Data-poor fragrance chemicals: Environment tier II assessment

01 September 2015

CAS Registry Numbers: 6502-23-4, 7774-82-5, 142-83-6, 52844-21-0, 3613-30-7, 7775-00-0, 65405-84-7, 33885-51-7, 93981-63-6, 605-85-6, 1333-52-4, 68459-99-4, 10316-66-2, 7549-37-3, 40910-49-4, 6379-73-3, 68213-86-5, 2114-29-6, 101-85-9

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Preface

This assessment was carried out by staff of the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) using the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework.

The IMAP framework addresses the human health and environmental impacts of previously unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory).

The framework was developed with significant input from stakeholders and provides a more rapid, flexible and transparent approach for the assessment of chemicals listed on the Inventory.

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

The IMAP framework is a science and risk-based model designed to align the assessment effort with the human health and environmental impacts of chemicals. It has three tiers of assessment, with the assessment effort increasing with each tier. The Tier I assessment is a high throughput approach using tabulated electronic data. The Tier II assessment is an evaluation of risk on a substance-by-substance or chemical category-by-category basis. Tier III assessments are conducted to address specific concerns that could not be resolved during the Tier II assessment.

These assessments are carried out by staff employed by the Australian Government Department of Health and the Australian Government Department of the Environment and Energy. The human health and environment risk assessments are conducted and published separately, using information available at the time, and may be undertaken at different tiers.

This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

For more detail on this program please visit: www.nicnas.gov.au.

Disclaimer

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Acronyms & Abbreviations

Grouping Rationale

This Tier II assessment considers the environmental risks of nineteen organic chemicals that may have uses as fragrance ingredients in Australia.

The group comprises a range of aldehydes, ketones, acetals, ethers, acetates and alcohols. Available information indicates that these chemicals may be used as fragrance ingredients with diverse applications in personal care products including perfumes and colognes, hair products, soaps, deodorants, and cleaning products in Australia. These products are often released to sewers and air as a normal part of their use in domestic and commercial situations. Any use of these substances as fragrance ingredients therefore has the potential to result in environmental exposure through direct volatilisation and through a common pathway involving releases of the chemicals in the treated effluents and biosolids produced by sewage treatment plants.

These chemicals have been grouped together due their similar assumed use pattern and resulting common potential pathways for release into the environment, and because there are limited experimental data available regarding their environmental fate and effects.

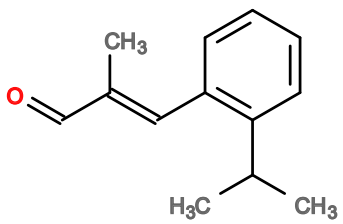
The Tier I environmental risk assessments of each of these chemicals were conducted assuming a default annual introduction volume of 100 tonnes in accordance with the IMAP Framework. The risks arising from use of these volumes of the chemicals were characterised using a standard emission scenario involving release into the environment through sewage treatment plants and values for environmental hazard properties that were calculated using standard Quantitative Structure-Activity (Property) Relationship (QSA(P)R) models. The use of modelling to estimate values for critical hazard properties was necessary in most cases because there were generally no readily available measured values for critical environmental fate and ecotoxicity

characteristics. The results of these standard risk analyses indicated that use of the chemicals in this group based on the default annual introduction volume may result in hazardous concentrations of these chemicals in surface waters.

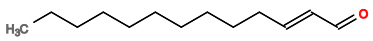
This Tier II group assessment includes further refinement of the risk characterisation for these chemicals where possible, and outlines the most significant data gaps that would need to be addressed to further refine the risk assessment.

