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PRIORITISATION OF CHEMICALS USING THE INTEGRATED APPROACHES FOR TESTING AND ASSESSMENT (IATA)-BASED ECOLOGICAL RISK CLASSIFICATION

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Series on Testing and Assessment

No. 291

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OECD Environment Directorate,
Environment, Health and Safety Division
2, rue André-Pascal
75775 Paris cedex 16
France
Fax : (33-1) 44 30 61 80
E-mail : ehscont@oecd.org

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FOREWORD

OECD member countries have been making efforts to expand the use of alternative methods in assessing chemicals. The OECD has been developing guidance documents and tools for the use of alternative methods such as (Q)SAR, chemical categories and Adverse Outcome Pathways (AOPs) as a part of Integrated Approaches for Testing and Assessment (IATA). There is a need for the investigation of the practical applicability of these methods/tools for different aspects of regulatory decision-making, and to build upon case studies and assessment experience across jurisdictions.

The objective of the IATA Case Studies Project is to increase experience with the use of IATA by developing case studies, which constitute examples of predictions that are fit for regulatory use. The aim is to create common understanding of using novel methodologies and the generation of considerations/guidance stemming from these case studies.

This case study was developed by Canada for illustrating practical use of IATA and submitted to the 2017 review cycle of the IATA Case Studies Project. This case study was reviewed by the project team. The document was endorsed at the 2nd meeting of the Working Party on Hazard Assessment in June 2018.

The following three case studies were also reviewed in the project in 2017 and are published with this case study:

1. CASE STUDY ON THE USE OF INTEGRATED APPROACHES FOR TESTING AND ASSESSMENT (IATA) FOR ESTROGENICITY OF THE SUBSTITUTED PHENOLS CLASSIFICATION, ENV/JM/MONO(2018)26, Series on Testing & Assessment No. 290.
2. CASE STUDY ON GROUPING AND READ-ACROSS FOR NANOMATERIALS GENOTOXICITY OF NANO-TiO2, ENV/JM/MONO(2018)28, Series on Testing & Assessment No. 292.
3. A CASE STUDY ON THE USE OF INTEGRATED APPROACHES FOR TESTING AND ASSESSMENT FOR SUB-CHRONIC REPEATED-DOSE TOXICITY OF SIMPLE ARYL ALCOHOL ALKYL CARBOXYLIC ESTERS: READ-ACROSS, ENV/JM/MONO(2018)29, Series on Testing & Assessment No. 293.

These case studies are illustrative examples, and their publication as OECD monographs does not translate into direct acceptance of the methodologies for regulatory purposes across OECD countries. In addition, these cases studies should not be interpreted as official regulatory decisions made by the authoring member countries.

A considerations document summarizing the learnings and lessons of the review experience of the case studies is published with the case studies:

> REPORT ON CONSIDERATIONS FROM CASE STUDIES ON INTEGRATED APPROACHES FOR TESTING AND ASSESSMENT (IATA) -Third Review Cycle (2017)- ENV/JM/MONO(2018)25, Series on Testing & Assessment No. 289.

This document is published under the responsibility of the Joint Meeting of the Chemicals Committee and Working Party on Chemicals, Pesticides and Biotechnology.

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INTRODUCTION

In Canada, the Ecological Risk Classification (ERC) approach, which employs concepts of an Integrated Approaches for Testing and Assessment (IATA), was used to prioritise several hundred organic substances. This was done in an effort to identify ecological priorities for regulatory action with greater efficiency. The ERC is based on chemical profiling, and is therefore a departure from traditional PBiT criteria-based prioritisation methods. The application of the ERC approach in prioritisation captures *chemicals that have the greatest potential to cause adverse effects*. It also identifies substances of low concern with increased confidence. Consequently, it enables the use of tailored regulatory approaches, from time-intensive detailed risk assessment to less resource-intensive, including class assessment, rapid screening, or tracking of use patterns and quantities.

1. PURPOSE

Identifying and prioritizing chemical substances for regulatory action is fundamental to the management of chemicals. The purpose of this paper is to describe a novel prioritisation approach based on an IATA, called the Ecological Risk Classification (ERC) approach, which has been used by Environment and Climate Change Canada (ECCC) to identify priorities for ecological risk assessment under the *Canadian Environmental Protection Act, 1999* (CEPA) (Canada 1999). This paper focuses on ecological priorities for chemical risk assessment. An analysis of advantages, limitations and uncertainties for the ERC approach is presented. Profiles of three substances, *phenol, 2-(1-methylpropyl)-4,6-dinitro-* (CAS RN 88-85-7); *phosphoric acid, triphenyl ester* (CAS RN 115-86-6); and *benzenamine, N-phenyl-* (CAS RN 122-39-4), identified by ERC as high, moderate, and low priorities, respectively, are provided as examples to illustrate hazard and exposure prioritisation profiles and risk classification.

Through the 2006 Categorisation (a prioritisation scheme using persistence, bioaccumulation and inherent toxicity (PBiT) criteria, and consideration of the greatest potential for exposure to humans or health effects of concern including carcinogenicity, genotoxicity and developmental or reproductive toxicity), the Government of Canada identified approximately 4 300 of the 23 000 chemical substances on the Canadian Domestic Substance List (DSL) as meeting the criteria for further attention. This could include risk assessment, research and/or measures to control their use or release. In the first two phases of Chemicals Management Plan (CMP), nearly 2 800 substances have been addressed (by means of risk assessment and, as required, risk management), including the highest and moderate priorities identified as PBiT, and PiT or BiT, respectively. The third phase of the CMP, launched in May 2016, will address the remaining approximately 1500 priority chemicals by 2020. It is within Canada's Strategic Approach to International Chemicals Management (SAICM) commitment to complete assessment of the DSL priorities by 2020 (ECCC [modified 2016a]). Six hundred and forty out of the 1500 priority chemicals identified for the third phase of CMP are organic substances, and these include 448 discrete substances and 192 substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCBs).

In the effort to further prioritise and evaluate the 640 organic substances for risk assessment with greater efficiency, the ERC approach was developed by ECCC (ECCC 2016).

The ERC is a risk-based prioritisation approach that employs a weighted consideration of multiple descriptors to establish both the hazard (potency) and the exposure profiles to determine a risk classification of a chemical substance. Hazard profiles are established based principally on descriptors regarding mode of toxic action, chemical reactivity, food web-derived internal toxicity thresholds, bioavailability, and chemical and biological activity. Descriptors considered in the exposure profiles include potential emission rate, overall persistence, and long-range transport potential. A risk matrix is used to assign a low, moderate or high level of potential concern for substances based on their specific hazard and exposure profiles.

The various lines of evidence underlying the risk classification in ERC identify substances as warranting further evaluation of their potential to cause harm to the environment or as having a low likelihood of causing harm to the environment. The application of the ERC approach in prioritisation captures *chemicals that have the greatest potential to cause adverse effects*, and enables the use of tailored regulatory approaches, which can vary from detailed risk assessment of individual substances to less resource-intensive, including class assessment or rapid screening, or to defer to tracking of use patterns with the goal of priority status re-evaluation as dictated by new information. The ERC science approach document, which identifies high, moderate and low risk profiles among the 640 organic substances, was published by ECCC in July 2016 (ECCC 2016).

While the focus of this paper is on the ERC, a retrospective analysis of prioritisation approaches using the PBiT criteria and the IATA-based ERC, based on a subset of 433 discrete organic substances of the 640 organic priorities, is presented in Annex A.

2. PRIORITISATION OF CHEMICALS USING AN IATA-BASED ERC APPROACH

The ERC is a risk-based approach that uses multiple descriptors for both hazard and exposure, and applies a weight-of-evidence for determining risk classification. ERC considers the mechanisms and modes of action through which chemicals exert their toxicity, and includes non-apical toxicity endpoints. Hazard profiles are established based principally on the mode of toxic action, chemical reactivity, food web-derived internal toxicity thresholds, bioavailability, and chemical and biological activity. Exposure profiles are also composed of multiple descriptors and include substance quantities in commerce, overall persistence, and long-range transport in air and environmental emission rates. The various lines of evidence are combined to identify substances of higher potency and increased potential for exposure in various environmental media. This approach reduces the overall uncertainty with risk classification compared to one that relies on a single metric in a single medium (e.g., LC_{50}) for classification.

The ERC approach involves the following steps:

a Data gathering

b Hazard and exposure profiling based on several descriptors

c The preliminary classifications of hazard and exposure using qualifiers of 1 , 2 and 3 to rank substances as having low, moderate or high potential for hazard and exposure

d Examination of the preliminary hazard classification for adjustment based on consideration of classification consistency, special classes of chemicals (e.g. quaternary ammonium compounds), potent reactivity, terrestrial hazard, and margin of exposure

e Assignment of low, moderate or high risk classification according to a risk classification matrix based on substance hazard and exposure profiles

f Verification of risk classification and, if need, adjustment based on exposure considerations for near-field exposure and low regional emissions

The framework for the Ecological Risk Classification of organic substances is illustrated in Figure 1.

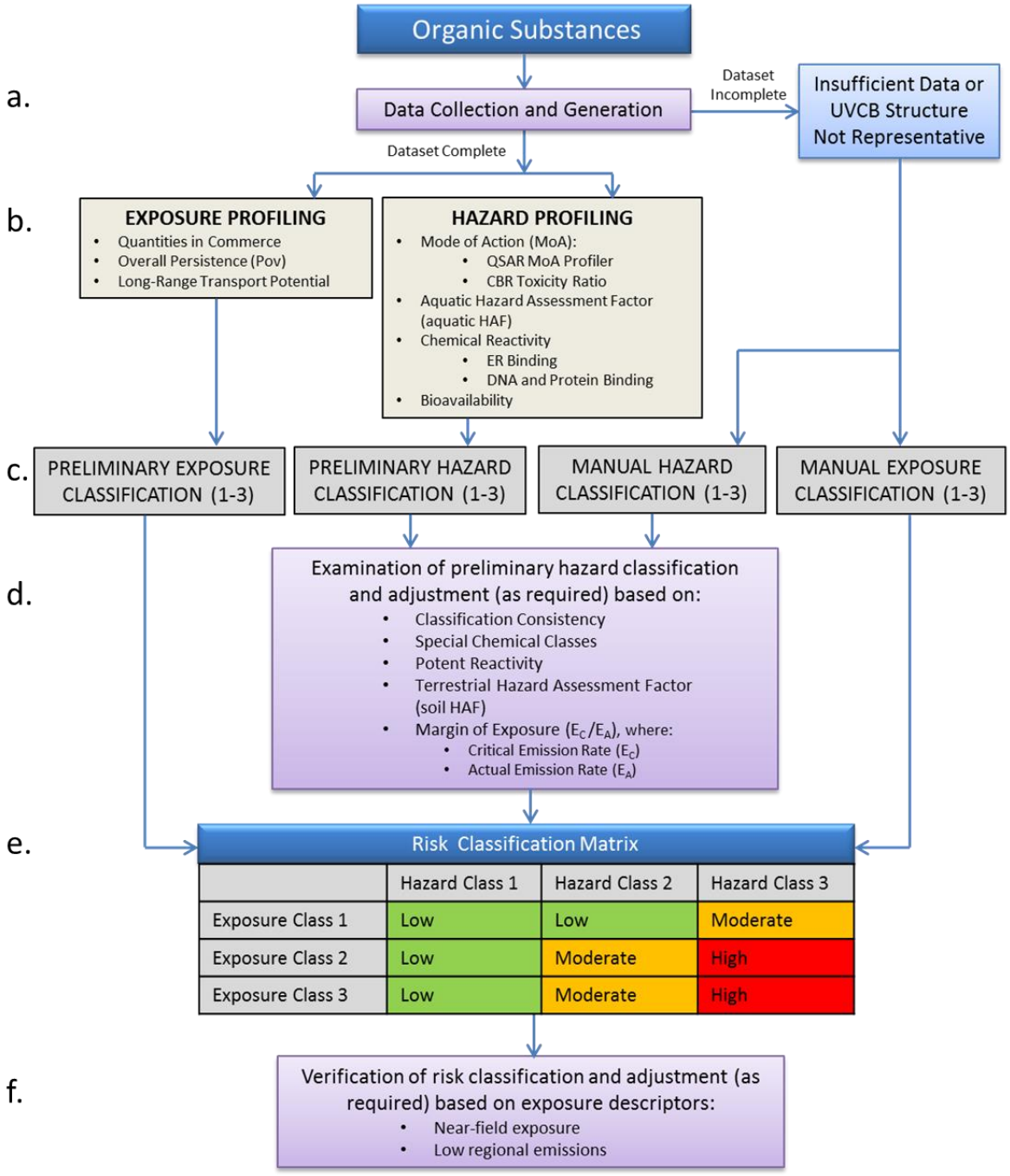


Figure 1. Framework for the ecological risk classification of 640 organic substances

2.1. Data gathering

To complete substance hazard and exposure profiles in ERC for the organic chemicals identified as priorities for regulatory action, various data were collected and generated. The substance import and manufacture quantities in Canada were gathered from surveys of Canadian industry for the years 2009 and 2012 (DSL Inventory Updates; Canada 2009 and 2012). Data on the physical-chemical properties, fate (e.g., chemical half-lives in various media and biota, partition coefficients, and fish bioconcentration factors), acute fish ecotoxicity, were collected from scientific literature or empirical databases (e.g., PhysProp c2013), and were generated using selected Quantitative Structure Activity Relationship (QSAR), mass-balance, and bioaccumulation models. Modelled data were generated using various QSAR models and expert systems for all organic substances with acceptable two-dimensional chemical structures represented by a simplified molecular-input line-entry system (SMILES) notation. Models and expert systems used in ERC are listed in Annex B.

For UVCB substances, a single representative chemical structure was chosen to represent the substance. In many cases, a conservative representative chemical structure was chosen to represent an entire UVCB substance (e.g., where variation of the UVCB components was known or predictable). In cases where individual structures were deemed inappropriate for modelling, a read-across approach was used to fill-in data gaps.

Data collected and generated for discrete and UVCB organic substances are summarised in the ERC spreadsheet, provided in Annex C.

2.2. Hazard and exposure profiling in the ERC approach

Profiling of hazard was based on four key hazard descriptors. Additional hazard descriptors were used as supporting information to verify the quality of the ecotoxicity data and to gain further understanding of the mode of action. Profiling of exposure was based on three key descriptors.

In several instances, mainly for complex UVCB organic substances, a manual classification of hazard and exposure was required due to insufficiency of available data (see Figure 1). The manual approach was mainly applied to the more complex UVCB organic substances. In particular, critical data gaps included the lack of knowledge on the two-dimensional representative structure of a substance, difficult to model substances falling outside of the models' domain of applicability, or lack of empirical data to fulfil data requirements for the ERC. Manual classification involved consideration of read-across empirical data from close analogues. All hazard low-concern UVCBs were closely checked for classification consistency and were also subject to adjustment of risk classification.

Hazard profiling

The aim of hazard profiling was to identify chemicals that are bioavailable and have the potential to cause adverse effects from interaction with biological tissues through various mechanisms, including baseline toxicity (non-specific toxicity or narcosis via cell membrane perturbation) and specific modes of action (e.g., steroid receptor binding, enzyme inhibition). Non-baseline substances are typically more potent than chemicals that only exert baseline toxicity, and require lower exposures to exert

adverse effects. Therefore, recognizing baseline and non-baseline toxicities is useful for classifying hazardous substances (OECD 2014; Wu et al. 2010; Mackay et al. 2014a), and it is the focus of the substance hazard profile in ERC.

The hazard profiling approach also minimises the chance of underestimating hazard classification from limited ecotoxicity data based on a single medium of exposure (e.g., water) because internal concentrations (body or tissue residues) are also considered. Hence, exposures and potential risks of chemicals that exhibit bioaccumulation or biomagnification in food webs are more appropriately evaluated.

ERC hazard profiles are established based mainly on four descriptors, including:

1) Mode of Action (QSAR MoA profiler, CBR Toxicity Ratio)
2) Hazard Assessment Factor (HAF)
3) Chemical reactivity (ER binding, DNA and protein binding)
4) Bioavailability

Additional hazard descriptors were used as supporting evidence for a reactive mode of action or to verify the quality of the available ecotoxicity data, and did not factor directly into substance hazard classification. These included:

1) Chemical activity
2) Chemical reactivity (AR binding and EDKB)
3) Bioactivity

1) Mode of Action (MoA)

In ERC, substance MoA was profiled using QSAR structural profiling and critical body residue (CBR) ratios.

QSAR structural profiling was applied using the OECD Toolbox (2015) which contains two profilers: the Verharr profiler based on the ToxTree software, and the OASIS MoA profiler. These profilers categorise MoA based on pass/fail structural rules.

Mode of action was also determined using critical body residue (CBR) toxicity ratios. The CBR toxicity ratio refers to the difference in tissue concentration between a baseline toxicant and a tissue concentration of a chemical exerting a more specific MoA (e.g., Maeder et al. 2004, Escher et al. 2011, Arnot 2014). A median CBR of 3.0 mmol/kg associated with acute lethality and a median CBR of 0.3 mmol/kg associated with chronic lethality are used for the acute and chronic thresholds for baseline narcosis, respectively (McCarty and Mackay 1993, McCarty et al. 2013). Thus, if 3.0 mmol/kg divided by the tissue residue concentration calculated using an acute LC_{50} (i.e., $CBR_{fishLC50}$) is greater than 10, a chemical is expected to be more potent than a narcotic chemical. This is because the concentration in the tissue necessary to cause death is lower than that for a narcotic chemical. Since CBRs are calculated based on fish bioconcentration factors (BCF) and fish toxicity data (LC_{50} values), extrapolation to other species remains uncertain.

2) Hazard Assessment Factor (HAF)

The hazard assessment factor (HAF) integrates into a single value environmental emission rates and chemical fate properties (i.e., environmental degradation half-lives and biotransformation half-lives in vertebrate species), food web bioaccumulation, and toxicity (hazard data) (Arnot and Mackay 2008).

HAFs are calculated as the ratio between the dose in representative food web organisms based on a unit default emission rate (C_U) and the dose associated with acute lethality (C_T). HAFs were estimated using the RAIDAR model (RAIDAR 2011) in aquatic and terrestrial food webs based on a default emission rate (1 kg/hr) to each of these media, and the calculated CBR values (used also to derive CBR toxicity ratios to inform the MoA). The HAF can be used to rank chemicals by their intrinsic ability to result in a dose (indicative of either a narcotic (3 mmol/kg) or non-narcotic mode of action (less than 3 mmol/kg)), which exceeds a critical internal threshold.

The HAF threshold values in ERC were selected based on examination of HAF distribution and HAF correlation with higher levels of inherent aquatic toxicity. HAFs greater than 10^{-3} represent approximately 23% of the HAF distribution and are associated with the most potent chemicals and high hazard. HAFs of 10^{-6} to 10^{-3} represent approximately 35% of the distribution are associated with potent chemicals or moderate hazard. HAFs of less than 10^{-6} are associated with low hazard and less potent chemicals.

3) Chemical reactivity (ER binding, DNA and protein binding)

Chemical reactivity is a broad term that refers to the ability of a chemical to undergo changes according to the environmental system in which it resides. Here, we refer to reactivity as a chemical's potential to undergo interactions with biological tissues beyond baseline narcotic interactions, i.e., non-specific weak interactions with cell membrane surfaces. If the chemical has an intrinsic ability to interact with biological systems through more specific binding mechanisms (hydrogen bonding, charge-transfer or covalent binding), the potency of the chemicals is expected to be greater than baseline toxicity (Mackay et al. 2009).

In ERC, profiling of chemical reactivity included protein, DNA, and estrogen receptor binding, as well and androgen receptor binding (used as supporting information only). These are generally considered to be precautionary models in that binding results do not necessarily reflect adverse outcomes.

Profiling of covalent interactions with protein and DNA was conducted using protein and DNA mechanistic profilers in the OECD QSAR Toolbox (v3.4) (OECD QSAR Toolbox 2015). Protein binding is typically associated with skin sensitisation in mammals but has been shown to be indicative of a non-passive mechanism of uptake and distribution in other organisms (Princz et al. 2014) and to correlate with aquatic toxicity (Roberts et al. 2010, Schultz et al. 2010). DNA binding can lead to genetic damage through, for example, adduct formation and is a well-known initiating event for genotoxicity.

Estrogen receptor (ER) binding was predicted to capture potential endocrine-mediated effects. ER binding was predicted with the OECD QSAR Toolbox structural rule-based ER profiler (OECD QSAR Toolbox 2015). The model output classifies chemicals as binders or non-binders depending on molecular weight and structural characteristics such as the presence of amino, hydroxyl, and cyclic groups. The model

outputs provide five qualitative ER binding affinity ranges: very strong, strong, moderate, weak, and non-binders.

4) Bioavailability

Bioavailability relates the quantity of a substance absorbed by the organism compared to the quantity of substance to which the organism is exposed. It has been shown that dietary assimilation efficiency, bioconcentration, bioaccumulation and biomagnification factors in non-human organisms decrease for substances with higher log K_{ow} values (above log K_{ow} of approximately 8.0) (Kelly et al. 2004; Arnot and Gobas 2006; Arnot and Quinn 2014) . Currently, QSAR models are unable to provide reliable estimates of aquatic toxicity for substances with a log K_{ow} above 8 primarily due to the lack of observed acute or chronic effects at or above this log K_{ow}. Thus, a simple rule of log K_{ow} or log D (the log dissociation constant is applied to ionogenic substances) greater than 10 was used to indicate very low aquatic and terrestrial bioavailability.

5) Chemical activity

The thermodynamic equilibrium criterion of chemical activity can be used to help identify substances acting via a baseline MoA as well as more specific MoAs (Mackay et al. 2009). In ERC, chemical activities were used as supporting information for MoA profiling and to verify the quality of the available ecotoxicity data.

Here we define chemical activity to be the fraction of solubility in water associated with median lethal effects (LC_{50}) in aquatic organisms. Chemical activity (unitless) can be calculated as fish LC_{50} divided by water solubility. A chemical activity of 0.01 to 0.1 in water has been associated with baseline narcosis (Mackay et al. 2014a). Calculated activities just below 0.01 could suggest subtle chronic effects and activities far below 0.01 could suggest a MoA more potent than baseline narcosis. Activities greater than one indicate a potential error with the ecotoxicity data as solubility limits in water have been exceeded.

In ERC, chemical activities were calculated for substances with log K_{ow} values greater than 2 since very soluble substances are not amenable to this approach and their calculated chemical activities would appear unrealistically low. Due to the lack of empirical ecotoxicity data, many LC_{50} values and most water solubility values were estimated using QSARs; as a result chemical activity estimates can be uncertain.

6) Chemical reactivity (AR binding and EDKB)

Androgen receptor (AR) binding was profiled using the TIMES model (TIMES 2014). The AR binding results were not used directly to classify hazard in the ERC, because the domain of applicability of AR binding in the TIMES model is restricted and many chemicals were identified as being out of the model domain. *In silico* AR binding affinities were considered as additional supporting information to gain understanding of the mode of action. Model outputs are grouped into four relative binding affinity (RBA) ranges reflecting the chemical potency: highly active with RBA>10%; moderate with 0.1%<RBA<10%; low with 0.001%<RBA<0.1% and non-active with RBA<0.001% (LMC Oasis2017).

The ERC also includes the *in vitro* assay Endocrine Disruption Knowledge Base (EDKB) from the US FDA (Ding et al. 2010). EDKB data are used as supporting information in ERC.

7) Bioactivity

Bioactivity is a broad term meaning the effect of a chemical on any living tissue. Bioactivity can be determined using high-throughput *in vitro* assays such as those developed by the US EPA under the ToxCast and Tox21 programs (US EPA [updated 2016a]). ToxCast screens chemicals in over 700 high-throughput assays that cover a range of high-level cell responses and approximately 300 signalling pathways (US EPA [updated 2016b]). A response (i.e., activity) could indicate that a particular pathway represented by the assay was triggered from the chemical exposure. However, this does not necessarily represent a definitive adverse outcome, but rather another type of *in vitro* level alert (e.g., oxidative stress, mitotic arrest, impaired enzyme functioning). Consequently, the ERC uses both the ToxCast and Tox21 databases as supporting information, and not directly to classify hazard. Similarly, the MoATox database from the US EPA (Baron et al. 2015) was incorporated to provide empirical insight into mode of toxic action, where information was available.

Exposure profiling

A weighted approach to exposure profiling was used to address the uncertainty associated with reliance on a single quantitative estimation of chemical release to define exposure to organisms. This helps to mitigate the possibility of over or underestimation of risk classification from relying on a single metric (Stahl and Cimorelli 2013).

In ERC, the purpose of the exposure profile is to determine the probability of organisms coming into contact with an organic substance released to the aquatic or terrestrial environment in Canada. Similar to the ERC hazard profile, multiple descriptors were used to weigh this probability, and included:

1) Quantities in commerce
2) Overall persistence (Pov)
3) Long-range transport in air

1) Quantities in commerce

Data on substance quantities in commerce (kg/yr) were gathered for all 640 organic substances. These data consist of chemical import and/or manufacture volumes in Canada, and were collected from recent regulatory surveys for the years 2009 and 2012 (Canada 2009, Canada 2012). Exact import and manufacture quantities reported in response to the surveys are considered confidential business information, and are therefore masked by using broad quantity ranges when described.

Quantity data for most of the 640 organic substances came from the 2012 DSL Inventory Update (Canada 2012). In general, higher chemical quantities can be related to a higher probability of widespread exposure upon release to the environment. In ERC, a quantity in commerce of 100 000 kg/year or greater is considered to contribute to the potential for high exposure.

2) Overall persistence (Pov)

Environmental presence of a substance is observed by its potential for degradation (i.e., persistence), partitioning in environmental media (its fate in the environment as determined by mass fraction partitioning) and its ability to travel far away from emission sources (long range transport).

Overall persistence (Pov), rather than medium-specific half-lives, has been advocated by many environmental chemists as the preferred metric for screening chemicals for persistence, (e.g., Webster et al. 1998, Gouin et al. 2000; Pennington 2001, Mackay et al. 2014b; OECD 2004). Pov is the sum of a chemical's half-lives in all environmental media weighted by the mass fraction of the chemical in the medium as determined using a multimedia fate model (Webster et al. 1998; Klasmeier et al. 2006; Wegmann et al. 2009). Pov only includes the reaction rate of a chemical (i.e., degradation), and does not consider advection out of a model environment as removal from the environment.

In ERC, Pov was calculated for 640 organic substances using the RAIDAR model (RAIDAR 2011) with an assumption of 100% releases to water, given that water represents the predominant entry point into the environment for industrial chemicals. A Pov greater than 60 days is considered to be of high potential for exposure. The value reflects typical persistence criteria for water in some jurisdictions (e.g., 60 days criteria in the European Union) and chronic aquatic toxicity test durations (i.e., 21 days).

3) Long-range transport in air

The long-range transport potential (LRTP) in air was determined using calculated or observed air half-lives and air-water partition coefficients (log K_{aw}). Combining these substance-specific properties identifies those substances expected to partition to air and potentially undergo long-range transport. The use of the air half-life is considered to be a precautionary approach because the deposition of the substance, which could limit the travel distance in air, is not taken into account. A half-life greater than 2 days in air and log K_{aw} greater than 10^{-6} are considered to represent high exposure potential.

It is noted that long-range transport in water was not considered, owing to the difficulties of identifying a suitable evaluative receiving water body for environments across Canada (e.g., the Great Lakes or rivers of varying sizes and depths). Also the OECD LRTP and Pov Screening Tool (OECD 2009) was not used to model the long-range transport in air in ERC because the model cannot account for air transport as a function of releases to water.

2.3. Preliminary classification of hazard and exposure

Classification criteria were developed to assign a numerical score, from 1 to 3, to both the hazard and exposure profiles of each organic substance. This was done to classify the organic substances as having low, moderate, or high potential for hazard and for exposure, where 1 is classified as low, 2 as moderate and 3 as high.

While some of the classification criteria are similar in concept (e.g., HAF and CBR toxicity ratio), they use different algorithms and are applied for different purposes, such as in characterizing the mode of action or for determining food web hazard. Classification criteria are also applied in a step-wise manner to avoid double counting of descriptors. This provides a precautionary fail-safe mechanism for classification.

Classification was dependent on the number and type of descriptors triggered in each profile. The preliminary classification of organic substances was subsequently verified and adjusted, if required, based on additional hazard descriptors (see Figure 1).

Preliminary hazard classification criteria

Three hazard classification criteria were used to rank organic substances into the 3 preliminary Hazard Classes based on formalised rules. These criteria included:

- Estrogen receptor binding affinity
- CBR toxicity ratio and MoA profile
- Aquatic HAF and log K_{ow}/log D

For classification into a particular Hazard Class at least one hazard criterion must be met. Each criterion has a specific range associated the particular Hazard Class. Figure 2 is a decision diagram for determining Hazard Class 1, 2 or 3 chemicals based on the criteria and the formalised rules for each Hazard Class.

