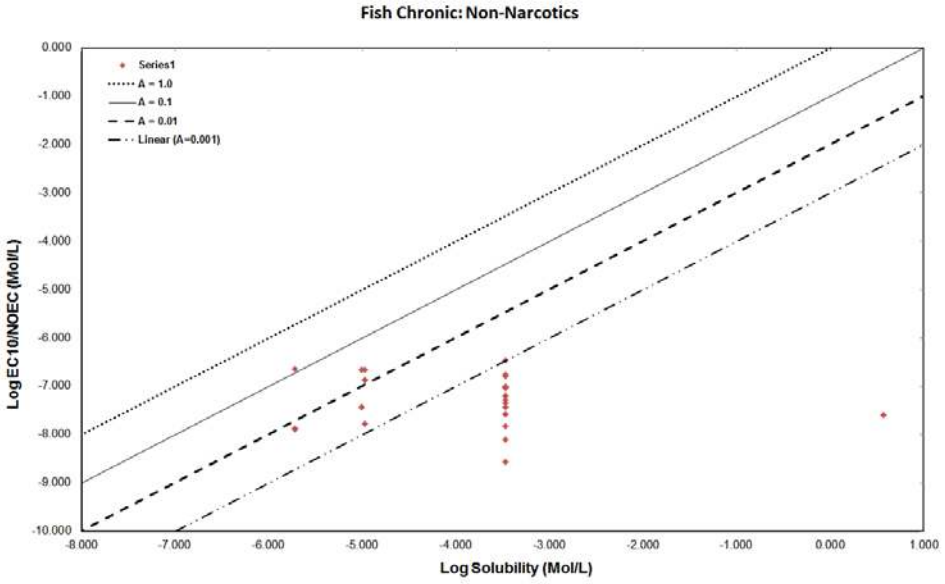
3.4 Fish chronic toxicity data

Fish chronic data are presented in Figure 5. More data are available for low solubility MoA 1 chemicals, perhaps due to a lack of acute narcosis with such substances. The chronic intercept is decreased by approximately 0.5 log units versus fish acute data (to -2.65 from -2.22), which is consistent with chronic effects occurring at lower concentrations. Interpretations of plots for MoA 2, as well as MoA 3 and 4 are not possible due to a lack of availability of high quality data.

Figure 5: Fish chronic toxicity: MoA 1, MoA 2, MoA 3 / 4



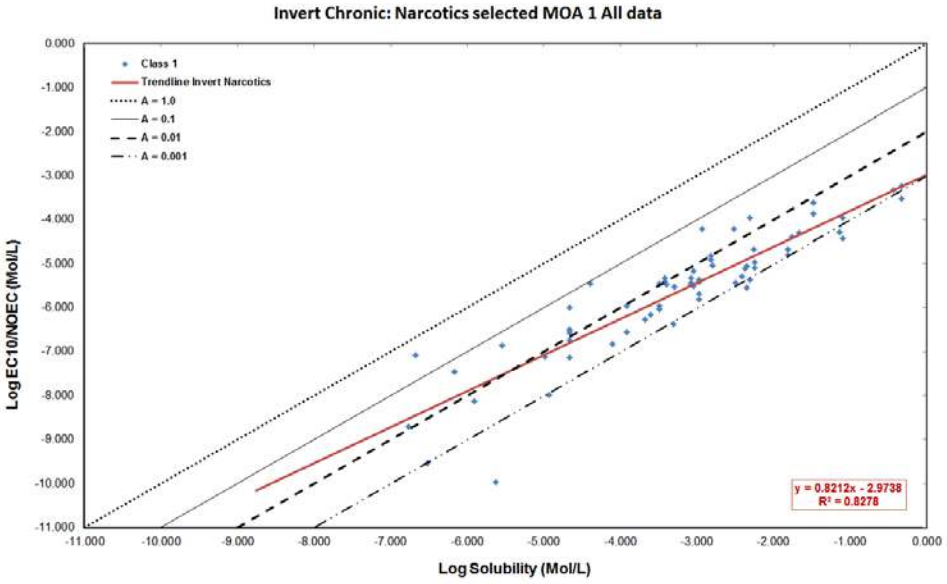


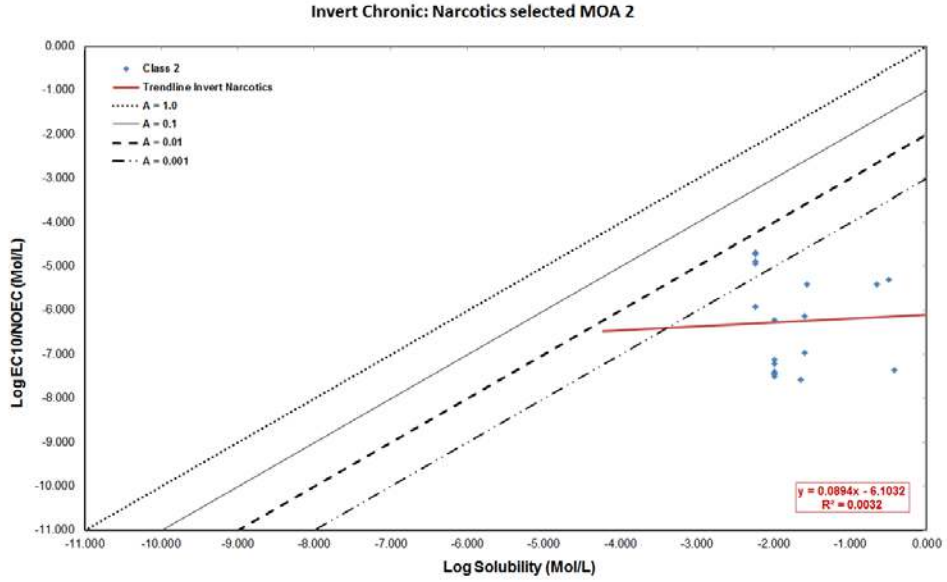


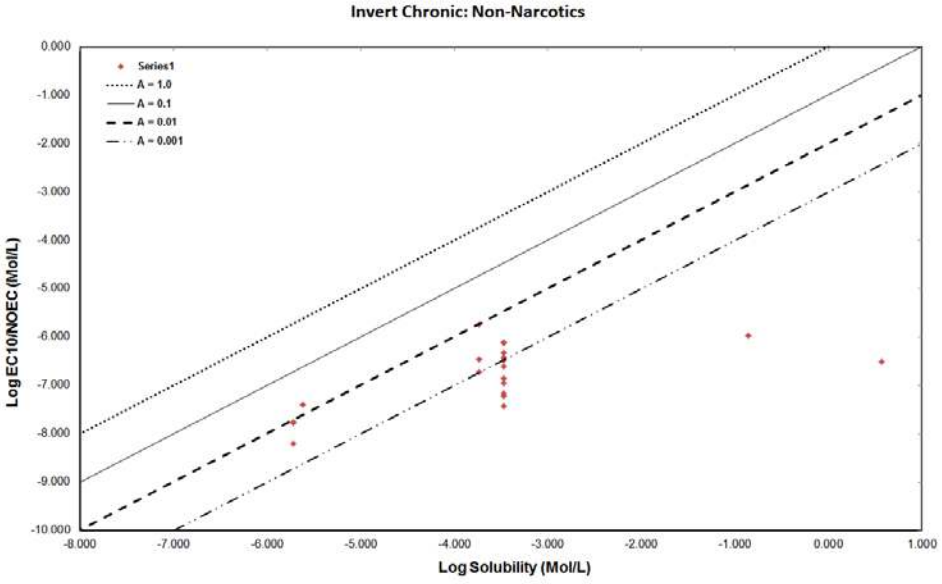
3.5 Invertebrate chronic toxicity data

Invertebrate chronic data are presented in Figure 6. For MoA 1, the data appear to scatter with decreased solubility, perhaps reflecting the experimental challenges in maintaining constant aqueous concentrations in invertebrate tests. As with fish, a lack of availability of high quality data and limited range of solubilies made interpretation of the MoA 2 difficult.

Figure 6: Invertebrate chronic toxicity: MoA 1, MoA 2, MoA 3 / 4



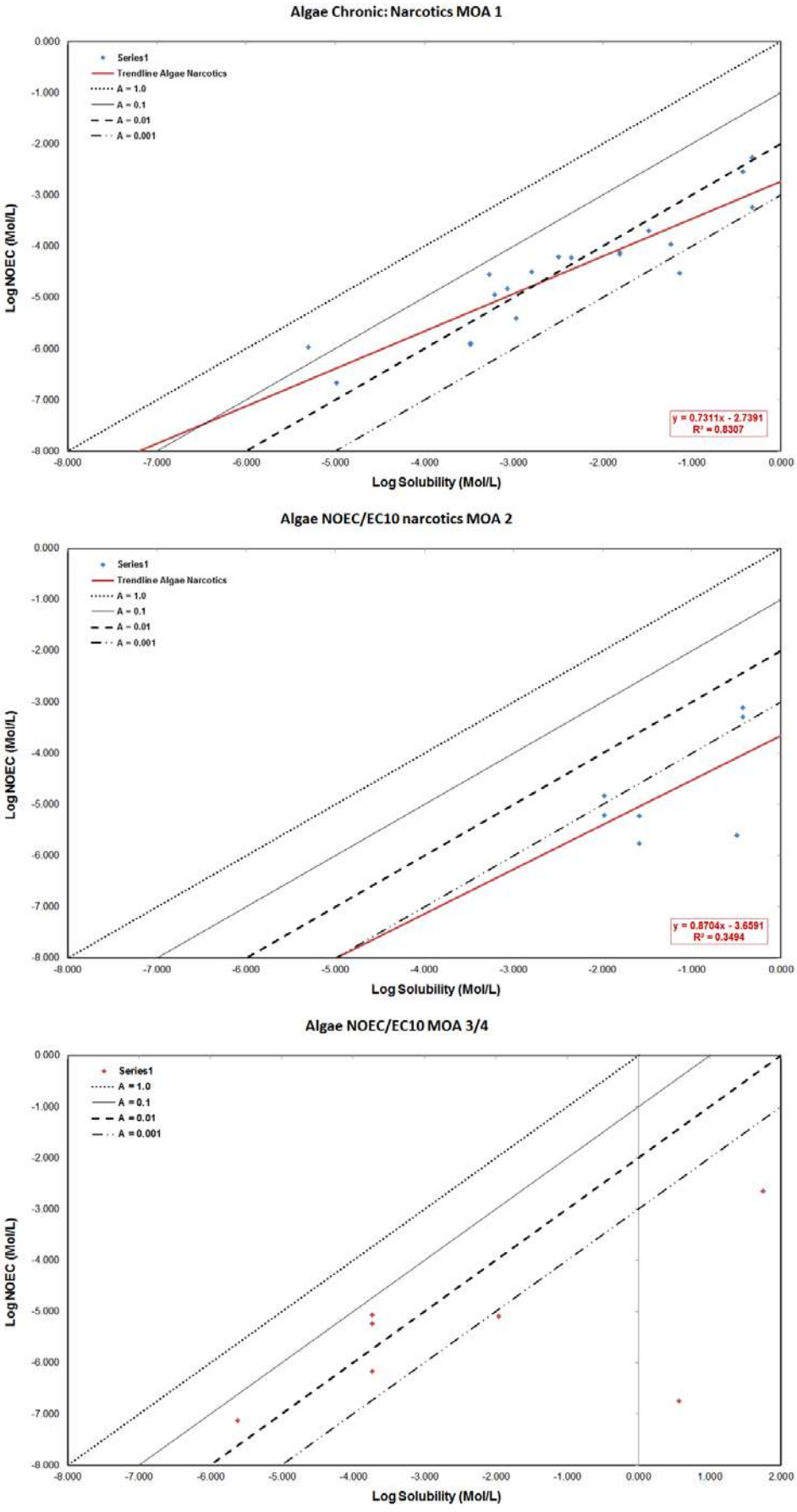




3.6 Algal NOEC/EC10 toxicity data

Algal NOEC/EC10 data are presented in Figure 7. Slopes for the algal EC50 and NOEC/EC10 MoA 1 plots are similar, probably because the NOECs were derived from the same studies as the EC50s presented in Section 3.3. Minimal availability of high quality data and a limited range of solubilities, make interpretation of non-MoA 1 algal plots difficult.

Figure 7: Algal NOEC/EC10 toxicity: MoA 1, MoA 2, MoA 3 / 4



4. DISCUSSIONS AND CONCLUSIONS

There are few previous studies addressing the potential use of activity as an indicator of toxicity which are directly applicable to standard regulatory ecological risk assessment, but the number is increasing (Reichenberg and Mayer, 2006; Smith *et al*, 2010). The work carried out by the aforementioned authors and others (Ferguson, 1939; Mackay *et al*, 2009) has therefore clarified and demonstrated the value of this approach but there still exists a paucity of quality data available for both physico-chemical properties and ecotoxicity. Moreover, generally the narcotic modes of action have been taken together in the dataset while the activities of MoA 2 appear to be slightly higher than those of MoA 1. The impact of pH on ionising chemicals and relative toxicity of the ionised and unionised forms may be a confounding factor when included in the same dataset. In this work, standard regulatory guideline studies on fish, invertebrates and algae have been used and the resulting activities compared for four MoAs separately. The major emphasis has been placed on the MoA 1 chemicals for which data were more readily available and verifiable (increasing confidence in their validity). Less emphasis has been placed on MoA 2 substances for which fewer data were available and due to their ionising potential, over a shorter solubility range with higher variability in results than MoA 1 chemicals.