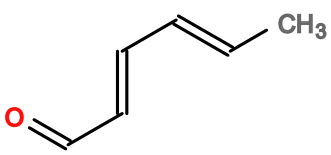
Chemical Identity

Alpha, Beta Unsaturated Aldehydes

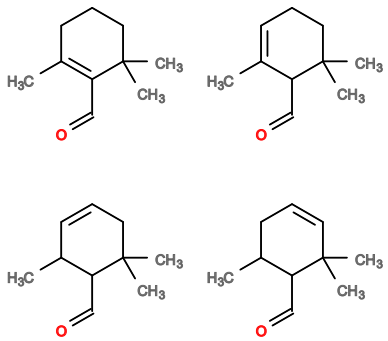
CAS RN	6502-23-4
Chemical Name	2-Propenal, 2-methyl-3-[2-(1-methylethyl)phenyl]-
Synonyms	o-isopropyl-α-methylcinnamaldehyde
Structural Formula	
Molecular Formula	$C_{13}H_{16}O$
Molecular Weight (g/mol)	188.27
SMILES	c1(C(C)C)c(/C=C\(C)C=O)cccc1

CAS RN	7774-82-5
Chemical Name	2-Tridecenal

Synonyms	2-tridecenal
Structural Formula	
Molecular Formula	$C_{13}H_{24}O$
Molecular Weight (g/mol)	196.33
SMILES	C(=O)/C=C/CCCCCCCCCC

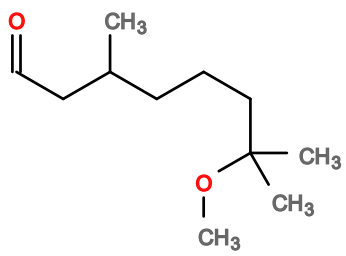
CAS RN	142-83-6
Chemical Name	2,4-Hexadienal, (E,E)-
Synonyms	(*E*,*E*)-2,4-hexadienal *trans*,*trans*-2,4-hexadienal sorbic aldehyde sorbaldehyde
Structural Formula	
Molecular Formula	C_6H_8O
Molecular Weight (g/mol)	96.13

SMILES	C(=O)\C=C\C=C\C

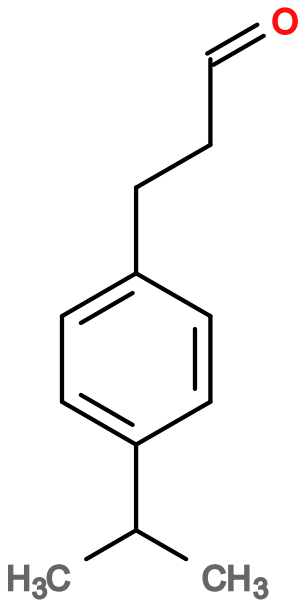
CAS RN	52844-21-0
Chemical Name	Cyclohexenecarboxaldehyde, 2,6,6-trimethyl-
Synonyms	cyclocitral 2,6,6-trimethylcyclohexenecarboxaldehyde
Structural Formula	
Molecular Formula	$C_{10}H_{16}O$
Molecular Weight (g/mol)	152.23
SMILES	C1(C)(C)C(C=O)=C(C)CCC1 C1(C)(C)C(C=O)C(C)C=CC1 C1(C)(C)C(C=O)C(C)=CCC1 C1(C)(C)C(C=O)C(C)CC=C1

Other Aldehydes

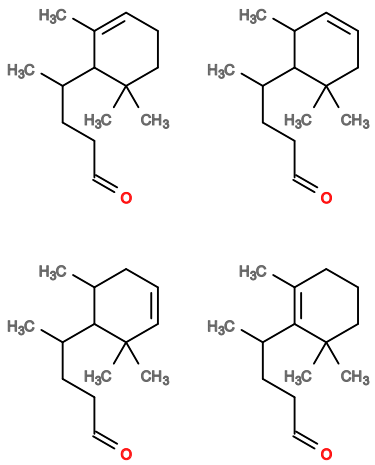
CAS RN	3613-30-7

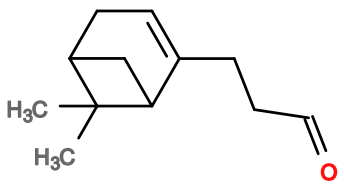
Chemical Name	Octanal, 7-methoxy-3,7-dimethyl-
Synonyms	methoxycitronellal
Structural Formula	
Molecular Formula	$C_{11}H_{22}O_2$
Molecular Weight (g/mol)	186.29
SMILES	C(C)(C)(CCCC(C)CC=O)OC