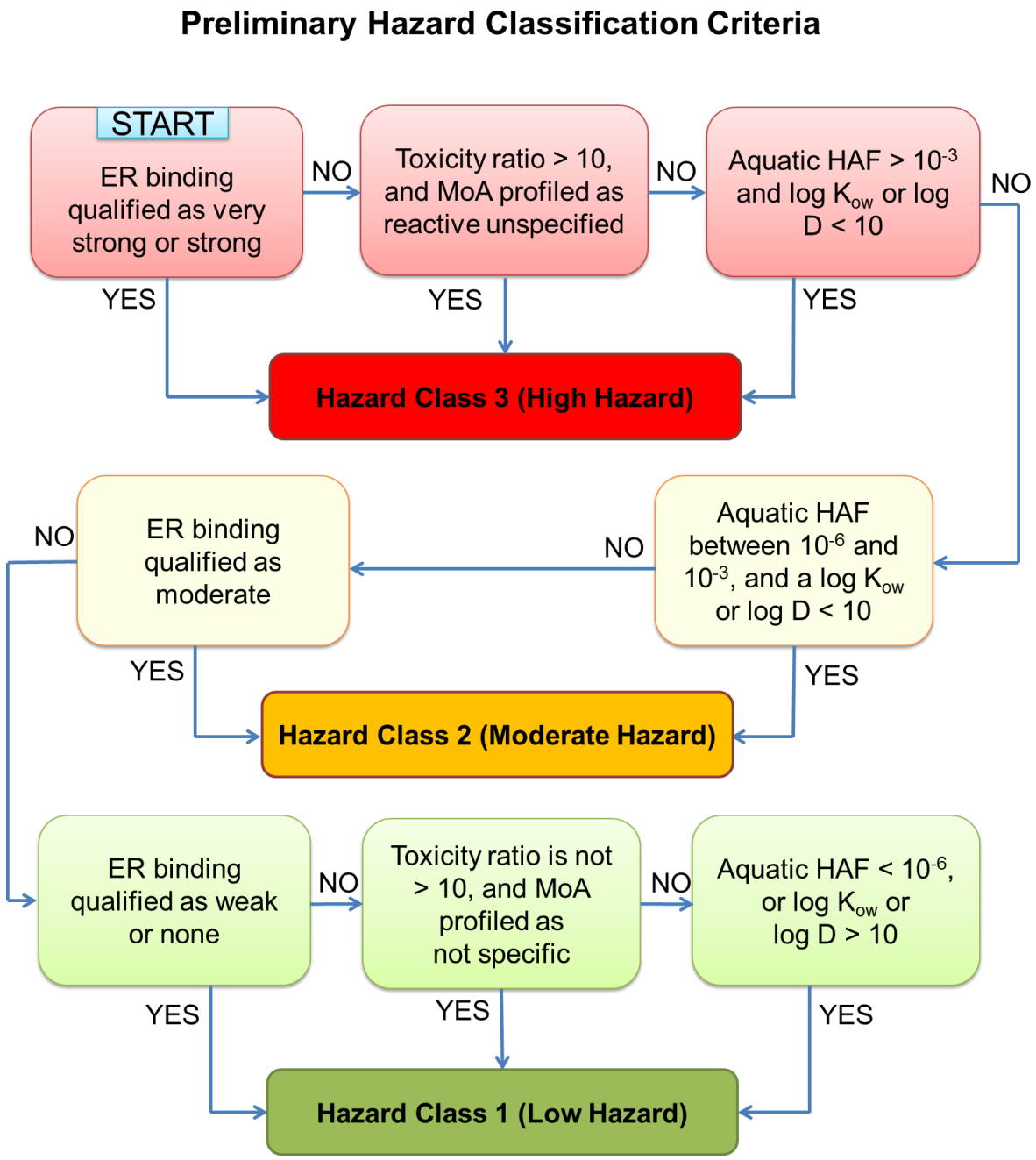


Figure 2. Decision diagram for determining preliminary hazard classification criteria in ERC

Hazard Class 3 substances are profiled to be the most reactive and potentially the most potent of the 640 organics. They are identified having the potential to exert "non-baseline toxicity" or "excess toxicity to baseline", and also include some polar and non-polar narcotics with high food web accumulation potential.

Toxicity ratios for substances classified as Hazard Class 2 are generally less than 10 suggesting they act through baseline mode of action. However, many also profile as "reactive unspecified", suggesting some uncertainty with the MoA, and some degree of potency greater than baseline.

Chemicals classified as Hazard Class 1 are mainly weak acids, ethers, short chain esters, alcohols, amides and ketones. These groups of substances are generally not considered to present significant ecological hazard.

Preliminary exposure classification criteria

Preliminary exposure classification criteria used to rank organic substances into the 3 preliminary Exposure Classes were applied according to formalised rules and included:

- Long-range transport potential in air determined by the half-life in air and log K_{aw}
- Overall persistence (Pov) and substance quantity in commerce

For classification into a particular Exposure Class at least one exposure criterion must be met. Each criterion has a specific range associated the particular Exposure Class. Exposure Class 1 substances are those that do not meet any of the Class 3 and 2 criteria. Figure 3 is a decision diagram for determining Exposure Class 1, 2 or 3 chemicals based on the criteria and the formalised rules for each Exposure Class.

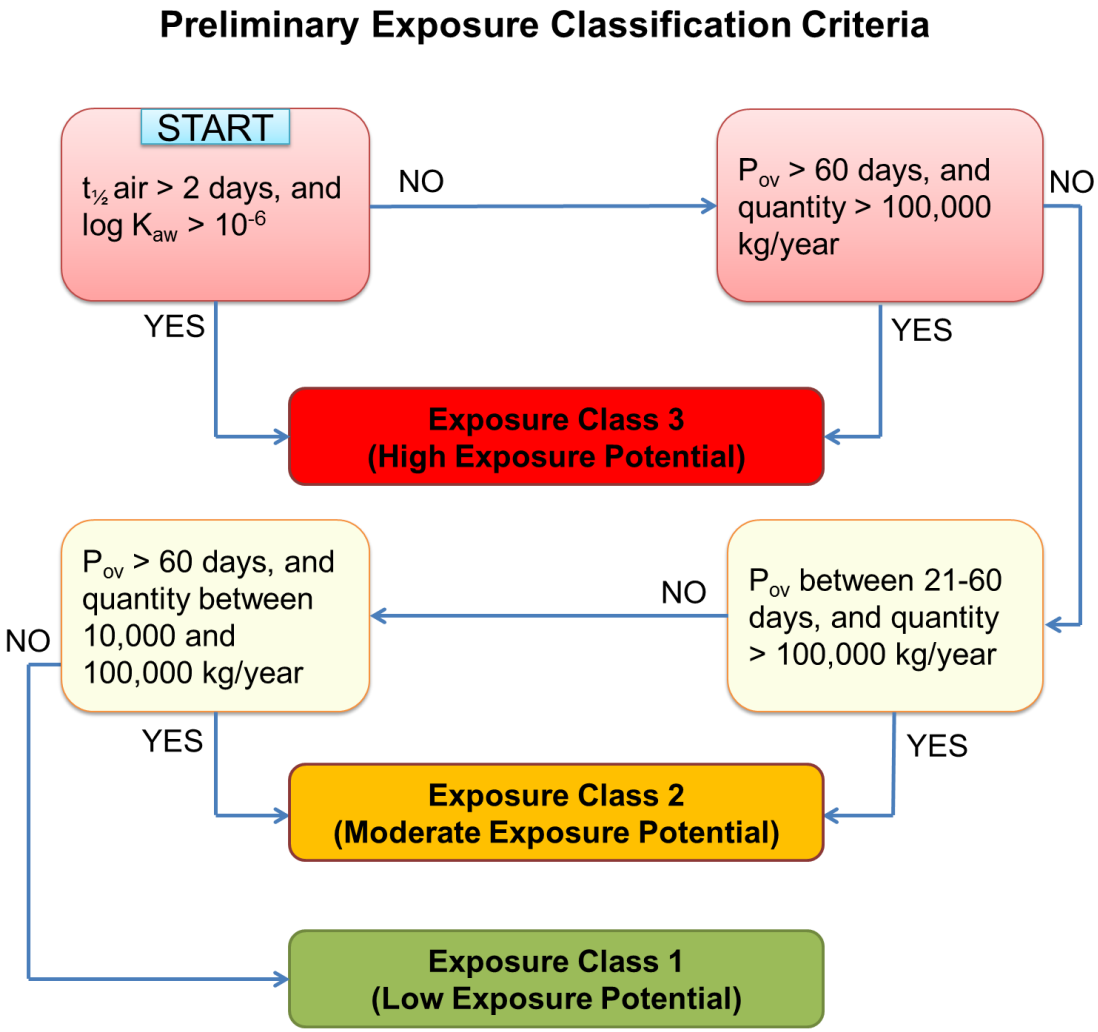


Figure 3. Decision diagram for determining preliminary exposure classification criteria in ERC

Substances classified in Exposure Class 3 are expected to have a longer residence time in the environment (i.e., longer Pov), may undergo long-range transport in air or have been imported or manufactured in high quantities in Canada. Therefore, the spatial and temporal scale of potential exposure in the environment for these chemicals is the highest.

Classification at Exposure Class 2 captures substances with longer residence time in the environment (i.e. longer Pov) but lower reported quantities in commerce, or shorter reaction residence time but greater reported quantities in commerce. Exposure Class 2 substances are not expected to undergo long-range transport in air.

Substances in Exposure Class 1 present a low spatial and/or temporal extent of potential exposure and are not expected to undergo long-range transport in air.

2.4. Examination and adjustment of preliminary classification

Preliminary classification of hazard and exposure relies heavily on modelled parameters generated in the ERC approach. While empirical data were used when available and multiple descriptors for hazard and exposure have been considered in a tiered weight-of-evidence approach, it is recognised that there is some uncertainty with the preliminary classification results.

To reduce the potential for over- or under-estimation of hazard in the preliminary classification five additional judgement rules were applied. They consisted of checking for classification consistency of chemical classes, manual classification of special classes of chemicals, accounting for potent reactivity, examining hazard to soil from application of biosolids and the margin of exposure. These rules were applied outside of the preliminary classification step to allow for use of judgement when applying them (such as when a rule is only intended to be applied to a subset of substances) and to give them additional weight. The preliminary classification could be adjusted based on any one of the rules, with the first four rules below take precedence over the fifth. In most cases, the impact of these rules affects substances classified as preliminary Hazard Class 1 substances, with re-classification to Hazard Class 2, and thus is precautionary and minimises potential underestimation of risk of low hazard substances.

1. Classification Consistency: Classification results for substance groups were examined more closely in cases where a single CAS RN within the group appeared to be an outlier compared with the other structurally similar members of the group. If there was sufficient rationale to adjust the outlier result (e.g., due to model error), the differing classification was adjusted to be consistent with the group.

2. Manual Classification of Special Chemical Classes: To avoid potential error with current predictive approaches, manual classification to a minimum Hazard Class 2 was applied to substance classes known to be potent and ionogenic, and typically falling outside of model domain of applicability. Hazard Class 3 classification was always retained. Substance classes manually classified in ERC were quaternary ammonium compounds and nitro musks.

3. Potent Reactivity: If both protein and DNA binding alerts were triggered, substances were manually classified at minimum as Hazard Class 2.

4. Terrestrial Hazard: This rule considers hazard from agricultural amendment practice of WWTS biosolids application to soil. If the soil HAF was greater than 10^{-4},

substances were manually classified at minimum as Hazard Class 2. This soil HAF threshold was selected in order to equate it to a preliminary Hazard Class 2 triggered by the aquatic HAF criterion.

5. Margin of Exposure (MoE) (a ratio of the critical to actual emission rates; E_C/E_A):

A margin of exposure (MoE) was determined based on two emission rates, the actual emission rate (EA), and the critical emission rate (EC) to water generated by the RAIDAR model (RAIDAR 2011).

The actual emission rate (E_A) is the term used in ERC for the emission rate to water after waste water treatment system (WWTS) removal. E_A (kg/yr) to the aquatic environment was calculated based on the 2012 DSL Inventory Update import or manufacture volumes (Canada 2012) after determining percentage removal in a modelled WWTS. The ERC conservatively assumes that 100% of the chemical quantity reported to be in commerce can be released to a WWTS, without consideration of the fraction actually released as a function of a substance's use pattern (which would typically be less than 100%). Removal in WWTS, as a function of biodegradation and adsorption to biosolids, was estimated using the SimpleTreat model (SimpleTreat 1997). WWTS removal was used to determine the emission rate to water after treatment as well as the fraction of chemical quantity that could be applied to agricultural lands in association with biosolids.

The critical emission rate (E_C) is the rate of emission to water (kg/yr) that could result in a risk (i.e., exceed the critical toxicity body burden) to the various representative species in the food web and the most sensitive aquatic species, identified in the RAIDAR model. The critical emission rate assumes a default rate (E_U) of 1 kg/hr, and is calculated as E_U/HAF.

The ratio of the critical emission rate to actual the emission rate (i.e., E_C/E_A) provides a MoE, and is similar to the concept of a MoE used in human health studies.

For baseline substances, if the MoE was greater than 10,000, hazard classification was lowered to Hazard Class 1. This rule was applied to the preliminary hazard classification and not the preliminary exposure classification because MoE is calculated using the aquatic HAF and is therefore most sensitive to the HAF (i.e., a substance has lower hazard because it cannot reach critical levels in biota associated with adverse effects).

2.5. Risk classification matrix

Following adjustment of the preliminary hazard and exposure classifications, a risk matrix was used to classify high, moderate, and low levels of potential for risk. Table 1 lists the possible risk outcomes from combinations of hazard and exposure classifications. Colours red, yellow and green are used to highlight the high, moderate and low concern categories, respectively.

Table 1. Risk classification matrix according to hazard and exposure classifications

	Hazard Class 1	Hazard Class 2	Hazard Class 3
Exposure Class 1	Low	Low	Moderate
Exposure Class 2	Low	Moderate	High
Exposure Class 3	Low	Moderate	High

Organic substances of higher risk concern are generally characterised as being more potent from a hazard perspective and having a greater potential for widespread continuous exposure. Substances of higher risk concern generally have moderate to quantities in commerce, have longer reaction residence times in the environment (months or longer), may be transported over long distances in air, and are potentially very potent substances beyond baseline toxicity. Substances in the moderate risk classification generally have a relatively short predicted reaction residence time in the environment (less than months, often days), do not undergo long range transport in air and are generally baseline substances (e.g., alcohols, esters, acids, alkanes) with lower reactivity. Organic substances classified as being of low risk concern are generally characterised as being less potent from a hazard perspective and having a lower potential for widespread continuous exposure.

2.6. Adjustment of risk classification

Risk classification outcomes were verified to determine possible overestimation or underestimation of potential risk considering two exposure scenarios: low emission rate and near-field (i.e., local) exposure.

1. **Low emission rate:** To address possible overestimation of risk, the risk classification outcome for substances which had a regional rate of emission to water estimated to be less than 1 000 kg/yr after wastewater treatment was adjusted to low risk based on low potential for exposure. This was performed because the likelihood of risk is very low at this rate of emission, particularly when the emission is dispersed over a wide spatial scale (e.g., 100 000 km^2 is used in the RAIDAR model (RAIDAR 2011). In addition, the ERC uses the total reported quantities in commerce as the emission rate to a WWTS, whereas it is very likely that only a fraction of the total reported quantity is actually released to the WWTS.

2. **Near-field (local) exposure:** Given that exposure and hazard classification is, in part, based on regional scale model results (from RAIDAR (2011)), local field exposures may not be fully accounted for in classification of potential for risk. To account for this situation, an additional near-field risk-based evaluation of all substances classified as low risk was performed to address the higher concentrations that may occur close to the point of discharge of a substance in the aquatic environment.

The aquatic release scenario for near-field exposure involved applying a generic scenario to estimate local aquatic exposure. While the generic aquatic exposure scenario has been developed to be conservative overall, the level of conservatism applied to individual parameters was selected to be moderate, since it is recognised that:

- a high level of conservatism applied to each parameter can easily compound into an excessively conservative overall exposure scenario;
- it is very unlikely that each parameter would be "worst case" at the same time; and
- interdependence of some parameters exists.

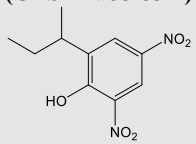
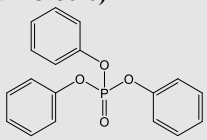
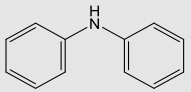
The description of the aquatic release scenario, equation and parameters used are summarised in ECCC (2016).

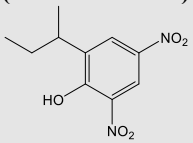
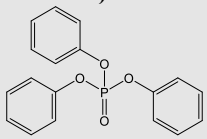
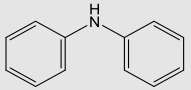
3. RESULTS OF ERC PRIORITISATION

3.1. ERC results for three example substances

The profiles of three discrete organic substances, identified by ERC as high, moderate, and low, respectively, are shown as examples to illustrate the ERC outcomes. The high risk profiled substance, phenol, 2-(1-methylpropyl)-4,6-dinitro- (CAS RN 88-85-7), is a restricted pesticide that also has an industrial application in Canada. The moderate risk profiled, phosphoric acid, triphenyl ester (CAS RN 115-86-6), is used as a plasticiser, smoke suppressant, and a fire retardant in a variety of products. The low risk profiled substance, benzenamine, N-phenyl- (CAS RN 122-39-4), is used as an antioxidant, including in lubricants and fuels. Table 2 shows the complete set of hazard and exposure descriptors used by the ERC approach, with colours red, yellow and green used to highlight the high, moderate and low concern hazard and exposure descriptors, respectively, and the final risk classification. Bolded descriptors were considered directly by the ERC approach; others were used as supporting evidence.

Table 2. Ecological Risk Classification for three example substances

Descriptor[1]			**Phenol, 2-(1-methylpropyl)-4,6-dinitro- (CAS RN 88-85-7)** 	**Phosphoric acid, triphenyl ester (CAS RN 115-86-6)** 	**Benzenamine, N-phenyl- (CAS RN 122-39-4)** 
b. Hazard	Mode of action	**OASIS MoA profiler**	Phenols and Anilines	Reactive unspecified	Base surface narcotics
		MoATox database by US EPA	Electron transport inhibition	Narcosis	Narcosis
		CBR toxicity ratio[2]	398	0.17	0.92
		Chemical activity[3]	10^{-7}	0.23	0.01
	HAF[4]	**Aquatic food web**	0.002	$4.6x10^{-6}$	$9.6x10^{-5}$
	Chemical reactivity	**ER binding**	Non-binder, impaired OH or NH_2 group	Non-binder, without OH or NH_2 group	Non-binder, without OH or NH2 group
		DNA binding	Structural alert for genotoxic carcinogenicity	No alert	No alert
		Protein binding	No alert	No alert	No alert
		AR binding	0.001<RBA<0.1	Not active	N/A
	Bioavailability	**log K_{ow} or log D**	3.56 (Bioavailable)	4.59 (Bioavailable)	3.50 (Bioavailable)
	Bioactivity[5]	ToxCast	Bioactive	N/A	Bioactive
		Tox21	Bioactive	N/A	Bioactive
b. Exposure	Exposure	**Quantities in commerce after WWTP removal (kt)**	0.1-1	0.01-0.1	0.1-1
		Overall persistence (hours)	3,825	792	1,080
		Half-life in air (hours)	63.6	23.7	1.3
c.	Preliminary hazard classification result		3	1	2
	Preliminary exposure classification result		3	1	1
d.		**Classification consistency**	N/A	N/A	N/A
		Special classes	N/A	N/A	N/A

			Descriptor[1]	Phenol, 2-(1-methylpropyl)-4,6-dinitro- (CAS RN 88-85-7) 	Phosphoric acid, triphenyl ester (CAS RN 115-86-6) 	Benzenamine, N-phenyl- (CAS RN 122-39-4) 
	Preliminary classification adjustments	**Potent reactivity**		Low	Low	Low
		HAF[4] Terrestrial food web		$5.2x10^{-3}$	$2.3x10^{-7}$	$1.4x10^{-5}$
		Margin of exposure[6]		10-100	10,000-100,000	100-1,000
e.	Risk classification matrix result			High (near and far field risk)	Low (mostly near field risk)	Low (mostly near field risk)
f.	Risk classification adjustment			N/A	Local RQ > 10	N/A
Final	Final classification result			High	Moderate (mostly near field risk)	Low

Abbreviations: not applicable (N/A); relative binding affinity (RBA); concentration of a substance that is estimated to be lethal to 50% of the test organisms (LC_{50}); molecular weight (MW); hazard assessment factor (HAF); waste water treatment plant (WWTP)

[1] Bolded descriptors were considered directly by the ERC approach; others were used as supporting evidence.

[2] CBR toxicity ratio = $CBR_{narcosis} \div CBR_{fishLC50}$ = 3.0 mmol/kg ÷ [(Fish LC_{50} × BCF) ÷ MW]

[3] Chemical activity = Fish LC_{50} ÷ WS

[4] HAF = CU ÷ CT, where:

CU (mol/m^3 or mmol/kg) is the tissue residue concentration in most sensitive aquatic or terrestrial foodweb organism based on a default unit emission rate of 1kg/h into the aquatic or terrestrial environment.

CT (mol/m^3 or mmol/kg) is the critical body residue (CBR) associated with median lethality for the most sensitive organism in the foodweb identified by the RAIDAR model. The CT is calculated as (LC_{50} × K_{ow} x 5%) ÷ MW

[5] US EPA [updated 2016a]; ToxCast and Tox21 data accessed for ERC in 2014

[6] Margin of Exposure (MoE) = E_C/E_A, where:

E_C is the critical emission rate (kt/yr), calculated as $E_U \div$ HAF [E_U is a default emission rate of 1 kg/h]

E_A is the actual emission rate (kt/yr)

3.2. Summary of the ERC results for 640 organic substances

Application of the ERC approach to further prioritise the remaining substances in CMP allowed ECCC to identify substances with the highest potential to cause adverse effects, as well as substances of low concern, and to apply appropriate regulatory approaches for their evaluation. To facilitate assessment, substances were grouped based on either similarity of chemical structures (e.g., hindered phenols) or similar types of use (e.g., flame retardants).

Five percent of the 640 organic substances were classified as having a high risk potential, 16% as moderate risk potential, and 79% as low risk potential (see Table 3). The high risk potential substances represent 13 chemical groupings and two individual substances (see Table 4), and are proposed for detailed risk assessment. For reasons of precaution and the potential for substitution, a number of moderate risk potential substances will also undergo a similar risk assessment. As a result, a total of 14% of the organic substances evaluated by the ERC approach are proposed for detailed risk assessment in the third phase of CMP. The information found in the ERC hazard and exposure profiles will be used as lines of evidence in those risk assessments.

For the remaining moderate risk potential substances (7% of the organic substances), use patterns and quantitates in commence will be tracked and their priority status re-evaluated if new information becomes available.

Risk assessment for the low risk potential substances, identified as low-volume chemicals in Canada, but classified as having high hazard (Class 3) potential, or ability to trigger hazard alerts, are not proposed at this time. These substances are identified for tracking of use patterns and re-evaluation of priority status based on new information.

Risk classification outcomes for the 640 organic substances by CAS RN are summarised in Appendices B to D in ECCC (2016). Table 4 summarises the overall risk classification of these substances and the anticipated regulatory actions in the third phase of CMP.

Table 3. Risk classification and regulatory action for 640 organic substances in the third phase of CMP

Risk Classification	Percent (%)	Regulatory action
High	5	To be evaluated in risk assessments
Moderate and member of high risk classification substance group	9	To be evaluated in risk assessments together with substances classified as having high potential for ecological risk
Moderate but not member of high risk classification substance group	7	To be evaluated using rapid screening approaches and tracking of use patterns; priority status to be re-evaluated if new information becomes available
Low	79	Use pattern data is proposed to be collected for those substances which were classified as high hazard by ERC and their priority status to be re-evaluated if new information becomes available

Table 4. Substances and substance groups prioritised for risk assessment

Individual Substance or Substance Groups	Number of discrete substances	Number of UVCB substances
Aliphatic amines	2	5
Alkyl aryl sulfonates/LABS and derivatives	4	12
Benzotriazoles & benzothiazoles	8	0
Carboxylic acid anhydrides	0	2
Dithiophosphate alkyl esters	0	3
Flame retardants	6	3
Hindered phenols	10	1
Naphthalene sulfonic acids and salts	5	0
Nitro musks	2	0
Phenol, 2-(1-methylpropyl)-4,6-dinitro-	1	0
Phenol, 4-(1,1,3,3-tetramethylbutyl)-	1	0
Quaternary ammonium compounds	2	10
Resins & rosins	0	8
Thiocarbamates	2	0
Triarylmethanes	6	0

3.3. Uncertainties identified in the ERC approach

The ERC generally reflects a realistically conservative or precautionary approach where consistency of descriptors adds to a weight of evidence for classification. The weighted approach used in ERC minimises the potential for both over or under estimation of hazard and exposure classification subsequent to risk classification. To avoid introducing overly conservative descriptors, values of central tendency rather than those from extremes of a distribution have been used and include median values for aquatic toxicity (i.e., LC_{50} values), CBRs, emission rates and HAFs. Nonetheless, uncertainties associated with profiling of hazard and exposure remain, given the use of models and prevalence of data gaps, and are acknowledged in Table 5.

Table 5. Uncertainties associated with profiling of hazard and exposure in ERC

	Factor	Uncertainty	Comment
Uncertainty Associated with the Hazard Descriptors	Model domain applicability	Medium	Applicability of each model's domain was not checked for each of the profiled chemicals as it is very time intensive and some models do not specify this information. However, this is not perceived to undermine risk classification results by the ERC approach since ERC is based on the weight-of-evidence approach which reduced the impact of uncertainties by not relying on a single hazard or exposure metric (i.e., a consensus approach was used). In some cases, model results could not be generated (due to limitations of the model domain) or were not available for all organic substances (e.g., androgen binding) and results were considered only as supporting information.

	Factor	Uncertainty	Comment
	Error with empirical or modelled acute toxicity values	Medium	The impact of this error is mitigated by the fact that overestimation of median lethality will result in a conservative CBR values, toxicity ratios and HAFs. Conversely, error with underestimation of median lethality is partly mitigated through the use of multiple hazard descriptors.
	Substances with low water solubility and high K_{ow} are difficult to model for fish LC_{50} data	Low	Fish LC_{50} data were required to generate some of the metrics, however, there are few reliable empirical LC_{50} data for high K_{ow} substances. In addition, they are not easily amenable to modelling because they may overpredict acute aquatic toxicity. Similarly, few measured data were available for ionogenic substances, and the difficulty with their profiling remains. Adjustment made to certain models allowed for generation of acceptable results; however, assessment uncertainty is generally greater for these substances than for the neutral substances. The CBR approach mitigates the error associated with classifying substances solely based on external concentrations.
	Extrapolating from mechanistic data to an adverse outcome in an organism	Medium	The models used for profiling chemical reactivity (i.e., receptor binding affinity, DNA and protein binding) and for bioactivity results (i.e., high throughput *in vitro* assays) suggest a potential for interaction with biological tissues. However, apical endpoints may or may not be realised depending on the fate and toxicokinetics of the substance. As a result, protein and DNA binding results that are supported by more than one profiler in the OECD QSAR Toolbox were considered and applied as an adjustment to the preliminary hazard classification and bioactivity results were considered only as supporting information.
Uncertainty Associated with the Exposure Descriptors	Fluctuations to the quantities in commerce	Low	Changes in substance quantities could result in significant changes in classification of exposure. The ERC approach considers current exposure and risk in Canada and may not reflect future trends. Therefore, import and manufacture quantities, and use patterns of low and moderate concern substances with a high hazard classification are proposed to be tracked to identify quantity increases and future trends.
	Prediction of long-range transport in air	Low	Air transport is based predominantly on chemical half-life in air. Some classes of substances may undergo transport in air based on sorption to fine particles in air (e.g., certain organic flame retardants). Although well correlated with long-range air transport, the half-life approach used in the ERC cannot account for this transport process and thus far-field concerns may be underestimated for some classes of organic substances. Therefore, a risk classification adjustment that considers near-field exposure is applied to substances with short environmental residence time and travel distance.

3.4. Conclusion

The ERC is a novel approach developed to increase efficiency in prioritizing chemicals for ecological risk assessment. It creates chemical-specific hazard and exposure profiles by integrating information from multiple data sources (e.g. *in silico*, *in*

chemico, *in vivo*, read-across), and draws on the concepts of an Integrated Approach for Testing and Assessment (IATA). ERC uses formalised rules to classify the hazard and exposure profiles into respective levels of concern. Supporting information, read-across approaches, and manual classification relied on professional judgment. The hazard and exposure classifications are then integrated together to create a final risk classification of high, medium, or low, which forms the basis for prioritisation.

The ERC approach is anticipated to improve identification of substances with the greatest potential to cause harm to the environment in both the near and far field, as well as increase confidence in lower-concern outcomes. The multiple hazard and exposure descriptors that underlie the risk classification define a wide toxicological space, identify the most potent substances, and directly consider the spatial and temporal scale of exposure.

Application of the ERC allowed Canada to identify the most suitable, fit-for- purpose regulatory action for the prioritised chemicals. In the Canadian regulatory decision context, the ERC was used to tailor regulatory assessment approaches based on the potential for risk. This included recommendations for detailed risk assessment of individual substances to less resource-intensive activities, such as class assessments and rapid screening, or tracking use patterns with the goal of re-prioritizing as dictated by new information.

3.5. Future direction

As the third phase of CMP is set to conclude in 2020, ECCC has begun planning future chemicals management initiatives including prioritisation of chemicals for assessment post 2020. It is anticipated that the ERC approach described here will continue to be used as a prioritisation tool. With new scientific developments in computational toxicology and advancements in regulatory science, updates to the ERC approach are also anticipated. These updates may consider additional information that could be used in profiling of hazard and exposure (e.g., other sources of data or databases, MoA alerts, QSARs).

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ANNEX A

Retrospective analysis of prioritisation approaches using PBiT hazard criteria versus the ERC based on hazard and exposure criteria

Categorisation of the Canadian DSL using the ecological and human health criteria was completed in 2006 and resulted in 4,300 of 23,000 substances being identified for further assessment activity. Ecological categorisation was based on the regulatory criteria for persistence (P) and bioaccumulation (B) as set out in the Persistence and Bioaccumulation Regulations of CEPA (Canada 2000), and a chosen threshold for inherent toxicity to non-human organisms (Robinson et al. 2004).

This approach allowed ECCC to prioritise substances for assessment based on their hazard profile, with the highest ecological priorities defined and referred to as "PBiT" substances. The PBiT criteria are specified in Table 6. Human health priorities were identified based on inherent toxicity and the greatest potential for exposure to humans or on the classification by other national or international agencies for having health effects of concern including carcinogenicity, genotoxicity, developmental or reproductive toxicity (ECCC [modified 2014).

Results of DSL Categorisation are available through an online ECCC search engine (ECCC [modified 2016]) and eChemPortal (eChemPortal [accessed 2017a]).

Table 6. Categorisation criteria for persistence (P), bioaccumulation (B) and inherent toxicity (iT)

Persistence (P)		**Bioaccumulation (B)**	**Inherent toxicity (iT)**	
Air	Half-life ≥ 2 days	BAF ≥ 5000 or BCF ≥ 5000 or $\log K_{ow} \geq 5$	Acute Exposure	LC_{50}, EC_{50} ≤ 1 mg/L
Water, Soil	Half-life ≥ 182 days		Chronic Exposure	NOEC ≤ 0.1 mg/L
Sediment	Half-life ≥ 365 days			

Abbreviations: BAF, bioaccumulation factor; BCF, bioconcentration factor; log K_{ow}, octanol-water partition coefficient; LC_{50}, the concentration of a substance that is estimated to be lethal to 50% of the test organisms; EC_{50}, the concentration of a substance that is estimated to cause some effect on 50% of the test organisms; NOEC, the no observed effect concentration is the highest concentration in a toxicity test not causing a statistically significant effect in comparison to the controls

Due to the magnitude of the task to categorise the 23 000 substances on the DSL in the timeframe specified by CEPA (Canada 1999), substance hazard profiles were typically based on one empirical or modelled acute median lethal effects endpoint (e.g., 96-hour LC_{50}) for an aquatic species, typically daphnids or fish. Where there were data gaps or information was simply not available, categorisation relied on the use of QSAR models or other available methods including the use of analogue and read-across data to establish descriptors for degradation, bioaccumulation and aquatic effects.