The objectives of this study were to examine possible relationships between activity as sub-cooled liquid solubility and aquatic toxicity using an evaluated experimental dataset. In principle the aquatic toxicity data should fit within the same regression equation for all species for MoA 1 and 2 substances assuming that equilibrium has been reached (Mackay *et al*, 2009). This was tested by separating the data into the three trophic levels: fish, invertebrates and algae; and then comparing these relationships separately for MoAs 1 and 2 in order to maximise the precision. Furthermore, as mentioned earlier, most studies have focussed upon the acute toxicity but the activity for chronic toxicity remained to be elucidated. In this study, considerable effort was made to validate the dataset by using, for the most part, values classified in the available databases as Klimisch 1 and 2 (Klimisch *et al*, 1997). These data were then further scrutinised. The data used in this exercise are considered fit for purpose although in a few cases significant differences between endpoint values exist for the same substance. An example of this is 1,4-dichlorobenzene for which only 7 studies out of 15 on fish were judged valid by this ECETOC task force and the results nevertheless varied by a factor of 10 (from 1.12 mg L^{-1} for a study on *O. mykiss* to 11.7 mg L^{-1} for *P. promelas*). Correcting for temperature used in the studies in this case does not improve the result. Fortunately, such wide variability within trophic level data was the exception rather than the rule. The physico-chemical parameters, both (sub-cooled) solubility and melting point were also subject to variation. They are not used as a regulatory threshold for classification and labelling or risk assessment under current practice of EU risk assessment and so may tend to be seen as 'dossier fillers' such that the attention to quality may be less than required for accurate activity determination. It was therefore difficult for the authors to determine whether the data used here were accurate or an approximation. Despite these drawbacks, the data quality in this publication are considered to be generally acceptable, allowing an in depth assessment. Nevertheless, the development of high quality toxicity data as a training or validation set for activity calculations is the only way to achieve certainty in predictions based on activities.

Quantitative studies on activity evaluating a wide variety of chemical structures are rare, and limited to recent studies due to the reanimation of the topic in ecotoxicology and risk assessment

(Mayer and Holmstrup, 2008; Mackay *et al*, 2009; Smith *et al*, 2010; Engraff *et al*, 2011). The intent of the present study was to evaluate whether the principle of activity holds true for a high quality dataset. The extent to which current guideline-based studies, which have not been performed with this aim in mind and therefore, may contain experimental deficiencies, can still be used to provide accurate toxicity data which fit with the activity concept have also been considered here.

In practice, this has meant that approximately two thirds of the current data are not fit for purpose (all the studies in the ECHA disseminated dataset which did not meet Klimisch 1 or 2 and 30% of the data which apparently attained the score but were still found to have methodological difficulties for the purpose of this study). Nevertheless, the remaining data were of sufficient quality for use where and, while there is still variability in the results of standard studies, it seems that well executed aquatic toxicity tests in most cases (at solubilities that are > 0.1 mmol L-1) fit well with the concept of activity for MoA 1.

The imperfect fits to the regression lines could be due to several sources: lack of high quality solubility, melting point and/or ecotoxicity, lack of sufficient experimental duration to achieve equilibrium and to some extent for chronic data, the use of NOECs rather than a more appropriate statistical method to calculate the value. For very low solubility substances (< 0.1 mmol L^{-1}) analytical and dosing methods become less accurate due to adsorption of the test substance (to equipment, food and faeces) and due to inappropriate methodology that fails to account for the truly dissolved fraction of the chemical. Alternatively, constant dosing methods employing solid phase technology that currently are being used more frequently (Smith *et al*, 2010) together with chromatography techniques have made significant improvements in terms of sample analysis turn-around time and limit of quantitation over the last decade. It is therefore possible that appropriate analytical methodologies that are now available will provide the definitive database from which an appropriate QSAR could be developed and both acute and chronic ecotoxicity could be predicted, at least for MoA 1 chemicals and potentially also for MoA 2. The potential for experimental reduction in risk assessment is significant if the substance under evaluation can be accurately determined as having only baseline toxicity (or in the case of polar chemicals, slightly higher toxicity). In such cases the number of experimental studies could be limited to a screening evaluation.

- ***Accounting for MoAs***

In order to plot activities accurately, it was essential to determine the modes of action of the substance in the dataset. Data were attributed a score according to the Verhaar and modified Verhaar method (Verhaar e*t al*, 1992; 2000; Enoch *et al*, 2008), using the online ToxTree software (Patlewicz *et al*, 2008). Both the original and modified methods were used to verify the data. Some differences in the two methods were noted. For example, the original Verhaar method classification for certain compounds indicates a non-polar narcosis mode of action while the modified Verhaar classification assigns them to a specific mode of action, which was not justified by the activity of these substances as they fell within the expected limits of activity for classification as MoA 1.

In certain cases, results in the present study were found to be in conflict with existing publications. For example, Su *et al* (2012) found slightly higher toxicity than baseline for nitrobenzene to *Tetrahymena pyriformis* which they considered equated to MoA 2 toxicity. Here, no such toxicity was noted for fish, invertebrates or algae for this compound, thus it was classified as MoA 1. Despite the expected polarity of this substance the appearance of certain structures can be misleading. The solubility of

nitrobenzene (1,900 g m^{-3}) is comparable to that of other singly substituted benzene rings such as chlorobenzene (502 g m^{-3}) and toluene (526 g m^{-3}) despite nitrobenzene possessing a greater dipole (4.22 D) than chlorobenzene (1.69 D) and a much greater dipole moment than toluene (0.36 D). In comparison, aniline has a solubility of 35,000 g m^{-3} and phenol a value of 70,000 g m^{-3}, while the dipole moments (1.53 D and 1.45 D respectively) are lower than that of nitrobenzene (Nelson *et al,* 1967). However, the hydrogen bonding ability of both aniline and phenol is significantly greater than that of nitrobenzene, due to the strong H-bond donating and accepting nature of phenol and aniline. Nitrobenzene is a weak H-bond acceptor only and the solubility is thereby reduced. Thus the substance was reclassified as a non-polar narcotic in line with the toxicity (activity) exhibited.

Some substances were classified by observation of their similarity with other compounds (e.g. 2-nitrotoluene and 4-nitrotoluene reclassified as MoA 1 as read-across from 3-nitrotoluene on the basis of the above justification) and provided much better fits in the new MoA classes. Certain other substances such as hexachlorobutadiene also do not seem to fit with the MoA 3 prediction (modified Verhaar) and both acute and chronic data on this substance are consistent with MoA 1 classification. This is also the case for hexachlorobenzene (classified as MoA 4 under modified Verhaar but reclassified as MoA 1 in this exercise as was recommended by the original Verhaar method).

Nevertheless, it should be noted that MoA allocation is still not an exact science and certain data presented here may be re-classified under a new scheme.

- ***Equilibrium, steady state and variability within the dataset***

Excluding external influences (such as addition of food to the test vessels during a chronic study), we would predict that regression slopes and intercepts are the same for fish, invertebrates and algae and if equilibrium / steady state has been reached in all cases there should be no difference between slopes of acute and chronic plots.

According to Mackay *et al* (2009) the ratio between activity and liquid solubility is in the range of 0.01 to 0.1 for more soluble chemicals increasing from 0.1 to 1 for more hydrophobic substances. Thus, the slope is not 1 as predicted by a constant activity hypothesis but closer to 0.8. This suggests that more hydrophobic substances appear to require higher activities and so are less toxic than predicted. Several explanations are provided by the authors to account for this difference: metabolic biotransformation rates reducing body burdens, reduced bioavailability with increasing hydrophobicity, co-solvents introducing confounding factors, inherent sensitivity of different species, increased activity coefficient of large hydrophobic molecules in the lipid phase or the fact that the tests may not reach equilibrium within the allotted study duration.

To explore these options in more depth, comparisons can be made between slopes of higher and lower solubility compounds and also between slopes for acute and chronic data. For MoA 1 substances, regression lines of acute graphs tend to a slope between 0.6 and 0.75 and those of chronic data between 0.7 and 0.90. Thus activity (read as slope) is closer to the predicted constant activity hypothesis slope value of 1 for chronic than for acute studies. This could be due to a greater chance for equilibrium to be reached during chronic exposures.

To determine whether the slopes of the graphs may be reduced by failure to reach equilibrium within the test duration for low solubility substances, it was necessary to first obtain an approximate value for the equilibrium time at various log K_{OW} values using the method proposed in OECD 305 (OECD, 2012). These could then be related to the solubility data. In the case of the fish MoA 1 plot, three fish studies are not expected to have reached equilibrium as their log K_{OW} was > 4 ($S_L < 10^{-4}$). When the three S_L values less than 10^{-4} are removed the slope for fish effectively increases from 0.73 to 0.77.

The chronic fish regression slope is slightly higher than that found by Mackay *et al* with a value of 0.87, close to the predicted constant activity hypothesis slope of 1. Nevertheless, the data were verified that the equilibrium time was not exceeded as several of the chronic studies had durations of 28 days or less (see *O. latipes,* where the endpoint, development, was measured at 17 days). Using Equation 2, for a log K_{OW} value for fish of 6.0 the 95% equilibrium time was 31 days. This value corresponds to a log solubility of approximately -6.3 for our data (see Figure 1) and all but one of the endpoint values were well below this figure. The log K_{OW} of the shorter (less than 28 day) studies did not exceed 5.4. The lowest solubility value (for benzo(k)fluoranthene at 0.0008 mg L^{-1}) was a 42 day growth study on *D. rerio* and as the value was slightly lower than the regression line, it would seem that equilibrium had also been reached within the duration of this study. Overall, it would seem that the fish had reached equilibrium within the timeframe of the chronic studies.

Time to equilibrium for *Daphnia* neonates was estimated using a modified calculation from Parkerton *et al* (2008) (Equation 5), a literature daphnia respiration rate and neonate weight (Chopelet *et al*, 2008), literature *Daphnia* growth rate constant for neonates (from days 1-9) (Guan and Wang, 2006). The denominator of equation 5 in Parkerton *et al* (2008) contains a term for fecal egestion. This term was omitted in our calculations below, as the impact of fecal egestion on *Daphnia* neonates is expected to be minimal given the small mass of the organisms.

$$t_{90} = \frac{2.3}{k_2 + k_m + k_G} \quad \text{..... Equation 5}$$

Where t_{90} = time required to approach 90% of steady-state *Daphnia* concentration (days)

k_m = biotransformation rate of substance; 0.1 day^{-1} (Parkerton *et al*, 2008)

k_G = growth rate of 1-9 day old *Daphnia*; 0.218 day^{-1}(Chopelet *et al*, 2008)

k_2 = elimination rate of test substance = $\frac{k_1}{LK_{ow}}$ (Parkerton *et al*, 2008)

L = lipid fraction = 3%; default lipid fraction for zooplankton (US EPA, 2009)

k_1 = uptake clearance of chemical into fish = $\frac{r_{ox}}{C_{ox}}$ (Parkerton *et al*, 2008)

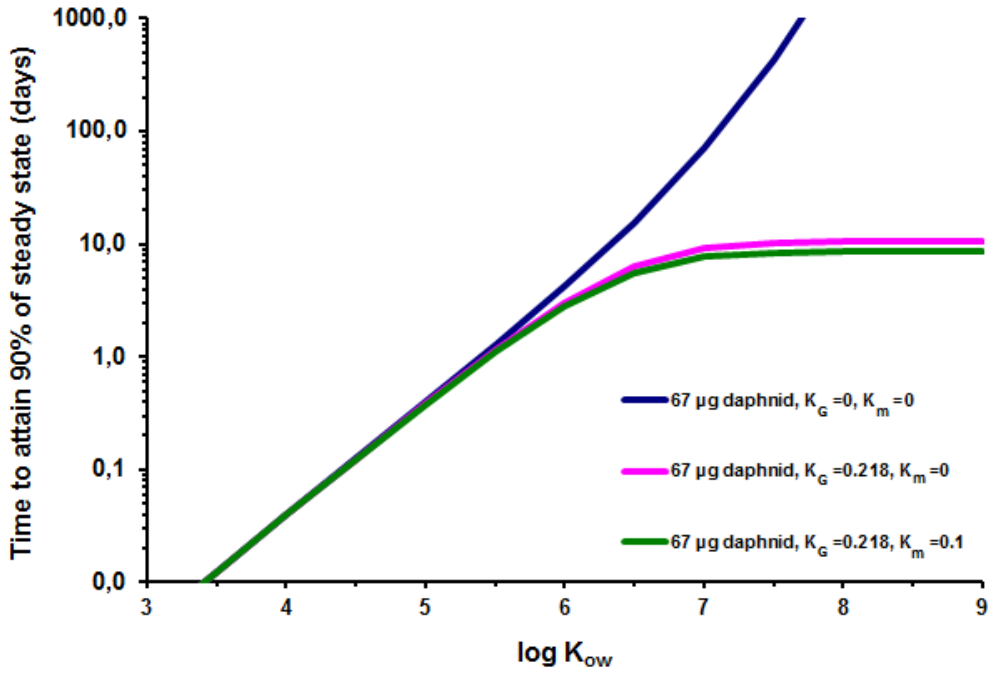
r_{ox} = respiration rate; 0.14 g O_2 g wet^{-1} day^{-1} (Chopelet *et al*, 2008)

C_{ox} = dissolved oxygen concentration; 0.008 g O_2 day^{-1}

Equation 5 was used to create three plots using values for k_G and k_m (Figure 8). The plots in Figure 8 show that for high log K_{OW} substances, daphnid growth rates allow for 90% of steady state to be reached in approximately seven days assuming k_m = 0.1. Note that this k_m is likely to overestimate that in *Daphnia.* However, as seen in Figure 8, growth rate is the major influence on t_{90}. If k_m is set to zero, t_{90} reaches a plateau at approximately 10 days, well inside the duration of OECD 211 (OECD, 2008). These data indicate

that it is likely that equilibrium is reached for substances, including highly hydrophobic substances, within ten days assuming that constant concentrations of substance are met.

Figure 8: Predicted time for Daphnia neonates to accumulate 90% of steady state in studies aquatic toxicity studies with different growth and metabolism scenarios



In this study for acute test data on invertebrates the slope increases from 0.59 to 0.73 if S_L values lower than 10^{-5} mol/L are removed. One hypothesis for this is that it is difficult to maintain constant, accurate concentrations for poorly soluble substances, and that incorrect analytical measurements cause a deviation from the expected slope.