CAS RN	7775-00-0
Chemical Name	Benzenepropanal, 4-(1-methylethyl)-
Synonyms	cuminyl acetaldehyde 3-*p*-cumenyl propionaldehyde
Structural Formula	

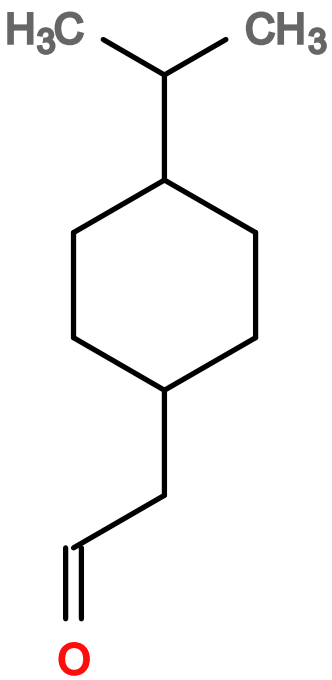
	
Molecular Formula	$C_{12}H_{16}O$
Molecular Weight (g/mol)	176.25
SMILES	c1(C(C)C)ccc(CCC=O)cc1

CAS RN	65405-84-7
Chemical Name	Cyclohexenebutanal, .alpha.,2,2,6-tetramethyl-
Synonyms	cetonal
Structural Formula	

	
Molecular Formula	$C_{14}H_{24}O$
Molecular Weight (g/mol)	208.34
SMILES	C1(C)(C)C(C(C)CCC=O)C(C)=CCC1 C1(C)(C)C(C(C)CCC=O)C(C)CC=C1 C1(C)(C)C(C(C)CCC=O)C(C)C=CC1 C1(C)(C)C(C(C)CCC=O)=C(C)CCC1

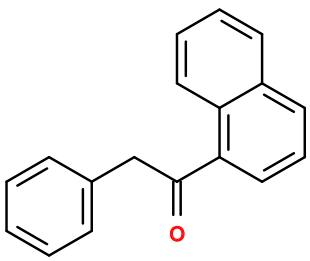
CAS RN	33885-51-7
Chemical Name	Bicyclo[3.1.1]hept-2-ene-2-propanal, 6,6-dimethyl-
Synonyms	pinoacetaldehyde homonopal
Structural Formula	

Molecular Formula	$C_{12}H_{18}O$
Molecular Weight (g/mol)	178.27
SMILES	C1(CCC=O)C2C(C)(C)C(CC=1)C2

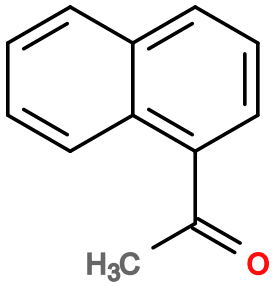
CAS RN	93981-63-6
Chemical Name	Cyclohexaneacetaldehyde, 4-(1-methylethyl)-
Synonyms	4-(isopropyl) cyclohexane acetaldehyde
Structural Formula	
Molecular Formula	$C_{11}H_{20}O$
Molecular Weight	168.28

(g/mol)	
SMILES	C(C)(C)C1CCC(CC=O)CC1

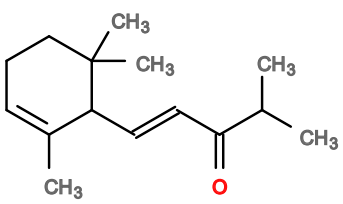
Aryl Ketones

CAS RN	605-85-6
Chemical Name	Ethanone, 1-(1-naphthalenyl)-2-phenyl-
Synonyms	1-(1-naphthalenyl)-2-phenylethanone
Structural Formula	
Molecular Formula	$C_{18}H_{14}O$
Molecular Weight (g/mol)	246.30
SMILES	C(=O)(c1c2c(cccc2)ccc1)Cc1ccccc1