Experience assessing these substances in the first and second phases of CMP over the last 10 years has revealed that fewer than 20% of organic compounds captured as priority substances using the PBiT ecological Categorisation approach (i.e., PiT, BiT, or PBiT) resulted in toxic conclusions under CEPA. For the third phase of CMP, the

ERC approach based on an IATA was used to prioritise the remaining 640 organic substances for ecological risk assessment.

A comparison of the results from prioritisation approaches using PBiT criteria and the ERC approach was conducted to investigate whether classification between the two approaches would be different and whether greater efficiency in risk assessment may be gained by prioritisation using an IATA. Unlike the PBiT approach, the ERC also considers the potential for exposure.

A subset of 433 discrete organic substances of the 640 organics was used for the comparison. There were approximately 448 discrete organic substances among the 640 priorities, but 15 discrete organic substances did not have the 2006 Categorisation result and could not be included in the analysis. As well, UVCB organics were excluded from the analysis since most of them were manually classified in ERC.

Compared with PBiT, the ERC approach resulted in fewer substances being classified as high or moderate priorities (approximately 41% less, 70/169), and more substances classified as low priority (approximately 37% more, 363/264) (Figure 4). This is in line with the expectation that the IATA-based ERC approach will better identify substances of true ecological concern (i.e., reduce false positives), enabling more efficiency in risk assessment. Classification as high or moderate priority typically designates that a full risk assessment of a substance will be undertaken.

The substances prioritised as high/moderate by the ERC approach have greater parity with PBiT human health priorities, that is, with those substances originally categorised as "Not iT" (to non-human organisms) (Figure 4). This indicates that the ERC approach more effectively captures substances with higher hazard potential. As further illustrated in Figure 4, the majority of substances considered high/moderate priorities by ERC (approximately 66%, or 47 substances) did not meet the original PBiT ecological categorisation criteria, or a categorisation conclusion could not be made due to QSAR limitations (i.e., "uncertain" conclusion). These results further suggest that the IATA approach is better able to identify substances of greatest hazard potential, and is able to classify substances that were previously unclassifiable by considering a variety of metrics which overcomes limitations of certain QSAR models.

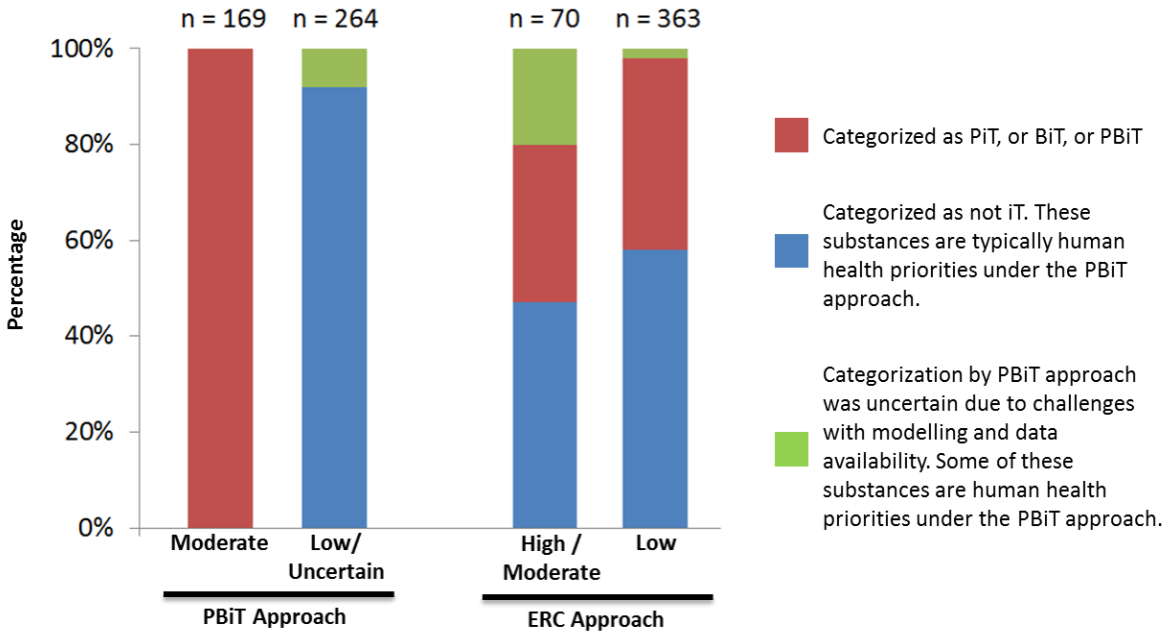


Figure 4. Comparison of prioritisation results using the PBiT and the ERC approaches

ANNEX B

List of models and expert systems used in ERC

		Name	Version	Description	Use in ERC	Reference
GENERAL SOFTWARE		OECD QSAR Toolbox	3.4	Software that includes databases of empirical data and various physico-chemical and hazard profiler models	Collecting empirical data and profiling for hazard-based descriptors	OECD QSAR Toolbox 2015
		EPI Suite	4.11	EPI Suite is a physical-chemical property and environmental fate estimation program.	Estimating physical-chemical properties, fate, acute ecotoxicity	EPI Suite c2000-2012
EXPOSURE PROFILING	**Persistence**	AOPWIN	1.92	atmospheric, gas-phase reaction predictor in EPI Suite v4.11	Determining half-life in air	EPI Suite c2000-2012
		RAIDAR (Risk Assessment, Identification and Ranking) model	2.5	An evaluative, regional-scale, mass balance model for screening level exposure and risk assessment. Model includes approaches suitable for ionogenic substances (Armitage et al. 2013: Arnot 2011: Arnot 2014) .	Overall Persistence (Pov)	RAIDAR 2011
		BIOWIN	4.10	Biodegradation Probability Program for Microsoft Windows in EPISUITE v4.11	Generating biodegradation half-lives for input into RAIDAR model	EPI Suite c2000-2012
	Emission Rate	SimpleTreat	3.0	Software program developed by The National Institute for Public Health and the Environment (RIVM) for sewage treatment plant removal predictions	Wastewater removal rate predictions (%)	SimpleTreat 1997
FATE	**Physico-chemical properties**	ACD/Percepta	Build 2920 2016	*In Silico* Prediction of Physicochemical, ADME, and Toxicity Properties	Log D at pH=7 (log Kow) Water solubility	ACD/Percepta c1997-2012
		HENRYWIN	3.2	Henry's law constant predictor in EPISUITE v4.11	Air-water partition coefficient	EPI Suite c2000-2012

		Name	Version	Description	Use in ERC	Reference
	Bioaccumulation	BCFBAF	3.01	Bioaccumulation Program for Microsoft Windows [estimation model] in EPISUITE v4.11	Bioconcentration factor	EPI Suite c2000-2012
		Iterative Fragment Selection (RAIDAR)	2.5	Prediction model for determining biotransformation rates. Model includes approaches suitable for ionogenic substances (Armitage et al. 2013: Arnot 2011: Arnot 2014) .	Half life (1 kg fish) Half life (1 kg mammal)	RAIDAR 2011
HAZARD	**Aquatic Toxicity**	Ecological Structure Activity Relationships Class Program (ECOSAR)	1.11	Predictive software that estimates acute and chronic aquatic toxicity in EPI Suite v4.11	Acute Fish LC_{50}	EPI Suite c2000-2012
	Endocrine Effects	Estrogen Receptor (ER) Profiler	2.2	ER binding profiling scheme is based on structural and parametric rules. In OECD QSAR Toolbox v3.3	Profiling Estrogen receptor binding	OECD QSAR Toolbox 2015
		Tissue Metabolism Simulator (TIMES)	2.27.15	TIMES is a metabolic predictor. It also includes models for predicting androgen receptor (AR) binding affinity	Profiling Androgen receptor binding	TIMES 2014
	Mode of Action (MOA)	OASIS MOA Profiler	3.0	This profile divides chemicals in different categories according to their acute toxic mode of action. In OECD QSAR Toolbox v3.3	Determining whether the MOA falls into a known category	OECD QSAR Toolbox 2015
		Acute aquatic toxicity MOA Verhaar Profiler	3.2	Profiler for Acute aquatic toxicity classification based on the Toxtree software. In OECD QSAR Toolbox v3.3	Determining whether the MOA is different than baseline narcosis	OECD QSAR Toolbox 2015
	Protein and	Protein Binding by DPRA Cysteine peptide depletion	1.0	This profiler is based on data derived from Direct Peptide Reactivity Assay (DPRA). In OECD QSAR Toolbox v3.3	Determining potential for binding proteins	OECD QSAR Toolbox 2015

		Name	Version	Description	Use in ERC	Reference
		Protein Binding by DPRA Lysine peptide depletion	1.0	This profiler is based on data derived from Direct Peptide Reactivity Assay (DPRA). In OECD QSAR Toolbox v3.3	Determining potential for binding proteins	OECD QSAR Toolbox 2015
		Protein binding by OASIS	1.3	This profiler scans for structural alerts responsible for interaction with proteins. In OECD QSAR Toolbox v3.3	Determining potential for binding proteins	OECD QSAR Toolbox 2015
		Protein binding by OECD	2.3	Structural alert-based profiler. In OECD QSAR Toolbox v3.3	Determining potential for binding proteins	OECD QSAR Toolbox 2015
		DNA binding by OASIS	1.3	The profiler is based on AMES Mutagenicity model part of OASIS TIMES system. In OECD QSAR Toolbox v3.3	Determining potential for binding DNA	OECD QSAR Toolbox 2015
		DNA binding by OECD	2.3	Structural alert-based profiler. In OECD QSAR Toolbox v3.3	Determining potential for binding DNA	OECD QSAR Toolbox 2015
		Carcinogenicity (genotox and nongenotox) alerts by ISS	2.3	Structural alert-based profiler based on the Toxtree software. In OECD QSAR Toolbox v3.3	Determining potential for interacting with DNA and/or chromosomes	OECD QSAR Toolbox 2015
		DNA alerts for AMES, MN (micro nucleus) and CA (chromosomal aberration) by OASIS	1.3	Structural alert-based profiler part of OASIS TIMES system. in OECD QSAR Toolbox v3.3	Determining potential for interfering with genetic material and/or inducing mutations	OECD QSAR Toolbox 2015
		in vitro mutagenicity (Ames test) alerts by ISS	2.3	Structural alert-based profiler based on the Toxtree software. In OECD QSAR Toolbox v3.3	Determining potential for inducing genetic mutations	OECD QSAR Toolbox 2015
		in vivo mutagenicity (Micronucleus) alerts by ISS	2.3	Structural alert-based profiler based on the Toxtree software. In OECD QSAR Toolbox v3.3	Determining potential for inducing genetic mutations	OECD QSAR Toolbox 2015
		Chromosomal aberration by OASIS	1.1	Structural alert-based profiler based on the Toxtree software. In OECD QSAR Toolbox v3.3	Determining potential for inducing genetic mutations	OECD QSAR Toolbox 2015

		Name	Version	Description	Use in ERC	Reference
	Food web Hazard Assessment Factor (HAF)	Risk Assessment, Identification and Ranking model (RAIDAR)	2.5	An evaluative, regional-scale, mass balance model for screening level exposure and risk assessment. Model includes approaches suitable for ionogenic substances (Armitage et al. 2013: Arnot 2011: Arnot 2014).	Predicting HAF for water and soil	RAIDAR 2011

ANNEX C

ERC spreadsheet for evaluation of 640 discrete and UVCB organic substances.

Supporting Documentation:

Data Used to Create Substance-Specific Hazard and Exposure Profiles and Assign Risk Classifications

Information in support of the Science Approach Document: Ecological Risk Classification of Organic Substances.

Environment and Climate Change Canada
2016

This document contains additional details of information that is summarized or referenced in the Science Approach Document: Ecological Risk Classification of Organic Substances (ERC). Relevant data were identified up to October, 2015. *More specifically, this document includes critical data and considerations used to create substance-specific profiles and classifications associated with hazard, exposure and risk, as well as identification of potential need for tracking of future use patterns.*	
In the Science Approach Document: Ecological Risk Classification of Organic Substances, this document is referenced as: *[ECCC] Environment and Climate Change Canada. 2016a. Gatineau (QC): ECCC. Data used to create substance-specific hazard and exposure profiles and assign risk classifications. Available from: substances@ec.gc.ca.*	

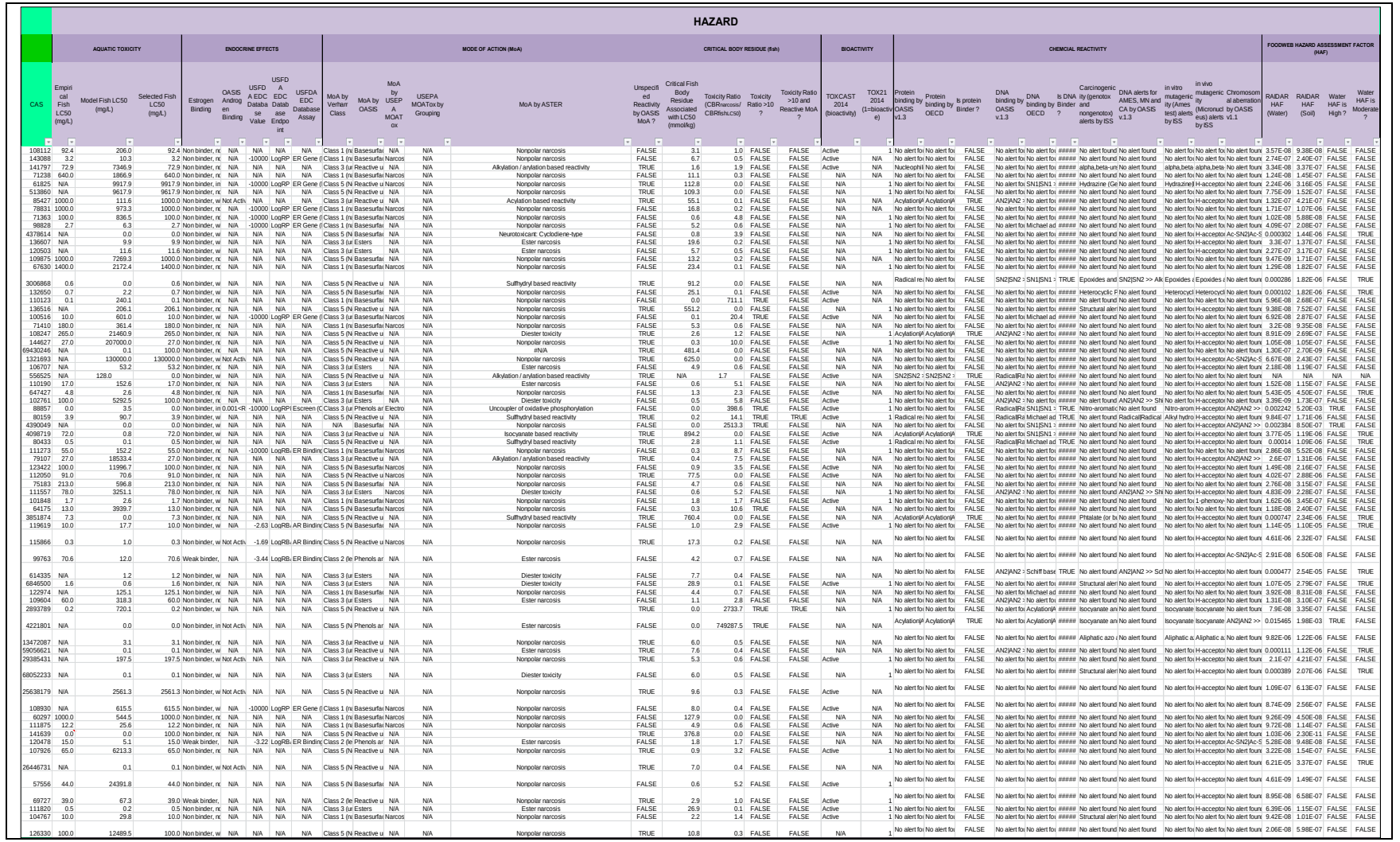
NOTES
Values reported in this document are typically model outputs unless otherwise noted.
Values for Annual Tonnage and Ratio of Critical Emmission to Actual Emission (margin of exposure) have been converted into orders of magnitude to protect Confidential Business Information (CBI)

LEGEND

SYMBOL OR MARKER	DEFINITION
N/A	No Data Available or Not Able to Model
?	Unknown
	Classification consistency rule applied

ACRONYM	DEFINITION
ACD Median LogD	[Predictive Model] Estimates the value of the octanol-water distribution constant, as the logarithmic ratio (logD), from structure at median pH (7) [by Advanced Chemistry Development]
AMES, MN and CA	Ames mutagenicity, Chromosomal Aberration and Micronucleus
BCF	Bioconcentration Factor
CBR	Critical Body Residue
DPRA	Direct Peptide Reactivity Assay
ECOSAR	[Predictive Model] Ecological Structure Activity Relationships
HAF	Hazard Assessment Factor (generated in RAIDAR)
ISS	Istituto Superiore di Sanita, Rome, Italy
KOWWIN	[Predictive Model] Estimates the log octanol-water partition coefficient, log KOW, of chemicals using an atom/fragment contribution method (by US EPA).
LC50	Median Lethal Dose
LogKaw	Air-water partition coefficient
LogKow	Octanol-water partition coefficient
RAIDAR	Risk Assessment IDentification And Ranking model
SMILES	Simplified Molecular-Input Line-Entry System
TIMES	[Predictive Model] TIssue MEtabolism Simulator (by OASIS)
TOX21 2014	Toxicology in the 21st Century (2014) [US EPA]
TOXCAST 2014	Toxicity Forecaster (2014) [US EPA]
USEPA	United States Environmental Protection Agency
USFDA EDC	United States Food and Drug Administration Electronic Data Capture
WWTP	Wastewater Treatment Plant

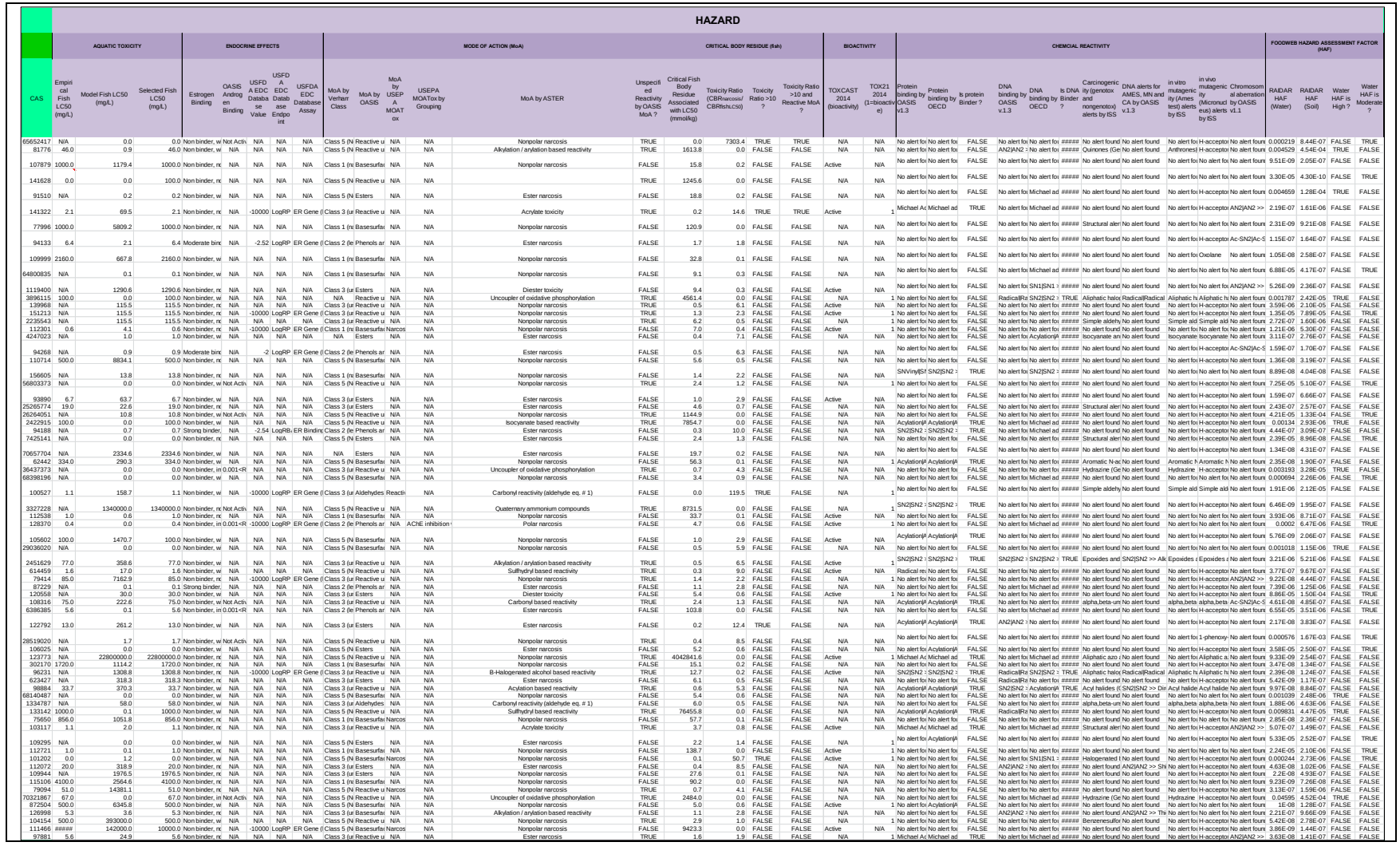
CHEMICAL IDENTITY					EXPOSURE									FATE																				
SUBSTANCE AND GROUPING FOR CMP					PERSISTENCE				EMISSION RATE (EA)					PHYSICO-CHEMICAL PROPERTIES														BIOACCUMULATION								
CAS	CMP Phase 3 Group	Substance Name	SMILES	Molecular Weight (g/mol)	Overall Persistence (hours)	Critically Long Overall Persistence	Selected Air Half life (hours)	Critically Long Half Life in Air	WWTP Removal (%)	Annual Tonnage (kilotonnes)	Annual tonnage after WWTP Removal (kilotonnes)	Large value for tonnage	Moderate value for tonnage	Low value for tonnage	Empirical LogKow	ACD Median Log D @ pH 7	Selected LogKow	ACD Water Sol. @ pH 7 (mg/L)	Empirical Water Sol. SRC Database (mg/L)	Empirical Water Sol. REACH Database (mg/L)	Selected Water Sol (mg/L)	LogK aw	Model BCF 5% Lipid Fish (L/kg)	Empirical BCF 5% Lipid Fish (L/kg)	Selected BCF 5% Lipid Fish (L/kg)	Half-Life 1 kg Mammal (days)	Half-life 1 kg Fish (days)								
108112	Alcohols	2-Pentanol, 4-methyl-	CC(CC(O)	102.2	3,012	FALSE	285.00	TRUE	81.5	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	9.2	1.6	9.2	10948.2	N/A	N/A	10948.2	-2.7	3.4	N/A	3.4	0.9	12.5								
143088	Alcohols	1-Nonanol	CCCCCC	144.3	176	FALSE	285.0	TRUE	81.9	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	3.8	4.0	3.8	112.0	N/A	N/A	112.0	-2.9	300.0	N/A	300.0	1.0	30.2								
141797	Ketones	3-Penten-2-one, 4-methyl-	CC(=CC(=	98.2	441	FALSE	273.0	TRUE	81.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	1.4	1.4	4590.5	N/A	N/A	4590.5	-2.8	2.1	N/A	2.1	1.3	17.2								
71238	Alcohols	1-Propanol	CCCO	60.1	244	FALSE	46.9	TRUE	82.5	1 - 10	1 - 10	TRUE	FALSE	FALSE	0.3	0.3	0.3	161747.8	1000000	N/A	1000000.0	-3.5	1.0	N/A	1.0	1.0	4.2								
61825	Triazoles	1H-1,2,4-Triazol-3-amine	Nc1n[nH]c	84.1	877	FALSE	46.5	TRUE	61.5	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	-1.0	-0.7	-1.0	84390.5	280000	280000	280000.0	-11.0	1.0	N/A	1.0	0.8	2.2								
513860	Ketones	2-Butanone, 3-hydroxy-	CC(=O)C(	88.1	312	FALSE	43.8	TRUE	82.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	-0.3	-0.3	749896.2	N/A	N/A	749896.2	-3.4	1.0	N/A	1.0	0.4	2.3								
85427	Carboxylic acid anhydrides	1,3-Isobenzofurandione, hexahydro-	O=C1OC(	154.2	751	FALSE	37.7	FALSE	61.5	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	0.3	0.3	16518.9	N/A	N/A	16518.9	-3.1	8.5	N/A	8.5	0.0	23.6								
78831	Alcohols	1-Propanol, 2-methyl-	OCC(C)C	74.1	292	FALSE	37.3	FALSE	82.4	10 - 100	1 - 10	TRUE	FALSE	FALSE	0.8	0.7	0.8	67599.7	N/A	N/A	67599.7	-3.4	1.2	N/A	1.2	0.8	6.4								
71363	Alcohols	1-Butanol	CCCCO	74.1	154	FALSE	37.2	FALSE	82.4	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	0.9	0.8	0.9	37148.8	63200	N/A	63200.0	-3.4	1.3	0.5	0.5	1.0	6.1								
98828	Arenes	Benzene, (1-methylethyl)-	CC(c1ccc(	120.2	215	FALSE	37.2	FALSE	27.1	1 - 10	1 - 10	TRUE	FALSE	FALSE	3.7	3.7	3.7	47.9	N/A	N/A	47.9	-0.3	233.3	N/A	233.3	1.5	56.3								
4378614	Pigments and Dyes	Dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-	Brc1cc2c3	464.1	22,918	TRUE	36.2	FALSE	83.8	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.8	6.8	0.0	N/A	N/A	0.0	-10.2	29981.0	N/A	29981.0	73.6	125.9								
136607	Benzoates	Benzoic acid, butyl ester	CCCCOC(	178.2	182	FALSE	49.4	TRUE	81.7	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	3.8	3.6	3.8	219.3	N/A	N/A	219.3	-2.8	352.1	N/A	352.1	0.9	7.3								
120503	Benzoates	Benzoic acid, 2-methylpropyl ester	CC(COC(=	178.2	326	FALSE	49.5	TRUE	81.8	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	3.6	3.6	257.6	N/A	N/A	257.6	-2.5	87.5	N/A	87.5	0.7	12.5								
109875	INDIVIDUAL - Methane, dime	Methane, dimethoxy-	COCOC	76.1	465	FALSE	50.5	TRUE	79.1	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	0.2	0.2	355920.3	N/A	N/A	355920.3	-2.2	1.0	N/A	1.0	0.8	5.4								
67630	Alcohols	2-Propanol	CC(O)C	60.1	285	FALSE	35.3	FALSE	82.5	10 - 100	10 - 100	TRUE	FALSE	FALSE	0.1	0.2	0.1	173315.9	1000000	N/A	1000000.0	-3.5	1.0	N/A	1.0	0.8	4.4								
3006868	Organic peroxides	Peroxide, cyclohexylidenebis[(1,1-dimethylethyl)	CC(OOC1	260.4	11,534	TRUE	31.8	FALSE	80.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	4.8	4.8	9.7	N/A	N/A	9.7	-1.6	37096.4	N/A	37096.4	4.7	101.9								
132650	Heterocycles	Dibenzothiophene	c1ccc2c(c	184.3	1,089	FALSE	31.7	FALSE	72.1	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	4.4	4.4	4.4	2.5	N/A	N/A	2.5	-2.9	1204.3	6606.9	6606.9	2.8	514.3								
110123	Ketones	2-Hexanone, 5-methyl-	CC(CCC(=	114.2	361	FALSE	31.4	FALSE	79.3	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	1.9	1.8	1.9	8464.7	N/A	N/A	8464.7	-2.2	4.8	N/A	4.8	0.5	23.0								
136516	2-EHA and derivatives	Hexanoic acid, 2-ethyl-, calcium salt	CCCCC(C	144.2	199	FALSE	31.4	FALSE	82.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	2.6	0.5	2.6	563767.1	N/A	N/A	563767.1	-3.9	385.8	N/A	385.8	0.4	22.2								
100516	Alcohols	Benzenemethanol	OCc1ccccc	108.1	334	FALSE	31.1	FALSE	82.7	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	1.1	1.2	1.1	24209.0	N/A	N/A	24209.0	-4.9	1.6	N/A	1.6	1.1	5.1								
71410	Alcohols	1-Pentanol	CCCCCO	88.2	159	FALSE	30.9	FALSE	82.3	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	1.5	1.6	1.5	9020.1	22000	N/A	22000.0	-3.3	2.6	N/A	2.6	1.0	8.6								
108247	INDIVIDUAL - Acetic acid, an	Acetic acid, anhydride	CC(=O)OC	102.1	346	FALSE	53.50	TRUE	61.3	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	4.4	0.0	4.4	134579.0	N/A	N/A	134579.0	-3.6	1.0	N/A	1.0	0.2	3.3								
144627	Carboxylic acids	Ethanedioic acid	OC(=O)C(	90.0	162	FALSE	53.5	TRUE	82.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	-5.8	-5.8	1000024.9	N/A	N/A	1000024.9	-8.2	1.0	N/A	1.0	0.2	1.0								
69430246	Siloxanes	Cyclosiloxanes, di-Me	C[Si](C)(C	222.5	348	FALSE	53.5	TRUE	90.0	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	4.4	3.0	4.4	1.6	N/A	N/A	1.6	0.4	14.7	N/A	14.7	1.4	26.0								
1321693	Naphthalene sulfonic acids a	Naphthalenesulfonic acid, sodium salt	OS(=O)(=C	208.2	1,102	FALSE	54.0	TRUE	61.5	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	0.6	-2.7	0.6	117018.1	N/A	N/A	117018.1	-8.0	1.0	N/A	1.0	1.7	9.7								
106707	Esters	Hexanoic acid, methyl ester	CCCCCC(	130.2	136	FALSE	54.4	TRUE	76.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	2.5	2.5	1133.9	N/A	N/A	1133.9	-1.8	12.1	N/A	12.1	0.6	8.6								
556525	Epoxides & glycidyl ethers	Oxiranemethanol	OCC1CO1	74.1	N/A	N/A	55.1	TRUE	0.0	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	-0.7	-0.7	707444.6	N/A	N/A	707444.6	-6.6	1.0	N/A	1.0	20.0	20.0								
110190	Esters	Acetic acid, 2-methylpropyl ester	CC(COC(=	116.2	210	FALSE	55.8	TRUE	75.6	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	1.8	1.7	1.8	4842.3	N/A	N/A	4842.3	-1.7	4.0	N/A	4.0	0.5	6.9								
647427	INDIVIDUAL - 1-Octanol, 3,3,4	1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-	CCCC(C(	364.1	1,100	FALSE	61.4	TRUE	33.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	4.5	4.3	4.5	2.6	N/A	N/A	2.6	0.8	15752.6	99.0	99.0	1424.7	498.3								
102761	Esters	1,2,3-Propanetriol, triacetate	CC(=O)OC	202.3	130	FALSE	30.2	FALSE	82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	0.3	0.4	0.3	30120.5	N/A	N/A	30120.5	-6.3	1.0	N/A	1.0	0.1	0.8								
88857	INDIVIDUAL - Phenol, 2-(1-m	Phenol, 2-(1-methylpropyl)-4,6-dinitro-	CCC(c1cc	240.2	3,825	TRUE	63.6	TRUE	14.2	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	3.6	0.6	3.6	43390.6	N/A	N/A	43390.6	-4.7	2.5	64.6	64.6	9.8	8.4								
80159	Organic peroxides	Hydroperoxide, 1-methyl-1-phenylethyl	OOC(c1cc	152.2	944	FALSE	29.7	FALSE	14.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.6	2.6	2357.2	N/A	N/A	2357.2	-5.7	8.3	N/A	8.3	1.5	8.4								
4390049	INDIVIDUAL - Nonane, 2,2,4,	Nonane, 2,2,4,4,6,8,8-heptamethyl-	CC(C)(C(	226.5	21,233	TRUE	29.6	FALSE	83.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	7.1	7.1	1.4	N/A	N/A	1.4	3.1	14375.5	177.8	177.8	2.0	4911.5								
4098719	Isocyanates	Cyclohexane, 5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethyl-	O=C=NCC	222.3	3,505	TRUE	29.1	FALSE	54.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	4.5	4.5	82.6	N/A	N/A	82.6	-2.6	2760.7	N/A	2760.7	2.4	79.3								
80433	Organic peroxides	Peroxide, bis(1-methyl-1-phenylethyl)	CC(c1ccc(	270.4	8,675	TRUE	27.7	FALSE	74.9	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	5.5	5.4	5.5	1.3	N/A	N/A	1.3	-2.7	144.1	1607.7	1607.7	3.3	74.3								
111273	Alcohols	1-Hexanol	CCCCCC(	102.2	163	FALSE	26.4	FALSE	82.2	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	2.0	1.9	2.0	5879.5	N/A	N/A	5879.5	-3.2	6.4	0.6	0.6	1.0	11.6								
79107	Acrylates/methylacrylates	2-Propenoic acid	OC(=O)C=	72.1	216	FALSE	26.4	FALSE	82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	0.4	2.3	0.4	1000023.7	N/A	N/A	1000023.7	-4.8	1.1	N/A	1.1	0.4	5.5								
123422	Ketones	2-Pentanone, 4-hydroxy-4-methyl-	CC(=O)CC	116.2	760	FALSE	65.2	TRUE	32.3	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	0.2	0.2	192774.8	N/A	N/A	192774.8	-5.0	1.0	N/A	1.0	0.9	3.2								
112050	Carboxylic acids	Nonanoic acid	CCCCCC(	158.2	169	FALSE	26.3	FALSE	82.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	3.4	1.2	3.4	21797.7	N/A	N/A	21797.7	-4.2	134.8	N/A	134.8	0.5	29.1								
75183	Thiols	Methane, thiobis-	CSC	62.1	75	FALSE	67.2	TRUE	65.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	1.3	1.3	4935.6	N/A	N/A	4935.6	-1.2	1.4	N/A	1.4	1.3	14.0								
111557	Esters	1,2-Ethanediol, diacetate	CC(=O)OC	146.1	156	FALSE	68.3	TRUE	82.7	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	0.4	0.4	55561.3	N/A	N/A	55561.3	-5.5	1.1	N/A	1.1	0.2	0.8								
101848	Ethers	Benzene, 1,1'-oxybis-	c1ccc(cc1)	560.8	309	FALSE	26.1	FALSE	59.1	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	4.2	4.0	4.2	72.6	N/A	N/A	72.6	-1.9	173.5	594.0	594.0	18.7	61.8								
64175	INDIVIDUAL - Ethanol	Ethanol	CCO	46.1	237	FALSE	71.8	TRUE	82.6	100 - 1,000	100 - 1,000	TRUE	FALSE	FALSE	-0.3	-0.2	-0.3	271271.1	1000000	N/A	1000000.0	-3.7	1.0	N/A	1.0	1.0	3.1								
3851874	Organic peroxides	Peroxide, bis(3,5,5-trimethyl-1-oxohexyl)	CC(CC(C)	314.5	17,179	TRUE	23.9	FALSE	83.6	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	5.8	5.8	3.4	N/A	N/A	3.4	-0.7	32756.6	N/A	32756.6	0.4	272.4								
119619	INDIVIDUAL - Benzophenone	Methanone, diphenyl-	O=C(c1cc	182.2	630	FALSE	72.2	TRUE	62.1	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	3.2	3.0	3.2	69.3	N/A	N/A	69.3	-4.1	2.9	18.8	18.8	1.0	5.1								
115866	Flame Retardants	Phosphoric acid, triphenyl ester	O=P(Oc(cc	326.3	792	FALSE	23.7	FALSE	48.6	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	4.6	4.1	4.6	1.3	N/A	N/A	1.3	-3.9	74.3	18900.0	18900.0	1.8	16.5								
99763	Parabens	Benzoic acid, 4-hydroxy-, methyl ester	O=C(OC)c	152.2	283	FALSE	23.2	FALSE	82.8	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	2.0	2.1	2.0	1672.1	N/A	N/A	1672.1	-6.8	9.1	N/A	9.1	0.8	1.6								
614335	Benzoates	1,2,3-Propanetriol, tribenzoate	O=C(c1cc(	404.4	258	FALSE	22.5	FALSE	88.2	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	5.6	5.6	1.4	N/A	N/A	1.4	-9.3	2641.0	N/A	2641.0	0.5	1.2								
6846500	Esters	Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propa	CC(C(=O)(	286.4	638	FALSE	22.4	FALSE	58.5	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	4.1	4.1	15.7	N/A	N/A	15.7	-3.4	3923.4	5340.0	5340.0	0.4	19.8								
122974	Alcohols	Benzenepropanol	OCCCc1c	136.2	380	FALSE	22.2	FALSE	82.7	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	1.9	1.8	1.9	4208.7	N/A	N/A	4208.7	-5.1	4.8	N/A	4.8	1.1	10.4								
109604	Esters	Acetic acid, propyl ester	CCCOC(=	102.1	201	FALSE	80.3	TRUE	78.5	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	1.2	1.4	1.2	11999.4	N/A	N/A	11999.4	-2.1	1.8	N/A	1.8	0.6	2.3								
2893789	Cyanurates	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3-dichloro-, sodium salt	O=c1n(Cl)c	198.0	1,057	FALSE	85.6	TRUE	61.5	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-2.2	-2.2	910512.5	N/A	N/A	910512.5	-9.9	1.0	N/A	1.0	2.6	0.8								
4221801	Hindered phenols	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2,4-bis(1,1-dim	O=C(Oc(c(	438.6	6,670	TRUE	21.7	FALSE	83.6	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	9.0	9.0	0.0	N/A	N/A	0.0	N/A	269.8	N/A	269.8	N/A	N/A								
13472087	Nitriles	Butanenitrile, 2,2'-azobis[2-methyl-	CCC(N=N(	192.3	2,093	TRUE	86.5	TRUE	17.3	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	2.4	2.4	167.5	N/A	N/A	167.5	-8.0	368.5	N/A	368.5	10.9	68.0								
59056621	Terpenes & Terpenoids	2,3b-Methano-3bH-cyclopenta[1,3]cyclopropa[1,2]benzene-4-meth	CC(=O)OC	276.4	3,975	TRUE	21.4	FALSE	75.5	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.5	5.5	0.3	N/A	N/A	0.3	-1.7	15752.6	N/A	15752.6	0.6	140.7								
29385431	Benzotriazoles & benzothiazo	1H-Benzotriazole, 4(or 5)-methyl-	Cc1cccc2(	133.2	658	FALSE	93.5	TRUE	61.2	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	1.7	1.7	4487.9	N/A	N/A	4487.9	-5.2	3.6	N/A	3.6	1.6	19.3								
68052233	Benzoates	1,3-Pentanediol, 2,2,4-trimethyl-, dibenzoate	O=C(c1cc(	354.5	2,659	TRUE	21.4	FALSE	81.0	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	5.8	5.8	1.4	N/A	N/A	1.4	-5.3	28713.2	N/A	28713.2	0.9	17.1								
25638179	Naphthalene sulfonic acids a	Naphthalenesulfonic acid, butyl-, sodium salt	CCCCc1c	264.3	974	FALSE	21.3	FALSE	61.6	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	-0.3	-0.3	20510.0	N/A	N/A	20510.0	-7.6	1.0	N/A	1.0	3.4	38.8								
108930	Alcohols	Cyclohexanol	O=C1CCC	98.2	450	FALSE	21.2	FALSE	82.4	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	0.8	0.9	0.8	12643.3	N/A	42000	42000.0	-3.4	1.3	N/A	1.3	0.5	10.1								
60297	Ethers	Ethane, 1,1'-oxybis-	CCOCC	74.1	272	FALSE	20.8	FALSE	68.4	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	0.9	1.2	0.9	38899.6	60400	N/A	60400.0	-1.3	1.3	9.5	9.5	1.5	15.2								
111875	Alcohols	1-Octanol	CCCCCC(	130.2	172	FALSE	20.5	FALSE	82.0	10 - 100	1 - 10	TRUE	FALSE	FALSE	3.0	3.0	3.0	683.5	N/A	N/A	683.5	-3.0	51.9	N/A	51.9	1.0	20.5								
141639	Siloxanes	Pentasiloxane, dodecamethyl-	C[Si](O[Si]	384.9	1,760	TRUE	95.1	TRUE	93.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	9.4	6.2	9.4	65.4	N/A	N/A	65.4	1.5	28713.2	1450.0	1450.0	2.9	28.0								
120478	Parabens	Benzoic acid, 4-hydroxy-, ethyl ester	O=C(OCC	166.2	293	FALSE	20.4	FALSE	82.9	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	2.5	2.5	2.5	936.6	N/A	N/A	936.6	-6.7	19.8	N/A	19.8	0.7	2.2								
107926	Carboxylic acids	Butanoic acid	CCCC(=O	88.1	1,760	FALSE	95.08	TRUE	82.7	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	9.4	-1.4	9.4	1000002.6	N/A	N/A	1000002.6	-4.7	1.3	N/A	1.3	0.5	6.2								
26446731	Flame Retardants	Phosphoric acid, bis(methylphenyl) phenyl ester	Cc1ccc(cc	354.4	4,015	TRUE	20.1	FALSE	79.5	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	4.7	4.7	0.4	N/A	N/A	0.4	-5.7	21885.9	N/A	21885.9	2.6	78.2								
57556	Alcohols	1,2-Propanediol	OCC(O)C	76.1	184	FALSE	20.0	FALSE	82.7	10 - 100	1 - 10	TRUE	FALSE	FALSE	-0.9	-1.0	-0.9	999891.4	1000000	N/A	1000000.0	-6.3	1.0	N/A	1.0	0.7	1.0								
69727	Salicylates	Benzoic acid, 2-hydroxy-	OC(=O)c1(	138.1	310	FALSE	19.7	FALSE	82.8	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	2.3	-0.8	2.3	999905.4	2240	N/A	2240.0	-6.5	10.2	N/A	10.2	0.1	2.4								
111820	Esters	Dodecanoic acid, methyl ester	CCCCCC(	214.4	266	FALSE	19.5	FALSE	86.2	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	5.4	5.5	5.4	5.9	N/A	N/A	5.9	-0.9	11077.3	N/A	11077.3	0.6	50.8								
104767	Alcohols	1-Hexanol, 2-ethyl-	CCCCC(C	130.2	201	FALSE	19.4	FALSE	82.1	10 - 100	1 - 10	TRUE	FALSE	FALSE	N/A	2.5	2.5	860.4	N/A	N/A	860.4	-3.0	28.3	N/A	28.3	1.5	21.1								
126330	Furan and derivatives	Thiophene, tetrahydro-, 1,1-dioxide	O=S1(=O)(	120.2	602	FALSE	19.3	FALSE	61.5	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	-0.8	-0.6	-0.8	15128.7	N/A	N/A	15128.7	-3.7	1.0	13.0	13.0	4.1	6.6								



| HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavalibility ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
108112	3	1	245456.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
143088	1	1	31933.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
141797	1	1	262007.8	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
71238	1	1	708270.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
61825	1	1	3914.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
513860	1	1	1130313.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
85427	1	1	66519.3	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
78831	1	1	51237.1	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
71363	1	1	858722.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
98828	1	1	21414.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4378614	1	2	29.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
136607	1	1	26551.6	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
120503	1	1	38612.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
109875	1	1	1925275.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
67630	1	1	681060.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3006868	2	2	30.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A			N/A	N/A
132650	1	2	86.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
110123	1	1	146988.3	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
136516	1	1	93432.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
100516	1	1	126609.3	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
71410	1	1	273450.1	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
108247	1	1	983060.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
144627	1	1	830813.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
69430246	1	1	66269.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1321693	3	1	131375.5	1,000,000 - 10,000,000	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
106707	1	1	401225.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
556525	N/A	N/A	N/A	N/A	N/A	N/A	FALSE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
110190	3	1	575541.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
647427	1	2	161.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
102761	1	1	2585891.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
88857	3	3	3.9	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	3	3	high (near and far field risk	N/A	N/A	N/A	N/A	N/A	N/A
80159	1	3	8905.2	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4390049	1	3	3.7	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4098719	1	2	232.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
80433	2	2	62.8	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A			N/A	N/A
111273	1	1	306309.2	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
79107	1	1	33644.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
123422	3	1	588945.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
112050	1	1	21783.3	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
75183	1	1	317045.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
111557	1	1	1813846.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
101848	1	1	5407.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
64175	3	1	741026.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
3851874	1	2	11.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
119619	1	2	769.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
115866	1	1	1898.7	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near fiel	local RQ >10	moderate (mostly near fiek	N/A	N/A	N/A	N/A
99763	1	1	301100.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
614335	1	2	18.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
6846500	1	2	815.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A			N/A	N/A
122974	1	1	223678.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
109604	3	1	667624.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
2893789	1	3	110876.3	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	local RQ <1	low (mostly near field)			N/A	N/A
4221801	2	3	0.6	1 - 10	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
13472087	2	1	892.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	greater potential for local ex	ERC classified this substan	N/A	N/A
59056621	1	2	78.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
29385431	1	1	41767.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
68052233	2	2	22.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
25638179	1	1	80307.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
108930	1	1	1002542.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
60297	1	1	946477.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
111875	1	1	90124.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
141639	1	1	8430.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
120478	1	1	165819.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
107926	1	1	271984.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
26446731	1	2	141.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
57556	1	1	1898515.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
69727	1	1	97836.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
111820	1	1	1370.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
104767	1	1	92985.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
126330	1	1	425879.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A

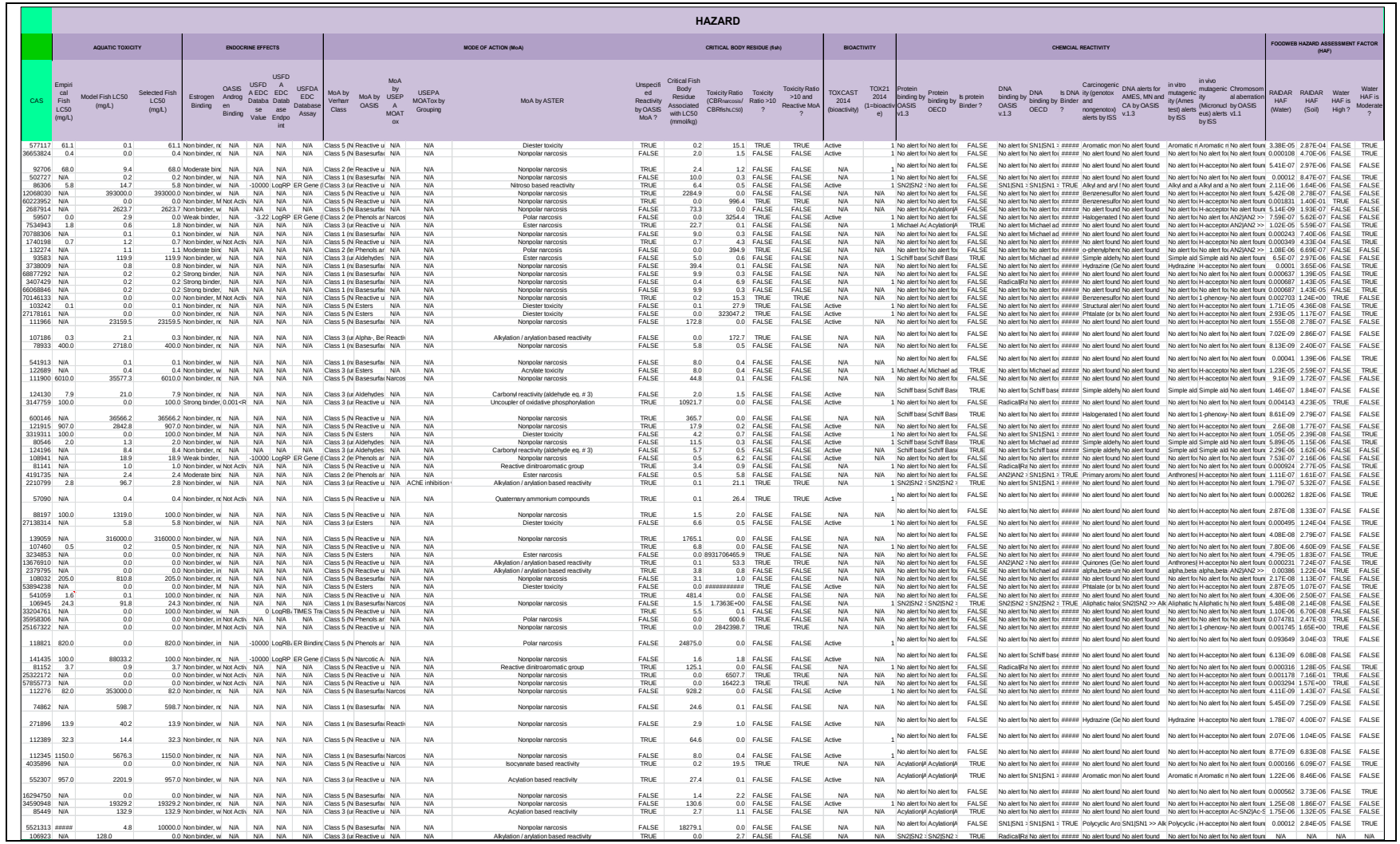
| CHEMICAL IDENTITY | | | | | EXPOSURE | | | | | | | | | | | | | | FATE | | | | | | | | | | | | | |



| HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE		AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailability ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
65652417	1	3	40.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
81776	2	3	1.9	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
107879	1	1	921073.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
141628	1	2	262.1	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
91510	1	3	1.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
141322	1	3	40026.4	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A			N/A	N/A
77996	1	1	3796909.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
94133	1	2	76132.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
109999	1	1	834349.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
64800835	1	2	127.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1119400	1	1	1666603.2	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3896115	1	3	4.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
139968	1	1	2441.7	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near fiel	local RQ >10	moderate (mostly near fiel	Moderate potential for risk;	ERC classified this substan	N/A	N/A
151213	1	2	650.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	moderate (mostly near fiel	local RQ >10	moderate (mostly near field)			N/A	N/A
2235543	1	1	32165.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112301	1	1	7207.5	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4247023	1	1	28169.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
94268	1	2	55201.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
110714	1	1	646255.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
156605	3	1	98587.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
56803373	2	2	120.8	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
93890	1	1	54989.6	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
25265774	1	1	36010.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
26264051	1	2	208.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	moderate (mostly near fiel	local RQ >10	moderate (mostly near fiel	N/A	N/A	N/A	N/A
2422915	1	3	6.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
94188	1	3	19738.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
7425141	1	2	366.3	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
70657704	1	1	654295.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
62442	1	1	373076.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3643737	1	3	2.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
68398196	1	2	12.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
100527	1	1	4592.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3327228	1	1	1356976.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
112538	1	1	2179.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
128370	1	2	43.0	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	moderate (mostly near fiel	local RQ >10	moderate (mostly near fiel	N/A	N/A	N/A	N/A
105602	1	1	1521315.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
29036020	1	3	8.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
2451629	3	1	2732.8	10,000 - 100,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A			N/A	N/A
614459	1	1	23254.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
79414	1	1	94992.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
87229	1	3	1184.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
120558	1	2	98.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
108316	3	1	190058.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
6386385	1	2	131.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
122792	1	1	402971.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
28519020	2	2	15.2	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
106025	1	2	244.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
123773	1	1	939350.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
302170	1	1	252363.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
96231	1	1	366948.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A			N/A	N/A
623427	1	1	1615371.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
98884	1	1	87889.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Low current exposure, but h	ERC classified this substan	N/A	N/A
68140487	1	3	8.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1334787	1	1	4658.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
133142	1	3	0.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
75650	3	1	307025.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
103117	1	1	17286.7	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near fiel	local RQ >10	moderate (mostly near field)			N/A	N/A
109295	1	2	164.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112721	1	2	343.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A			N/A	N/A
101202	1	2	35.9	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112072	1	1	189303.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
109944	1	1	398254.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
115106	3	1	948656.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
79094	3	1	28020.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A			N/A	N/A
70321867	1	3	0.2	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
872504	1	1	876053.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
126998	1	1	39713.2	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
104154	1	1	161494.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
111466	1	1	2270879.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
97881	1	1	241363.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A