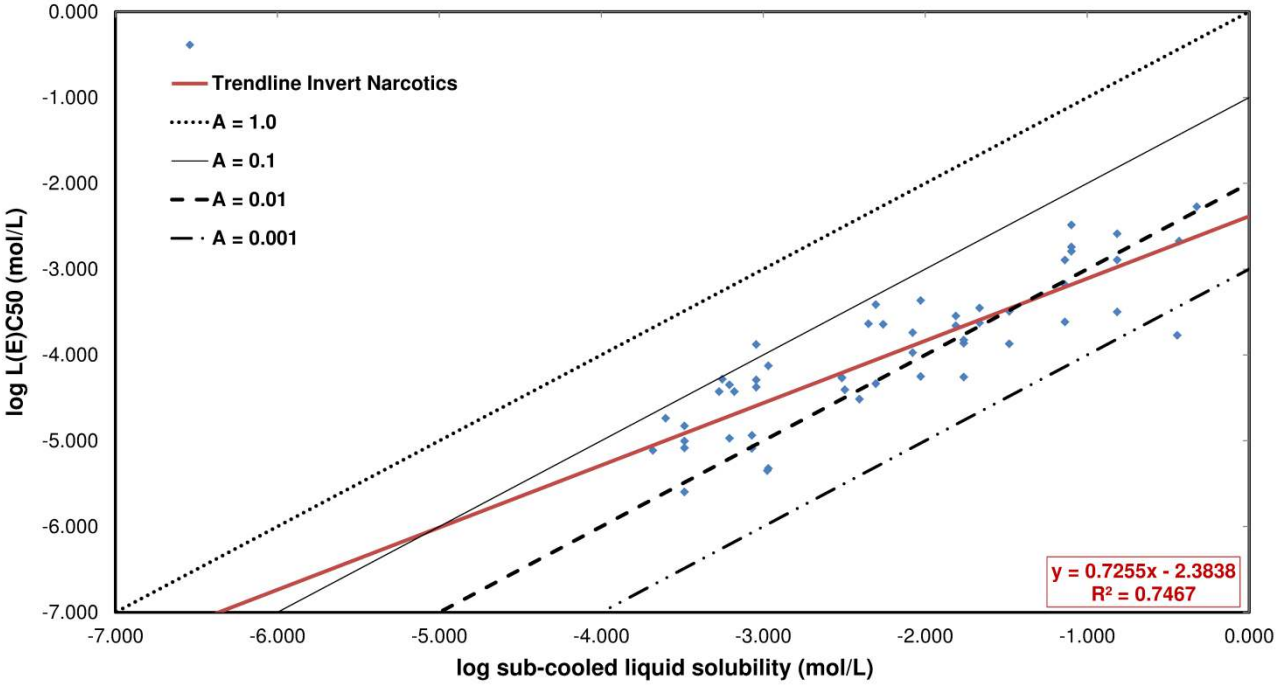
As the toxicity data for algae are based on assays on unicellular organisms, we would expect steady state to be reached over the 72 to 96 hours study period. The slope for algae was also 0.73 which supports this hypothesis.

For multicellular species in the acute dataset it is reasonable to assume that time to equilibrium is not always attained for substances with S_L lower than 10^{-5} mol L^{-1}.

As slopes of chronic data versus solubility tended to be higher than those of acute data, equilibrium may indeed be one of the factors influencing differences between the slopes for experimental and predicted data. Bioavailability was also considered by these authors to be a major influencing factor as the adsorption of low solubility substances to suspended solids may be inadvertently included in samples in many cases. While some of the other factors may also play a role in accounting for the remaining fraction of the slope, most of the other proposals made by Mackay *et al* (2009) would be most likely to account for data variability across the dataset rather than a systematic increase with hydrophobicity although it is recognised that co-solvents are more likely to be used for low solubility substances.

For chronic invertebrate studies, the slope is mostly based on 21 day daphnid reproduction studies, although some *Ceriodaphnia* 7 day data has been included and this test system may be less likely to achieve equilibration than the longer reproduction test for substances with a solubility less than 10^{-5} mol L^{-1}. The chronic test slope (MoA 1) is 0.82 with all data and this decreases slightly to 0.78 if substances at solubility < $10^{-5.5}$ mol L^{-1} are removed. Significant scatter was observed in data below this point suggesting that technical difficulties became increasingly serious at this low solubility level and the validity of the studies is questionable. Separating *Ceriodaphnia* data from all other chronic data leads to slopes of 0.7 for the longer term (non-*Ceriodaphnia*) data and approximately 1 for the *Ceriodaphnia* data. It would therefore appear that there are systematic methodological differences between these two study designs. In this case the longer term data has almost the same slope as the rectified acute invertebrate regression line (with solubility < 10^{-5} mol L^{-1} removed) (Figure 9).

Figure 9: Invert Acute: Narcotics MoA 1



If the invertebrate acute non-polar narcotic data are separated by their degree of solubility, then large differences in slope can be observed. Figure 9 shows the acute invertebrate data with data points for substances with solubility lower than $10^{-4.4}$ mol L^{-1} removed. This changes the slope to 0.73 from 0.59. The new slope is similar to that observed for the chronic invertebrate data at 0.7 and is also closer to the acute fish and algae slopes. This indicates that at lower solubilities (< 10-4.4 mol L^{-1}), factors such as time to reach steady state are playing an increasingly significant role.

For algae, variability within the dataset is slightly greater and validity of the studies more difficult to conclude upon (due to the static design of the test). It is nonetheless reassuring that the slopes for EC50 and NOEC data for MoA 1 chemicals are similar as the time to equilibrium will not change for these endpoints and the slopes for both endpoints at 0.73, were not far from the values found for fish and invertebrates.

- ***Similarities between intercepts***

Intercepts for all studies were analysed and means of intercepts were found to be 2.2 (RSD 6.1% with $S_L < 10^{-4.4}$ mol L^{-1} removed) for acute fish and daphnid data and algal EC50 studies, and 2.79 (RSD 5.9% including all data) for chronic fish and daphnid data, and algal NOECs/EC10s. Differences of approximately half a log unit between acute and chronic studies were observed at the intercept.

For fish, due to the slight difference between acute and chronic slopes, the graphs diverge slightly with decreasing solubility. For algae and daphnids the difference between EC50 and NOECs remains more or less parallel until the activity of acute studies becomes attenuated, perhaps due to equilibrium not being attained.

A second intercept is the point at which S_L will be so low that it will cross the activity line at 1. As it is not possible to have an activity >1 this is the point at which equilibrium can never be reached regardless of the conditions of the study or the lifetime of the organism and the substance can be predicted as non-toxic regardless of the study duration (as an individual substance). Mayer and Reichenberg (2006) reported a melting point cut-off in toxicity, and the point at which the activity of 1 is exceeded occurs when S_L is between 10^{-8} and 10^{-9} mol L^{-1} can be described as the solubility cut-off.

- ***Differences between MoA***

This study has concentrated on narcosis and particularly non-polar narcosis. Nevertheless data for MoAs 2, 3 and 4 were included when available (Figure 2-7).

In order to further assess the ability for the activity concept to discriminate between baseline narcosis and specific modes of action, aquatic toxicity data were accessed from the publications by Verhaar *et al* (1992) and Russom *et al* (1997). Melting points and water solubilities for these substances were obtained from EPISuite v4.1 (measured values, where available, or estimated values were used) and converted to sub-cooled liquid solubilities using fugacity ratios (in the case of solids at room temperature) as described previously. These were then plotted against fish aquatic toxicity data. Substances that were not predicted to reach 80% of equilibrium within four days were removed from the datasets.

Figures 10 and 11 are different plots of the same data from Russom *et al* (1997) as the correlation between water solubility and toxicity, as well as the variability and range of activity values associated with the different toxicity classes.

Figure 10: Empirical mode of action assessment, modified from Russom* et al *(1997)

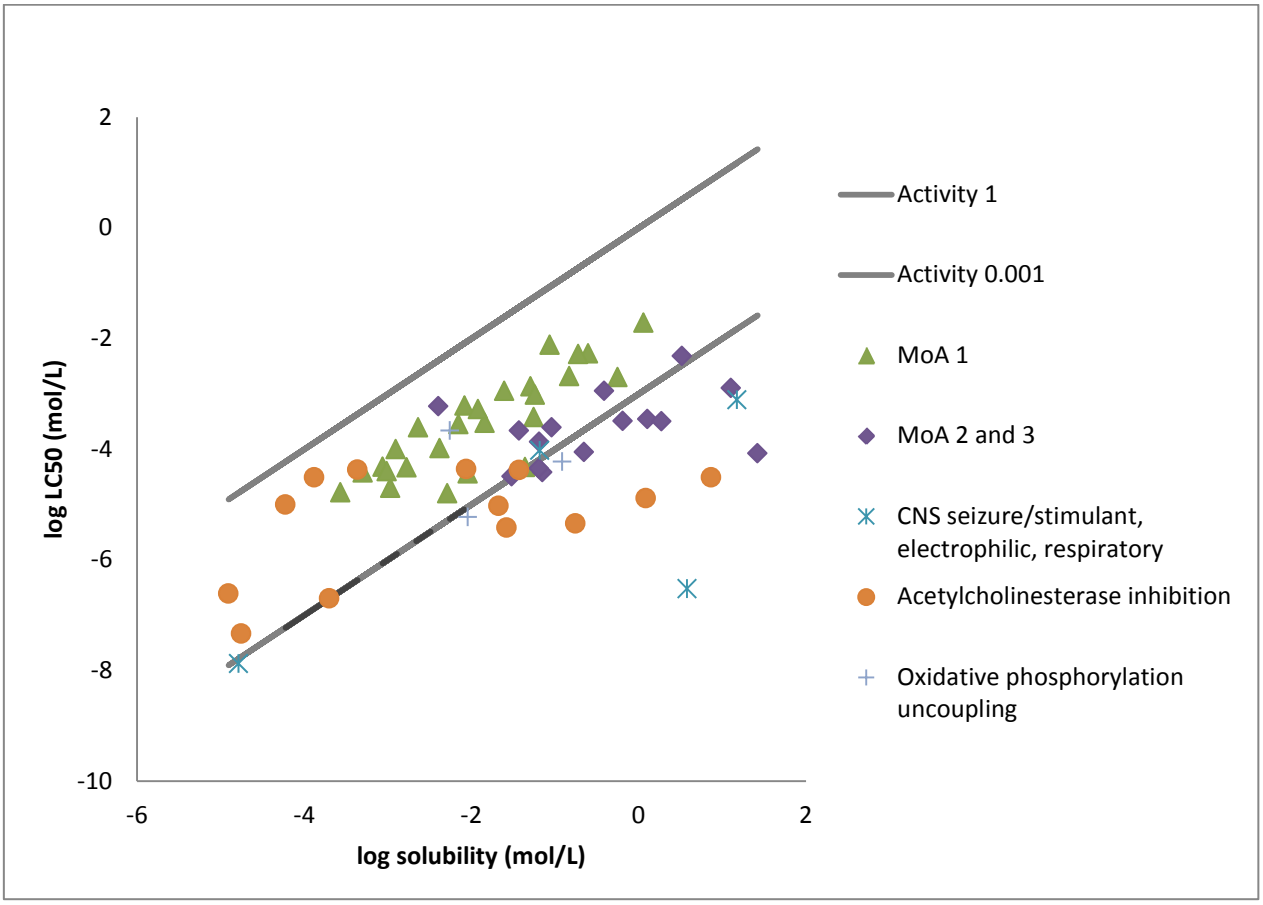
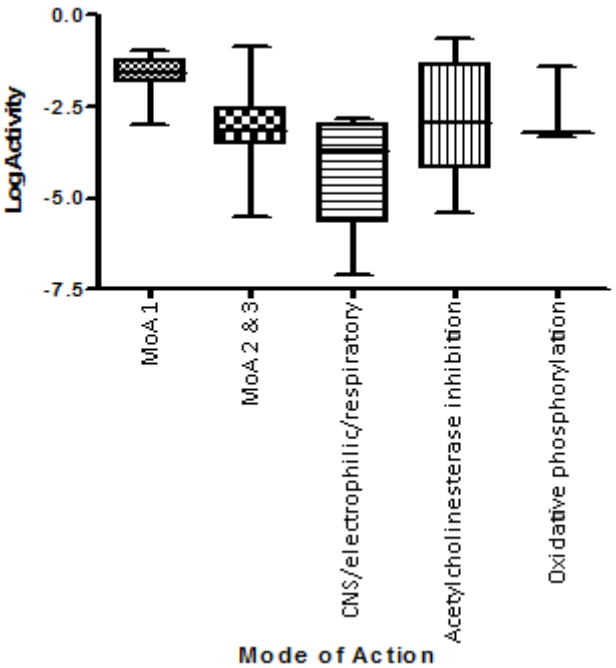
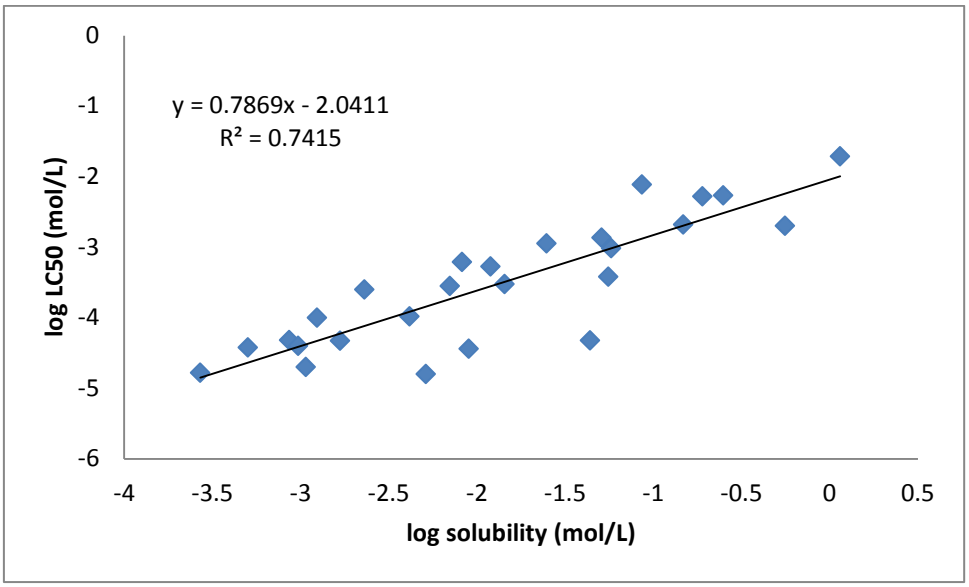


Figure 11: Activity of differently acting substances from Russom* et al *(1997)



The chemicals that exhibit baseline narcosis behave as expected, with all data points lying above the 0.001 activity line. These substances also show the smallest variability in the range of activities. In addition, there was a reasonably good correlation between the water solubility and LC50 data, suggesting that the changes in toxicity were largely explained by changes in water solubility (Figure 12). In addition, the slope of the regression (0.79) was similar to the one observed by Mackay *et al* (2009) and also to that for acute fish observed in this work (0.77).

Figure 12: MoA 1 data, modified from Russom* et al *(1997)



The other MoA substances generally lie close to or below the 0.001 activity line, but there are exceptions to this, most noticeably some chemicals that are classed as Narcosis II and III (MoA 2 and 3 as per Verhaar *et al*, 1992) and acetyl cholinesterase inhibitors. There are a number of possible reasons for these deviations.