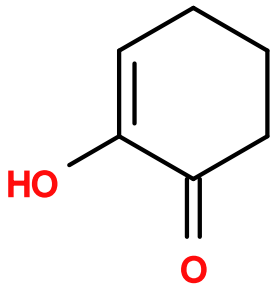
CAS RN	1333-52-4
Chemical Name	Ethanone, 1-(naphthalenyl)-

Synonyms	1-(naphthyl)ethan-1-one methyl naphthyl ketone
Structural Formula	
Molecular Formula	$C_{12}H_{10}O$
Molecular Weight (g/mol)	170.21
SMILES	C(C)(=O)c1c2c(cccc2)ccc1

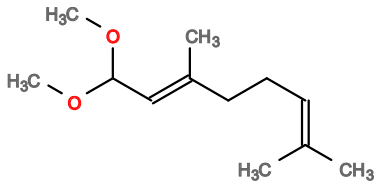
Alpha, Beta Unsaturated Ketones

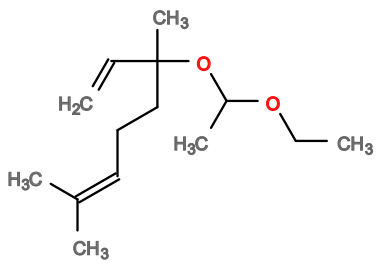
CAS RN	68459-99-4
Chemical Name	1-Penten-3-one, 4-methyl-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
Synonyms	dimethylionone
Structural Formula	

Molecular Formula	$C_{15}H_{24}O$
Molecular Weight (g/mol)	220.35
SMILES	C1(C)(C)C(\C=C\C(=O)C(C)C)C(C)=CCC1

CAS RN	10316-66-2
Chemical Name	2-Cyclohexen-1-one, 2-hydroxy-
Synonyms	2-hydroxy-2-cyclohexenone
Structural Formula	
Molecular Formula	$C_6H_8O_2$
Molecular Weight (g/mol)	112.13
SMILES	C1(=O)C(O)=CCCC1

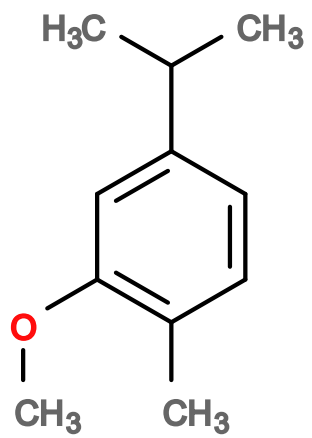
Acetals

CAS RN	7549-37-3
Chemical Name	2,6-Octadiene, 1,1-dimethoxy-3,7-dimethyl-
Synonyms	citral dimethyl acetal
Structural Formula	
Molecular Formula	$C_{12}H_{22}O_2$
Molecular Weight (g/mol)	198.30
SMILES	C\(C)(=C\C(OC)OC)CCC=C(C)C

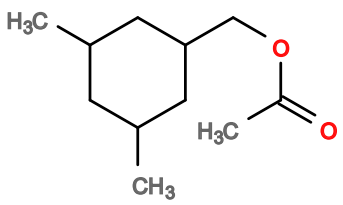
CAS RN	40910-49-4
Chemical Name	1,6-Octadiene, 3-(1-ethoxyethoxy)-3,7-dimethyl-
Synonyms	acetaldehyde ethyl linalyl acetal
Structural Formula	

Molecular Formula	$C_{14}H_{26}O_2$
Molecular Weight (g/mol)	226.36
SMILES	C(C)(C=C)(CCC=C(C)C)OC(C)OCC