| CHEMICAL IDENTITY | | | | | EXPOSURE | | | | | | | | | FATE | | | | | | | | |



HAZARD

	AQUATIC TOXICITY			ENDOCRINE EFFECTS					MODE OF ACTION (MoA)					CRITICAL BODY RESIDUE (fish)					BIOACTIVITY		CHEMICAL REACTIVITY								FOODWEB HAZARD ASSESSMENT FACTOR (HAF)			
CAS	Empirical Fish LC50 (mg/L)	Model Fish LC50 (mg/L)	Selected Fish LC50 (mg/L)	Estrogen Binding	OASIS Androgen Binding	USFDA EDC Database Value	USFDA EDC Database Endpoint	USFDA EDC Database Assay	MoA by Verhaar Class	MoA by OASIS	MoA by USEPA MOATox	USEPA MOATox by Grouping	MoA by ASTER	Unspecified Reactivity by OASIS MoA ?	Critical Fish Body Residue Associated with LC50 (mmol/kg)	Toxicity Ratio (CBRnarcosis/CBRfish,c50)	Toxicity Ratio >10 ?	Toxicity Ratio >10 and Reactive MoA ?	TOXCAST 2014 (bioactivity)	TOX21 2014 (1=bioactive)	Protein binding by OASIS v1.3	Protein binding by OECD	Is protein Binder ?	DNA binding by OASIS v.1.3	DNA binding by OECD	Is DNA Binder ?	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, MN and CA by OASIS v.1.3	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Chromosomal aberration by OASIS v1.1	RAIDAR HAF (Water)	RAIDAR HAF (Soil)	Water HAF is High ?	Water HAF is Moderate ?
577117	61.1	0.1	61.1	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Diester toxicity	TRUE	0.2	15.1	TRUE	TRUE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Aromatic mon	No alert found	No alert found	Aromatic n	Aromatic n	No alert found	3.38E-05	2.87E-04	FALSE	TRUE
36653824	0.4	0.0	0.4	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	2.0	1.5	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.000108	4.70E-06	FALSE	TRUE
92706	68.0	9.4	68.0	Moderate binc	N/A	N/A	N/A	N/A	Class 2 (le	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	2.4	1.2	FALSE	FALSE	N/A	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	5.41E-07	2.97E-06	FALSE	FALSE
502727	N/A	0.2	0.2	Non binder, w	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	10.0	0.3	FALSE	FALSE	N/A	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.00012	8.47E-07	FALSE	TRUE
86306	5.8	14.7	5.8	Non binder, w	N/A	-10000	LogRP	ER Gene ((	Class 3 (ur	Reactive u	N/A	N/A	Nitroso based reactivity	TRUE	6.4	0.5	FALSE	FALSE	Active	1	SN2|SN2 >	No alert fo	TRUE	SN1|SN1 >	SN1|SN1 >	TRUE	Alkyl and anyl	No alert found	Alkyl and a	Alkyl and a	No alert found	2.11E-06	1.64E-06	FALSE	FALSE
120680030	N/A	393000.0	393000.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	2284.9	0.0	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Benzenesulfor	No alert found	No alert found	H-acceptor	No alert found	5.42E-08	2.78E-07	FALSE	FALSE
60223952	N/A	0.0	0.0	Non binder, M	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	0.0	996.4	TRUE	TRUE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Benzenesulfor	No alert found	No alert found	H-acceptor	No alert found	0.001831	1.40E-01	TRUE	FALSE
2687914	N/A	2623.7	2623.7	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	73.3	0.0	FALSE	FALSE	N/A	N/A	No alert fo	Acylation|A	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	5.14E-09	1.93E-07	FALSE	FALSE
59507	0.0	2.9	0.0	Weak binder,	N/A	-3.22	LogRP	ER Gene ((	Class 2 (le	Phenols ar	Narcos	N/A	Polar narcosis	FALSE	0.0	3254.4	TRUE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Halogenated I	No alert found	No alert found	No alert fo	AN2	AN2 >>	7.59E-07	5.62E-07	FALSE	FALSE
7534943	1.8	0.6	1.8	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Reactive u	N/A	N/A	Ester narcosis	TRUE	22.7	0.1	FALSE	FALSE	N/A	1	Michael Ac	Acylation|A	TRUE	No alert fo	Michael ad	#####	No alert found	No alert found	No alert found	No alert fo	AN2|AN2 >>	1.02E-05	5.59E-07	FALSE	TRUE
70788306	N/A	0.1	0.1	Non binder, w	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	9.0	0.3	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	Michael ad	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000243	7.40E-06	FALSE	TRUE
1740198	0.7	1.2	0.7	Non binder, w	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	0.7	4.3	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000349	4.33E-04	FALSE	TRUE
132274	N/A	1.1	1.1	Moderate binc	N/A	N/A	N/A	N/A	Class 2 (le	Phenols ar	N/A	N/A	Polar narcosis	FALSE	0.0	394.9	TRUE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	o-phenylpheno	No alert found	No alert found	No alert fo	AN2	AN2 >>	1.08E-06	6.69E-07	FALSE	FALSE
93583	N/A	119.9	119.9	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Aldehydes	N/A	N/A	Ester narcosis	FALSE	5.0	0.6	FALSE	FALSE	N/A	1	Schiff base	Schiff Base	TRUE	No alert fo	Michael ad	#####	Simple aldehy	No alert found	Simple ald	Simple ald	No alert found	6.5E-07	2.97E-06	FALSE	FALSE
3738009	N/A	0.8	0.8	Non binder, w	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	39.4	0.1	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Hydrazine (Ge	No alert found	Hydrazine	H-acceptor	No alert found	0.0001	3.65E-06	FALSE	TRUE
68877292	N/A	0.2	0.2	Strong binder,	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	9.9	0.3	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000637	1.39E-05	FALSE	TRUE
3407429	N/A	0.2	0.2	Strong binder,	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	0.4	6.9	FALSE	FALSE	N/A	1	No alert fo	No alert fo	FALSE	Radical	Ra	No alert fo	#####	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000687	1.43E-05	FALSE	TRUE
66068846	N/A	0.2	0.2	Strong binder,	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	9.9	0.3	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000687	1.43E-05	FALSE	TRUE
70146133	N/A	0.0	0.0	Non binder, M	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	0.2	15.3	TRUE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Benzenesulfor	No alert found	No alert found	1-phenoxy	No alert found	0.002703	1.24E+00	TRUE	FALSE
103242	0.1	0.0	0.1	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Esters	N/A	N/A	Diester toxicity	FALSE	0.1	27.9	TRUE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Structural aler	No alert found	No alert found	H-acceptor	No alert found	1.71E-05	4.36E-08	FALSE	TRUE
27178161	N/A	0.0	0.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Esters	N/A	N/A	Diester toxicity	FALSE	0.0	323047.2	TRUE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Phtalate (or bi	No alert found	No alert found	H-acceptor	No alert found	2.93E-05	1.17E-07	FALSE	TRUE
111966	N/A	23159.5	23159.5	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	172.8	0.0	FALSE	FALSE	Active	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	1.55E-08	2.78E-07	FALSE	FALSE
107186	0.3	2.1	0.3	Non binder, no	N/A	N/A	N/A	N/A	Class 3 (ur	Alpha-, Be	Reactiv	N/A	Alkylation / arylation based reactivity	FALSE	0.0	172.7	TRUE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	7.02E-09	2.86E-07	FALSE	FALSE
78933	400.0	2718.0	400.0	Non binder, no	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	5.8	0.5	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	8.13E-09	2.40E-07	FALSE	FALSE
541913	N/A	0.1	0.1	Non binder, w	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	8.0	0.4	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.00041	1.39E-06	FALSE	TRUE
122689	N/A	0.4	0.4	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Esters	N/A	N/A	Acrylate toxicity	FALSE	8.0	0.4	FALSE	FALSE	N/A	1	Michael Ac	Michael ad	TRUE	No alert fo	Michael ad	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	1.23E-05	2.59E-07	FALSE	TRUE
111900	6010.0	35577.3	6010.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	Narcos	N/A	Nonpolar narcosis	FALSE	44.8	0.1	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	9.1E-09	1.72E-07	FALSE	FALSE
124130	7.9	21.0	7.9	Non binder, no	N/A	N/A	N/A	N/A	Class 3 (ur	Aldehydes	N/A	N/A	Carbonyl reactivity (aldehyde eq. # 3)	FALSE	2.0	1.5	FALSE	FALSE	Active	N/A	Schiff base	Schiff Base	TRUE	No alert fo	Schiff base	#####	Simple aldehy	No alert found	Simple ald	Simple ald	No alert found	1.46E-07	1.84E-07	FALSE	FALSE
3147759	100.0	0.0	100.0	Strong binder,	0.001<R	N/A	N/A	N/A	Class 3 (ur	Aldehydes	N/A	N/A	Uncoupler of oxidative phosphorylation	TRUE	10921.7	0.0	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	Radical|Ra	No alert fo	#####	No alert found	No alert found	No alert fo	No alert fo	No alert fo	No alert found	0.004143	4.23E-05	TRUE	FALSE
600146	N/A	36566.2	36566.2	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	365.7	0.0	FALSE	FALSE	N/A	N/A	Schiff base	Schiff Base	TRUE	No alert fo	No alert fo	#####	Halogenated I	No alert found	No alert found	1-phenoxy	No alert fo	No alert found	8.61E-09	2.79E-07	FALSE	FALSE
121915	907.0	2842.8	907.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	17.9	0.2	FALSE	FALSE	Active	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	2.6E-08	1.77E-07	FALSE	FALSE
3319311	100.0	0.0	100.0	Non binder, M	N/A	N/A	N/A	N/A	Class 5 (N	Esters	N/A	N/A	Diester toxicity	FALSE	4.2	0.7	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	SN1|SN1 >	SN1|SN1 >	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	1.05E-05	2.39E-08	FALSE	TRUE
80546	2.0	1.3	2.0	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Aldehydes	N/A	N/A	Nonpolar narcosis	FALSE	11.5	0.3	FALSE	FALSE	Active	1	Schiff base	Schiff Base	TRUE	No alert fo	Michael ad	#####	Simple aldehy	No alert found	Simple ald	Simple ald	No alert found	5.89E-05	1.15E-06	FALSE	TRUE
124196	N/A	8.4	8.4	Non binder, no	N/A	N/A	N/A	N/A	Class 3 (ur	Aldehydes	N/A	N/A	Carbonyl reactivity (aldehyde eq. # 3)	FALSE	5.7	0.5	FALSE	FALSE	Active	N/A	Schiff base	Schiff Base	TRUE	No alert fo	Schiff base	#####	Simple aldehy	No alert found	Simple ald	Simple ald	No alert found	2.29E-06	1.62E-06	FALSE	FALSE
108941	N/A	18.9	18.9	Weak binder,	N/A	-10000	LogRP	ER Gene ((	Class 2 (le	Phenols ar	N/A	N/A	Nonpolar narcosis	FALSE	0.5	6.2	FALSE	FALSE	N/A	None	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	7.53E-07	2.16E-06	FALSE	FALSE
81141	N/A	1.0	1.0	Non binder, w	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Reactive dinitroaromatic group	TRUE	3.4	0.9	FALSE	FALSE	N/A	1	No alert fo	No alert fo	FALSE	Radical|Ra	No alert fo	#####	No alert found	No alert found	No alert fo	No alert fo	No alert fo	No alert found	0.000924	2.77E-05	FALSE	TRUE
4191735	N/A	2.4	2.4	Moderate binc	N/A	N/A	N/A	N/A	Class 2 (le	Phenols ar	N/A	N/A	Ester narcosis	FALSE	0.5	5.8	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	AN2|AN2 >	SN1|SN1 >	TRUE	Primary aroma	No alert found	No alert found	Anthrones	H-acceptor	No alert found	1.11E-07	1.61E-07	FALSE	FALSE
2210799	2.8	96.7	2.8	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Reactive u	N/A	AChE inhibition	Alkylation / arylation based reactivity	TRUE	0.1	21.1	TRUE	TRUE	N/A	1	SN2|SN2 >	SN2|SN2 >	TRUE	No alert fo	SN1|SN1 >	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	1.79E-07	5.32E-07	FALSE	FALSE
57090	N/A	0.4	0.4	Non binder, M	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Quaternary ammonium compounds	TRUE	0.1	26.4	TRUE	TRUE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.000262	1.82E-06	FALSE	TRUE
88197	100.0	1319.0	100.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	1.5	2.0	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	2.87E-08	1.33E-07	FALSE	FALSE
27138314	N/A	5.8	5.8	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Esters	N/A	N/A	Diester toxicity	FALSE	6.6	0.5	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000495	1.24E-04	FALSE	TRUE
139059	N/A	316000.0	316000.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	1765.1	0.0	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	4.08E-08	2.79E-07	FALSE	FALSE
107460	0.5	0.2	0.5	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A		TRUE	6.8	0.0	FALSE	FALSE	N/A	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	7.80E-06	4.60E-09	FALSE	FALSE
3234853	N/A	0.0	0.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Esters	N/A	N/A	Ester narcosis	FALSE	0.0	8931706465.9	TRUE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	4.79E-05	1.83E-07	FALSE	TRUE
13676910	N/A	0.0	0.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Alkylation / arylation based reactivity	TRUE	0.1	53.3	TRUE	TRUE	N/A	N/A	No alert fo	No alert fo	FALSE	AN2|AN2 >	No alert fo	#####	Quinones (Ge	No alert found	No alert found	Anthrones	H-acceptor	No alert found	0.000231	7.24E-07	FALSE	TRUE
2379795	N/A	0.0	0.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Alkylation / arylation based reactivity	TRUE	3.8	0.8	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	Michael ad	Michael ad	#####	alpha,beta-un	No alert found	AN2	AN2 >>	0.00386	1.22E-04	TRUE	FALSE
108032	205.0	810.8	205.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	3.1	1.0	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	2.17E-08	1.13E-07	FALSE	FALSE
53894238	N/A	0.0	0.0	Non binder, M	N/A	N/A	N/A	N/A	Class 5 (N	Esters	N/A	N/A	Diester toxicity	FALSE	0.0	##########	TRUE	FALSE	Active	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Phtalate (or bi	No alert found	No alert found	H-acceptor	No alert found	2.87E-05	1.07E-07	FALSE	TRUE
541059	1.6	0.1	100.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A		TRUE	481.4	0.0	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	4.30E-06	2.50E-07	FALSE	FALSE
106945	24.3	91.8	24.3	Non binder, no	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	Narcos	N/A	Nonpolar narcosis	FALSE	1.5	1.7363E+00	FALSE	FALSE	N/A	1	SN2|SN2 >	SN2|SN2 >	TRUE	SN2|SN2 >	SN2|SN2 >	TRUE	Aliphatic halo	SN2|SN2 >>	Alk	Aliphatic ha	Aliphatic ha	No alert found	5.48E-08	2.14E-08	FALSE	FALSE
33204761	N/A	0.0	100.0	Non binder, w	N/A	0	LogRB,	TIMES Tra	Class 5 (N	Reactive u	N/A	N/A		TRUE	5.5	0.1	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	1.10E-06	6.70E-08	FALSE	FALSE
35958306	N/A	0.0	0.0	Non binder, in	Not Activ	N/A	N/A	N/A	Class 5 (N	Phenols ar	N/A	N/A	Polar narcosis	FALSE	0.0	600.6	TRUE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.074781	2.47E-03	TRUE	FALSE
25167322	N/A	0.0	0.0	Non binder, M	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	0.0	2842398.7	TRUE	TRUE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	1-phenoxy	No alert found	0.001745	1.65E-00	TRUE	FALSE
118821	820.0	0.0	820.0	Non binder, in	N/A	-10000	LogRB,	ER Binding	Class 5 (N	Phenols ar	N/A	N/A	Polar narcosis	FALSE	24875.0	0.0	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.093649	3.04E-03	TRUE	FALSE
141435	100.0	88033.2	100.0	Non binder, no	N/A	-10000	LogRP	ER Gene ((	Class 5 (N	Reactive u	Narcotic A	N/A	Nonpolar narcosis	FALSE	1.6	1.8	FALSE	FALSE	Active	N/A	No alert fo	No alert fo	FALSE	Schiff base	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	6.13E-09	6.08E-08	FALSE	FALSE
81152	3.7	0.9	3.7	Non binder, w	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Reactive dinitroaromatic group	TRUE	125.1	0.0	FALSE	FALSE	N/A	1	No alert fo	No alert fo	FALSE	Radical|Ra	No alert fo	#####	No alert found	No alert found	No alert fo	No alert fo	No alert fo	No alert found	0.000316	1.28E-05	FALSE	TRUE
25322172	N/A	0.0	0.0	Non binder, w	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	0.0	6507.7	TRUE	TRUE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.001178	7.16E-01	TRUE	FALSE
57855773	N/A	0.0	0.0	Non binder, w	Not Activ	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	0.0	16422.3	TRUE	TRUE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.003294	1.57E+00	TRUE	FALSE
112276	82.0	353000.0	82.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	Narcos	N/A	Nonpolar narcosis	FALSE	928.2	0.0	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	4.11E-09	1.43E-07	FALSE	FALSE
74862	N/A	598.7	598.7	Non binder, no	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	24.6	0.1	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	5.45E-09	7.25E-09	FALSE	FALSE
271896	13.9	40.2	13.9	Non binder, w	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	Reactiv	N/A	Nonpolar narcosis	FALSE	2.9	1.0	FALSE	FALSE	Active	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	Hydrazine (Ge	No alert found	Hydrazine	H-acceptor	No alert found	1.78E-07	4.00E-07	FALSE	FALSE
112389	32.3	14.4	32.3	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Nonpolar narcosis	TRUE	64.6	0.0	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	2.07E-06	1.04E-05	FALSE	FALSE
112345	1150.0	5676.3	1150.0	Non binder, no	N/A	N/A	N/A	N/A	Class 1 (n	Basesurfac	Narcos	N/A	Nonpolar narcosis	FALSE	8.0	0.4	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	8.77E-09	6.83E-08	FALSE	FALSE
4035896	N/A	0.0	0.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Reactive u	N/A	N/A	Isocyanate based reactivity	TRUE	0.2	19.5	TRUE	TRUE	N/A	N/A	No alert fo	Acylation|A	TRUE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	H-acceptor	No alert found	0.000166	6.09E-07	FALSE	TRUE
552307	957.0	2201.9	957.0	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Reactive u	N/A	N/A	Acylation based reactivity	TRUE	27.4	0.1	FALSE	FALSE	Active	N/A	Acylation|A	Acylation|A	TRUE	No alert fo	SN1|SN1 >	#####	Aromatic mon	No alert found	No alert found	Aromatic n	Aromatic n	No alert found	1.22E-06	8.46E-06	FALSE	FALSE
16294750	N/A	0.0	0.0	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	1.4	2.2	FALSE	FALSE	N/A	N/A	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	0.000562	3.73E-06	FALSE	TRUE
34590948	N/A	19329.2	19329.2	Non binder, no	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	130.6	0.0	FALSE	FALSE	Active	1	No alert fo	No alert fo	FALSE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	No alert fo	No alert found	1.25E-08	1.86E-07	FALSE	FALSE
85449	N/A	132.9	132.9	Non binder, w	Not Activ	N/A	N/A	N/A	Class 3 (ur	Reactive u	N/A	N/A	Acylation based reactivity	TRUE	2.7	1.1	FALSE	FALSE	N/A	N/A	Acylation|A	Acylation|A	TRUE	No alert fo	No alert fo	#####	No alert found	No alert found	No alert found	No alert fo	Ac-SN2	Ac-S	1.75E-06	1.32E-05	FALSE	FALSE
5521313	#####	4.8	10000.0	Non binder, w	N/A	N/A	N/A	N/A	Class 5 (N	Basesurfac	N/A	N/A	Nonpolar narcosis	FALSE	18279.1	0.0	FALSE	FALSE	N/A	N/A	No alert fo	Acylation|A	FALSE	SN1|SN1 >	SN1|SN1 >	TRUE	Polycyclic Aro	SN1|SN1 >>	Alk	Polycyclic A	H-acceptor	No alert found	0.00012	2.84E-05	FALSE	TRUE
106923	N/A	128.0	0.0	Non binder, w	N/A	N/A	N/A	N/A	Class 3 (ur	Reactive u	N/A	N/A	Alkylation / arylation based reactivity	TRUE	0.0	2.7	FALSE	FALSE	N/A	N/A	SN2|SN2 >	SN2|SN2 >	TRUE	Radical|Ra	No alert fo	#####	No alert found	No alert found	No alert fo	No alert fo	No alert fo	No alert found	N/A	N/A	N/A	N/A

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS							RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailability ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
577117	1	2	259.4	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
36653824	1	2	50.5	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
92706	1	2	16187.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
502727	1	2	73.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
86306	1	1	4154.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
12068030	1	1	161494.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
60223952	2	3	4.8	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
2687914	1	1	1705306.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
59507	1	1	11539.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
7534943	1	2	862.5	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
70788306	1	2	33.7	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1740198	1	2	25.1	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
132274	1	2	8103.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
93583	1	1	13484.8	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3738009	1	2	87.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
68877292	1	3	13.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
3407429	1	3	12.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
66068846	1	3	12.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
70146133	2	3	3.2	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
103242	1	2	511.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
27178161	3	2	299.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A			N/A	N/A
111966	1	1	565378.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
107186	1	1	1247860.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
78933	3	1	1077487.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
541913	1	2	21.3	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
122689	1	2	711.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
111900	1	1	963104.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
124130	1	1	60179.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3147759	1	3	2.1	100 - 1,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
600146	1	1	1017606.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
121915	3	1	336659.5	100,000 - 1,000,000	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3319311	1	1	835.7	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
80546	1	2	148.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
124196	1	1	3832.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
108941	1	1	11634.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
81141	1	2	9.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
4191735	1	2	79146.0	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
2210799	1	3	48978.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	local RQ <1	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
57090	1	3	33.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
88197	1	1	304778.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
27138314	1	2	17.7	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
139059	1	1	214912.2	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
107460	1	1	1127.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3234853	1	1	182.8	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
13676910	1	3	38.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
2379795	1	3	1.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
108032	1	1	404570.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
53894238	1	1	304.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
541059	1	1	2047.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
106945	1	1	159741.6	1,000,000 - 10,000,000	N/A	FALSE	TRUE	TRUE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A			N/A	N/A
33204761	1	1	7924.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
35958306	1	3	0.1	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
25167322	2	3	5.0	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
118821	1	3	0.1	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
141435	1	1	1428135.3	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
81152	1	2	27.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
25322172	1	3	7.4	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
57855773	1	3	2.7	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
112276	1	1	2133142.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
74862	1	1	1606426.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
271896	1	1	49091.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112389	1	1	4224.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112345	1	1	998565.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4035896	1	3	52.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
552307	3	1	7167.5	1,000 - 10,000	FALSE	TRUE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
16294750	1	2	15.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
34590948	1	1	698753.7	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
85449	3	1	5018.8	1,000 - 10,000	FALSE	TRUE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
5521313	2	2	72.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
106923	N/A	N/A	N/A	N/A	N/A	N/A	FALSE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A

| CHEMICAL IDENTITY | | | | | EXPOSURE | | | | | | | | | | | | FATE | | | | | | | | | | | |

| HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE		AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emissio n High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailability ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
110009	1	1	321760.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
98544	1	1	3498.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
149304	1	3	13858.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
2492264	1	3	659.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
139071	1	3	630.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
29761215	2	2	318.4	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
79436	1	1	11971.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
140669	2	3	51.8	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
123546	1	1	96447.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
118569	1	3	41.0	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A			N/A	N/A
2082793	3	1	0.3	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	3	1	low (up to far field)	N/A	N/A			N/A	N/A
25103586	1	2	91.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A			N/A	N/A
78671	2	1	12585.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
139082	1	3	86.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
112492	1	1	1005525.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
60242	1	1	1019789.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
64197	3	3	102495.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
95318	1	2	191.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
67561	3	1	618461.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
32072961	3	3	31.8	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
25155231	1	2	19.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
124414	1	1	618461.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
64186	3	1	99622.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
596032	1	3	90.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
96764	1	3	57.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
128392	1	2	102.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	moderate (mostly near fiel	local RQ >10	moderate (mostly near fiel	N/A	N/A	N/A	N/A
120401	1	1	32130.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
28777982	3	3	74.7	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
43048084	1	2	67.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112607	1	1	1814798.3	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
94109098	1	1	705.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
142789	1	1	46487.6	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
108101	1	1	424307.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
2627954	1	2	552.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
76039	1	2	386.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
67633572	1	2	46.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
124301	1	2	11.8	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	moderate (mostly near fiel	local RQ >10	moderate (mostly near fiel	N/A	N/A	N/A	N/A
19720457	1	3	0.7	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
108918	1	1	54794.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
141537	3	1	209769.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
75003	3	1	316286.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A			N/A	N/A
68425616	1	3	2.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
78400	1	1	2554573.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
5089225	1	3	0.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
77474	1	3	2.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
17418585	1	3	75.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
74964	1	1	390715.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Low current exposure, but h	ERC classified this substan	N/A	N/A
79209	1	1	2017462.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
107313	1	1	428332.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4051632	1	3	0.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
41484359	2	1	0.7	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	2	1	low (mostly near field)	N/A	N/A			N/A	N/A
546281	1	2	9.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
121142	2	2	14.1	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
107153	1	1	150943.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
1139306	1	2	93.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
79743	1	3	19.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
431038	1	1	949783.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
14233375	1	3	3.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
127684	2	1	95562.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
4151513	1	3	18.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
97530	1	1	59985.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
298077	1	2	33.0	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
124403	1	1	319174.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
38640629	1	2	21.4	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
7576650	1	2	86.7	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
26544387	1	2	63.1	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
25550985	1	3	12.3	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
25619561	2	3	1.6	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
7779502	1	3	1.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
28645514	1	3	1.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A

CHEMICAL IDENTITY					EXPOSURE											FATE																	
SUBSTANCE AND GROUPING FOR CMP					PERSISTENCE					EMISSION RATE (EA)						PHYSICO-CHEMICAL PROPERTIES											BIOACCUMULATION					
CAS	CMP Phase 3 Group	Substance Name	SMILES	Molecular Weight (g/mol)	Overall Persistence (hours)	Critically Long Overall Persistence	Selected Air Half life (hours)	Critically Long Half Life in Air		WWTP Removal (%)	Annual Tonnage (kilotonnes)	Annual tonnage after WWTP Removal (kilotonnes)	Large value for tonnage	Moderate value for tonnage	Low value for tonnage	Empirical LogKow	ACD Median Log D @ pH 7	Selected LogKow	ACD Water Sol. @ pH 7 (mg/L)	Empirical Water Sol. SRC Database (mg/L)	Empirical Water Sol. REACH Database (mg/L)	Selected Water Sol (mg/L)	LogKaw	Model BCF 5% Lipid Fish (L/kg)	Empirical BCF 5% Lipid Fish (L/kg)	Selected BCF 5% Lipid Fish (L/kg)	Half-Life 1 kg Mammal (days)	Half-life 1 kg Fish (days)					
5718263	Pigments and Dyes	1H-Indole-5-carboxylic acid, 2-[(1,5-dihydro-3-methyl-5-oxo-1-phen	COC(=O)c	415.5	19,079	TRUE	3.5	FALSE		83.2	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	3.6	3.6	1.8	N/A	N/A	1.8	-10.3	40453.5	N/A	40453.5	43.7	33.2					
95556	Aromatic Amines	Phenol, 2-amino-	Nc1ccccc1	109.1	796	FALSE	3.5	FALSE		61.5	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	0.6	0.7	0.6	8157.0	N/A	N/A	8157.0	-8.1	1.2	N/A	1.2	0.2	1.4					
36443682	Hindered phenols	Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-,	O=C(CCc1	586.8	7,126	TRUE	3.4	FALSE		80.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	6.6	6.6	0.1	N/A	N/A	0.1	N/A	517.6	12.0	12.0	N/A	N/A					
120241	Eugenol and Isoeugenol deriv	Benzeneacetic acid, 2-methoxy-4-(1-propenyl)phenyl ester	CC=Cc1cc	282.3	754	FALSE	3.4	FALSE		52.5	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	3.9	3.9	2.1	N/A	N/A	2.1	-5.0	2416.4	N/A	2416.4	0.4	86.8					
101144	Aromatic Amines	Benzenamine, 4,4'-methylenebis[2-chloro-	Nc1ccc(Cc	267.0	N/A	N/A	3.3	FALSE		0.0	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	3.7	3.7	10.2	N/A	N/A	10.2	-8.9	199.0	398.0	398.0	0.4	0.4					
126136	INDIVIDUAL - α-D-Glucopyra	α-D-Glucopyranoside, 6-O-acetyl-1,3,4-tris-O-(2-methyl-1-oxopropy	CC(=O)OC	846.9	651	FALSE	3.3	FALSE		69.5	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	7.3	7.3	2.6	N/A	N/A	2.6	-24.8	5083.7	N/A	5083.7	0.0	0.8					
37609259	Musks (Macro/Poly cyclic)	5-Cyclohexadecen-1-one	O=C1CCC	236.4	3,927	TRUE	3.2	FALSE		79.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.2	5.2	24.2	N/A	N/A	24.2	-1.5	22552.0	N/A	22552.0	0.5	707.4					
95330	Benzotriazoles & benzothiazo	2-Benzothiazolesulfenamide, N-cyclohexyl-	N(c(c(S1)c	264.4	1,423	FALSE	3.2	FALSE		18.8	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.2	4.2	36.5	N/A	N/A	36.5	N/A	90.4	N/A	90.4	N/A	N/A					
301020	Fatty amides	9-Octadecenamide, (Z)-	CCCCCC(	281.5	1,481	TRUE	3.2	FALSE		85.5	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	6.8	6.8	1.0	N/A	N/A	1.0	-4.4	40198.3	N/A	40198.3	0.6	163.2					
542461	Musks (Macro/Poly cyclic)	9-Cycloheptadecen-1-one, (Z)-	O=C1CCC	250.4	5,264	TRUE	3.2	FALSE		82.5	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.8	5.8	8.1	N/A	N/A	8.1	-1.4	37759.1	N/A	19796.3	0.5	1023.9					
103833	Aliphatic amines	Benzenemethanamine, N,N-dimethyl-	CN(Cc1cc	135.2	1,278	FALSE	3.1	FALSE		17.3	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	2.0	0.0	2.0	925117.3	N/A	N/A	925117.3	-3.9	5.8	25.4	25.4	1.5	7.6					
100005	Nitrobenzenes	Benzene, 1-chloro-4-nitro-	Clc1ccc(cc	157.6	2,209	TRUE	1497.4	TRUE		14.1	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	2.4	2.5	2.4	321.7	N/A	N/A	321.7	-3.7	11.1	112.2	112.2	6.9	24.9					
4174098	Heterocycles	3H-Pyrazol-3-one, 2,4-dihydro-4-[(5-hydroxy-3-methyl-1-phenyl-1H-	CC1=NN(C	358.4	2,170	TRUE	3.1	FALSE		35.7	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.8	2.8	6.6	N/A	N/A	6.6	-16.5	8057.0	N/A	8057.0	17.7	18.6					
53980884	Fatty acids and salts	2-Cyclohexene-1-octanoic acid, 5(or 6)-carboxy-4-hexyl-	CCCCCC(	352.5	193	FALSE	3.1	FALSE		83.2	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.0	2.0	19225.1	N/A	N/A	19225.1	-8.0	32210.4	N/A	32210.4	0.1	144.4					
77098	Furan and derivatives	1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-	Oc1ccc(cc	318.3	813	FALSE	3.1	FALSE		15.1	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	2.4	3.1	2.4	119.0	N/A	N/A	119.0	-13.4	59.5	N/A	59.5	2.6	13.1					
120116	Eugenol and Isoeugenol deriv	Benzene, 2-methoxy-1-(phenylmethoxy)-4-(1-propenyl)-	CC=Cc1cc	254.3	851	FALSE	3.0	FALSE		51.1	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.1	4.1	3.5	N/A	N/A	3.5	-4.3	2260.1	N/A	2260.1	1.4	210.5					
112845	Fatty amides	13-Docosenamide, (Z)-	CCCCCC(	337.6	2,067	TRUE	3.0	FALSE		84.0	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	8.2	8.2	0.2	N/A	N/A	0.2	-3.9	5920.0	N/A	5920.0	0.6	516.0					
5064313	INDIVIDUAL - Nitrilotriacetic a	Glycine, N,N-bis(carboxymethyl)-, trisodium salt	OC(=O)CN	191.1	198	FALSE	2.9	FALSE		82.7	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	-5.9	-5.9	1000112.5	N/A	N/A	1000112.5	-14.3	1.0	N/A	1.0	0.1	0.8					
100403	INDIVIDUAL - Cyclohexene, 4	Cyclohexene, 4-ethenyl-	C=CC1CC	108.2	137	FALSE	2.9	FALSE		27.3	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	3.9	3.3	3.9	56.8	N/A	N/A	56.8	0.3	53.7	254.8	254.8	0.8	29.3					
80568	Terpenes & Terpenoids	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-	CC1=CCC	136.2	529	FALSE	2.8	FALSE		30.6	1 - 10	1 - 10	TRUE	FALSE	FALSE	4.8	4.1	4.8	71.5	N/A	N/A	71.5	1.1	3293.5	N/A	3293.5	2.0	249.7					
28984692	Heterocycles	4,4(5H)-Oxazoledimethanol, 2-(heptadecenyl)-	CCCCCC(	367.6	414	FALSE	2.8	FALSE		88.9	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.0	6.0	0.9	N/A	N/A	0.9	-6.6	21172.2	N/A	21172.2	1.2	151.1					
111422	Alkanolamines	Ethanol, 2,2'-iminobis-	OCCNCC(	105.1	145	FALSE	2.8	FALSE		82.7	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	-1.4	-3.1	-1.4	999885.2	N/A	N/A	999885.2	-8.8	1.0	N/A	1.0	1.0	0.8					
470406	Terpenes & Terpenoids	Cyclopropa[d]naphthalene, 1,1a,4,4a,5,6,7,8-octahydro-2,4a,8,8-te	CC1=CC(	204.4	20,668	TRUE	2.8	FALSE		75.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.1	6.1	0.4	N/A	N/A	0.4	0.9	32671.6	N/A	32671.6	4.2	502.9					
1533455	Stilbenes	Benzoxazole, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis-	c1ccc2c(c:	414.5	16,015	TRUE	2.7	FALSE		83.9	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.5	6.5	0.0	N/A	N/A	0.0	-12.3	20228.5	N/A	20228.5	3.8	7325.9					
3846717	Benzotriazoles & benzothiazo	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-	N/A	N/A	N/A	N/A	N/A	N/A		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A					
101371	Cyanurates	1,3,5-Triazine, 2,4,6-tris(2-propenyloxy)-	C=CCOc1	74.1	487	FALSE	2.7	FALSE		43.1	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.2	2.2	1847.8	N/A	N/A	1847.8	-4.8	8391.5	N/A	8391.5	2.9	84.4					
469614	Terpenes & Terpenoids	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramet	CC1=CCC	204.4	12,973	TRUE	2.7	FALSE		76.7	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	5.9	5.9	58.9	N/A	N/A	58.9	0.9	19935.8	N/A	19935.8	2.3	720.5					
639996	Terpenes & Terpenoids	Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)	C=CC1(C)	222.4	7,803	TRUE	2.6	FALSE		76.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.5	4.5	7.5	N/A	N/A	7.5	-2.8	14145.8	N/A	14145.8	0.1	225.2					
78422	Flame Retardants	Phosphoric acid, tris(2-ethylhexyl) ester	CCCCC(C	434.7	1,475	TRUE	2.6	FALSE		84.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	9.0	9.0	0.1	N/A	N/A	0.1	-5.5	1.0	22.0	22.0	10.4	38.6					
2478208	Pigments and Dyes	1H-Benz[de]isoquinoline-1,3(2H)-dione, 6-amino-2-(2,4-dimethylph	Cc1ccc(c(c	316.4	3,559	TRUE	2.6	FALSE		5.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	2.9	2.9	3.6	N/A	N/A	3.6	-10.0	19.0	N/A	19.0	5.1	39.6					
27193868	INDIVIDUAL - Dodecylphenol	Phenol, dodecyl-	CCCCCC(	262.4	657	FALSE	2.6	FALSE		82.2	< 0.0000001	< 0.0000001	FALSE	FALSE	TRUE	N/A	7.6	7.6	0.1	N/A	N/A	0.1	-3.2	21172.2	N/A	21172.2	0.7	239.5					
100378	Alkanolamines	Ethanol, 2-(diethylamino)-	OCCN(CC	117.2	604	FALSE	2.6	FALSE		82.8	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-2.0	-2.0	999973.5	N/A	N/A	999973.5	-6.9	1.0	7.8	7.8	1.5	1.5					
112696	Aliphatic amines	1-Hexadecanamine, N,N-dimethyl-	CCCCCC(	269.5	2,531	TRUE	2.6	FALSE		77.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	5.2	5.2	35.5	N/A	N/A	35.5	-1.0	22398.3	N/A	22398.3	1.3	266.2					
21564170	Benzotriazoles & benzothiazo	Thiocyanic acid, (2-benzothiazolylthio)methyl ester	N#CSCSc	238.3	1,275	FALSE	2.5	FALSE		17.2	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	3.3	2.9	3.3	168.7	N/A	N/A	168.7	-9.6	11.0	292.6	292.6	12.2	7.4					
66072386	Epoxides & glycidyl ethers	Oxirane, 2,2',2''-(methylidynetris(phenyleneoxymethylene))tris-	c1ccc(c(c1	460.5	7,331	TRUE	2.5	FALSE		51.0	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	3.3	3.3	20.6	N/A	N/A	20.6	-13.5	2700.2	N/A	2700.2	57.5	30.7					
13680358	Aromatic Amines	Benzenamine, 4,4'-methylenebis[2,6-diethyl-	CCc1cc(C	310.5	8,987	TRUE	2.5	FALSE		38.6	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.5	4.5	130.4	N/A	N/A	130.4	-7.9	38357.6	N/A	38357.6	31.2	26.6					
98000	Furan and derivatives	2-Furanmethanol	OCc1ccco	98.1	359	FALSE	2.5	FALSE		82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	0.3	0.2	0.3	27648.3	N/A	N/A	27648.3	-5.5	1.0	N/A	1.0	0.8	2.9					
6511399	Terpenes & Terpenoids	3-Cyclopentene-1-butanol, α,β,2,2,3-pentamethyl-	CC(CCC(	210.4	2,156	TRUE	2.4	FALSE		68.1	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	4.5	4.5	39.2	N/A	N/A	39.2	-2.7	6553.1	N/A	6553.1	2.6	114.4					
24448202	Acrylates/methylacrylates	2-Propenoic acid, 2-methyl-, (1-methylethylidene)bis(4,1-phenylene	O=C(C(=C	452.6	2,957	TRUE	2.4	FALSE		83.4	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	6.4	6.4	0.2	N/A	N/A	0.2	-9.1	40284.6	N/A	40284.6	1.3	72.0					
112903	Aliphatic amines	9-Octadecen-1-amine, (Z)-	CCCCCC(	267.5	753	FALSE	2.4	FALSE		87.5	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	4.0	4.0	374.1	N/A	N/A	374.1	-1.5	20228.5	N/A	20228.5	1.2	1129.0					
29350730	Terpenes & Terpenoids	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1α,4a	CC1CCC2	206.4	3,658	TRUE	2.4	FALSE		77.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.2	6.2	1.1	N/A	N/A	1.1	1.3	36861.9	N/A	36861.9	2.3	2002.4					
102716	Alkanolamines	Ethanol, 2,2',2''-nitrilotris-	OCCN(CC	344.9	242	FALSE	2.3	FALSE		82.7	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	-1.0	-2.0	-1.0	1000079.7	N/A	N/A	1000079.7	-10.5	1.0	3.9	3.9	0.6	0.8					
68966381	Alkyl imidazolines and salts	1H-Imidazole-1-ethanol, 4,5-dihydro-2-isoheptadecyl-	OCCN1C(	352.6	1,849	TRUE	2.3	FALSE		81.8	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.2	5.2	126.4	N/A	N/A	126.4	-6.6	16790.9	N/A	16790.9	0.8	270.0					
471534	Terpenes & Terpenoids	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo, (3β,20β)	O=C1C=C	470.7	7,677	TRUE	2.3	FALSE		3.4	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.2	4.2	9.8	N/A	N/A	9.8	-11.1	1.0	N/A	1.0	1.3	951.8					
4572092	Terpenes & Terpenoids	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-, compd. wit	O=C1C=C	470.7	7,677	TRUE	2.3	FALSE		3.4	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.2	4.2	9.8	N/A	N/A	9.8	-11.1	36071.8	N/A	36071.8	1.3	951.8					
31135576	Alkyl imidazolines and salts	1H-Benzimidazolesulfonic acid, 2-heptadecyl-1-[(sulfophenyl)methy	CCCCCC(	606.8	4,892	TRUE	2.3	FALSE		68.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	3.2	3.2	2.6	N/A	N/A	2.6	-15.2	7422.5	N/A	7422.5	8.6	224.3					
26266773	Resins & rosins	1-Phenanthrenemethanol, dodecahydro-1,4a-dimethyl-7-(1-methyle	OCC1(C)C	290.5	9,848	TRUE	2.3	FALSE		82.6	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.5	6.5	0.6	N/A	N/A	0.6	-2.7	37966.0	N/A	37966.0	4.2	699.2					
4979322	Benzotriazoles & benzothiazo	2-Benzothiazolesulfenamide, N,N-dicyclohexyl-	C1CCC(C	346.6	870	FALSE	2.3	FALSE		44.6	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	4.8	6.1	4.8	1.1	N/A	N/A	1.1	-7.0	26996.0	1140.0	1140.0	3.6	62.5					
78217	Quaternary ammonium comp	Morpholinium, 4-ethyl-4-hexadecyl-, ethyl sulfate	CCCCCC(	341.6	4,628	TRUE	2.3	FALSE		83.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	2.8	2.8	0.1	N/A	N/A	0.1	-11.2	34190.8	N/A	34190.8	N/A	562.2					
134098	Aromatic Amines	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, 2-aminobenzoate	CC1CCC(	275.4	1,551	TRUE	2.2	FALSE		42.5	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.5	5.5	0.5	N/A	N/A	0.5	-5.5	37096.4	N/A	37096.4	0.8	77.2					
80584903	Benzotriazoles & benzothiazo	1H-Benzotriazole-1-methanamine, N,N-bis(2-ethylhexyl)-4-methyl-	CCCCC(C	386.6	9,017	TRUE	2.2	FALSE		83.9	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	7.5	7.5	0.6	N/A	N/A	0.6	-5.4	17600.2	N/A	17600.2	8.6	555.0					
80595740	Benzotriazoles & benzothiazo	1H-Benzotriazole-1-methanamine, N,N-bis(2-ethylhexyl)-5-methyl-	CCCCC(C	386.6	9,017	TRUE	2.2	FALSE		83.9	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	7.5	7.5	0.6	N/A	N/A	0.6	-5.4	17600.2	N/A	17600.2	4.1	555.0					
94270867	Benzotriazoles & benzothiazo	1H-Benzotriazole-1-methanamine, N,N-bis(2-ethylhexyl)-ar-methyl-	CCCCC(C	386.6	9,017	TRUE	2.2	FALSE		83.9	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	7.5	7.5	0.6	N/A	N/A	0.6	-5.4	17600.2	N/A	17600.2	4.1	555.0					
101962	Aromatic Amines	1,4-Benzenediamine, N,N'-bis(1-methylpropyl)-	CCC(Nc1c	215.9	2,371	TRUE	2.2	FALSE		16.8	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	1.9	1.9	15492.5	N/A	N/A	15492.5	-6.1	161.9	N/A	161.9	7.5	20.9					
632519	Arenes	Benzene, 1,1',1'',1'''-(1,2-ethenediylidene)tetrakis-	c1ccc(cc1)	332.5	1,549	TRUE	2.2	FALSE		82.9	0.00001 - 0.0001	0.000001 - 0.0	FALSE	FALSE	TRUE	N/A	7.3	7.3	0.0	N/A	N/A	0.0	-5.0	39943.5	N/A	39943.5	8.0	334.4					
514512	Terpenes & Terpenoids	4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-	CC1CCC2	204.4	14,175	TRUE	2.2	FALSE		72.0	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.5	5.5	6.8	N/A	N/A	6.8	1.0	24244.2	N/A	24244.2	1.1	703.8					
77736	INDIVIDUAL - 4,7-Methano-1	4,7-Methano-1H-indene, 3a,4,7,7a-tetrahydro-	C1=CC2C	132.2	268	FALSE	2.2	FALSE		19.7	10 - 100	10 - 100	TRUE	FALSE	FALSE	N/A	3.0	3.0	98.0	N/A	N/A	98.0	0.4	74.6	678.9	678.9	0.0	236.9					
118967	Nitrobenzenes	Benzene, 2-methyl-1,3,5-trinitro-	O=N(=O)c:	227.1	6,576	TRUE	1865.8	TRUE		4.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	1.6	1.8	1.6	140.1	N/A	115	115.0	-6.1	3.0	338.0	338.0	2.3	7.9					
489849	Terpenes & Terpenoids	Azulene, 1,4-dimethyl-7-(1-methylethyl)-	CC(c1ccc(	198.3	2,704	TRUE	2.2	FALSE		76.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.1	5.1	2.4	N/A	N/A	2.4	-1.3	26306.2	N/A	26306.2	3.6	902.3					
489407	Terpenes & Terpenoids	1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetra	CC1CCC2	204.4	16,651	TRUE	2.1	FALSE		76.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.3	6.3	1.2	N/A	N/A	1.2	1.0	34481.8	N/A	34481.8	1.1	1284.4					