Many of the Narcosis II and III substances are ionisable and it is therefore possible that the correlation between water solubility and toxicity has been influenced by the pH conditions under which the measurements were made. No agreement has been reached whether or not there is an underlying difference between baseline and polar narcosis, with Roberts and Costello (2003) proposing there is a difference, due to differences in physical chemistry, and Vaes *et al* (1998) suggesting there is no difference. These latter authors demonstrated that for a set of polar substances, unionised at physiological pH there was no real difference between polar and non-polar narcosis mechanisms in aquatic toxicity when plotted against log K_{DMPC} (DMPC = 1,2-dimyristoyl-sn-glycero-3-phosphocholine) instead of log K_{OW} and indicated that the approach could be used to account for differences in LC50 between MoAs 1 and 2. Thus in their opinion there was no real difference in mode of action between polar and non-polar narcotics. However, these hypotheses are based purely on relations between aquatic toxicity and K_{OW} or K_{DMPC}, with no reference being made to the role ionisation might play.

Su *et al* (2012) in their work on toxicity of polar and non-polar narcotics supported the work of Vaes *et al* (1998) preferring to use the term 'baseline' narcotic toxicity rather than 'non-polar' narcotic toxicity, because it transparently presents the effect of hydrophobicity on toxicity and the relationship between the hydrophobic parameter log K_{OW} and toxicity. According to the authors, the difference between the toxicity of

polar and non-polar narcotics disappears by inclusion of a polarity descriptor (e.g. K_{DMPC}) as well as the hydrophobic parameter log K_{OW}. However, if log K_{OW} is just another way of representing activity, then it follows that the plots of activity versus liquid solubility for polar chemicals should also have slopes similar to those of baseline narcotics but the intercept should be different. This was not found in this study (Figures 2-7) where slopes were inconsistent for all graphs, acute or chronic, for the set of polar substances used so it is not possible to support the proposals of Vaes *et al* (1998) or Su *et al* (2012) with this work.

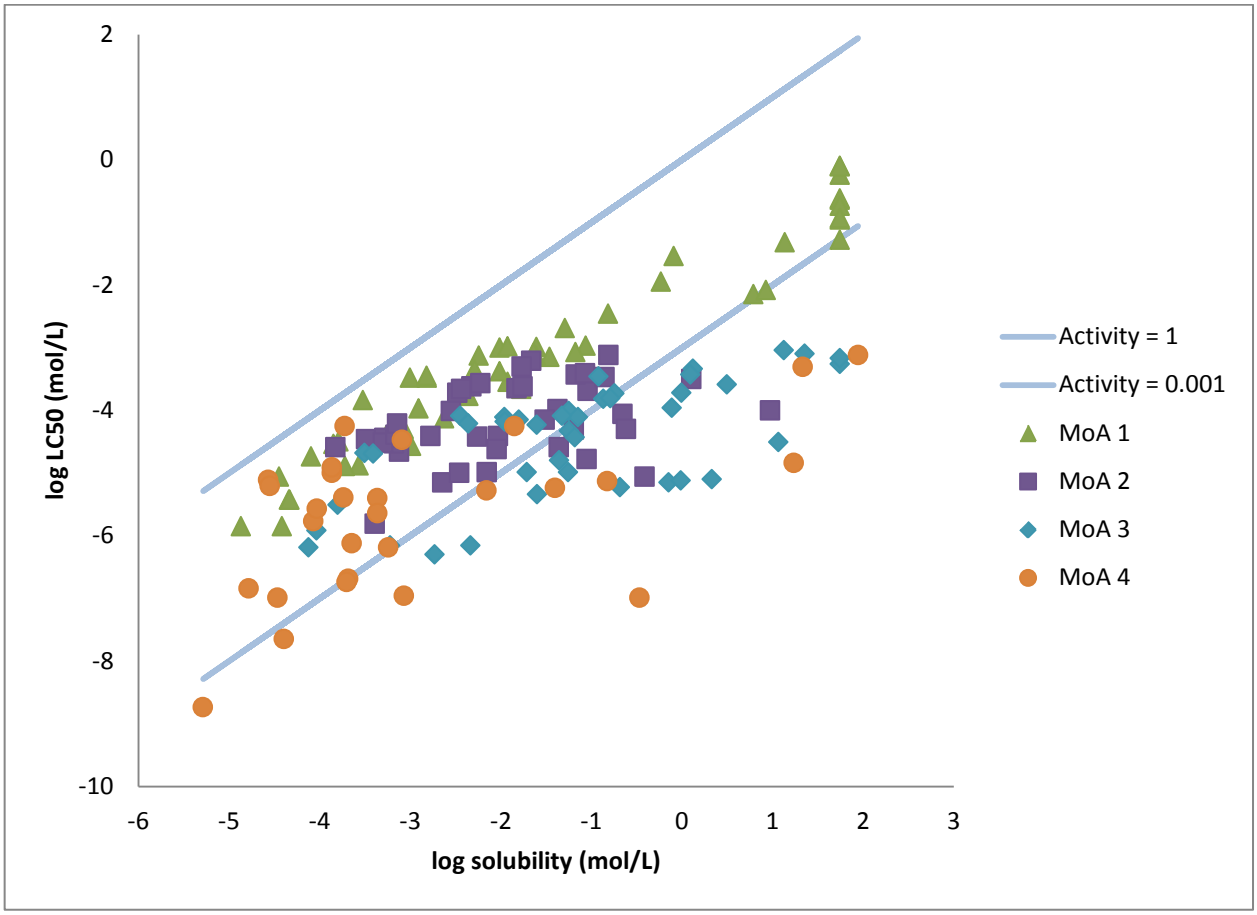
In case of the acetyl cholinesterase inhibitors, malathion, disulfoton, diazinon show activities that are noticeably higher than the 0.001 activity threshold. For these substances it is possible that within the 96 h exposure period, the lethal endpoint observed has been largely due to narcotic effects, rather than acetyl cholinesterase inhibition. However, a more plausible explanation is the fact that between aquatic species there can be considerable variation in the toxic potency of chemicals (i.e. due to differences in metabolic capacity) that have a specific mode of action. For example, for malathion it has been shown that for the fathead minnow (*Pimephales promelas*) and goldfish (*Carassius auratus*), the toxicity is much less than for trout species (Department of Fish and Game, California, 1998). Some of the data compiled for malathion are presented in Table 3.

Table 3: State of California, The Resources Agency, Department of Fish and Game (1998) Hazard assessment of the insecticide Malathion to aquatic life in the Sacramento-San Joaquin river system, Office of Spill Prevention and Response Administrative Report 98-2

Species	Malathion toxicity, 96 h LC50 (µg/L)	Activity
Bluegill (*Lepomis macrochirus*)	30 – 100	0.0002 – 0.0008
Brook trout (*Salvelinus fontinalis*)	120	0.0008
Brown trout (*Salmo trutta*)	101	0.0007
Daphnia magna (48 h EC50)	1	7×10^{-6}
Goldfish (*Carassius auratus*)	10700	0.075
Fathead minnow (*Pimephales promelas*)	8650 – 11000	0.06 – 0.08

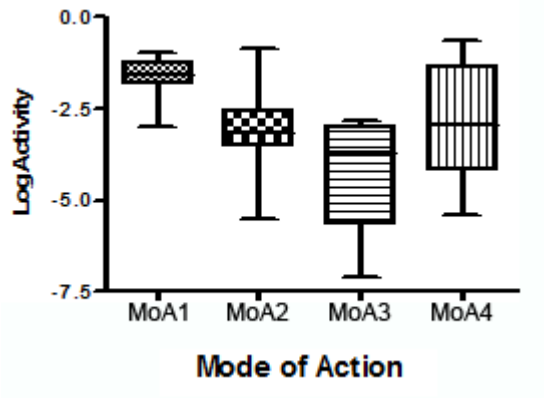
The data from Verhaar *et al* (1992) was also plotted as described above. Figure 13 below shows the dataset with substances not reaching 80% of equilibrium within the acute exposure period removed, and water-miscible substances adjusted according to their pseudo solubility (Mackay, 2001).

Figure 13: Empirical mode of action assessment, modified from Verhaar* et al *(1992)



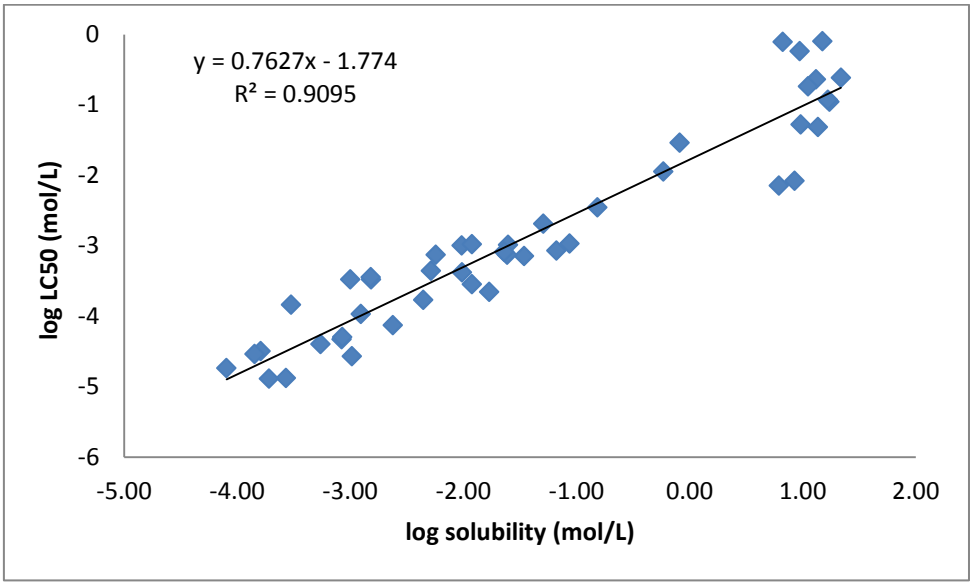
As seen with the Russom dataset, the lowest variability in the activity values was seen for MoA 1 substances, the others showing much greater variability (Figure 14).

Figure 14: Activity of differently acting substances from Verhaar* et al *(1992)



Like the Russom data and the dataset from this study, a very good correlation between water solubility and LC50 was observed for Verhaar's Class 1 substances with a slope of 0.762 and an R^2 of 0.91.

Figure 15: MoA 1 data, modified from Verhaar* et al *(1992), adjusted for chemicals t_{80} > 4 days



In contrast, there were very poor correlations for MoA 2 (R^2 = 0.16, slope = 0.27), MoA 3 (R^2 = 0.50, slope = 0.40) and MoA 4 substances (R^2 = 0.34, slope = 0.38). This is in agreement with the concept that for specifically acting toxicants, water solubility is a poor descriptor of toxicity.

It is important to mention that 50% of the data considered valid (Klimisch 1 and 2) in ECHA-disseminated dossiers were found in this study to be flawed and therefore were not used. This highlights that limitations around data quality are still quite prevalent. This applies to water solubility and melting point data, as well as ecotoxicity data, since these values are critical for establishing these relationships. Due to inherent variability between and within laboratories, care must be taken in the development of high quality data. However, as high correlations for MoA 1 chemicals were observed for this study, the development of such data is possible. The similarities in the fish acute slope between the Russom *et al* (1997), Verhaar *et al* (1992) and this dataset support this. It is recommended to consider the development of high quality toxicity data using purpose-built study methodologies accounting for time to steady state, and measurement of concentrations in the test organism as well as the exposure medium. These may also be designed in accordance with the mode of action. Such work is underway (Mayer and Reichenberg, 2006; Mayer and Holmstrup, 2008; Engraff *et al*, 2011; Smith *et al*, 2013; Schmidt *et al*, 2013).

Polar narcotics pose a new source of methodological challenges and these will need to be considered in the study design and should be separated from non-polar narcotics. The toxicity of MoA 3 and 4 chemicals may be less easy to predict using an activity-based method and it is recommended to concentrate first on MoA 1 and 2 for which high quality QSARs could be produced within a reasonable timeframe. The task force also propose further work in order to obtain better MoA predictions.

GLOSSARY

Acute toxicity	The harmful properties of a substance which are demonstrated within a short period of exposure (e.g. hours for algae or days for fish and crustaceans).
Chronic toxicity	The harmful properties of a substance which are demonstrated only after long-term exposure in relation to the life of the organism.
Critical body burden (CBB)	The term is used in this report to encompass the various terms used by different authors, including critical body / tissue residue, residue-based toxicity, internal effects concentration etc. It relates to the highest tissue concentration having no effect as well as the 'lowest concentration' causing some significant effect (equating to a LOEC).
EC_{50}	Median effect concentration (generating an effect response in 50% of the test population). Where the endpoint is lethality, this is known as the LC_{50}.
EC_{10}	Median effect concentration (generating an effect response in 10% of the test population), regarded in the TGD as being of similar value as the NOEC. The EC_{10} can be based on a population endpoint that is used to for risk assessment application, such as survival, growth or reproduction (termed the $^{adverse}EC_{10}$), or on a biomarker response (termed the $^{biomarker}EC_{10}$).
Fugacity and fugacity capacity	The term fugacity was introduced in 1901 by G.N. Lewis and is most often regarded as the 'escaping tendency' of a chemical from a particular environmental compartment (e.g. water, soil, air, biota, etc). Fugacity (F) has units of pressure, generally pascals (Pa), and can be related to phase concentrations. For any particular environmental phase (e.g. water, soil, air, or biota) there is a corresponding 'fugacity capacity' with units of mol/m^3-Pa and is denoted by Z. The relationship between fugacity, fugacity capacity and chemical concentration (C) is defined by the equation: C=Z*F Environmental compartments in equilibrium with each other have equal fucagity values (i.e. the tendency to leave one compartment and enter a second is equal to the tendency to leave the second and enter the first). High fugacity equals high propensity to migrate.