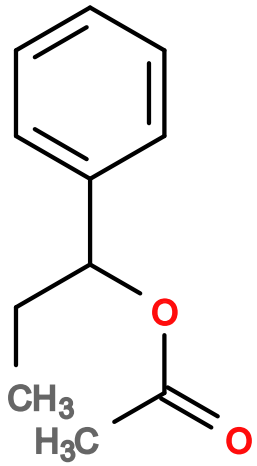
Ethers

CAS RN	6379-73-3
Chemical Name	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-
Synonyms	carvacryl methyl ether
Structural Formula	
Molecular Formula	$C_{11}H_{16}O$
Molecular Weight (g/mol)	164.24
SMILES	c1(C)c(OC)cc(C(C)C)cc1

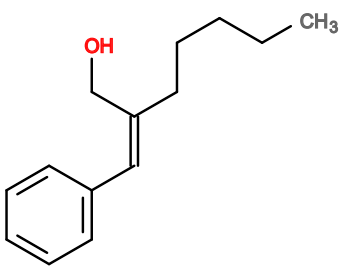
Acetates

CAS RN	68213-86-5
Chemical Name	Cyclohexanemethanol, 3,5-dimethyl-, acetate
Synonyms	3,5-dimethylcyclohexylmethyl acetate
Structural Formula	
Molecular Formula	$C_{11}H_{20}O_2$
Molecular Weight (g/mol)	184.28
SMILES	C(C)(=O)OCC1CC(C)CC(C)C1

CAS RN	2114-29-6
Chemical Name	Benzenemethanol, .alpha.-ethyl-, acetate
Synonyms	1-phenyl propyl acetate
Structural Formula	

	
Molecular Formula	$C_{11}H_{14}O_2$
Molecular Weight (g/mol)	178.23
SMILES	c1(C(CC)OC(C)=O)ccccc1

Alcohols

CAS RN	101-85-9
Chemical Name	1-Heptanol, 2-(phenylmethylene)-
Synonyms	α-amylcinnamyl alcohol
Structural Formula	

Molecular Formula	$C_{14}H_{20}O$
Molecular Weight (g/mol)	204.31
SMILES	c1(C=C(CCCCC)CO)ccccc1

Physical and Chemical Properties

Limited measured chemical property data are available for the substances in this group. They are a mixed group of low to moderate molecular weight neutral organic substances with polar functional groups including aldehydes, ketones, acetals, ethers, acetates and alcohols. Based on the available calculated and experimental values for key chemical properties, most substances in this group are expected to have some volatility and to be at least slightly soluble in water (ECHA, 2015a; LMC, 2013; US EPA, 2008):

Physical Form	liquids and solids
Melting Point	-56–≤ 130.85°C (calc. and exp.)
Vapour Pressure	0.00122–172 Pa (calc.)
Water Solubility	0.6–36 198 mg/L (calc. and exp.)
Ionisable in the Environment?	no
log K_{ow}	1.23 to >5.9 (calc. and exp.)

Some of the chemicals in this group have only moderate solubility in water and relatively high volatility, which suggests that they may be volatile from water and moist soil. For example, carvacryl methyl ether (CAS RN 6379-73-3) has a calculated Henry's Law constant of 1080 Pa-m^3/mol (US EPA, 2008).

The acetals in this group, citral dimethyl acetal (CAS RN 7549-37-3) and acetaldehyde ethyl linalyl acetal (CAS RN 40910-49-4), are susceptible to rapid hydrolysis under acid conditions (pH 1.2). However, available information indicates that hydrolysis of acetals will be significantly slower at near neutral pH which is considered to be more representative of likely environmental exposure conditions (European Food Safety Authority, 2011).

Import, Manufacture and Use

Australia

No specific Australian use, import, or manufacturing information has been identified.