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	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emissio n High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailability ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
5718263	1	3	1.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
95556	1	3	79672.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
36443682	1	3	1.4	100 - 1,000	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
120241	1	1	1554.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
101144	N/A	3	N/A	N/A	FALSE	N/A	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A			N/A	N/A
126136	1	1	4552.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
37609259	1	2	17.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
95330	1	1	4928.0	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
301020	2	2	204.0	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
542461	1	3	6.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
103833	1	1	19506.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
100005	1	2	863.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
4174098	1	3	57.1	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
53980884	1	2	115.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	greater potential for local ex	ERC classified this substan	N/A	N/A
77098	1	3	4721.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
120116	1	2	356.2	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112845	3	2	95.8	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
5064313	1	1	270316.0	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
100403	1	1	17842.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
80568	1	2	878.4	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
28984692	1	3	39.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
111422	1	1	436335.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
470406	1	3	4.3	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
1533455	1	3	0.0	100 - 1,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
3846717	2	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	2	3	high (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
101371	1	2	458.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
469614	1	2	9.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
639996	1	3	4.3	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
78422	1	2	410.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
2478208	1	3	212.0	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
27193868	1	3	12.0	< 0.0000001	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
100378	1	1	215203.0	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112696	2	3	7.1	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
21564170	1	3	22.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
66072386	1	3	0.1	1,000 - 10,000	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
13680358	1	3	2.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
98000	1	1	313932.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
65113997	1	2	197.0	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
24448202	1	2	232.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
112903	1	3	5.3	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
29350730	1	3	8.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
102716	1	1	3146535.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
68966381	1	3	10.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
471534	1	3	0.1	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
4572092	1	3	0.1	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
31135576	1	3	1.5	10,000 - 100,000	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
26266773	1	3	1.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
4979322	1	2	28.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
78217	1	2	18.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	2	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
134098	1	3	13.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
80584903	1	3	1.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
80595740	1	3	1.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
94270867	1	3	1.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
101962	2	2	12.6	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
632519	1	2	61.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
514512	1	3	6.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
77736	1	1	9174.4	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
118967	2	2	66.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
489849	1	2	10.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
489407	1	3	2.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A

| CHEMICAL IDENTITY | | | | | EXPOSURE | | | | | | | | | | | | FATE | | | | | | | | | | | |

| HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailability ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
288880	1	1	616571.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
63449683	1	3	423.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
65405847	1	2	195.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
122203	1	1	2710463.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
66327546	1	2	256.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
15708415	1	1	N/A	N/A	TRUE	N/A	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3081149	1	3	6.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
7159905	1	3	3.6	10,000 - 100,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
78513	1	3	34495.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
96695	1	3	1.1	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
22451736	1	2	39.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
489861	1	2	17.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
2475458	1	3	1770.1	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
27136738	1	3	13.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
21265509	2	1	N/A	N/A	TRUE	N/A	TRUE	FALSE	FALSE	TRUE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
110918	1	1	297742.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
96457	1	1	972338.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1335940	1	2	151.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
7779308	1	2	151.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
87445	1	3	7.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
15647082	1	1	6098.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
111400	1	1	623937.2	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
4630073	1	3	7.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
5285609	1	3	1.0	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
1.08E+08	1	2	43.3	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
57976	1	2	14.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
95385	1	3	15.8	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A			N/A	N/A
21652277	1	3	15.8	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
91667	1	1	3708.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
110850	1	1	1922328.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3691121	1	3	7.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
95545	1	3	53158.1	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
60004	1	1	121852.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
64028	1	1	990308.7	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
6408726	1	3	3.8	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
463401	1	3	2.0	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
19286750	1	3	18.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
91441	1	1	12183.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A
25428437	1	2	31.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
122394	1	2	90.4	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
81481	1	3	6.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
108463	1	1	89197.2	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
87661	1	1	51522.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
121697	1	1	4656.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
2387033	1	3	3.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
74884	1	3	710731.6	>100,000,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
15791783	1	3	5.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
85609	1	3	0.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
52474609	1	2	306.3	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
58965665	1	1	42.8	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
52475862	1	2	306.3	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
37677148	1	1	947.0	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1843034	1	3	0.1	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
28173593	1	3	1.0	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
117986	1	2	58.7	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
101906	1	1	405615.0	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	Low current exposure, but h	ERC classified this substan	N/A	N/A
42373046	1	3	6.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
1843056	1	3	43.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A			N/A	N/A
2669469	1	3	28.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
793248	3	2	34.7	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A			N/A	N/A

CHEMICAL IDENTITY					EXPOSURE										FATE																	
SUBSTANCE AND GROUPING FOR CMP					PERSISTENCE				EMISSION RATE (EA)						PHYSICO-CHEMCIAL PROPERTIES								BIOACCUMULATION										
CAS	CMP Phase 3 Group	Substance Name	SMILES	Molecular Weight (g/mol)	Overall Persistence (hours)	Critically Long Overall Persistence	Selected Air Half life (hours)	Critically Long Half Life in Air	WWTP Removal (%)	Annual Tonnage (kilotonnes)	Annual tonnage after WWTP Removal (kilotonnes)	Large value for tonnage	Moderate value for tonnage	Low value for tonnage	Empirical LogKow	ACD Median Log D @ pH 7	Selected LogKow	ACD Water Sol. @ pH 7 (mg/L)	Empirical Water Sol. SRC Database (mg/L)	Empirical Water Sol. REACH Database (mg/L)	Selected Water Sol (mg/L)	LogKaw	Model BCF 5% Lipid Fish (L/kg)	Empirical BCF 5% Lipid Fish (L/kg)	Selected BCF 5% Lipid Fish (L/kg)	Half-Life 1 kg Mammal (days)	Half-life 1 kg Fish (days)						
6858497	Pigments and Dyes	Propanedinitrile, [[4-[ethyl[2-[[(phenylamino)carbonyl]oxy]ethyl]amin	CCN(c1cc	374.5	5,016	TRUE	1.1	FALSE	51.0	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.6	4.6	2.0	N/A	N/A	2.0	-14.3	2700.2	N/A	2700.2	40.7	4.1						
88846	Terpenes & Terpenoids	Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethyl)de	CC(=C1C(	204.4	2,667	TRUE	1.1	FALSE	82.8	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.6	5.6	3.0	N/A	N/A	3.0	1.7	38349.3	N/A	38349.3	2.1	1934.9						
90937	INDIVIDUAL - Methanone, bis	Methanone, bis[4-(diethylamino)phenyl]-	CCN(c1cc	324.5	7,350	TRUE	1.1	FALSE	24.0	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	5.0	5.0	36.5	N/A	N/A	36.5	-7.2	12423.0	N/A	12423.0	0.3	43.6						
72391243	Anthraquinones	Benzenesulfonic acid, [[(chloroacetyl)amino]methyl][4-[[4-(cyclohex	ClCC(=O)N	688.2	13,819	TRUE	1.1	FALSE	1.2	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	1.0	1.0	3.1	N/A	N/A	3.1	-28.3	519.1	N/A	519.1	148.8	2.8						
28768323	Epoxides & glycidyl ethers	Oxiranemethanamine, N,N'-(methylenedi-4,1-phenylene)bis[N-(oxir	O1CC1CN	422.5	21,321	TRUE	1.0	FALSE	1.6	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	2.5	2.5	475.9	N/A	N/A	475.9	-14.5	18.2	N/A	18.2	9.9	3.4						
121824	Triazoles	1,3,5-Triazine, hexahydro-1,3,5-trinitro-	O=N(=O)N	222.1	1,148	FALSE	1.0	FALSE	13.8	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	0.9	-1.2	0.9	1307.9	N/A	59.7	59.7	-9.1	1.3	13.0	13.0	0.0	0.9						
150607	Thiols	Disulfide, bis(phenylmethyl)	S(Cc1ccc	246.4	1,110	FALSE	1.0	FALSE	70.9	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.0	5.0	4.4	N/A	N/A	4.4	-3.5	8737.8	N/A	8737.8	5.2	75.9						
68310076	Pigments and Dyes	Xanthylium, 3,6-bis(ethylamino)-9-[2-(methoxycarbonyl)phenyl]-2,7-	CCNC1CC	442.7	2,362	TRUE	1.0	FALSE	47.7	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	1.0	1.0	20083.8	N/A	N/A	20083.8	-12.2	1.0	N/A	1.0	4.3	499.4						
3426435	Stilbenes	Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-methoxy-6-(phe	COc1nc(Nc	770.8	38,946	TRUE	1.0	FALSE	41.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	-3.5	-3.5	313.2	N/A	N/A	313.2	-34.1	543.4	1.0	1.0	67.3	3.9						
75058	Nitriles	Acetonitrile	CC#N	41.1	474	FALSE	9933.6	TRUE	81.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	-0.3	-0.2	-0.3	55377.6	N/A	N/A	55377.6	-2.9	1.0	N/A	1.0	1.5	7.1						
12224985	Pigments and Dyes	Xanthylium, 9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-di	CCNC1CC	456.7	2,994	TRUE	1.0	FALSE	56.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	1.4	1.4	12485.1	N/A	N/A	12485.1	-12.0	1.0	N/A	1.0	5.8	666.0						
80083405	Pigments and Dyes	Xanthylium, 9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-di	CCNC1CC	456.7	2,994	TRUE	1.0	FALSE	56.7	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	1.4	1.4	12485.1	N/A	N/A	12485.1	-12.0	1.0	N/A	1.0	5.8	666.0						
75627122	Pigments and Dyes	Xanthylium, 3,6-bis(ethylamino)-9-[2-(methoxycarbonyl)phenyl]-2,7-	CCNC1CC	448.7	2,362	TRUE	1.0	FALSE	47.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	0.7	0.7	43595.2	N/A	N/A	43595.2	-11.1	1.0	N/A	1.0	0.7	1051.6						
17627440	Terpenes & Terpenoids	Cyclohexene, 4-(1,5-dimethyl-1,4-hexadienyl)-1-methyl-	CC(=CCC	204.4	292	FALSE	1.0	FALSE	82.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.5	5.5	2.7	N/A	N/A	2.7	1.9	32210.4	N/A	32210.4	16.3	844.5						
63022093	Pigments and Dyes	Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, molybdatep	CCNC1CC	488.8	5,028	TRUE	0.9	FALSE	76.7	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	1.8	1.8	7698.1	N/A	N/A	7698.1	-11.1	1.0	N/A	1.0	0.5	1643.7						
1.02E+08	Pigments and Dyes	Xanthylium, 3,6-bis(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-, n	CCN(C1C(	470.7	18,368	TRUE	0.9	FALSE	53.7	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	1.8	1.8	17661.7	N/A	N/A	17661.7	-11.5	1.0	N/A	1.0	3.5	77.8						
1326030	Pigments and Dyes	Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, molybdatet	CCN(C1C(	456.7	9,277	TRUE	0.9	FALSE	0.8	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.2	2.2	4295.3	N/A	N/A	4295.3	-14.0	1.0	N/A	1.0	3.1	73.7						
62973799	Pigments and Dyes	Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, molybdatet	CCN(C1C(	456.7	9,277	TRUE	0.9	FALSE	0.8	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	2.2	2.2	4295.3	N/A	N/A	4295.3	-14.0	1.0	N/A	1.0	3.1	73.7						
15827608	INDIVIDUAL - Phosphonic ac	Phosphonic acid, [[(phosphonomethyl)imino]bis[2,1-ethanediylnitrilo	OP(=O)(CI	573.2	23,114	TRUE	0.9	FALSE	82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-19.5	-19.5	1000011.9	N/A	N/A	1000011.9	0.0	1.0	N/A	1.0	2.1	0.8						
495625	Terpenes & Terpenoids	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl-	CC(=CCC	204.4	349	FALSE	0.9	FALSE	83.4	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.8	5.8	1.9	N/A	N/A	1.9	2.0	28574.8	N/A	28574.8	12.1	759.3						
1113219	Terpenes & Terpenoids	1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)-	C=CC(CC	290.5	10,805	TRUE	0.9	FALSE	84.0	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	6.6	6.6	1.2	N/A	N/A	1.2	-1.5	11505.1	N/A	11505.1	58.2	929.7						
67970	Vitamins & derivatives	9,10-Secocholesta-5,7,10(19)-trien-3-ol, (3β,5Z,7E)-	CC(CCCC	384.7	12,256	TRUE	0.9	FALSE	84.0	0.0000001 - 0.000001	< 0.0000001	FALSE	FALSE	TRUE	N/A	8.7	8.7	0.3	N/A	N/A	0.3	-2.0	142.2	N/A	142.2	38.3	6991.4						
116314	Vitamins & derivatives	Retinal	O=CC=C((	284.5	6,025	TRUE	0.8	FALSE	83.9	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	5.8	5.8	1.1	N/A	N/A	1.1	-1.3	18017.2	N/A	18017.2	17.5	5471.6						
73984937	Thiols	1,3,4-Thiadiazole-2(3H)-thione, 5-(tert-dodecyldithio)-	S=c1[nH]nc	350.6	2,467	TRUE	0.8	FALSE	10.0	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	4.7	4.7	24.6	N/A	N/A	24.6	-3.5	39783.2	N/A	39783.2	8.1	112.9						
120785	Benzotriazoles & benzothiaz	Benzothiazole, 2,2'-dithiobis-	c1ccc2c(c1	332.5	4,233	TRUE	0.8	FALSE	51.4	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	5.4	5.4	3.6	N/A	10	10.0	-11.0	2.8	55.7	55.7	19.9	9.4						
3089110	Triazoles	1,3,5-Triazine-2,4,6-triamine, N,N,N',N',N'',N''-hexakis(methoxyme	COCN(c1r	390.4	32,881	TRUE	0.8	FALSE	0.7	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	1.5	1.5	3904.4	N/A	N/A	3904.4	-9.9	2.3	1.9	1.9	3.1	0.8						
90302	Aromatic Amines	1-Naphthalenamine, N-phenyl-	c1ccc(cc1)	219.3	2,095	TRUE	0.7	FALSE	34.1	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	4.2	4.3	4.2	12.1	N/A	N/A	12.1	-5.4	800.4	4000.0	4000.0	3.7	164.8						
137268	Thiocarbamates	Thioperoxydicarbonic diamide [(H2N)C(S)]2S2), tetramethyl-	CN(C(=S)S	240.4	1,404	FALSE	0.7	FALSE	17.1	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	1.7	1.9	1.7	25.8	N/A	30	30.0	-5.1	2.3	4.6	4.6	11.2	5.0						
13082478	Pigments and Dyes	Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, hydroxide	O=C(O)c4(	444.6	3,873	TRUE	0.7	FALSE	33.3	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	2.0	2.0	0.0	N/A	N/A	0.0	0.0	31102.2	N/A	31102.2	N/A	945.2						
68268	Vitamins & derivatives	Retinol	OCC=C(C	286.5	5,528	TRUE	0.6	FALSE	78.2	0.0000001 - 0.000001	< 0.0000001	FALSE	FALSE	TRUE	5.7	6.0	5.7	4.3	N/A	N/A	4.3	-2.3	18073.5	N/A	18073.5	13.8	1079.0						
16090021	Stilbenes	Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-(4-morpholinyl)-	OS(=O)(=C	881.0	55,268	TRUE	0.6	FALSE	82.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	1.5	-4.6	1.5	57.3	N/A	1900	1900.0	-41.5	2.2	1.0	1.0	7.0	0.8						
3844459	Triarylmethanes	Benzenemethanaminium, N-ethyl-N-[4-[[4-[ethyl((3-sulfophenyl)meth	CC[N+](=C	750.9	16,921	TRUE	0.6	FALSE	1.1	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-6.2	-6.2	0.0	N/A	N/A	0.0	-34.2	1.0	N/A	1.0	N/A	14.1						
630206	Alkyl or aryl halides	Ethane, 1,1,1,2-tetrachloro-	ClCC(Cl)(C	167.9	9,177	TRUE	10483.2	TRUE	3.2	0.0001 - 0.001	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	2.7	2.7	638.1	N/A	N/A	638.1	-1.0	44.3	N/A	44.3	88.7	79.0						
4193559	Stilbenes	Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-[bis(2-hydroxye	OCCN(c1r	919.0	50,635	TRUE	0.6	FALSE	4.1	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-5.9	-5.9	3873.6	N/A	N/A	3873.6	0.0	1.4	1.0	1.0	8.4	0.8						
1324761	Triarylmethanes	Benzenesulfonic acid, [[4-[[4-(phenylamino)phenyl][4-(phenylimino)-	OS(=O)(=C	595.7	5,731	TRUE	0.6	FALSE	5.5	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	2.5	2.5	0.6	N/A	N/A	0.6	-15.1	30734.1	N/A	30734.1	36.5	383.2						
569642	Triarylmethanes	Methanaminium, N-[4-[[4-(dimethylamino)phenyl]phenylmethylene]-;	C[N+](=C1	330.5	3,675	TRUE	0.6	FALSE	6.9	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	0.2	0.2	22.2	N/A	N/A	22.2	-13.3	1.2	N/A	1.2	N/A	89.0						
548629	Triarylmethanes	Methanaminium, N-[4-[bis[4-(dimethylamino)phenyl]methylene]-2,5-	C[N+](=C1	373.6	8,174	TRUE	0.6	FALSE	7.3	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	0.2	0.2	8.6	N/A	N/A	8.6	-15.1	1.1	N/A	1.1	N/A	86.7						
632995	Triarylmethanes	Benzenamine, 4-[[4-aminophenyl](4-imino-2,5-cyclohexadien-1-yli	NC1C=CC	303.4	3,967	TRUE	0.5	FALSE	6.7	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	0.8	0.8	17.1	N/A	N/A	17.1	-13.0	43.3	N/A	43.3	5.7	52.8						
2390592	Triarylmethanes	Ethanaminium, N-[4-[bis[4-(diethylamino)phenyl]methylene]-2,5-cyc	CC[N+](=C	457.7	14,960	TRUE	0.5	FALSE	33.6	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	1.6	1.6	0.0	N/A	N/A	0.0	-14.4	432.5	N/A	432.5	N/A	592.7						
100970	Heterocycles	1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane	C1N2CN3(	140.2	8,637	TRUE	0.5	FALSE	4.6	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	1.0	1.0	1000013.8	N/A	N/A	1000013.8	-7.2	1.0	N/A	1.0	0.6	0.8						
58713216	Aliphatic amines	1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane, hydrochloride	C1N2CN3(	140.2	8,637	TRUE	0.5	FALSE	4.6	0.0001 - 0.001	0.00001 - 0.0	FALSE	FALSE	TRUE	N/A	1.0	1.0	1000013.8	N/A	N/A	1000013.8	-7.2	1.0	N/A	1.0	0.6	0.8						
4080313	Hexamethylenetetramine	3,5,7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane, 1-(3-chloro-2-prop	ClC=CC[N	216.7	9,000	TRUE	0.5	FALSE	4.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-1.8	-1.8	999899.1	N/A	304000	304000.0	-7.3	1.0	N/A	1.0	N/A	0.8						
51229788	Hexamethylenetetramine	3,5,7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane, 1-(3-chloro-2-prop	ClC=CC[N	216.7	9,000	TRUE	0.5	FALSE	4.6	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	-1.8	-1.8	999899.1	N/A	N/A	999899.1	-7.3	1.0	N/A	1.0	N/A	0.8						
2390605	Triarylmethanes	Ethanaminium, N-[4-[[4-(diethylamino)phenyl][4-(ethylamino)-1-napl	CC(/N=[C(	479.7	13,115	TRUE	0.5	FALSE	34.7	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.1	2.1	0.0	N/A	N/A	0.0	-16.8	581.9	N/A	581.9	N/A	1660.0						
68814028	Pigments and Dyes	Ethanaminium, N-[4-[bis[4-(diethylamino)phenyl]methylene]-2,5-cyc	CCN(C1C(	457.7	21,837	TRUE	0.4	FALSE	74.9	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	5.2	5.2	1.9	N/A	N/A	1.9	-8.3	1.0	N/A	1.0	2.4	736.1						
68409665	Pigments and Dyes	Ethanaminium, N-[4-[[4-(diethylamino)phenyl][4-(ethylamino)-1-napl	CCNc1ccc	479.7	17,394	TRUE	0.4	FALSE	70.7	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	5.5	5.5	0.6	N/A	N/A	0.6	-10.8	1.0	N/A	1.0	17.5	2556.0						
120547	Thiocarbamates	Piperidine, 1,1'-(tetrathiodicarbonothioyl)bis-	S=C(N1CC	384.7	2,705	TRUE	0.4	FALSE	14.9	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	2.8	5.0	2.8	0.7	N/A	10	10.0	-2.6	3.1	35.2	35.2	17.4	11.4						
7235407	Vitamins & derivatives	β,β-Carotene	CC(=CC=(	536.9	4,363	TRUE	0.3	FALSE	84.0	0.001 - 0.01	0.0001 - 0.00	FALSE	FALSE	TRUE	N/A	13.6	13.6	0.0	N/A	N/A	0.0	3.6	0.9	N/A	0.9	374.7	303578.7						

| HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER	
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION	
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High ?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavalibility ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)
6858497	1	3	4.8	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
88846	1	2	9.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
90937	1	3	8.4	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
72391243	1	3	0.9	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
28768323	1	3	0.3	1,000 - 10,000	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
121824	1	3	2042.8	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	local RQ <1	low (mostly near field)			N/A	N/A
150607	1	2	379.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
68310076	1	2	9.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3426435	1	3	0.3	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
75058	1	1	709305.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
12224985	1	3	2.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
80083405	1	3	2.9	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
75627122	1	3	5.0	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
17627440	1	2	143.0	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
63022093	1	3	1.3	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
1.02E+08	1	3	1.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
1326030	1	3	1.6	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	Moderate potential for risk;	ERC classified this substan	N/A	N/A
62973799	1	3	1.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
15827608	2	1	18617.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
495625	1	2	140.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
1113219	1	3	0.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
67970	1	3	0.1	1,000,000 - 10,000,000	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
116314	1	3	1.1	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
73984937	1	3	3.0	10,000 - 100,000	TRUE	FALSE	FALSE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
120785	3	2	193.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
3089110	3	1	7684.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A			N/A	N/A
90302	3	2	253.7	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A			N/A	N/A
137268	1	3	0.4	1 - 10	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
13082478	1	3	0.5	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
68268	1	3	0.7	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
16090021	1	2	24.1	1,000 - 10,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
3844459	2	2	106.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
630206	1	1	13986.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
4193559	2	2	82.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
1324761	2	3	1.9	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
569642	2	3	4.1	100 - 1,000	N/A	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
548629	2	3	5.3	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A
632995	1	3	13.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but p	ERC classified this substan	N/A	N/A
2390592	1	3	0.2	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
100970	3	1	89765.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A
58713216	1	1	7842.3	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for subs	ERC classified this substan	N/A	N/A
4080313	2	1	131471.8	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
51229788	1	1	131471.8	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A
2390605	1	3	0.1	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	moderate (mostly near fiel	N/A	N/A	N/A	N/A	N/A	N/A
68814028	1	3	0.1	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
68409665	1	3	0.0	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after \	low (mostly near field)	Low current exposure, but h	ERC classified this substan	N/A	N/A
120547	3	3	39654.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	3	high (near and far field risk	N/A	N/A	N/A	N/A	N/A	N/A
7235407	1	1	46.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A