Lowest-Observed Effect Concentration (LOEC)	This can be based on a population adverse effect measurement such as decreased survival, growth or reproduction (termed the ^{adverse}LOEC) or possibly on water biomarker response (termed the ^{biomarker}LOEC).
Mechanism of action	A complete and detailed understanding of each and every step in the sequence of events that leads to a toxic outcome, underlying the MoA.
Mode of action (MoA)	A common set of physiological and behavioural signs that characterise a type of adverse biological response (Escher and Hermens, 2002), where the major (but not all) biochemical steps are understood.
Mode of action (Type 1)	Non polar narcotic substances: Narcosis (or baseline) toxicity is believed to be the result of reversible and non-specific disturbance of membrane integrity and function resulting from the partitioning of the chemical into biological membranes (Escher and Hermens, 2002). Because the effects are not specific to particular chemical structures, this can be considered the minimum (or baseline) toxicity that any chemical will display, if it is not obscured by greater toxicity through other modes of action. This MoA is therefore displayed by chemicals that are 'inert' in terms of chemical or biological reactivity, and by interactions with specific biological receptors.
Mode of action (Type 2)	Polar narcotic substances: This group consists of more polar but essentially non-reactive substances such as substituted phenols and anilines which ionise to some extent depending on pH and display slightly greater toxicity (external concentration) than would be predicted by 'baseline' toxicity QSARs. They are often characterised as possessing hydrogen bond donor acidity.
Mode of action (Type 3)	Reactive substances: Reactive substances are considered as a group that includes diverse modes of action resulting from non-selective reactions with biomolecular structures and consequently displaying enhanced toxicity (lower CBBs) compared with baseline narcotics (Verhaar *et al.,* 1992). This group also includes chemicals that are metabolically activated into reactive substances. Of particular importance are electrophilic substances that react with amino, hydroxyl and sulphydryl groups within proteins and DNA (Hermens, 1990), such as certain carbonyls, epoxides, nitriles, hydrazines, acid anhydrides and aldehydes.
Mode of action (Type 4)	Specifically active receptor-active substances: Specifically acting chemicals can be classified by their interaction with one of four major protein targets i.e. (a) receptors; (b) ion channels; (c) enzymes and (d) transporters (Rang *et al*, 2003).

No-Observed Effect Concentration (NOEC)	The highest concentration below the LOEC where the stated effect was not observed. The effect can be based on a population endpoint which is used to for risk assessment application, such as survival, growth or reproduction (termed the ^{adverse}NOEC) or possibly on a biomarker response (termed the ^{biomarker}NOEC).
Vapour pressure	The pressure exerted by a chemical in the vapour phase in equilibrium with its solid or liquid form. It provides an indication of the relative tendency of a substance to volatilise from the pure state. Typical units are mm Hg, torr, or in Hg.
Water Solubility (S)	The maximum amount of a chemical that can be dissolved in a given amount of pure water at standard conditions of temperature and pressure. Typical units are mg/L, g/L.

ABBREVIATIONS

CBB	Critical body burden
CBR	Critical body residue
DNA	Deoxyribonucleic acid
DDT	Dichlorodiphenyltrichloroethane
EC50	Acute toxicity expressed as the concentration that induces an effect in 50% of the exposed population
ERA	Environmental risk assessment
F	Fugacity ratio
K_{ow}	Octanol-water partition coefficient
LC50	Lethal concentration required to kill 50% of the exposed population
LOEC	Lowest observed effect concentration
MoA	Mode of action
NOEC	No observed effect concentration
ppLFERs	Polyparameter linear free energy relationships
QSAR	Quantitative structure-activity relationship
RSD	Relative standard deviation
TLM	Target lipid model
Z	Fugacity capacity

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APPENDIX A: THE ACTIVITY CONCEPT AND THE RELATIONSHIP BETWEEN FUGACITY/ACTIVITY WITH TOXICITY AND CRITICAL BODY BURDEN (CBB)

Chemical activity and lipid volume fraction are dose metrics that have direct relationships to disruptive narcotic concentrations in cell membranes are chemical activity and the volume fraction in lipid. Chemical activity and lipid volume fraction provide other insights and applications for toxicity test data; however, these metrics are also constrained by some of the same technical issues discussed for critical body residue data earlier in the report. Chemical activity (a, unitless) is closely related to the lipid based critical body residue as activity in the lipid phase is a product of the chemical's mole fraction in the lipid and the activity coefficient in that phase (Ferguson, 1939). The activity coefficients of nonpolar narcotics in octanol (often an assumed surrogate for organic phase toxicity target sites) are relatively constant (Mackay *et al*, 2009; 2011). Chemical activity is directly related to concentration. For example, the chemical activity in water is the fraction of saturation of the chemical's liquid state water solubility. Activity thus expresses the proximity to saturation directly and can readily identify inadvertent experimental supersaturation in various phases (i.e. water and air). It also can explain the apparent non-toxicity of high melting point solid solutes such as hexachlorobenzene because these chemicals cannot achieve an activity coefficient of 1.0 in aqueous solution (Escher and Fenner, 2011), being constrained to lower activities and lower lipid concentrations by the low fugacity ratio. Chemical activity can be measured or estimated in the physical environment or in organisms (Mayer and Reichenberg, 2006; Mayer *et al*, 2009; Jahnke *et al*, 2011), calculated from toxicity test exposure concentrations or fugacities in water or air (Ferguson, 1939; Mackay *et al*, 2009) or calculated using multimedia mass balance models, thus providing a direct link to environmental fate, exposure, and toxicity evaluations in screening-level risk assessment (Mackay and Arnot, 2011).

When considering the activity and fugacity concepts discussed in Chapter 1, it is important to understand whether the chemical under consideration is a solid, liquid or vapour at the environmental temperature. In particular, for those substances that are solid at the ambient temperature, there is a need to establish what the super-cooled liquid vapour pressure is. This is defined as the vapour pressure that a solid would have at ambient temperature (e.g. 25°C) if it were a liquid at 25°C. The super-cooled liquid vapour pressure cannot be measured directly but can be calculated or measured indirectly using gas chromatographic retention times (Mackay, 2001). Correlations exist between the vapour pressure of substances in the solid state and their super-cooled liquid counterparts. The ratio between the solid vapour pressure and the super-cooled liquid vapour pressure is called the fugacity ratio (F). The fugacity ratio can be approximated with knowledge of the substance melting point (Yalkowsky *et al*, 1979; Cole and Mackay, 2000) as:

$$F = \exp[-6.79(T_M/T-1)] \quad \text{Equation 1}$$

where T_M is the melting point in Kelvin and T is the ambient temperature. The constant value of -6.79 is derived by dividing a typical value of 56 J mol^{-1} K assumed for entropy of fusion (ΔS_{fus}) with the gas constant (R = 8.314 J mol^{-1} K^{-1}). For example, solid naphthalene has a melting point of 318 K and a water solubility of 0.24 mol m^{-3} at 25°C. Its estimated fugacity ratio (F) is 0.634 and thus its hypothetical (and unmeasureable) liquid solubility is therefore 0.24/0.634 mol m^{-3} or 0.382 mol m^{-3}. Further information on more accurate determination of fugacity ratios (F) can be found in Yalkowsky *et al* (1979) and Mackay (2001).

In simple terms, fugacity can be viewed as a measure of the tendency of a component of a liquid mixture to escape, or vaporise, from the mixture. The fugacity of a component in a mixture is essentially the pressure that it exerts in the vapour phase when in equilibrium with the liquid mixture. The fugacity of a substance can be deduced for a chemical in solution from its concentration. At concentrations low enough to negate intermolecular interactions between solute molecules, fugacity and concentration are linearly related by C = Zf, where C is the concentration (mol/m^3), f is the fugacity (Pa) and Z is termed the fugacity capacity (mol/m^3 Pa). The fugacity capacity in (Z_w) water can be deduced from the Henry's law constant (H, Pa m^3/mol) where $Z_w = 1/H$.

The fugacity capacity in water can be defined as $1/v_w\gamma_i f_R$; where v_w is the molar volume of water, f_R the reference fugacity and γ_i is the activity coefficient of a particular chemical i. The reference fugacity is the fugacity that the solute will tend to in the pure liquid state when the mole fraction is 1.0 and γ_i is also 1.0. It is therefore the fugacity of the pure liquid solute at the temperature and pressure of the system. In a similar way, the fugacity capacity for octanol can be defined as $Z_o = 1/v_o\gamma_i f_R$, where v_o is the molar volume of octanol. This is further elaborated below.

When considering the potential for toxicity of non-polar narcotic substances, the property of interest is the hydrophobicity of the substance. The fundamental determinant of hydrophobicity is the solute's activity coefficient (γ_i) in water. This property can be viewed as the ratio of the activity (or fugacity) of the solute to the activity (or fugacity) that the solute would have if it were in a solution consisting entirely of pure solute. The activity coefficient can also be regarded as the inverse expression of solubility, where a solute that is only sparingly soluble in a solvent (e.g. water), will have a high activity coefficient. When expressed as a mole fraction, the activity coefficient is the reciprocal of the solubility (Mackay, 2001). Substances with an activity coefficient that is less than 20 can be considered highly soluble in water, or even miscible. Mackay (2001) defined a pseudo-solubility as $1/\gamma_i v_s$. For a substance that is miscible in water, which will then behave like an ideal liquid where $\gamma_i = 1.0$, the solubility approaches $1/v_s$ which is the density of the solvent (mol/m^3). Mackay has estimated this as 55,500 mol/m^3 for water (10^6 g/m^3 / 18 g/mol), or 55.5 mol/L. In comparison, a

poorly water soluble substance, like DDT (water solubility of 5.5 µg/L; 10^{-7} mol/L) has an activity coefficient (γ_i) of over 500,000. Table A1 from Mackay *et al* (2009) defines the relationships between the above parameters.

Table A1: Dependence and relationships of substance physicochemical properties with its activity coefficient in water (γ_w) as an indicator of hydrophobicity

Property	Relationships to γ_w
Fugacity ratio **F**, i.e. ratio of solid to liquid solubility (**S**) or vapour pressure (**P**) at temperature **T** (K)	$F = P_S^S/P_L^S = S_S^S/S_L^S \approx \exp^{(6.79(1-T_M/T))} \approx 10^{(0.01(298-T_M))}$ T_M is melting point (*K*) if $T_M < T$, $F = 1.0$
Solubility of liquid state chemical in water S_L^S (mol m^{-3})	$S_L^S = 1/(\gamma_w v_w)$ where v_W is molar volume of water (18 x 10^{-6} m^3 mol^{-1})
Solubility of solid state chemical in water S_S^S (mol m^{-3})	$S_S^S = FS_L^S = F/(\gamma_w v_w)$
Octanol-water partition coefficient K_{ow}	$K_{ow} = \gamma_w v/(\gamma_o v_o)$ where γ_o is the activity coefficient in octanol and v_o is the molar volume of water-saturated octanol (126.6 x 10^{-6} m^3 mol^{-1})

A suite of other useful substance property parameters (K_{OA}, K_{AW}, solubility in air / vapour pressure etc.) which describe the behaviour of substances in the environment, are dependent upon the activity coefficient of that substance in different media (e.g. water, air, soil and sediment). When partition coefficients e.g. octanol-water (K_{OW}), but also air-water (K_{AW}), and octanol-air (K_{OA}) are used, the fugacity ratio (F) does not need to be factored in as is the case for the solubility of solids since F cancels out between the concentration ratios in the two media. These additional partition coefficient parameters are useful in the application of multimedia environmental distribution models and have been discussed extensively in the literature (Mackay *et al*, 2009).

The concept of activity has proven to be extremely useful in providing a framework for directly comparing the toxic potency of chemicals in both air- and water-breathing animals (Reichenberg and Mayer, 2006; Mackay *et al*, 2009) and that are measured or predicted in the environment. Measured concentrations from bioassays were converted to activities in water by comparison to the saturation concentration (i.e. water solubility of the liquid-state chemical). For poorly defined phases such as biota or sediments, the concentrations could be converted into fugacities using the appropriate Z values. Multimedia models in many cases have fugacity as the output, and fugacities or concentrations can be converted to activities and can be compared with the activity levels required to cause acute or chronic toxicity in a variety of water and air-respiring organisms, i.e. risk characterisation using the chemical activity concept, rather than concentrations.

When chemical concentration is expressed as quantity per unit weight or volume (e.g. mg kg^{-1} and mg L^{-1}) it is often difficult, and not scientifically meaningful (Mackay *et al*, 2009), to compare the toxic potency of chemicals to organisms in environmental media (e.g. air, water, soil, sediment). As mentioned above, these units are external metrics which cannot be used to accurately describe the critical body burden) found to cause effects in various organisms. Unfortunately, the toxicological literature has rarely incorporated this knowledge and has instead made extensive use of external dose metrics in this manner that cannot be easily compared (Mackay *et al*, 2009). The standardised use of molar concentration ($mol \cdot L^{-1}$) normalises potency for chemicals with different molecular weights. However, two different chemical structures with the same mode of action (MoA), such as benzene and naphthalene present at the same molar concentration can appear to have vastly different (eco)toxicities and therefore this approach is considered a major cause of fragmentation in the approach to assess chemicals for environmental hazard (Mackay *et al*, 2009).

In a recent study present study, McCarty *et al* (2013) calculated chemical activity from the evaluated critical body residue data (n¼161 observations for 29 chemicals) using 2 methods: from estimated chemical fugacities in the test organisms and chemical solubilities in membranes. McCarty *et al* (2013) assumed that all types of biological lipids are equivalent to octanol in their capacity to dissolve the test chemicals. Details of the fugacity concept and activity calculations have been described elsewhere (Mackay, 2001; Mackay *et al*, 2009). For the first approach, fugacity capacities for lipid were calculated using octanol as a surrogate for lipid (ZL, moles per cubic meter lipid pascals) and fugacities (f, pascals) were calculated from the lipid-normalised critical body residues (moles per cubic meter lipid) as f¼C/Z (Mackay, 2001). Chemical activities were then calculated from the fugacities using liquid-state vapour pressures for the solutes (PL, pascals) as f/PL. For the second approach, liquid-state chemical solubilities in lipid (SL, moles per cubic meter lipid) were estimated assuming a constant activity coefficient in octanol for all chemicals and the water-saturated molar volume of octanol (vO, 126.6 $x10^{-6}$ m3/mol). Chemical activities were then calculated as critical body residue-lipid/SL. For chemicals that are solids at 25 8C, the liquid-state, subcooled PL and SL properties can be calculated from the solid-state estimates and the fugacity ratios as described elsewhere (Mackay *et al*, 2009). Henry's law constants, octanol/water partition coefficient (K_{OW}), and melting point data required for these calculations can be obtained from EPI Suite 4.1 (US EPA, 2011) with measured data selected preferentially over quantitative structure–activity relationship predictions. It is recognised that the true liquid-state vapour pressures and lipid and solubilities in octanol will differ to some degree from these approximations. Despite differences in the chemical activity estimation methods, approximately 80% of the activities for the same data point were within a factor of 3.