International

Available information indicates that the chemicals in this group may be used as fragrances in a range of products internationally. Most are listed on the International Fragrance Association (IFRA) Transparency List, which identifies chemicals used as fragrances by member companies (IFRA, 2015). Others are listed on the European Union (EU) Cosmetic Ingredients and Substances Database (CosIng) (European Commission, 2013), or share structural characteristics with other chemicals identified in fragrance compositions (Rastogi, et al., 1998).

Some of the chemicals in the group such as methyl naphthyl ketone (CAS RN 1333-52-4), methoxycitronellal (CAS RN 3613-30-7) and carvacryl methyl ether are reported to be used internationally in domestic cleaning and washing products (NICNAS, 2015; Nordic Council of Ministers, 2015).

Other industrial applications have been reported for some of the chemicals in the group. For example, (*E*,*E*)-2,4-hexadienal (CAS RN 142-83-6) is used as a chemical intermediate (WHO, 2013). However, use in fragrance formulations is the focus of this assessment due to the extent of potential environmental emissions that may result from this use pattern.

Environmental Regulatory Status

Australia

The use of the chemicals in this group is not subject to any specific national environmental regulations.

United Nations

The chemicals in this group are not currently identified as Persistent Organic Pollutants (UNEP, 2001), ozone depleting substances (UNEP, 1987), or hazardous substances for the purpose of international trade (UNEP & FAO, 1998).

OECD

The chemicals in this group have not been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP) (OECD, 2013).

Canada

The chemicals in this group are not listed under Schedule 1 (the Toxic Substances List) of the *Canadian Environmental Protection Act 1999*(CEPA 1999) (Government of Canada, 2013).

The majority of the chemicals in this group are listed on the Canadian Domestic Substances List (DSL) (Environment Canada, 2013a). Of the 18 chemicals that are listed, none of the chemicals were found to be Persistent (P), Bioaccumulative (B) and Inherently Toxic to the Environment (iT_E) during the categorization of the DSL. One chemical (2-tridecanal, CAS RN 7774-82-5) was found to be iT_E and two chemicals (cetonal and dimethylionone, CAS RNs 65405-84-7 and 68459-99-4) were found to be B

and iT_E. The two chemicals were prioritised for further assessment. Dimethylionone has been assessed under the Rapid Screening Approach, but cetonal is yet to undergo further assessment (Environment Canada, 2013b).

European Union

Most of the chemicals in this group (18 substances) have been pre-registered for use in the European Union under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2015b), but only one chemical (cetonal) has undergone the full registration process (ECHA, 2015a).

United States of America

Most of the chemicals in this group (17 substances) are listed on the inventory of chemicals manufactured or processed in the USA, as published under the *Toxic Substances Control Act 1976* (TSCA) (US EPA, 2014).

Environmental Exposure

Available international use data indicate that the majority of the chemicals in this group have use as fragrances, which are incorporated into a range of product types (European Commission, 2013; IFRA, 2015). The formulations of such products on the Australian market are assumed to not differ significantly from those found internationally. Therefore, the chemicals in this group may be found in a range of products available for use in Australia. This may include personal care products including perfumes, cosmetics, deodorants, food-stuffs and domestic and industrial cleaners.

Chemicals used as fragrances are typically released to sewer as a normal part of their domestic applications. During treatment in sewage treatment plants (STPs), chemicals may degrade by abiotic and/or biological processes, volatilise to the air compartment, partition to sludge, or remain in effluent (Struijs, 1996). Depending on the removal efficiencies for individual substances in sewage treatment plants, some fraction of the quantity of chemicals in waste water entering STPs can be emitted to the air compartment, to soil through application of biosolids to agricultural land, or to rivers or oceans in treated effluent. Once released to the environment, the chemicals in this group are expected to partition to the air, soil, sediment and water compartments, depending on their individual partitioning properties.