CHEMICAL IDENTITY					EXPOSURE											FATE																					
SUBSTANCE AND GROUPING FOR CMP					PERSISTENCE				EMISSION RATE (EA)							PHYSICO-CHEMICAL PROPERTIES												BIOACCUMULATION									
CAS	CMP Phase 3 Group	Substance Name	SMILES	Molecular Weight (g/mol)	Overall Persistence (hours)	Critically Long Overall Persistence	Selected Air Half-Life (hours)	Critically Long Half Life in Air	WWTP Removal (%)	Annual Tonnage (kilotonnes)	Annual tonnage WWTP removal (kilotonnes)	Large value for tonnage	Moderate value for tonnage	Low value for tonnage	Empirical LogKow	ACD Median LogD @ pH 7	Selected LogKow	ACD Water Sol. @ pH 7	Empirical Water Sol. SRC Database (mg/L)	Empirical Water Sol. REACH Database (mg/L)	Selected Water Sol (mg/L)	LogKaw		Model BCF 5% Fish (L/kg)	Empirical BCF 5% Lipid Fish (L/kg)	Selected BCF 5% Lipid Fish (L/kg)	Half-Life 1 kg Mammal (days)	Half-life 1 kg Fish (days)									
1328047	Inorganic - Aluminum	C.I Pigment Violet 5:1	c12C(=O)(	320.3	1165.8	TRUE	84.0	TRUE	14.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	-2.0	-2.0	69378.2	N/A	N/A	69378.2			1.0	N/A	1.0											
68551428	Inorganic - Manganese	Fatty acids, C6-19-branched, m	CC(C)C(C	172.3	824.9	FALSE	36.1	FALSE	61.4	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.1	1.1	4394.4	N/A	N/A	4394.4			1167.3	N/A	1167.3											
61789364	Naphthenic acids and salts	Naphthenic acids, calcium salts	OC(=O)CC	128.2	267.0	FALSE	35.1	FALSE	82.73969862	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	-0.2	-0.2	58611.5	N/A	N/A	58611.5	-4.4		1.0	N/A	1.0	0.3	16.2									
1338245	Naphthenic acids and salts	Naphthenic acids	OC(=O)CC	128.2	267.0	FALSE	286.0	TRUE	82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-0.2	-0.2	58611.5	N/A	N/A	58611.5			14.0	N/A	14.0											
8005036	Pigments and Dyes	C.I. Acid Black 2	N/A	N/A	N/A	TRUE	35.0	FALSE	N/A	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1.0	N/A	1.0											
8013012	INDIVIDUAL - Yeast, ext.	Yeast, ext.	NC[P](C(	146.1	184.3	FALSE	35.0	FALSE	82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			109.1	N/A	109.1											
8016817	Resins & rosins	Tall-oil pitch	CCC(CCC	414.7	18518.7	TRUE	35.0	FALSE	84.0	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	9.4	9.4	0.0	N/A	N/A	0.0			2145.6	N/A	2145.6											
8024439	Terpenes & Terpenoids	Perfumes and Essences, jasmir	CC(=O)CC	150.2	317.2	FALSE	35.0	FALSE	82.4	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.9	1.9	1192.9	3100.0	N/A	3100.0			6.7	N/A	6.7											
8031036	Terpenes & Terpenoids	Oils, mimosa	CCCCCC	238.4	2832.7	TRUE	35.0	FALSE	84.0	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	8.2	8.2	0.1	N/A	N/A	0.1			42571.1	N/A	42571.1											
9015547	Proteins and derivatives	Protein hydrolyzates	CC(C)CC(	131.2	272.1	FALSE	35.0	FALSE	61.5	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			17.0	N/A	17.0											
11103574	Vitamins & derivatives	Vitamin A	OCC1C(O	180.1	108.4	FALSE	35.0	FALSE	82.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	-2.8	-2.8	385166.4	500000.0	N/A	500000.0			1.0	N/A	1.0											
61790496	INDIVIDUAL - Oils, lard, sulfuriz	Oils, lard, sulfurized	N/A	N/A	N/A	FALSE	35.0	FALSE	N/A	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1000.0	N/A	1000.0											
66071941	INDIVIDUAL - Corn, steep liquo	Corn, steep liquor	CC(C)CC(	131.2	272.1	FALSE	35.0	FALSE	61.5	100 - 1,000	N/A	TRUE	FALSE	FALSE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			618.9	N/A	618.9											
66241110	Pigments and Dyes	C.I Leuco Sulphur Black 1	Nc1cc2c(c	614.8	32320.6	TRUE	35.0	FALSE	1.8	0.01 - 0.1	N/A	FALSE	TRUE	FALSE	N/A	1.2	1.2	0.1	N/A	N/A	0.1			1.5	N/A	1.5											
68122861	Alkyl imidazolines and salts	Imidazolium compounds, 4,5-dih	CCCCCC(	603.0	3593.3	TRUE	35.0	FALSE	84.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			822.7	N/A	822.7											
68442977	Alkyl imidazolines and salts	1H-Imidazole-1-ethanamine, 4,5	CCCCCC(	349.6	1032.5	FALSE	35.0	FALSE	80.6	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	3.5	3.5	712.5	N/A	N/A	712.5			19172.2	N/A	19172.2											
68953582	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	536.0	982.8	FALSE	35.0	FALSE	84.0	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	14.1	14.1	0.0	N/A	N/A	N/A			1.0	N/A	1.0											
71011240	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	424.1	N/A	N/A	35.0	FALSE	N/A	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1.0	N/A	1.0											
71011251	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	424.1	N/A	N/A	35.0	FALSE	N/A	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1420.3	N/A	1420.3											
71011262	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	424.1	N/A	N/A	35.0	FALSE	N/A	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			703.1	N/A	703.1											
71486798	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, mono-C1	CC(C)CC(	705.2	8947.6	TRUE	35.0	FALSE	9.2	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	12.5	12.5	0.0	N/A	N/A	0.0			1.0	N/A	1.0											
84012157	Salicylates	Birch, Betula alba, ext.	COC(=O)c	152.1	239.5	FALSE	35.0	FALSE	80.6	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	2.4	2.4	1239.0	700.0	N/A	700.0			20.1	N/A	20.1											
8008933	Terpenes & Terpenoids	Oils, wormwood	CC(C)C12	152.2	520.3	FALSE	50.1	TRUE	12.9	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	2.5	2.5	348.8	N/A	N/A	348.8			23.2	N/A	23.2											
84082542	Terpenes & Terpenoids	Ivy, Hedera helix, ext.	CCCCCC(	244.4	476.9	FALSE	35.0	FALSE	76.2	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	6.4	6.4	1.4	N/A	N/A	1.4			16375.0	N/A	16375.0											
84696242	INDIVIDUAL - Lotus corniculata	Lotus corniculatus, ext.	Oc1ccc(C	270.2	512.5	FALSE	35.0	FALSE	14.8	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.7	1.7	550.4	N/A	N/A	550.4			32.8	N/A	32.8											
84696479	Eugenol and Isoeugenol derivat	Rose, Rosa canina, ext.	COc1cc(C	164.2	525.1	FALSE	35.0	FALSE	61.8	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	2.5	2.5	1366.4	N/A	N/A	1366.4			5.6	N/A	5.6											
84961671	Terpenes & Terpenoids	Verbena officinalis, ext.	CC(P-)1(C	388.3	355.4	FALSE	35.0	FALSE	82.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	211000.0	N/A	211000.0			1.0	N/A	1.0											
90028663	Fatty acids and salts	Evening primrose, Oenothera bi	CCCCCC(	280.4	248.3	FALSE	35.0	FALSE	83.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	4.5	4.5	852.8	N/A	N/A	852.8			17851.0	N/A	17851.0											
90045366	Terpenes & Terpenoids	Ginkgo biloba, ext.	CC(P+)1C	578.5	300.2	FALSE	35.0	FALSE	82.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1.0	N/A	1.0											
90045388	Terpenes & Terpenoids	Ginseng, Panax quinquefolium,	N/A	N/A	N/A	FALSE	35.0	FALSE	N/A	0.0001 - 0.001	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1000.0	N/A	1000.0											
92044876	Fatty acids and salts	Fatty acids, coco, 2-ethylhexyl e	CCCCCC(	312.5	744.6	FALSE	35.0	FALSE	83.9	0.001 - 0.01	N/A	FALSE	FALSE	TRUE	8.0	8.3	8.0	0.0	N/A	N/A	0.0			1.0	N/A	1.0											
92113310	Proteins and derivatives	Collagens, hydrolyzates	CC(C)CC(	131.2	272.1	FALSE	35.0	FALSE	61.5	0.01 - 0.1	N/A	FALSE	TRUE	FALSE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			640.0	N/A	640.0											
111174631	Proteins and derivatives	Protein hydrolyzates, leather, ex	CC(C)CC(	302.9	5991.8	TRUE	35.0	FALSE	83.5	0.0001 - 0.001	N/A	FALSE	FALSE	TRUE	N/A	8.1	8.1	1.1	N/A	N/A	1.1			10129.7	N/A	10129.7											
115340802	Quaternary ammonium compou	1-Propanaminium, 3-amino-N-(	CCCCCC(	394.7	6300.3	TRUE	35.0	FALSE	84.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	5.6	5.6	260.8	N/A	N/A	260.8			1502.2	N/A	1502.2											
8022966	Terpenes & Terpenoids	Oils, jasmine	COC(=O)c	136.1	279.6	FALSE	304.1	N/A	81.9	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	2.1	2.1	1300.2	2100.0	N/A	2100.0	n/a		7.4	N/A	7.4											
119345016	Phosphoric acid derivatives	Phosphorous trichloride, reactio	CC(C)(C)c	1035.4	45514.6	TRUE	35.0	FALSE	84.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	23.5	23.5	0.0	N/A	N/A	N/A			925.2	N/A	925.2											
129828235	INDIVIDUAL - Fatty acids, tall-oi	Fatty acids, tall-oil, reaction proc	CCCCCC(	312.3	216.0	FALSE	35.0	FALSE	85.5	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	4.7	4.7	3.5	2.7	N/A	2.7			352.9	N/A	352.9											
164288522	Terpenes & Terpenoids	Cork tree, Phellodendron amure	CC(C)=CC	136.2	72.2	FALSE	35.0	FALSE	32.5	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	4.4	4.4	69378.2	5.6	N/A	5.6			3484.1	N/A	3484.1											
68603156	Alcohols	Alcohols, C6-12	CCCCCC	102.2	162.9	FALSE	26.4	FALSE	82.21020838	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	2.0	1.9	2.0	5879.5	N/A	6260.0	6260.0	-3.2		6.4	N/A	6.4	1.0	11.6									
8002093	Terpenes & Terpenoids	Oils, pine	CC1(C)C2	154.2	779.0	FALSE	22.5	FALSE	32.6	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	2.6	2.6	809.5	N/A	N/A	809.5			2.1	N/A	2.1											
68987428	Arenes	Benzene, ethylenated, residues	c1ccc(cc1)	182.3	393.1	FALSE	21.4	FALSE	53.37338612	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	4.8	4.5	4.8	3.1	N/A	N/A	3.1	-1.6		2259.8	N/A	2259.8	2.0	115.8									
12001853	Inorganic - Zinc	Naphthenic acids, zinc salts	OC(=O)CC	128.2	267.0	FALSE	20.4	FALSE	82.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	-0.2	-0.2	58611.5	N/A	N/A	58611.5			4157.3	N/A	4157.3											
68411303	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, C10-13-a	CC(C)CC(	312.5	2438.1	TRUE	19.2	FALSE	14.2	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	1.2	1.2	25398.4	N/A	N/A	25398.4			1.0	N/A	1.0											
68584225	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, C10-16-a	CCCCCC(	298.4	890.0	FALSE	19.0	FALSE	61.62818111	1 - 10	1 - 10	TRUE	FALSE	FALSE	N/A	1.4	1.4	609.3	N/A	N/A	609.3	-5.8		321.3	N/A	321.3	4.4	64.7									
68649003	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, mono-C9	CCCC(CC	298.4	2010.2	TRUE	18.3	FALSE	14.1980185	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	0.9	0.9	19717.9	N/A	N/A	19717.9	-5.8		4564.6	N/A	4564.6	6.3	91.8									
90218352	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, dodecyl-,	CC(c1ccc(	326.5	2521.2	TRUE	15.2	FALSE	14.3131163	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	1.0	1.0	25344.1	N/A	N/A	25344.1	-5.6		168.9	N/A	168.9	5.3	179.5									
67774747	Linear Alkyl Benzenes (LAB) ar	Benzene, C10-13-alkyl derivs.	c1ccc(CC(	232.4	4157.9	TRUE	14.9	FALSE	83.9	0.1 - 1	N/A	FALSE	TRUE	FALSE	N/A	7.9	7.9	0.0	N/A	N/A	0.0			208.0	N/A	208.0											
68442693	Linear Alkyl Benzenes (LAB) ar	Benzene, mono-C10-14-alkyl de	c1ccc(CC(	218.4	3361.4	TRUE	14.9	FALSE	83.4	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	7.5	7.5	0.0	N/A	N/A	0.0			462.0	N/A	462.0											
68952352	Phosphoric acid derivatives	Tar acids, cresylic, Ph phosphat	O=P(OC2	354.4	4016.1	TRUE	14.5	FALSE	79.5	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	4.7	4.7	0.4	N/A	N/A	0.4			1631.0	N/A	1631.0											
68909182	Heterocycles	Pyridinium, 1-(phenylmethyl)-, Cl	CC1c2ccHv	213.3	590.9	FALSE	14.1	FALSE	12.4106268	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	-1.0	-1.0	70.3	N/A	N/A	70.3	-9.1		1.0	N/A	1.0	N/A	10.2									
68783368	Inorganic - Lithium	Fatty acids, C16-22, lithium salt	CCCCCC(	256.4	197.9	FALSE	13.8	FALSE	82.7	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	7.2	4.8	7.2	11.2	0.0	N/A	0.0			1.7	N/A	1.7											
68783379	Inorganic - Lithium	Fatty acids, C16-18, lithium salt	CCCCCC(	256.4	197.9	FALSE	13.8	FALSE	82.7	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	7.2	4.8	7.2	11.2	0.0	N/A	0.0			9.2	N/A	9.2											
68082359	Epoxides & glycidyl ethers	Fatty acids, soya, epoxidized, M	CCCCCC(	340.5	2011.6	FALSE	13.6	FALSE	88.4	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	5.7	5.7	15.9	N/A	N/A	15.9			154.0	N/A	154.0											
68439576	Alkyl Sulfates and Olefin Sulfon	Sulfonic acids, C14-16-alkane h	CCCCCC(	292.5	387.6	FALSE	13.1	FALSE	82.79177792	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	1.3	1.3	232.7	N/A	N/A	232.7	-4.6		1.0	N/A	1.0	2.5	68.6									
68648873	Linear Alkyl Benzenes (LAB) ar	Benzene, C10-16-alkyl derivs.	c1ccccc1C	218.4	3361.4	TRUE	12.8	FALSE	83.4	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	7.5	7.5	0.0	N/A	N/A	0.0			3.0	N/A	3.0											
8024053	Benzoates	Oils, tuberose	CC(C)C1C	260.4	2064.7	TRUE	12.7	FALSE	83.3	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	5.7	5.7	4.5	N/A	N/A	4.5			10415.9	N/A	10415.9											
67762305	Alcohols	Alcohols, C14-18	CCCCCC	214.4	601.7	FALSE	12.2	FALSE	86.77104874	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	6.0	6.2	6.0	0.1	N/A	0.2	0.2	-2.2		39053.2	N/A	39053.2	1.0	118.7									
8046193	Resins & rosins	Storax (balsam)	OC(=O)C=	148.2	295.4	FALSE	11.6	FALSE	82.8	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-0.3	-0.3	147138.7	570.0	N/A	570.0			7.7	N/A	7.7											
68647585	Inorganic - Aluminum	Aluminum, benzoate hydroxyde	CCCCCC(	284.5	211.2	FALSE	11.0	FALSE	84.3	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	5.9	5.9	1.5	0.6	N/A	0.6			1534.9	N/A	1534.9											
68411325	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, dodecyl-,	CC(CC(c1	376.6	3030.0	TRUE	10.9	FALSE	14.50699894	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	2.2	2.2	335.4	N/A	N/A	335.4	-6.6		17749.4	N/A	17749.4	4.1	605.4									
61790485	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, petroleum, bariu	CC(C)C(C	324.5	2944.3	TRUE	10.7	FALSE	14.3	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	1.1	1.1	10742.0	N/A	N/A	10742.0			431.0	N/A	431.0											
68890993	Linear Alkyl Benzenes (LAB) ar	Benzene, mono-C10-16-alkyl de	CCCCCC(	218.4	3361.4	TRUE	10.6	FALSE	83.4	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	7.5	7.5	0.0	N/A	N/A	0.0			462.0	N/A	462.0											
68649116	INDIVIDUAL - 1-Decene, dimer	1-Decene, dimer, hydrogenated	CCCCCC(	282.6	7721.7	TRUE	10.1	FALSE	83.9974213	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	10.7	10.7	0.0	N/A	N/A	0.0	3.6		202.4	N/A	202.4	1.7	3754.6									
125328645	Nitriles	Nitriles, rape-oil, hydrogenated	CCCCCC	321.6	2175.5	TRUE	10.0	FALSE	84.0	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	9.6	9.6	0.0	N/A	N/A	N/A			2619.6	N/A	2619.6											
8024064	Aldehydes	Oils, vanilla	COc1cc(C	152.1	191.8	FALSE	9.4	FALSE	82.8	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	1.2	1.2	1.2	4883.9	11000.0	N/A	11000.0			11.7	N/A	11.7											
68515606	Trimellitates	1,2,4-Benzenetricarboxylic acid,	CCCC(CC	504.7	2761.6	TRUE	9.0	FALSE	83.99796949	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	9.2	9.2	0.1	N/A	N/A	0.1	-5.0		221.6	N/A	221.6	2.0	131.0									
8050155	Resins & rosins	Resin acids and Rosin acids, hy	CC(C)C1C	320.5	9259.4	TRUE	8.8	FALSE	83.5	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	7.1	7.1	0.3	N/A	3.6	3.6			36.3	N/A	36.3											
61788725	Epoxides & glycidyl ethers	Fatty acids, tall-oil, epoxidized, (	CCCCCC(	410.7	1438.9	FALSE	8.7	FALSE	84.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	9.4	9.4	0.0	N/A	N/A	0.0			30.8	N/A	30.8											
1328514	Inorganic - Copper	C.I. Solvent Blue 38	N/A	N/A	N/A	TRUE	8.6	FALSE	N/A	0.0001 - 0.001	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	N/A	N/A	0.0	N/A	N/A	N/A			1.0	N/A	1.0											
8021394	INDIVIDUAL - Creosote, wood	Creosote, wood	c1(O)c(OC	124.1	368.2	FALSE	8.6	FALSE	82.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.3	1.3	5301.5	N/A	N/A	5301.5			2.0	N/A	2.0											

| HAZARD | | |

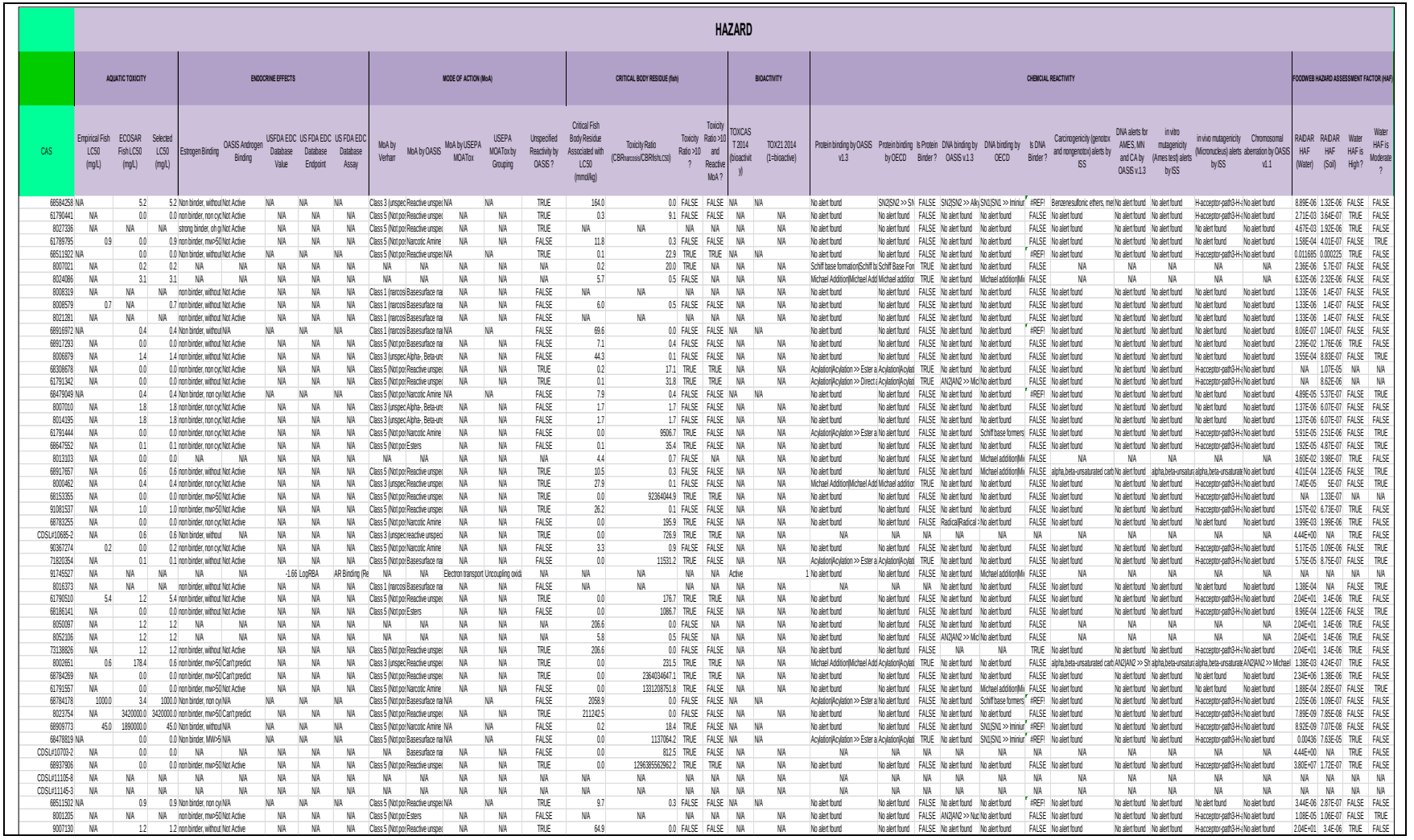
	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER		
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM COMPOUNDS	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION		
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavalibility ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification (including manual classification)	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)	UVCB Model Result Acceptance
1328047	1	N/A	185022.3	>100,000,000	TRUE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Not found	accept model result if appropriate
68551428	1		982.1	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	N/A	N/A	Accepted given low volume
61789364	1	1	89262.8	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	No	C1=CC=C	?
1338245	1	1	89259.5	1,000,000 - 10,000,000	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	1	2	moderate (mostly near field)	local RQ >10	moderate (mostly near field)			No	:=CC2=C1	accept model result if appropriate
8005036	1	N/A	N/A	N/A	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	No (no SM	C1=CC=C	Accepted given low volume
8013012	1	N/A	1020505.6	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted
8016817	2	3	0.0	0.01 - 0.1	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	C[C@@]1(	Accepted
8024439	1	1	466769.1	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC(=CCC	Accepted
8031036	2	N/A	14.2	1,000 - 10,000	FALSE	FALSE	TRUE	N/A	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	COC1=CC	Accepted
9015547	1	N/A	3539836.6	>100,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	No	Accepted given low volume
11103574	1	1	9306418.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	Not neede	Accepted
61790496	1	N/A	N/A	N/A	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	Not availat	Not availat	Accepted given low volume
66071941	1	N/A	3539836.6	10,000 - 100,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not availat	accept model result if appropriate
66241110	2	N/A	0.5	10 - 100	FALSE	FALSE	TRUE	TRUE	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	Yes	Not neede	Accepted
68122861	1	1	110.4	10,000 - 100,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted
68442977	1	N/A	1.8	100 - 1,000	FALSE	FALSE	TRUE	N/A	FALSE	FALSE	1	2	moderate (mostly near field)	local RQ >10	moderate (mostly near field)	Moderate potential for risk; m	ERC classified this substance	Yes	Not neede	Accepted
68953582	1	1	10.5	10 - 100	FALSE	FALSE	TRUE	FALSE	TRUE	TRUE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	accept model result if appropriate
71011240	N/A	N/A	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	Available	Accepted
71011251	N/A	N/A	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	Accepted given low volume
71011262	N/A	N/A	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	Available	Accepted
71486798	2	1	0.0	< 0.0000001	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	2	1	low (mostly near field)	N/A	N/A	Possible substitute for substa	ERC classified this substance	Yes	CC(c1cc(	Accepted
84012157	1	1	168824.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC(=C)C1	Accepted
8008933	1	1	28703.5	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC(=CCC	Accepted
84082542	1	1	128.7	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	No	CC1C(C(C	Accepted given low volume
84696242	1	3	24250.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Available	accept model result if appropriate
84696479	1	N/A	119995.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	OCC(c(cc(	Accepted
84961671	1	1	6120631.3	>100,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	CC1CCC2	Accepted
90028663	1	3	3.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	CCCCC(C	Accepted
90045366	1	1	1886718.2	>100,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Oc1cc(O)c	Accepted given low volume
90045388	1	N/A	N/A	N/A	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	No (no SM	CC(=CCC	Accepted given low volume
92044876	1	1	343.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	Not Neede	Accepted given low volume
92113310	1	N/A	3539836.6	>100,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not found	Accepted given low volume
111174631	1	3	1.4	10,000 - 100,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Not found	Accepted given low volume
115340802	1	1	91.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Not found	Accepted given low volume
8022966	3	1	313602.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	C1=CC=C	Accepted
119345016	1	1	0.0	< 0.0000001	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not found	Accepted given low volume
129828235	1	1	8502.8	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	Not found	Accepted given low volume
164288522	1	1	14543.7	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC(C1CC	Accepted
68603156	1	1	27102.2	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	?
8002093	1	N/A	15768.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC1=CCC	Accepted
68987428	1	1	1494.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	?
12001853	1	1	89259.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near field)	local RQ >10	moderate (mostly near field)	Moderate potential for risk; m	ERC classified this substance	No	C1=CC=C	Accepted
68411303	2	3	0.7	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	[Na][+] O=	Accepted
68584225	1	1	1896.3	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near field)	local RQ >10	moderate (mostly near field)	N/A	N/A	Yes	O=S(C(C(=	?
68649003	2	3	3.9	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	Probably n	CCCCCC(	?
90218352	3	2	9.8	10 - 100	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	3	2	moderate (up to far field)	N/A	N/A	N/A	N/A	No (no pro	CC(C)N[+]	?
67774747	2	N/A	17.2	100 - 1,000	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A			N/A	N/A	accept model result if appropriate
68442693	1	N/A	24.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Possible substitute for substa	ERC classified this substance	N/A	N/A	accept model result if appropriate
68952352	1	N/A	63.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	2	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	N/A	N/A	accept model result if appropriate
68900182	1	1	2280.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			N/A	N/A	?
68783368	1	3	0.0	0.1 - 1	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	Yes	Available	Accepted given low volume
68783379	1	3	0.0	0.1 - 1	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	Yes	Available	Accepted given low volume
68082359	1	N/A	293.9	10,000,000 - 100,000,000	TRUE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	accept model result if appropriate
68439576	1	3	1053.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A			N/A	N/A	?
68648873	1	N/A	24.2	10,000 - 100,000	TRUE	FALSE	TRUE	N/A	FALSE	FALSE	1	1	moderate (mostly near field)	local RQ >10	moderate (mostly near field)	Moderate potential for risk; m	ERC classified this substance	N/A	N/A	accept model result if appropriate
8024053	3	N/A	210.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	No	O=C(c1cc(	Accepted given low volume
67762305	1	2	343.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A			Yes	Not neede	?
8046193	1	1	147381.0	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	O=C(/C=C	Accepted
68647585	1	3	0.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	Accepted given low volume
68411325	3	3	1.5	1 - 10	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	3	3	high (near and far field risk)	N/A	N/A	N/A	N/A	Yes	CC(C)OC(	?
61790485	2	N/A	116.2	1,000 - 10,000	FALSE	FALSE	TRUE	N/A	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	No	Available	accept model result if appropriate
68890993	1	N/A	24.2	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Possible substitute for substa	ERC classified this substance	N/A	N/A	accept model result if appropriate
68649116	1	1	20.0	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	unknown	Not found	?
125328645	2	1	152.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted given low volume
8024064	1	N/A	891904.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	C1=CC(=(	Accepted
68515606	1	2	273.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	?
8050155	1	3	8.1	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted given low volume
61788725	1	3	0.0	1 - 10	FALSE	FALSE	TRUE	TRUE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	Accepted given low volume
1328514	1	N/A	N/A	N/A	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Not found	accept model result if appropriate
8021394	1	N/A	395447.6	>100,000,000	TRUE	FALSE	FALSE	N/A	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	Not found	accept model result if appropriate