APPENDIX B: DATABASE

Table 4: Fish Acute

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1-Hexanol	111-27-3	OCCCCCC	O	Class 1		-1.239	-3.023
1-Heptanol	111-70-6	OCCCCCCC	O	Class 1		-1.947	-3.485
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1		-2.373	-4.001
1-Nonanol	143-08	OCCCCCCCCC	O	Class 1		-3.052	-4.419
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1		-3.603	-4.838

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1-Undecanol	112-42-5	OCCCCCCCCCCC	O	Class 1		-4.333	-5.236
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-5.270
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.561
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1		-0.444	-2.153
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.371
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.118
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.186
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.643
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.933
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.411
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.817
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.064
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.369
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.202
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.227
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-2.994

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-3.801
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.915
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.667
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.509
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.474
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.521
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.521
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.093
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-3.843
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.296
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.862
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.935
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.924
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-4.879
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.281
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.468

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.207
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.118
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.544
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.099
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.544
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.419
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.845
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.845
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.985
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.969
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.960
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.977
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.451
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.917
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.915
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.958

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.797
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.715
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-4.754
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.403
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-4.080
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.448
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.513
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.377
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.607
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.499
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.666
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.523
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-4.398
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-4.229
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.269
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1		-3.253	-4.177

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.589
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.122
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.116
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.268
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-3.884
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.124
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.257
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.481
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.240
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.763
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.126
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.319
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.812	-3.015
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-3.659
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-3.630
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.268

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-3.535
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 2		0.239	-3.519
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 2		0.239	-2.827
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.021
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.084
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.791
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.792
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.355
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.677
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.922
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.665
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.365
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.086
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.149
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.096
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.303

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.547
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.329
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.280
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.829
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.144
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.135
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.963
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.969
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.290
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.109
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.017
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.804
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.045
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.948
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.310
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.290

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.265
3-Chlorophenol	108-43-0	ClC1=CC(O)=CC=C1	N	Class 2		-0.610	-4.508
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.529
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.180
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.529
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.828
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.361
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.410
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.377
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.696
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.385
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.317
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.944
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.410
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-4.024
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-3.983

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Butyraldehyde	123-72-8	O=CCCC	N	Class 3		-0.159	-3.446
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.416
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.462
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.036
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.462
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.906
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.911
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.416
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.763
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	
4-Chlorobenzaldehyde	104-88-1	ClC1=CC=C(C=O)C=C1	N	Class 3		-1.966	-4.805
Benzaldehyde	100-52-7	O=Cc(cccc1)c1	N	Class 3		-1.184	-3.977
Acetaldehyde	75-07-0	O=CC	N	Class 3		1.744	-2.920
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.458
Hexenal	66-25-1	O=CCCCCC	N	Class 3		-1.223	-3.855
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-3.978

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Salicylaldehyde	90-02-8	O=Cc(c(O)ccc1)c1	N	Class 3		-0.856	-4.883
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.001
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.268
Endosulfan	115-29-7	ClC2=C(Cl)C3(Cl)C1COS(=O)OCC1C2(Cl)C3(Cl)Cl	N	Class 4		-5.659	-8.530
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.780
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.773
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.458
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.572
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.703
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.210
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.174
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.342
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-8.095
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.996
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.572

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.233
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.509
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.032
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-8.163
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.851
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.708
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.318
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.589
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.631
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.260
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-4.260
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.121
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-8.233
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.948
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.118
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.896
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.868
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.916
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.294
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.374
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.948

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.169
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.072
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.937
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.374
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.314
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-9.294
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.403
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.050
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.998
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.456

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.429
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.087
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.001
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.319
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.581
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.662
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.787
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.754
Methyl acetate	79-20-9	O=C(OC)C	N	Class 5		0.516	-2.393
Trifluralin	1582-09-8	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)	N	Class 5		-4.691	-6.571

Table 5: Invertebrate Acute

A = 1.0		**A = 0.1**		**A = 0.01**		**A = 0.001**	
1	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	**CAS #**	**SMILES**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**Updated in this report**	**log S_L (mol/L)**	**Invert log L(E)C50 (mol/L)**
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1		-3.603	-4.737
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-5.384
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.710
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1		-0.444	-3.770
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.672
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.271

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
PBDE	32534-81-9	Brc1cc(c(cc1Oc2c(cc(cc2)Br)Br)Br)Br	O	Class 1			
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-3.498
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.892
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.587
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-2.894
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.179
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.614
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-3.643
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.973
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.739
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.290
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.375
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-3.877
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.791
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.740
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.485

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-5.113
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.088
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.937
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.322
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.126
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.348
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.863
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.827
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-4.256
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.596
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.003
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-4.827
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.083
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.365
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-4.250
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.870

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.492
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.492
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-3.636
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-4.427
n-Heptane	142-82-5	CCCCCCCC	O	Class 1		-4.469	-4.825
n-Octane	111-65-9	CCCCCCCCC	O	Class 1		-5.238	-5.581
n-Octane	111-65-11	CCCCCCCCC	O	Class 1		-5.238	-5.581
n-Octane	111-65-12	CCCCCCCCC	O	Class 1		-5.238	-5.478
n-Nonane	111-84-2	CCCCCCCCCC	O	Class 1		-5.766	-5.807
n-Nonane	111-84-3	CCCCCCCCCC	O	Class 1		-5.766	-5.807
2-Methylbutane	78-78-4	CC(C)CC	O	Class 1		-3.179	-4.427
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.971
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.348
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1		-3.253	-4.282
Dec-1-ene	872-05-9	CCCCCCCCC=C	O	Class 1			
Dodec-1-ene	112-41-4	CCCCCCCCCCC=C	O	Class 1			

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.626
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.452
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-3.412
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.334
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-4.969
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-4.646
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.746
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.546
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.659
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-4.405
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.268
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.262
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-4.514
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.317
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.350
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.376

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-5.765
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-5.765
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.248
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.766
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.940
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.371
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-4.482
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-4.905
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-5.154
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.899
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.848
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.931
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.812
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.762
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-3.417
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.704

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.397
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.848
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.566
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.033
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.747
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.240
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.694
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.317
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.393
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.711
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.496
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.426
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.277
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.166
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.160
Acetaldehyde	75-07-0	O=CC	N	Class 3		1.744	-2.885

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-4.442
Nonanal	124-19-6	O=CCCCCCCCC	N	Class 3		-3.126	-4.920
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.302
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.018
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.900
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.949
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.606
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.856
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.856
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.809
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-8.317
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-8.531
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.801
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.606
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.464
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.464

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-9.233
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.464
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.765
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.731
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.890
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.877
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.508
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.319
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.197
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.271
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.550
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.152
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-5.921
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.312
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5		-1.665	-3.626
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.239

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-4.926
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.453
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.280
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.540
Atrazine	1912-24-9	n(c(nc(n1)NC(C)C)NCC)c1Cl	N	Class 5		-2.321	-3.871

Table 6: Algae Acute

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
1-Hexanol	111-27-3	OCCCCCC	O	Class 1		-1.239	-3.106
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1		-2.373	-3.968
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.829
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1		-0.444	-3.535
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.335
Pentanol	94624-12-1	CC(CCC)O	O	Class 1		-0.591	-3.037
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.254
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.042

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.953
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-3.886
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.557
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-2.466
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-2.876
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.659
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.199
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.775
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.667
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-5.113
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-4.503
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-4.511
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.341
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.963
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-3.676
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.825
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.305
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.055

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.217
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-5.396
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.347
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.710
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.824
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.824
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.895
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.824
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.369
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-3.954
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-3.983
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-3.956
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1		-3.253	-4.272
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.136
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.143
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.842
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.835
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.643

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-3.795
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-3.795
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.993
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.010
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.507
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.940
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.010
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.927
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.359
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-2.726
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-2.094
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-3.188
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-4.139
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-3.984
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.528
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.033
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.867
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.829

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.704
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.168
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.556
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.410
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.264
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-2.879
3-Chlorophenol	108-43-0	ClC1=CC(O)=CC=C1	N	Class 2		-0.610	-3.647
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-3.647
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-3.529
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.109
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.127
4-Nitrophenol	100-02-7	N(=O)(=O)c(ccc(O)c1)c1	N	Class 2		0.028	-3.638
4-Nitrophenol	100-02-7	N(=O)(=O)c(ccc(O)c1)c1	N	Class 2		0.028	-4.126
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-5.963
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-4.595
4-Chlorobenzaldehyde	104-88-1	ClC1=CC=C(C=O)C=C1	N	Class 3		-1.966	-4.219
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.717
Atrazine	1912-24-9	n(c(nc(n1)NC(C)C)NCC)c1Cl	N	Class 5		-2.321	-6.700

Table 7: Fish Chronic

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-7.552
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.503
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.736
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.608
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.552
1-Methylphenanthrene	832-69-9	c1ccc2c3cccc(C)c3ccc2c1		Class 1		-4.884	-6.284
1,7-Dimethylphenanthrene	483-87-4	Cc3cccc2c3ccc1c2ccc(c1)C		Class 1		-5.488	-7.110
2,7-Dimethylphenanthrene	1576-69-8	c(cc(c1cc2)c(ccc3C)c2c3)c(c1)C		Class 1		-5.488	-7.201
2-Ethylphenanthrene	3674-74-6	c(ccc1c(ccc2CC)c3c2)cc1cc3		Class 1		-5.564	-6.917

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.818
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.459
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.818
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.126
Dibenzothiophene	132-65-0	s(c(c(c1cccc2)ccc3)c3)c12		Class 1		-4.366	-6.265
Retene	483-65-8	c(ccc1c(ccc2C(C)C)c3c2)c(C)c1cc3		Class 1		-6.531	
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-6.066
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-6.029
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.528
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.455
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-5.472
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-6.489
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-5.667
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-6.382
Benzo[a]pyrene	50-32-8	c(c(c(cc1)ccc2)c2cc3)(c3cc(c4ccc5)c5)c14		Class 1		-6.767	
Benzo[k]fluoranthene	207-08-9	c2ccc1cc3c(cc1c2)c4cccc5cccc3c45		Class 1		-7.074	-9.040
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-3.010

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.777
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-4.789
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-4.359
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.851
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.921
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-6.657
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-5.844
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.167
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.866
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.411
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.599
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.882
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.754
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.861
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-4.239
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-4.648
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.866

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.663
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-4.370
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.391
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-4.858
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.836
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-5.234
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-4.247
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1		
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-6.445
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-7.154
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-6.539
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.552
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-5.378
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-4.714
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-6.087
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-5.455
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.704

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.138
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.908
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.908
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.507
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-5.604
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.691
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-7.603
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-7.434
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.658
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.867
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.867
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.658
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.773
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.875
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.886
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.640
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-8.103
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.792
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.027
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.010
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.195
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.346
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.279
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.195
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.823
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.045
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.457
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.580
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.580
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.753
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.425
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-8.561

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.194
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.319
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-6.963
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-7.493
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-6.289

Table 8: Invertebrate Chronic

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1		-2.373	-5.115
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1		-3.603	-6.158
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-7.124
1-Tetradecanol	112-72-1	OCCCCCCCCCCCCCC	O	Class 1		-5.907	-8.127
1-Pentadecanol	629-76-5	OCCCCCCCCCCCCCCC	O	Class 1		-6.162	-7.467
1-Octadecanol	112-92-5	OCCCCCCCCCCCCCCCCCC	O	Class 1			
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-3.326
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-3.530
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-3.238

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-7.137
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.570
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.495
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.503
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.746
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-5.996
Perhydrophenanthrene		C(C(C(C(C1)CCC2)C2)CCC3)(C1)C3		Class 1		-6.671	-7.077
Benzene	71-43-2	c(cccc1)c1		Class 1		-1.096	-4.420
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-5.097
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.964
Ethylbenzene	100-41-4	c(cccc1)(c1)CC		Class 1		-2.798	-5.046
m-Xylene	108-38-3	c(cccc1C)(c1)C		Class 1		-2.819	-4.905
p-Xylene	106-423	c(ccc(c1)C)(c1)C		Class 1		-2.816	-4.830
Isopropylbenzene	98-82-8	c(cccc1)(c1)C(C)C		Class 1		-3.292	-5.536
1,3,5-Trimethylbenzene	108-67-8	c(cc(cc1C)C)(c1)C		Class 1		-3.397	-5.478
Biphenyl	92-52-2	c(c(cccc1)c1)(cccc2)c2		Class 1		-3.911	-5.958
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.397

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.330
Acenaphthylene	208-96-8	c1ccc2cccc3c2c1C=C3		Class 1		-3.308	-6.376
Acenaphthene	83--32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-6.565
Fluorene	86-73-7	c(c(c(c1ccc2)c2)ccc3)(c3)C1		Class 1		-4.104	-6.823
Pyrene	129-00-0	c(c(c(cc1)ccc2)c2cc3)(c1ccc4)c34		Class 1		-4.927	-7.984
Benzo[a]pyrene	50-32-8	c(c(c(cc1)ccc2)c2cc3)(c3cc(c4ccc5)c5)c14		Class 1		-6.767	-8.703
Benzo[ghi]perylene	191-24-2	c16cccc2ccc3ccc4ccc5cccc6c5c4c3c12		Class 1		-6.523	-9.528
Indeno(123cd)pyrene	193-39-5	c(c(c(c(ccc1)c2)c1cc3)c3cc4)(c2c(c5ccc6)c6)c45		Class 1			
Dibenz[ah]anthracene	53-70-3	c(c(c(c(c1)ccc2)c2)cc(c3c(c(c4)ccc5)c5)c4)(c1)c3		Class 1		-5.629	-9.967
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-4.278
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-4.682
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-5.512
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-5.175
Chlorobutane	109-69-3	ClCCCC	O	Class 1		-2.925	-4.218
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-3.954
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-6.259
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.328

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.435
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.468
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.825
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.690
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.427
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.368
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-4.386
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.459
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-6.028
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.958
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.870
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.620
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-5.546
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-5.050
Dec-1-ene	872-05-9	CCCCCCCCC=C	O	Class 1		-5.545	-6.859
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.675
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.811

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-5.438
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.218
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-5.292
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-4.306
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-3.949
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-5.365
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.462
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.732
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.896
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-5.919
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.942
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.692
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-6.961
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-6.128
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-7.367
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-5.311
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-7.577