Based on predicted degradation pathways and general information regarding metabolic processes, most chemicals in this group are expected to undergo ultimate degradation in the environment. However, available information suggests that many chemicals in this group will not be readily biodegradable. Experimental results from OECD Test Guideline studies for pinoacetaldehyde (CAS RN 33885-51-7) and cetonal demonstrate that these substances are not readily biodegradable (0% degradation in 28 days and 54% degradation in 29 days, respectively) (Seyfried and Boschung, 2014; ECHA, 2015a).

However, potential for persistence in the atmosphere is expected to be low. If released to air, the most volatile chemical in this group ((*E*,*E*)-2,4-hexadienal) is expected to be degraded through reaction with photochemically-produced hydroxyl radicals. The half-life for this reaction in air is estimated to be 1.96 hours (US EPA, 2008; US NLM, 2013). Other chemicals in this group, such as 1-(1-naphthalenyl)-2-phenylethanone (CAS RN 605-85-6), have similarly rapid estimated degradation half lives (5.085 hours) (US EPA, 2008).

No data are available to evaluate the potential for the chemicals in this group to bioaccumulate in aquatic or sediment-dwelling organisms. Most chemicals in this group have an octanol-water partition coefficient (K_{OW}) less than log K_{OW} 4.2. In addition, the chemicals in this group are, or are structurally similar to, naturally occurring substances which typically undergo rapid primary metabolism in exposed organisms. These metabolic processes generally yield more water soluble products, which are more easily excreted from the organism and therefore less likely to bioaccumulate. For example, cetonal, which has a log K_{OW} greater than 5.9, is predicted to undergo rapid primary metabolism to form a more soluble carboxylic acid (LMC, 2011). Based on the available information, the chemicals in this group are expected to have low potential for bioaccumulation.

Predicted Environmental Concentration (PEC)

No reported Australian environmental monitoring data were located for the chemicals in this group. In addition, no introduction volume information is available. In accordance with the IMAP Framework, a default use volume of 100 tonnes was applied for each chemical in this group (NICNAS, 2013). Chemical-by-chemical exposure modelling for the release of chemicals to surface waters in STP effluents, incorporating expected individual losses due to volatilisation and partitioning to sludge, were used to calculate riverine environmental concentrations based on this default introduction volume. In accordance with available information, no ready biodegradation was assumed.

Derived PECs for the chemicals in this group range from 9.4 to 85.04 µg/L. The lowest PEC derived was for cetonal due to its high lipophilicity and volatility (ECHA, 2015a), while the highest PEC derived was for 2-hydroxy-2-cyclohexenone (CAS RN 10316-66-2). This chemical is predicted to have high solubility in water and limited volatility (US EPA, 2008), and as a result calculated values indicate no removal in STPs.

Environmental Effects

Limited measured ecotoxicological data are available for the chemicals across this group.

The group comprises a range of aldehydes, ketones, acetals, ethers, acetates and alcohols. These chemicals primarily cause acute toxic effects through narcosis, but additional toxicological mechanisms can be present. Aldehydes, for example, can elicit toxic effects through the formation of Schiff bases and subsequent binding to DNA. Therefore, the reactivity of the aldehyde, and in turn its toxicity, are dependent on the reactivity of the carbonyl group. Profiling performed using the OECD QSAR Toolbox indicates that 10 chemicals in this group will form Schiff bases and, therefore, may cause toxic effects in the environment (LMC, 2013).

For this reason, it is not considered appropriate to use read across to fill gaps in the available ecotoxicity data, as the chemicals in this group may have different modes of action.

Acute toxicity

The following median effective concentration (EC50) value for the acute toxic effect of cetonal on aquatic invertebrates was the only measured toxicity value identified for chemicals in this group (LMC, 2013):

Taxon	Endpoint	Method
Invertebrates	48 h EC50 = 0.92 mg/L	Experimental *Daphnia magna* (Water flea) OECD TG 202 Immobilisation observed

Based on this value, cetonal has the potential to cause toxic effects in the environment. In addition, QSAR modelling for the remaining chemicals in this group indicates that these substances may also cause acute toxic effects in the environment. Most chemicals have predicted median lethal or median effective concentration values less than 1 mg/L, while the remainder are predicted to have values in the range of 1 to 20 mg/L (US EPA, 2008).