CHEMICAL IDENTITY					EXPOSURE										FATE																	
SUBSTANCE AND GROUPING FOR CMP					PERSISTENCE				EMISSION RATE (EA)						PHYSICO-CHEMICAL PROPERTIES										BIOACCUMULATION								
CAS	CMP Phase 3 Group	Substance Name	SMILES	Molecular Weight (g/mol)	Overall Persistence (hours)	Critically Long Overall Persistence	Selected Air Half-Life (hours)	Critically Long Half Life in Air	WWTP Removal (%)	Annual Tonnage (kilotonnes)	Annual tonnage WWTP removal (kilotonnes)	Large value for tonnage	Moderate value for tonnage	Low value for tonnage	Empirical LogKow	ACD Median LogD @ pH 7	Selected LogKow	ACD Water Sol. @ pH 7	Empirical Water Sol. SRC Database (mg/L)	Empirical Water Sol. REACH Database (mg/L)	Selected Water Sol (mg/L)	LogKaw		Model BCF 5% Fish (L/kg)	Empirical BCF 5% Lipid Fish (L/kg)	Selected BCF 5% Lipid Fish (L/kg)	Half-Life 1 kg Mammal (days)	Half-life 1 kg Fish (days)				
8001045	Musks (Macro/Poly cyclic)	Musks	CC1CCC(	238.4	4297.3	TRUE	8.6	FALSE	80.8	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	5.6	5.6	25.6	N/A	N/A	25.6			27431.1	N/A	27431.1						
61789013	Epoxides & glycidyl ethers	Fatty acids, tall-oil, epoxidized, 2	CCCCCC(	410.7	1767.3	TRUE	8.5	FALSE	84.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	9.3	9.3	0.0	N/A	N/A	0.0			242.0	N/A	242.0						
68584247	Alkyl aryl sulfonates/LABS and (	Benzenesulfonic acid, C10-16-a	CCCCCC(	339.5	6863.6	TRUE	8.1	FALSE	83.40097271	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	6.7	6.7	0.1	N/A	N/A	0.1	-3.0		8470.5	N/A	8470.5	8.4	341.4				
68990534	Esters	Glycerides, C14-22 mono-	CCCCCC(	302.4	130.1	FALSE	8.0	FALSE	87.9	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	5.4	5.4	0.3	N/A	N/A	0.3			210.7	N/A	210.7						
120547526	Epoxides & glycidyl ethers	Oxirane, mono[(C12-13-alkyloxy	CCCCCC(	254.5	3224.9	TRUE	7.9	FALSE	83.49987524	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	7.3	7.3	0.0	N/A	N/A	0.0	0.0		0.9	N/A	0.9	1.0	491.4				
68476039	Fatty acids and salts	Fatty acids, montan-wax	CCCCCC(	382.6	265.8	FALSE	7.9	FALSE	85.1	0.0001 - 0.001	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	8.4	8.4	0.0	N/A	N/A	0.0			1244.0	N/A	1244.0						
68955533	Aliphatic amines	Amines, C12-14-tert-alkyl	CCCCCC(	185.4	571.1	FALSE	7.9	FALSE	84.6875006	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	1.7	1.7	18441.3	N/A	N/A	18441.3	-2.2		125.9	N/A	125.9	1.3	121.5				
68937417	Flame Retardants	Phenol, isopropylated, phosphat	CC(c1ccc(	452.5	11538.1	TRUE	7.9	FALSE	83.9952853	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	7.1	7.1	0.1	N/A	N/A	0.1	-4.9		3594.6	N/A	3594.6	0.5	2748.9				
1338029	Inorganic - Copper	Naphthenic acids, copper salts	OC(=O)C(	128.2	267.0	FALSE	7.7	FALSE	82.7	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	-0.2	-0.2	58611.5	N/A	N/A	58611.5			1.0	N/A	1.0						
61789853	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, petroleum	OS(C1=C(	464.8	2699.8	TRUE	7.7	FALSE	15.6	0.0001 - 0.001	0.0001 - 0.001	FALSE	TRUE	N/A	5.2	5.2	25.5	N/A	N/A	25.5			35.0	N/A	35.0						
68608264	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, petroleum, sodiu	OS(C1=C(	464.8	2699.8	TRUE	7.7	FALSE	15.6	1 - 10	1 - 10	TRUE	FALSE	FALSE	N/A	5.2	5.2	25.5	N/A	N/A	25.5			35.0	N/A	35.0						
61790598	Aliphatic amines	Amines, hydrogenated tallow ali	HN(+)(CC(	328.5	1474.5	TRUE	7.7	FALSE	87.5	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	N/A	6.1	0.0	N/A	N/A	N/A			1261.5	N/A	1261.5						
68527015	Flame Retardants	Alkenes, C12-30 à-, bromo chlo	CCCC(C)(	281.7	7160.4	TRUE	7.4	FALSE	80.3286126	0.0001 - 0.001	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	5.7	5.7	9.1	N/A	N/A	9.1	0.3		40280.2	N/A	40280.2	12.8	626.9				
70775949	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, C10-18-alkane, (	CCCCCC(	354.6	4412.6	TRUE	6.5	FALSE	83.93809626	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	8.3	8.3	0.0	N/A	N/A	0.0	-2.6		32216.4	N/A	32216.4	4.5	599.5				
68640127	INDIVIDUAL - 1-Decene, tetram	1-Decene, tetramer, mixed with	CCCCCC(	422.8	26066.4	TRUE	6.4	FALSE	83.99819875	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	15.4	15.4	0.0	N/A	N/A	0.0	4.8		1.0	N/A	1.0	2.6	76359.2				
68391015	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	333.6	2911.6	TRUE	5.9	FALSE	83.56073515	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	3.0	3.0	0.0	N/A	N/A	0.0	-10.5		24198.2	N/A	24198.2	N/A	225.2				
68424851	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	333.6	2911.6	TRUE	5.9	FALSE	83.56073515	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	3.0	3.0	0.0	N/A	N/A	0.0	-10.5		3755.1	N/A	3755.1	N/A	225.2				
70955714	Terpenes & Terpenoids	Phenol, 2-methoxy-, reaction pro	COc1cc(cc	246.4	1326.5	FALSE	5.8	FALSE	34.86154934	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	4.1	4.1	60.5	N/A	N/A	60.5	-5.6		40.5	N/A	40.5	0.2	92.3				
70225057	Trimellitates	1,2,4-Benzenetricarboxylic acid,	CCCCCC(	673.0	523.8	FALSE	5.7	FALSE	83.99819877	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	16.7	16.7	0.0	N/A	N/A	0.0	-3.5		1.0	N/A	1.0	0.9	1266.2				
61788463	Aliphatic amines	Amines, coco alkyl	CCCCCC(	185.3	331.2	FALSE	5.6	FALSE	87.4	0.1 - 1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	1.7	1.7	16807.1	78.0	N/A	78.0			20684.8	N/A	20684.8						
68917759	Salicylates	Oils, wintergreen	CC(C)(C)(	1035.4	45514.6	TRUE	5.3	FALSE	84.0	0.0001 - 0.001	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	23.5	23.5	0.0	N/A	N/A	N/A			761.9	N/A	761.9						
68603429	Fatty amides	Amides, coco, N,N-bis(hydroxye	CCCCCC(	287.4	126.9	FALSE	5.2	FALSE	82.9	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	4.0	4.0	117.1	N/A	N/A	117.1			356.9	N/A	356.9						
CDSL#11053-1	Fatty amides	Fatty acids compounded with eit	N/A	N/A	4020.0	TRUE	5.0	FALSE	82	0.0001 - 0.001	0.00001 - 0.0001	N/A	N/A	TRUE	N/A	N/A	N/A	N/A	N/A	N/A	N/A			N/A	N/A	N/A						
CDSL#11555-8	Fatty amides	Fatty acids, reaction products wi	N/A	N/A	4020.0	TRUE	5.0	FALSE	82	0.01 - 0.1	0.001 - 0.01	N/A	N/A	TRUE	N/A	N/A	N/A	N/A	N/A	N/A	N/A			N/A	N/A	N/A						
L#11556-0 (85711531)	Fatty amides	Fatty acids, reaction products wi	N/A	N/A	4020.0	TRUE	5.0	FALSE	82	0.01 - 0.1	0.001 - 0.01	N/A	N/A	TRUE	N/A	N/A	N/A	N/A	N/A	N/A	N/A			N/A	N/A	N/A						CDS
CDSL#11557-1	Fatty amides	Fatty acids, reaction products wi	N/A	N/A	4020.0	TRUE	5.0	FALSE	82	0.01 - 0.1	0.001 - 0.01	N/A	N/A	TRUE	N/A	N/A	N/A	N/A	N/A	N/A	N/A			N/A	N/A	N/A						
61789773	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	418.2	N/A	N/A	4.9	FALSE	N/A	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	N/A	6.6	0.0	N/A	N/A	N/A			5.2	N/A	5.2						
73138451	Fatty acids and salts	Fatty acids, montan-wax, ethyler	CCCCCC(	366.6	1452.0	TRUE	4.8	FALSE	84.0	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	10.3	10.3	0.0	N/A	N/A	N/A			2970.2	N/A	2970.2						
61790292	Nitriles	Nitriles, tallow, hydrogenated	CCCCCC(	269.5	634.4	FALSE	4.7	FALSE	84.8	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	4.8	4.8	4.5	N/A	N/A	4.5			36.6	N/A	36.6						
8016884	Terpenes & Terpenoids	Oils, tarragon	CO[c1ccc((	148.2	378.1	FALSE	4.7	FALSE	17.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	3.1	3.1	363.8	178.0	N/A	178.0			18.7	N/A	18.7						
106276806	Pigments and Dyes	Benzoic acid, 2,3,4,5-tetrachlor	NHC1c1c(C	375.0	13569.0	TRUE	4.6	FALSE	9.441947198	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	3.6	3.6	0.4	N/A	N/A	0.4	-13.3		6.3	N/A	6.3	396.9	28.1				
8015778	Terpenes & Terpenoids	Oils, bois de rose	CC1(C)C2	136.2	486.9	FALSE	4.5	FALSE	20.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	3.9	3.9	45.1	N/A	N/A	45.1			714.8	N/A	714.8						
80939624	Aliphatic amines	Amines, C11-14-branched alkyl	CC(CC(C(	185.4	1174.7	FALSE	4.5	FALSE	67.82895562	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	0.6	0.6	151005.1	N/A	N/A	151005.1	-2.2		40.5	N/A	40.5	1.2	155.3				
61788894	Fatty acids and salts	Fatty acids, C18-unsatd., dimer	CCCCCC(	532.9	1317.7	FALSE	4.5	FALSE	84.0	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	12.4	12.4	0.0	N/A	N/A	N/A			1.0	N/A	1.0						
61788441	Hindered phenols	Phenol, styrenated	C=Cc1ccc	120.2	492.0	FALSE	4.4	FALSE	61.83519132	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.5	2.5	1149.0	N/A	N/A	1149.0	-4.9		21901.2	N/A	21901.2	0.2	14.8				
68783960	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, petroleum, calciu	CCCCCC(	390.7	485.8	FALSE	4.4	FALSE	82.9	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	4.6	4.6	1.2	N/A	N/A	1.2			160.0	N/A	160.0						
68391059	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	467.9	2748.7	TRUE	4.2	FALSE	83.99821408	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	7.4	7.4	0.0	N/A	N/A	0.0	-7.5		620.5	N/A	620.5	N/A	26595.7				
74499368	Anthraquinones	9,10-Anthracenedione, 1,4-dian	CCCCCN(	420.6	12907.3	TRUE	4.1	FALSE	83.99738556	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	7.7	7.7	0.0	N/A	N/A	0.0	-11.8		11068.7	N/A	11068.7	16.9	115.2				
174333803	Aldehydes	Benzaldehyde, 2-hydroxy-5-nonC	CCCC(CC	247.4	2177.9	TRUE	4.1	FALSE	59.27768818	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	4.7	4.7	62.5	N/A	N/A	62.5	-5.1		0.0	159.0	159.0	0.6	46.7				
68608322	Terpenes & Terpenoids	Terpenes and Terpenoids, ceda	CC1CCC2	204.3	12639.2	TRUE	4.0	FALSE	71.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	5.8	5.8	46.8	N/A	N/A	46.8			6141.2	N/A	6141.2						
8006788	Terpenes & Terpenoids	Oils, bay	COc1cc(C	164.2	525.1	FALSE	4.0	FALSE	61.8	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	2.5	2.5	1366.4	2460.0	N/A	2460.0			10.2	N/A	10.2						
61789864	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, petroleum, calciu	CC(C)(CC(	464.8	2699.8	TRUE	3.9	FALSE	15.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	5.2	5.2	25.5	N/A	N/A	25.5			35.0	N/A	35.0						
61789875	Alkyl aryl sulfonates/LABS and (	Sulfonic acids, petroleum, magn	CC(C)(CC(	464.8	2699.8	TRUE	3.9	FALSE	15.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	5.2	5.2	25.5	N/A	N/A	25.5			35.0	N/A	35.0						
61789808	Quaternary ammonium compou	Quaternary ammonium compou	CCCCCC(	586.5	N/A	N/A	3.7	FALSE	N/A	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	N/A	12.5	0.0	N/A	N/A	0.0	0.0		509.9	N/A	509.9						
70955349	Quaternary ammonium compou	Fatty acids, tall-oil, reaction pro	CCCCCC(	370.6	460.6	FALSE	3.6	FALSE	88.5	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	5.2	5.2	4.0	N/A	N/A	4.0			1516.9	N/A	1516.9						
61790281	Nitriles	Nitriles, tallow	CCCCCC(	263.4	1971.9	TRUE	3.5	FALSE	84.0	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	7.5	7.5	0.4	N/A	N/A	0.4			14804.5	N/A	14804.5						
90459624	Quaternary ammonium compou	Octadecanoic acid, reaction pro	CCCCCC(	367.7	3259.4	TRUE	3.5	FALSE	83.88992107	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.8	1.8	0.0	N/A	N/A	0.0	-14.3		18.3	N/A	18.3	N/A	1655.4				
68784123	Carboxylic acid anhydrides	2,5-Furandione, dihydro-, mono-	CCCC(CC	308.5	8831.2	TRUE	3.4	FALSE	83.9370408	1 - 10	0.1 - 1	TRUE	FALSE	FALSE	N/A	4.6	4.6	35.4	N/A	N/A	35.4	-1.4		15064.5	N/A	15064.5	1.9	332.4				
68604999	Phosphoric acid derivatives	Fatty acids, C18-unsatd., phosp	CCCCCC(	362.5	832.8	FALSE	3.4	FALSE	14.6	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.0	1.0	32036.0	N/A	N/A	32036.0			801.0	N/A	801.0						
111174619	Phosphoric acid derivatives	Alcohols, C8-16, reaction produ	CCCCCC(	434.7	522.7	FALSE	3.4	FALSE	82.90999134	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	6.4	6.4	0.9	N/A	N/A	0.9	-4.8		4008.6	N/A	4008.6	1.9	968.1				
61790123	Fatty acids and salts	Fatty acids, tall-oil	CCCCCC(	282.4	228.9	FALSE	3.4	FALSE	82.9	1 - 10	1 - 10	TRUE	FALSE	FALSE	7.6	5.2	7.6	103.2	N/A	N/A	103.2			18875.0	N/A	18875.0						
68139899	Fatty acids and salts	Fatty acids, tall-oil, maleated	CCCCCC(	378.5	434.6	FALSE	3.2	FALSE	63.3	0.01 - 0.1	N/A	FALSE	TRUE	FALSE	N/A	2.7	2.7	417.5	N/A	N/A	417.5			718.9	N/A	718.9						
8007087	Terpenes & Terpenoids	Oils, ginger	CC(C)CC(	294.4	310.2	FALSE	3.2	FALSE	83.0	0.1 - 1	0.01 - 0.1	FALSE	FALSE	FALSE	N/A	2.9	2.9	256.6	N/A	N/A	256.6			25.7	N/A	25.7						
8002264	Resins & rosins	Tall oil	CCCCCC(	282.4	228.9	FALSE	3.1	FALSE	82.9	10 - 100	1 - 10	TRUE	FALSE	FALSE	7.6	5.2	7.6	103.2	N/A	N/A	103.2			41773.5	N/A	41773.5						
72102400	Quaternary ammonium compou	1-Propanaminium, 3-amino-N-((	CCCCCC(	685.6	N/A	N/A	3.1	FALSE	N/A	0.00001 - 0.0001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	N/A	13.7	0.0	N/A	N/A	N/A			7.7	N/A	7.7						
61790601	Aliphatic amines	Amines, tallow alkyl, acetates	HN(+)(CC(	326.5	1717.5	TRUE	3.0	FALSE	83.4	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	N/A	5.9	0.0	N/A	N/A	N/A			1263.7	N/A	1263.7						
8006642	Terpenes & Terpenoids	Turpentine, oil	CC1=CCC	148.2	676.3	FALSE	2.9	FALSE	21.6	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	4.2	4.2	5.0	N/A	94.6	94.6			760.5	N/A	760.5						
9005907	Terpenes & Terpenoids	Turpentine	CC1=CCC	136.2	528.8	FALSE	2.8	FALSE	30.6	10 - 100	10 - 100	TRUE	FALSE	FALSE	N/A	4.1	4.1	71.5	N/A	N/A	71.5			1350.7	N/A	1350.7						
68527026	Flame Retardants	Alkenes, C12-24, chloro	CICCCCC(	200.8	3110.9	TRUE	2.8	FALSE	77.16371475	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	5.4	5.4	13.3	N/A	0.3	0.3	1.2		33193.3	N/A	33193.3	1.3	7.6				
68909206	INDIVIDUAL - Silanamine, 1,1,1	Silanamine, 1,1,1-trimethyl-N-(tr	C[Si](C)(C	161.4	889.7	FALSE	286.0	TRUE	21.2	0.1 - 1	0.1 - 1	TRUE	FALSE	FALSE	N/A	0.8	0.8	999963.5	N/A	N/A	999963.5	0.0		1.1	N/A	1.1						
8008524	Terpenes & Terpenoids	Oils, coriander	CC=CCC(	154.2	523.4	FALSE	2.8	FALSE	82.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	2.9	2.9	70.5	N/A	N/A	70.5			1533.0	N/A	1533.0						
8000279	Terpenes & Terpenoids	Oils, cedarwood	CC1CCC2	204.3	12973.2	TRUE	2.7	FALSE	76.7	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	5.9	5.9	58.9	N/A	N/A	58.9			28670.7	N/A	28670.7						
68990830	Terpenes & Terpenoids	Oils, cedarwood, Texan	CC1CCC2	204.3	12973.2	TRUE	2.7	FALSE	76.7	0.0001 - 0.001	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	5.9	5.9	58.9	N/A	N/A	58.9			46741.7	N/A	46741.7						
8016851	Terpenes & Terpenoids	Oils, tangerine	CC(CCC=	156.3	416.3	FALSE	2.6	FALSE	84.0	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	3.6	3.6	392.5	N/A	N/A	392.5			9049.6	N/A	9049.6						
37310831	Phosphoric acid derivatives	9-Octadecen-1-ol, (Z)-, phospha	CCCCCC(	348.5	721.9	FALSE	2.6	FALSE	14.92761256	0.0001 - 0.001	0.00001 - 0.0001	FALSE	FALSE	TRUE	N/A	1.9	1.9	8579.3	N/A	N/A	8579.3	-8.0		1.4	N/A	1.4	1.6	172.4				
8001614	Terpenes & Terpenoids	Balsams, copaiba	CC(C)C1C	204.3	4016.4	TRUE	2.6	FALSE	61.9	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	6.1	6.1	2.5	N/A	N/A	2.5			10097.4	N/A	10097.4						
64754956	Inorganic - Lithium	Castor oil, hydrogenated, lithium	CCCCCC(	939.4	418.0	FALSE	2.4	FALSE	84.0	0.001 - 0.01	0.0001 - 0.001	FALSE	FALSE	TRUE	N/A	17.3	17.3	0.0	N/A	N/A	N/A			12903.6	N/A	12903.6						
8050280	Resins & rosins	Rosin, maleated	CC(C)C1=	400.5	3783.7	TRUE	2.3	FALSE	9.0	0.001 - 0.01	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	2.1	2.1	93.8	N/A	N/A	93.8			60879.2	N/A	60879.2						
8022568	Terpenes & Terpenoids	Oils, sage	CC(C)=CC	154.2	829.4	FALSE	2.1	FALSE	15.1	0.01 - 0.1	0.01 - 0.1	FALSE	TRUE	FALSE	N/A	3.3	3.3	173.1	1590.0	N/A	1590.0			47.4	N/A	47.4						
68953800	Arenes	Benzene, mixed with toluene, de	c1ccccc1	78.1	155.9	FALSE	131.7	TRUE	10.12748542	10 - 100	10 - 100	TRUE	FALSE	FALSE	2.1	2.0	2.1	1708.9	N/A	1790.0	1790.0	-0.6		5.9	N/A	5.9	3.9	49.2				
61791319	Alkanolamines	Ethanol, 2,2'-iminobis-, N-coco d	CCCCCC(	273.4	358.7	FALSE	2.1	FALSE	85.8	0.01 - 0.1	0.001 - 0.01	FALSE	FALSE	TRUE	N/A	3.1	3.1	3402.4	N/A	N/A	3402.4			128.2	N/A	128.2						

| HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION						OTHER			
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE		AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM COMPOUNDS	BIOAVAILABILITY		FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION		
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kf/yt)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailibility ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification (including manual classification)	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)	UVCB Model Result Acceptance
8001045	1	N/A	8.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	Not found	Accepted
61789013	1	3	0.0	0.1 - 1	FALSE	FALSE	TRUE	TRUE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	Yes	CCCCCC	Accepted
68584247	2	2	23.3	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	Probably n	CCCCCC	?
68990534	1	1	10980.1	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted given low volume
120547526	1	3	25.6	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	CCCCCC	?
68476039	1	3	0.0	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	Yes	Not needed	Accepted given low volume
68955533	1	1	2594.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for substa	ERC classified this substance	Yes	Not needed	?
68937417	2	3	20.7	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A	?
1338029	1	1	89259.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near field)	local RQ >10	moderate (mostly near field)			Yes	C1=CC=C	Accepted
61789853	1	N/A	1.2	1,000 - 10,000	FALSE	FALSE	TRUE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	No	Available	accept model result if appropriate
68608264	3	N/A	1.2	0.1 - 1	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	3	3	high (near and far field risk)	N/A	N/A	N/A	N/A	N/A	N/A	accept model result if appropriate
61790598	2	3	0.5	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	CCCCCC	Accepted
68527015	1	2	9.2	10,000 - 100,000	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Longer car	?
70775949	2	3	25.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A	?
68649127	2	1	23.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC(C(CC(	?
68391015	2	2	86.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not Needed	?
68424851	3	2	20.8	100 - 1,000	FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	3	2	moderate (up to far field)	N/A	N/A	N/A	N/A	Yes	Not Needed	?
70955714	1	3	232.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Low current exposure, but po	ERC classified this substance	N/A	N/A	?
70225057	1	1	885.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	?
61788463	1	1	3079.0	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	moderate (mostly near field)	local RQ >10	moderate (mostly near field)	N/A	N/A	Yes	Not needed	Accepted
68917759	1	1	0.0	< 0.0000001	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	No	O=C(OC)c	Accepted given low volume
68603429	1	1	517313.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not needed	Accepted
CDSL#11053-1	1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CDSL#11555-8	1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SL#11556-0 (85711531)	1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CDSL#11557-1	1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	N/A
61789773	N/A	N/A	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	FALSE	3	3	high (near and far field risk)	N/A	N/A	N/A	N/A	Yes	Cl[-] CCC	Accepted
73138451	1	1	307.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted given low volume
61790292	1	3	5.1	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted given low volume
8016884	1	1	6032.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC(=CCC	Accepted
106276806	1	3	10.5	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	No (differe	COc1c(Cl)	?
8015778	1	1	1380.4	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	No	CC(=CCC	Accepted given low volume
80939624	1	1	1289.6	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	Possible substitute for substa	ERC classified this substance	Yes	Not found	?
61788894	1	1	463.4	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	No	C(=O)(O)C	Accepted given low volume
61788441	1	1	23024.2	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	C=CC1=CC	=C(C=C1)O)C=C	
68783960	1	N/A	8.2	1 - 10	FALSE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	accept model result if appropriate
68391059	1	3	15.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	1	3	moderate (mostly near field)	local RQ >10	moderate (mostly near field)	N/A	N/A	N/A	N/A	?
74499368	1	3	2.2	1,000 - 10,000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	?
174333803	1	3	17.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	local RQ <1	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	No	CCCC(C)(	?
68608322	1	3	7.5	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC1=CCC	Accepted
8006788	1	1	119995.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	O(C(CCC	Accepted
61789864	2	N/A	1.2	10 - 100	FALSE	FALSE	TRUE	N/A	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	No	Available	accept model result if appropriate
61789875	2	N/A	1.2	10 - 100	FALSE	FALSE	TRUE	N/A	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	No	Available	accept model result if appropriate
61789808	N/A	1	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	TRUE	3	3	high (near and far field risk)	N/A	N/A	N/A	N/A	Yes	Not needed	Accepted given low volume
70955349	1	1	1072.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	No	CCOS(=O	rejected
61790281	3	1	22.9	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted given low volume
90459624	1	3	1.5	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	?
68784123	3	2	20.9	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A	?
68604999	1	N/A	25.6	100,000 - 1,000,000	TRUE	FALSE	FALSE	N/A	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	accept model result if appropriate
111174619	1	3	9.0	100,000 - 1,000,000	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	No (no hex	CCCCCC	?
61790123	1	3	4.9	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A			Yes	Not needed	Accepted
68139899	1	3	0.0	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substance	No	Other cons	accept model result if appropriate
8007087	1	N/A	196359.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	No	CC1=CCC	Accepted given low volume
8002264	1	3	4.9	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted
72102400	N/A	1	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	TRUE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	Accepted given low volume
61790601	1	3	4.5	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	CCCCCC	Accepted
8006642	1	1	749.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC1=CCC	Accepted
9005907	1	N/A	930.4	10 - 100	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC1=CCC	Accepted
68527026	1	2	27.7	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Longer car	?
68909206	3	1	31207.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	Available	Accepted given low volume
8008524	1	1	10592.4	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC(=CCC	Accepted
8000279	1	3	1.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC1=CC=	Accepted
68990830	1	3	1.3	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC1=CCC	Accepted
8016851	1	N/A	5940.3	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	No	CC1=CCC	Accepted given low volume
37310831	1	3	8.4	10,000 - 100,000	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substance	N/A	N/A	?
8001614	2	1	73.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC1=CCC	Accepted
64754956	1	1	1317.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	No	CCCCCC	Accepted given low volume
8050280	1	3	0.0	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not needed	Accepted given low volume
8022568	1	1	11294.7	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	No	CC(=CCC	Accepted given low volume
68953800	3	1	58138.7	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A			N/A	N/A	?
61791319	1	1	29141.0	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CCCCCC	Accepted

| CHEMICAL IDENTITY | | | | | EXPOSURE | | | | | | | | | FATE | | | | | | | | |



| | HAZARD | | |

	PRELIMINARY CLASSIFICATION		PRELIMINARY CLASSIFICATION ADJUSTMENTS								RISK CLASSIFICATION							OTHER		
	EXPOSURE	HAZARD	MARGIN OF EXPOSURE			AIR-WATER PARTITIONING	TERRESTRIAL HAZARD	PROTEIN/DNA BINDING	QUATERNARY AMMONIUM COMPOUNDS	BIOAVAILABILITY	FINAL CLASSIFICATION					TRACKING		STRUCTURAL VERIFICATION		
CAS	Preliminary Exposure Classification	Preliminary Hazard Classification	Critical Emission Rate @ Default 1 kg/hr rate (kt/yr)	Ratio of Critical Emmission to Actual Emission (margin of exposure)	Ratio of Critical to Actual Emission High?	Critical air half-life but low LogKaw ?	Terrestrial HAF is Low ?	Protein and DNA Binder ?	Quaternary ammonium compound ?	Low Bioavailibility ?	Final Exposure Classification	Final Hazard Classification	Final Risk Classification (including manual classification)	Risk Classification Adjustment	Risk Adjustment Outcome	Track Use Pattern Flags	Track Use Pattern Flag Rationale	SMILES OK ? (UVCBs)	Alternative SMILES (UVCBs)	UVCB Model Result Acceptance
68584258	1	1	985.2	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A			Yes	CCCCCC(	?
61790441	1	3	3.2	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A			No	CCCCCC(	Accepted given low volume
8027336	1	N/A	1.9	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	Yes	CC(C)CC(	Accepted
61789795	1	1	55.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A			Yes	Not neede	Accepted
68511922	2	3	0.7	10 - 100	FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	CCCCCC(	?
8007021	1	N/A	3706.9	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	2	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	C=CC(CC	Accepted
8024086	1	N/A	1385.5	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	COC(C1=I	Accepted
8008319	1	N/A	6609.9	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	C(C(CC1(	Accepted
8008579	1	1	6609.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC(C)C12	Accepted
8021281	1	N/A	6609.9	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	C(C(CC1(	Accepted
68916972	1	1	10873.0	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	?
68917293	1	3	0.4	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	Yes	Not found	Accepted
8006879	1	1	24.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC1=CCC	Accepted
68308678	N/A	N/A	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	Available	Accepted
61791342	N/A	N/A	N/A	N/A	FALSE	N/A	TRUE	FALSE	TRUE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	N/A	N/A	Accepted given low volume
68479049	2	2	179.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	2	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC(C)CC(	?
8007010	1	1	6384.8	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CCCCCC(	Accepted
8014195	1	1	6384.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC1=CCC	Accepted
61791444	1	1	148.1	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted
68647552	1	1	455.6	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CCCCCC(	Accepted
8013103	1	N/A	0.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	No	CC1=CCC	Accepted given low volume
68917657	1	1	21.9	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	CC1(C2((	Accepted
8000462	1	1	118.4	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CC(CCC=	Accepted
68153355	N/A	1	N/A	N/A	FALSE	N/A	TRUE	FALSE	FALSE	TRUE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	Yes	More struc	Accepted
91081537	1	3	0.6	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	No	C[C@]1(C	Accepted given low volume
68783255	1	3	2.2	1,000 - 10,000	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted
CDSL#10685-2	1	3	0.0	0.01 - 0.1	FALSE	N/A	N/A	N/A	N/A	N/A	1	3	moderate (mostly near field)	N/A	N/A	Moderate potential for risk; m	ERC classified this substanc	N/A	N/A	N/A
90367274	1	1	169.5	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Possible substitute for substa	ERC classified this substanc	N/A	N/A	Accepted given low volume
71820354	1	1	152.4	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	Yes	Not neede	Accepted
91745527	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	1	3	low (mostly near field)	N/A	N/A			N/A	N/A	N/A
8016373	1	N/A	63.6	1,000,000 - 10,000,000	TRUE	FALSE	FALSE	N/A	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	N/A	N/A	accept model result if appropriate
61790510	2	3	0.0	0.01 - 0.1	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	Available	Accepted given low volume
68186141	1	1	9.8	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Possible substitute for substa	ERC classified this substanc	Yes	Not neede	Accepted given low volume
8050097	3	N/A	0.0	0.001 - 0.01	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	3	3	high (near and far field risk)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted given low volume
8052106	1	N/A	0.0	0.1 - 1	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted given low volume
73138826	1	3	0.0	1 - 10	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	Yes	Not Neede	Accepted given low volume
8002651	1	3	6.4	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	3	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	Low current exposure, but hig	ERC classified this substanc	Yes	CCC(CCC	Accepted
68784269	1	1	0.0	0.0000001 - 0.000001	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	Available	Accepted
61791557	1	1	46.5	100 - 1,000	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	Yes	[R]NCCC(	accept model result if appropriate
68784178	1	1	4271.5	10,000,000 - 100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	CCCCCC(	?
8023754	1	1	1110259.6	>100,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	only ~1,000 kg exposure after W	low (mostly near field)	N/A	N/A	No	CC1=CC=	accept model result if appropriate
68909773	3	1	981781.9	1,000,000 - 10,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	N/A	N/A	?
68478819	1	3	2.0	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	?
CDSL#10703-2	1	3	0.0	0.01 - 0.1	FALSE	FALSE	N/A	N/A	N/A	N/A	1	3	moderate (mostly near field)	N/A	N/A			N/A	N/A	N/A
68937906	1	1	0.0	< 0.0000001	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	1	1	low (mostly near field)	N/A	N/A	N/A	N/A	Yes	OCCCCC(	accept model result if appropriate
CDSL#11105-8	1	3	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	1	3	moderate (mostly near field)	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CDSL#11145-3	2	3	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	N/A	N/A	N/A
68511502	1	1	2545.1	100,000 - 1,000,000	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	1	1	low (mostly near field)	N/A	N/A	greater potential for local exp	ERC classified this substanc	Yes	Longer-chc	?
8001205	1	1	812.2	10,000 - 100,000	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	3	1	low (up to far field)	N/A	N/A	N/A	N/A	No	CCCCC=(	rejected
9007130	2	3	0.0	0.001 - 0.01	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	2	3	high (mostly near field risk)	N/A	N/A	N/A	N/A	Yes	Not neede	Accepted given low volume