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-5.406
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.397
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.511
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.210
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.431
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.461
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.130
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.227
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-5.410
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-5.310
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.520
Salicylaldehyde	90-02-8	O=Cc(c(O)ccc1)c1	N	Class 3		-0.856	-5.973
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-8.199
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.782
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.756

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.948
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.124
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.606
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.332
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.857
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.124
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.170
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.221
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.481
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.425
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.221
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.425
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.425
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.396
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.464

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.723
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.738
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.080
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.048
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-8.238
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-7.005
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-7.075

Table 9: Algae Chronic

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log EC10/NOEC (mol/L)
1-Hexanol	111-27-3	OCCCCCC	O	Class 1		-1.239	-3.968
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-6.668
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.969
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.543
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-3.238
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.273
Ethylbenzene	100-41-4	c(cccc1)(c1)CC		Class 1		-2.798	-4.495
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-4.521
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.825

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log EC10/NOEC (mol/L)
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.411
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.916
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.897
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.705
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-4.219
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-4.557
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.952
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.126
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.812	-4.161
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-4.218
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-5.604
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.225
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.756
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.106
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.288
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.210
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.829
Acetaldehyde	75-07-0	O=CC	N	Class 3		1.744	-2.644

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log EC10/NOEC (mol/L)
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.748
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-5.094
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.122
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.066
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.233
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.163
Atrazine	1912-24-9	n(c(nc(n1)NC(C)C)NCC)c1Cl	N	Class 5		-2.321	-7.292

Table 10: Polar K_{OW}s and Solubilities

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**Vw=**	**0.000018**	**mol/m^3**			**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
3	98-95-3	O	Class 2		123.0	1.9	20	20	1900	20	5.26	15.4471545	ECHA	L	-1.81115151	3596.49123	278.26			1	15.4472	-1.81115151
2-Nitrotoluene	88-72-2	O	Class 2		137.1	2.3	16	20	437	20	-9.3	3.18652472		L	-2.49668271	17434.5283	263.7			1	3.1865	-2.49668271
3-Nitrotoluene	99-08-1		Class 2		137.1	2.4	16	20	419	20	16.1	3.05616338	ECHA	L	-2.51482343	18178.2021	289.1			1	3.0562	-2.51482343
3-Nitrotoluene	99-08-1		Class 2		137.1	2.4	16	20	419	20	16.1	3.05616338	ECHA	L	-2.51482343	18178.2021	289.1			1	3.0562	-2.51482343
4-Nitrotoluene	99-99-0	O	Class 2		137.1	2.4	13	20	345	20	44.5	2.51567741		S	-2.59934505	14161.5327	317.5			0.64126526	3.9230	-2.40638277

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT												OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**		**log S_L (mol/L)**
4-Nitrochlorobenzene	100-00-5	O	Class 2		157.6	2.39	200	20	243	20	83	1.54226961	OECD SIDS dossier 2003	S	-2.8118397	9607.8915	356	Dugal M; Kirk-Othmer, 2005	0.26672326	5.782284			-2.23790059
Bisphenol-A	80-05-7	N	Class 2		228.3	3.4	4.12E-07		301		155	1.31844065	ECHA	S	-2.87993942	2178.97215	428		0.05171122	25.4962			-1.59352418
Aniline	62-53-3	N	Class 2		93.1	0.9	40	20	35000	20	-6.2	375.818748	ECHA	L	-0.42502156	147.825397	266.8		1	375.8187			-0.42502156
Nitroaniline	99-09-2	N	Class 2													#DIV/0!							
Phenol	108-95-2	N	Class 2		94.1	1.5	20	20	70000		40.6	743.810435		S	-0.12853773	52.3474343	313.6		0.70085822	1061.2852			0.02583209

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT										OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
																Vw=	**0.000018**	**mol/m^3**			
4-Nitrophenol	41092.0	N	Class 2													#DIV/0!					
2,4-Dinitrophenol	51-28-5	N	Class 2													#DIV/0!					
4,4'-Methylenedianiline	101-77-9	N	Class 2		198.3	1.6	0.00025		1010		90	5.09329299		S	-2.29300134	2480.39712	363		0.22740101	22.3978	-1.64979372
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	N	Class 2		142.6	3.09	27	20	2300	20	48	16.1301634	Publication 2002	S	-1.79236123	2039.35197	321	Publication 2002	0.59211145	27.241769	-1.56476469
3,4-Dichloroaniline	95-76-1	N	Class 2	Anilines (unhindered)	162.0	2.7	0.294		580	20	71.5	3.58024691	[1]	S	-2.44608702	5378.65493	344.5	Merck Index 2001	0.34662443	10.328894	-1.98594619

[1] European Union Risk Assessment Report: 3,4-dichloroaniline (3,4-DCA), Vol. 65

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT													OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**		**Solubility (mol/m^3)**	**Ref**			**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**Activity Coef (YW)**	**mol/m^3**	**Tm (MP in K)**	**Ref**			**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
2-Chlorophenol	95-57-8	N	Class 2		128.55	2.15	139		28500	20	9.3		221.703617	Chlor Euro Marine 2002	RA		L	-0.65422722			250.584795		282.3	Chlor Euro Marine 2002	RA		1	221.703617	-0.65422722
3-Chlorophenol	108-43-0	N	Class 2		128.55	2.50	125		26000	20	33.5		202.255932	Chlor Euro Marine 2019	RA		S	-0.69409873			226.315585		306.5	Chlor Euro Marine 2019	RA		0.82392605	245.478258	-0.60998697
4-Chlorophenol	106-48-9	N	Class 2		128.55	2.39	51		27100	20	43		210.812913	Chlor Euro Marine 2025	RA		S	-0.67610279			174.868366		316	Chlor Euro Marine 2025	RA		0.66356118	317.699288	-0.49798376
MoA 1																													

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1-Hexanol	111-27-3	O	Class 1		102.2				5900	20	-47.5	57.7299413		L	-1.23859888	**Activity Coef (YW)**	962.335217	**Tm (MP in K)**	225.5	**Ref**	1	57.7299	-1.23859888
1-Heptanol	111-70-6	O	Class 1		116.2				1313	20	-34	11.2994836		L	-1.9469414	**Activity Coef (YW)**	4916.64551	**Tm (MP in K)**	239	**Ref**	1	11.2995	-1.9469414
1-Octanol	111-87-5	O	Class 1		130.2				551		-16.25	4.23195084		L	-2.37345939	**Activity Coef (YW)**	13127.6467	**Tm (MP in K)**	256.75	**Ref**	1	4.2320	-2.37345939
1-Nonanol	143-08	O	Class 1		144.3				128	20	-5	0.88704089		L	-3.05205636	**Activity Coef (YW)**	62630.2083	**Tm (MP in K)**	268	**Ref**	1	0.8870	-3.05205636
1-Decanol	112-30-1	O	Class 1		158.3				39.5		6.4	0.24952622		L	-3.60288382	**Activity Coef (YW)**	222644.163	**Tm (MP in K)**	279.4	**Ref**	1	0.2495	-3.60288382

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT										OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**			**log S_L (mol/L)**
1-Undecanol	112-42-5	O	Class 1		172.3				8	20	14.3	0.04643064		L	-4.33319529	**Activity Coef (YW)**	1196527.78	**Tm (MP in K)**	287.3	**Ref**	**SS to S_L conversion**	-4.33319529
1-Dodecanol	112-53-8	O	Class 1		186.3				1.93	20	23.3	0.01035963		L	-4.98465555		5362694.3		296.3	1	0.0104	-4.98465555
1-Tridecanol	112-70-9	O	Class 1		200.4				0.38	20	30.6	0.00189621		S	-5.72211412		25788543		303.6	0.88020775	0.0022	-5.66669931
1-Tetradecanol	112-72-1	O	Class 1		214.4				0.191		39.5	0.00089086		S	-6.05019141		44816107.5		312.5	0.71864635	0.0012	-5.90670664
1-Pentadecanol	629-76-5	O	Class 1		228.4				0.102		44	0.00044658		S	-6.35009593		80687988.5		317	0.64861273	0.0007	-6.16208139

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**				**log S_L (mol/L)**
																Activity Coef (YW)	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**		
1-Hexadecanol	36653-82-4	O	Class 1		242.4				0.013		50	5.363E-05		S	-7.27058926	586042636	323		0.56573423	0.0001		-7.02320172
1-Octadecanol	112-92-5	O	Class 1		270.5	7.4			0.0011		58	4.0665E-06		S	-8.39077458	6440958786	331		0.4714639	0.0000		-8.06422303
Isotridecanol	27458-92-0	O	Class 1		200.37	5.19			1	20	-78	0.00499077		L	-5.3018327	11131666.7	195		1	0.0050		-5.3018327
Cyclohexanol	108-93-0	O	Class 1		100.16	1.25			36000	20	24	359.42492		L	-0.4439182	154.567901	297		1	359.4249		-0.4439182
Benzyl alcohol	100-51-6	O	Class 1		108.14	1.05			40000	20	-15.4	369.890882		L	-0.43192637	150.194444	257.6		1	369.8909		-0.43192637

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Pentanol	94624-12-1	O	Class 1		88.15	1.29, 1.51, 1.35			22600		-138	256.381168		L	-0.59111388	216.691249	135		1	256.3812	-0.59111388
tert-Butyl methyl ether	1634-04-4	O	Class 1		88.2	1.1	33000		41850	20	-108	474.758934	ECHA	L	-0.32352685	117.018452	165		1	474.7589	-0.32352685
PBDE	32534-81-9	O	Class 1		564.7	6.5	very low!		0.0024	20	-7	4.2503E-06		L	-8.37157578	1.3071E+10	266		1	0.0000	-8.37157578
Phenanthrene	85-01-8		Class 1		178.2	4.4			1.15		78	0.00645197		S	-5.19030733	2573790.74	351		0.2989086	0.0216	-4.66584574
1-Methylphenanthrene	832-69-9		Class 1		192.3	5.1			0.269		123	0.00139915		S	-5.85413666	4257013.01	396		0.10721136	0.0131	-4.88437748

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
1,7-Dimethylphenanthrene	483-87-4		Class 1		206.3	5.4			0.099		108.94	0.00047991		S	-6.31884298	17097871.8	381.94		0.14769697	0.0032	-5.48821456
2,7-Dimethylphenanthrene	1576-69-8		Class 1		206.3	5.4			0.099		108.94	0.00047991		S	-6.31884298	17097871.8	381.94		0.14769697	0.0032	-5.48821456
2-Ethylphenanthrene	3674-74-6		Class 1		206.3	5.4			0.096		102.68	0.00046536		S	-6.33220694	20335359.7	375.68		0.17034031	0.0027	-5.56352436
Perhydrophenanthrene			Class 1		192.4	5.2			0.041		20.83	0.00021315		L	-6.67130833	260636856	293.83		1	0.0002	-6.67130833
Benzene	71-43-2		Class 1		78.11	2.1			1790		80	22.9163999		S	-1.63985361	692.354475	353		0.2855929	80.2415	-1.09560101

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**				**log S_L (mol/L)**
Ethylbenzene	100-41-4		Class 1		106.2	3.2			169		-94.9	1.59178676		L	-2.79811511	**Activity Coef (YW)**	34901.3807	**Tm (MP in K)**	178.1	**Ref**	**Fugacity ratio (F)** 1	**SS to S_L conversion** 1.5918	-2.79811511
m-Xylene	108-38-3		Class 1		106.2	3.2			161		-47.8	1.5164359		L	-2.81917594		36635.6108		225.2		1	1.5164	-2.81917594
p-Xylene	106-423		Class 1		106.2	3.1			162		13.2	1.52585476		L	-2.8164868		36409.465		286.2		1	1.5259	-2.8164868
Isopropylbenzene	98-82-8		Class 1		120.2	3.7			61.3		-96	0.50998336		L	-3.29244399		108936.016		177		1	0.5100	-3.29244399
1,3,5-Trimethylbenzene	108-67-8		Class 1		120.2	3.4			48.2		-44.7	0.40099834		L	-3.39685743		138543.107		228.3		1	0.4010	-3.39685743

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m^3				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m^3)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m^3)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Biphenyl	92-52-2		Class 1		154.2	4.0			6.94		69	0.04500357		S	-4.34675307	452979.432	342		0.36694242	0.1226	-3.91135099
Dibenzothiophene	132-65-0		Class 1		184.3	4.2			1.47		99	0.00797786		S	-5.09811373	1289953.62	372		0.18523919	0.0431	-4.3658466
Dimethyl DBT	1207-12-1		Class 1		212.3	5.3			0.09		117	0.00042391		S	-6.37272794	16109025.6	390		0.12291753	0.0034	-5.46234178
Dimethyl phenanthrene	1576-67-6		Class 1		206.3	5.4			0.07133		109	0.00034578		S	-6.46120595	23697978.3	382		0.14749519	0.0023	-5.6299838
Retene	483-65-8		Class 1		234.3	6.4			0.00848		117	3.6187E-05		S	-7.44145057	188708692	390		0.12291753	0.0003	-6.53106441

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Retene	483-65-8		Class 1		234.3	6.4			0.00848		117	3.6187E-05		S	-7.44145057	188708692	390		0.12291753	0.0003	-6.53106441
7,12-DMBA	57-97-6		Class 1		256.4	6.6			0.061		154	0.00023796		S	-6.62350349	12351259.6	427		0.052903	0.0045	-5.34698376
Naphthalene	91-20-3		Class 1		128.2	3.2			31		45	0.2418474		S	-3.61645857	145638.445	318		0.63400103	0.3815	-3.41854854
Acenaphthylene	208-96-8		Class 1		152.2	3.9			16.1		92.5	0.10578187		S	-3.97558878	112815.793	365.5		0.21480957	0.4924	-3.30764241
Fluorene	86-73-7		Class 1		166.2	4.2			1.69		114.8	0.01016725		S	-4.99279657	706167.958	387.8		0.12923613	0.0787	-4.10418051

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT				Vw=	0.000018	mol/m^3				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m^3)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m^3)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Pyrene	129-00-0		Class 1		202.3	4.9			0.135		151.2	0.00066746		S	-6.17557623	4693441.44	424.2		0.05638813	0.0118	-4.92676391
Pyrene	129-00-0		Class 1		202.3	4.9			0.135		151.2	0.00066746		S	-6.17557623	4693441.44	424.2		0.05638813	0.0118	-4.92676391
Benz[a]anthracene	56-55-3		Class 1		228.3	5.8			0.0094		84	4.1174E-05		S	-7.38537806	351779840	357		0.26071463	0.0002	-6.80154345
Benzo[a]pyrene	50-32-8		Class 1		252.3	6.1			0.00162		6.4204E-06	6.4204E-06		S	-8.19243666	325245951	442		0.03758787	0.0002	-6.7674844
Benzo[ghi]perylene	191-24-2		Class 1		276.3	6.6			0.00026		278	9.4087E-07		S	-9.02647041	185197853	551		0.00313645	0.0003	-6.52290845

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m³)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m³)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m³**				**log S_L (mol/L)**
Benzo[k]fluoranthene	207-08-9		Class 1		252.32	6.11			0.0008		169	3.1706E-06		S	-8.49886169	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**		**Fugacity ratio (F)**	**SS to S_L conversion**	
Indeno(123cd)pyrene	193-39-5		Class 1		276.3	6.7			0.00019		163.6	6.8756E-07		S	-9.16269015	658623052	442			0.03758787	0.0001	-7.07390943
Dibenz[ah]anthracene	53-70-3		Class 1		278.4	6.8			0.00249		269.5	8.9453E-06		S	-8.04840748	3434797196	436.6			0.04250925	0.0000	-7.7911736
Dichloromethane	75-09-2	O	Class 1		84.926	1.25	58400	20	13000	25	-95	8.8756E-07		S	-8.04840748	23642031.4	542.5			0.00380671	0.0023	-5.62895729
Chloroform	67-66-3	O	Class 1		119.368	1.97	21100	20	8700	23	-63.5	153.074441	Horvath AL; Halogenated Hydrocarbons: Solubility-Miscibility With Water NY: Marcel Dekker (1982)	L	-0.81509732	362.931624	178	CRC handbook of chemistry and physics. 66th ed. Boca		1	153.074441	-0.81509732
												72.883855	Study, 1995	L	-1.13736866	762.247765	209.5	Merck Index 1976		1	72.883855	-1.13736866

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT													OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**		**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**		**Ref**		**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
Carbon tetrachloride	56-23-5	O	Class 1		153.81	2.83	12000	20	846		-23		5.50029257	Study, 2010	L	-2.25961421	**Activity Coef (YW)**	10100.4728	**Tm (MP in K)**	250	Dreisbach, R. R.;Martin, R. A., Ind. Eng. Chem., 41 (12),		1	5.500293	-2.25961421
Trichloroethylene	79-01-6	O	Class 1		131.5	2.53	9900	20	1100	20	-85		8.36501901	Mackay D, Shiu WY, Ma KC, 1993	L	-2.07753307		6641.41414		188	Merck Index 1989		1	8.365019	-2.07753307
Tetrachlorethylene	127-18-4	O	Class 1		165.9	2.53	2500		150		-22		0.90415913	CRC Handbook, 1994	L	-3.04375513		61444.4444		251	Merck Index 1989		1	0.904159	-3.04375513
Chlorobutane	109-69-3	O	Class 1		92.6	2.66	12060	20	110	20	-123		1.18841832	Study report, 2010	L	-2.92503066		46747.4747		150	Review article 1929		1	1.188418	-2.92503066
1,2-Dichloroethane	107-06-2	O	Class 1		99.0	1.45	10247		7900		-36		79.8366885	Banerjee, S.; Yalkowsky, S.H.; Valvani, *S. C. Environ. Sci. Technol.* 14, 1227 - 1229. 1980	L	-1.09779749		695.864979		237	Nabert, K., Schoen, G. (1963). Sicherheitstechnische Kenn zahlen brennbarer Gase und Daempfe, 2. Aufl., Deutscher Eichverlag GmbH, Braunschweig, 68.		1	79.836688	-1.09779749

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT												OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**			**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1,2,4-Trichlorobenzene	120-82-1	O	Class 1		181.5	4.05	26	20	37.8		17	0.20826446	Lide DR (ed.) CRC Handbook of Chemistry and Physics (82nd) 2001-2002	L	-3.68138483	**Activity Coef (YW)**	266754.85	**Tm (MP in K)**	290	Ullmann's Encyclopedia of Industrial Chemistry, Wiley-VCH Verlag GmbH & Co. KGaA, 2006	1	0.208264	-3.68138483
1,3-Dichlorobenzene	541-73-1	O	Class 1		147.0	3.44	188	20	125		-24.76	0.85034014	HSDB handbook 2009	L	-3.07040732		65333.3333		248.24	Merck Index 2006	1	0.850340	-3.07040732
1,4-Dichlorobenzene	106-46-7	O	Class 1		147.0	3.37	53		82.9		53.3	0.56394558	Lide DR (ed.) CRC Handbook of Chemistry and Physics (82nd) 2001-2002	S	-3.2487628		51694.888		326.3	Merck Index 2001	0.52475586	1.074682	-2.9687201
1,2-Dichlorobenzene	95-50-1	O	Class 1		147.0	3.38	208	20	155.8		-17.03	1.05986395	Banerjee S. 1984. Environ Sci. Technol. 16: 624-627	L	-2.97474988		52417.6294		255.97	Merck Index 2001	1	1.059864	-2.97474988
1,1,2,2-Tetrachloroethane	79-34-5	O	Class 1		167.9	2.39	650	20	2900	20	-44	17.277331	WHO CICAD3	L	-1.76252335		3215.51724		229		1	17.277331	-1.76252335

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**		**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1,2,3-Trichlorobenzene	87-61-6	O	Class 1		181.5	4.139	27.93		30.9		53.5	0.17029485	CRC Handbook of Chemistry and Physics, 82 ed.	S	-3.76879849	**Activity Coef (YW)**	170413.575	**Tm (MP in K)**	326.5	**Ref**	CRC Handbook of Chemistry and Physics, 76 ed.	0.52236997	0.326004	-3.48677669
1,1,1-Trichloroethane	71-55-6	O	Class 1		133.4	2.46	15500	20	1250	23	-33	9.37031484	Broholm K; Feenstra S, 1995	L	-2.02824582		5928.88889		240		ATSDR Toxicological profile for 1,1,1-	1	9.370315	-2.02824582
1,1,2-Trichloroethane	79-00-5	O	Class 1		133.4	1.89	2300	20	4400	20	-36	32.9835082	Handbook	L	-1.48170315		1684.34343		237		Merck Index 1986	1	32.983508	-1.48170315
Chlorobenzene	108-90-7	O	Class 1		112.6	2.84	11700	20	502	20	-46	4.45984364	Banerjee S *et al* 1984. Environ Sci Technol 18:587-591	L	-2.35068037		12456.8393		227		Thieme Römpp Online 2008	1	4.459844	-2.35068037
n-Pentane	109-66-0	O	Class 1		72.15	3.45	68400		38.5	20	-106.92	0.53361053	ESR RAR 2003	L	-3.27277561		104112.554		166.08			1	0.533611	-3.27277561

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
n-Hexane	110-54-3	O	Class 1		86.18	4.11	20200		9.5		-93.84	0.11023439	EHC Monograph 122, 1991	L	-3.95768288	503976.608	179.16		1	0.110234	-3.95768288
n-Heptane	142-82-5	O	Class 1		100.2	4.64	6110		3.4		-90.6	0.03393214	PhysProp Database	L	-4.4693888	1637254.9	182.4		1	0.033932	-4.4693888
n-Octane	111-65-9	O	Class 1		114.23	5.15	1800		0.66		-56.8	0.00577782	PhysProp Database	L	-5.23823624	9615319.87	216.2		1	0.005778	-5.23823624
n-Nonane	111-84-2	O	Class 1		128.26	5.65	571		0.22		-53.5	0.00171527	TPHC Vol 3	L	-5.76566855	32388888.9	219.5		1	0.001715	-5.76566855
n-Decane	124-18-5	O	Class 1		142.28	6.25	175		0.052		-29.7	0.00036548	PhysProp Database	L	-6.43714051	152008547	243.3		1	0.000365	-6.43714051

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT												OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**			**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
																Activity Coef (YW)	**Tm (MP in K)**	**Ref**					
n-Undecane	1120-21-4	O	Class 1		156.31	6.86	52.2		0.0044		-25.6	2.8149E-05	PhysProp Database	L	-7.55053409	1973611111	247.4				1	0.000028	-7.55053409
n-Dodecane	112-40-3	O	Class 1		170.34	7.41	15.4		0.0037		-9.6	2.1721E-05	PhysProp Database	L	-7.66311492	2557657658	263.4				1	0.000022	-7.66311492
n-Tridecane	629-50-5	O	Class 1		184.36	7.96	4.6		5.56E-04		-5.3	3.02E-06	ETC, 24, 9, 2382 (2005)	L	-8.52059191	1.8421E+10	267.7				1	0.000003	-8.52059191
2-Methylbutane	78-78-4	O	Class 1		72.15	2.72	91800		47.8		-159.9	6.63E-01	OECD SIDS C5 Aliphatics (McAuliffe 1966)	L	-3.17880844	83856.3459	113.1				1	0.662509	-3.17880844
Cyclopentane	287-92-3	O	Class 1		70.134	2.76	36230		156		-93.9	2.22431346	ECHA Database	L	-2.65280401	24976.4957	179.1				1	2.224313	-2.65280401

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**				**log S_L (mol/L)**
																Activity Coef (YW)	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**		
Cyclohexane	110-82-7	O	Class 1		84.1608	3.38	12400		52		6.5	0.61786485	ECHA Database	L	-3.20910651	89915.3846	279.5		1	0.617865		-3.20910651
Hex-1-ene	592-41-6	O	Class 1		84.16	3.39	24800		47	20	-139.8	0.55846008	ECHA Database	L	-3.25300787	99479.9054	133.2		1	0.558460		-3.25300787
Dec-1-ene	872-05-9	O	Class 1		140.27	5.62	210		0.4		-66.3	0.00285164	ETC, 24, 9, 2382 (2005)	L	-5.54490481	19481944.4	206.7		1	0.002852		-5.54490481
Dodec-1-ene	112-41-4	O	Class 1		168.32	6.7	20		0.032		-35.2	0.00019011	ETC, 24, 9, 2382 (2005)	L	-6.72098574	292222222	237.8		1	0.000190		-6.72098574
Tetradec-1-ene	1120-36-1	O	Class 1		196.38	7.08	1.65		0.0135		-12	6.8744E-05	ECHA Database	L	-7.16276349	808148148	261		1	0.000069		-7.16276349

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT				Vw=	0.000018	mol/m^3				OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
2-Ethoxyethyl acetate	111-15-9	N	Class 1		132.2	0.6	326		229000	20	-61	1732.74818		L	0.23873545	32.0621058	212		1	1732.7482	0.23873545

Table 11: K_{OW} v LC50

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1-Hexanol	111-27-3	OCCCCCC	O	Class 1	-1.239	-3.023	
1-Heptanol	111-70-6	OCCCCCCC	O	Class 1	-1.947	-3.485	
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1	-2.373	-4.001	
1-Nonanol	143-08	OCCCCCCCCC	O	Class 1	-3.052	-4.419	
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1	-3.603	-4.838	
1-Undecanol	112-42-5	OCCCCCCCCCCC	O	Class 1	-4.333	-5.236	
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1	-4.985	-5.270	
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1	-5.302	-5.561	5.19
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1	-0.444	-2.153	1.25
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1	-0.432	-2.371	1.05
Pentanol	94624-12-1	CC(CCC)O	O	Class 1	-0.591	-3.174	1.35
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1	-0.324	-2.118	1.1
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1	-0.324	-2.186	1.1
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.643	1.25

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.933	1.25
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.228	1.25
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.411	1.25
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.587	1.25
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.817	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.064	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.369	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.202	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.227	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-2.994	1.97
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1	-2.260	-3.801	2.83
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.915	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.667	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.380	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.403	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.509	2.53

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.474	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.294	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.341	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.521	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.521	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.093	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.106	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.311	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.757	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.843	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.296	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.955	2.53
Chlorobutane	109-69-3	ClCCCC	O	Class 1	-2.925	-3.113	2.66
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.862	1.45
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.362	1.45
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.935	1.45

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.924	1.45
1,2,4-Trichlorobenzene	120-82-1	CLC1CCC(CL)C(CL)C1	O	Class 1	-3.681	-4.879	4.05
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1	-3.070	-4.281	3.44
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1	-3.070	-4.468	3.44
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1	-3.070	-4.207	3.44
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-5.118	3.44
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-5.074	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-5.031	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.611	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.015	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.099	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.955	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.544	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.419	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.298	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.845	3.37

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.514	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.845	3.37
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.985	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.969	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.960	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.977	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.451	3.38
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.917	2.39
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.915	2.39
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.958	2.39
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.797	2.39
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1	-3.487	-5.715	4.139
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1	-3.487	-4.754	4.139
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.404	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-4.080	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.448	2.46

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.513	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.268	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.274	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.377	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.607	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-2.955	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.499	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.666	2.46
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1	-1.482	-3.523	1.89
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1	-2.351	-4.398	2.84
n-Pentane	109-66-0	CCCCCC	O	Class 1	-3.273	-4.229	3.45
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1	-3.209	-4.269	3.38
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1	-3.253	-4.177	3.39
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 1	0.239	-3.519	0.6
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 1	0.239	-2.827	0.6
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	-1.811	-3.126	1.9

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	-1.811	-3.319	1.9
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	-1.812	-3.015	1.9
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	-2.497	-3.387	2.3
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	-2.515	-3.630	2.4
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	-2.515	-4.268	2.4
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	-2.406	-3.305	2.4
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2	-2.238	-4.021	2.39
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2	-2.238	-4.084	2.39
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2	-2.238	-3.791	2.39
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2	-1.565	-4.792	3.09
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2	-1.565	-4.355	3.09
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2	-1.565	-4.677	3.09
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.922	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.665	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.365	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.086	2.7

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.149	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.096	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.303	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.547	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.329	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.280	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.829	2.7
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.144	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.135	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.963	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.969	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.290	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.109	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.017	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.804	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.045	2.15

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.948	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.310	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.290	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.265	2.15
3-Chlorophenol	108-43-0	ClC1=CC(O)=CC=C1	N	Class 2	-0.610	-4.508	2.50
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.529	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.180	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.529	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.828	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.361	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.410	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.377	2.39
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2	-1.594	-4.696	2.39
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2	-1.594	-4.385	3.4
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2	-1.594	-4.317	3.4
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2	-0.425	-3.944	0.9

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2	-0.425	-3.410	0.9
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2	0.026	-4.024	1.5
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2	-1.650	-3.983	1.6

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