Chronic toxicity

No reliable chronic aquatic ecotoxicity data were identified for the chemicals in this group.

Predicted No-Effect Concentration (PNEC)

Ecotoxicity values calculated using QSAR models for the most sensitive representative model organism were used to derive aquatic PNECs. These calculated acute ecotoxicity values ranged from 0.162 mg/L (predicted fish 96 h LC50 for cyclocitral) to 14.8 mg/L (predicted invertebrate 48 h LC50 for methyl naphthyl ketone). Using these values and an assessment factor of 1000, the PNEC values were determined to range from 0.162 to 14.8 µg/L.

An assessment factor of 1000 was selected as insufficient measured data were available to reliably characterise the trophic levels most sensitive to the aquatic toxicity of these chemicals, and because profiling results for the chemicals indicated potential for excess toxicity due to specific modes of action (EPHC, 2009).

Categorisation of Environmental Hazard

Categorisation according to domestic environmental hazard thresholds has not been performed in this assessment.

Risk Characterisation

Based on the PEC and PNEC values determined for the chemicals in this group, risk quotients (RQ = PEC ÷ PNEC) for the riverine compartment have been calculated. Derived RQ values for select chemicals in this group are presented below, with all chemicals in this group found to have an RQ value greater than one. An RQ greater than one indicates that the chemical may pose an unreasonable risk to the environment, as environmental concentrations may exceed levels that cause harmful effects:

Chemical	PEC (µg/L)	PNEC (µg/L)	RQ
methyl naphthyl ketone	81.64	14.8	5.52
cetonal	9.35	0.67	13.92
2-hydroxy-2-cyclohexenone	85.04	0.37	229.84
cyclocitral	69.73	0.16	435.81

Nevertheless, it is noted that the RQ values derived using the available information and default assumptions (EPHC, 2009; NICNAS, 2013) may not accurately represent the true risk posed by use of these chemicals in Australia. For example, work conducted during the categorization of the Canadian DSL indicates that cetonal, 2-hydroxy-2-cyclohexenone and cyclocitral are each used at less than one tonne per annum in Canada (Environment Canada, 2015). If these chemicals are used at a maximum of one tonne per annum in Australia, the PECs for these chemicals would be two orders of magnitude lower, reducing the RQ values to 0.14, 2.30 and 4.36, respectively.

Given the high reliance on modelling and default assumptions in this assessment, the RQ values derived for the chemicals in this group are taken to indicate that further refinement of the risk scenario is required.

Insufficient data are available to characterise the risks posed by the release of these chemicals to the sediment and soil compartments.

Key Findings

Available international use information suggests that the chemicals in this group may be used as fragrances in a range of products in Australia. Limited data are available for these substances, and no annual introduction volumes have been obtained. However, data that are available indicate that most chemicals in this group will not be readily biodegradable and have some potential for high ecotoxicity. Risk quotient values calculated using default volume assumptions, standard exposure models and modelled values for critical environmental hazard characteristics indicate that further refinement of the risk scenario is required.

Recommendations

It is recommended that all chemicals in this group be considered for assessment of environmental concerns at Tier III level under the IMAP framework. The Tier III environmental risk assessment of these chemicals will focus on outstanding areas of uncertainty in the assessment, including the extent of environmental exposure resulting from industrial use (including use as fragrances) in Australia, potential for ready biodegradation, and toxicity to aquatic and other organisms.

Categorisation of the chemicals in this group according to domestic hazard criteria will also be considered in a Tier III level assessment, in light of any additional hazard information obtained.

It is noted that some chemicals in this group (CAS RNs 3613-30-7, 7774-82-5, 33885-51-7, 52844-21-0, 93981-63-6, 101-85-9, 68459-99-4, and 6379-73-3) are recommended in the IMAP Human Health Tier II Assessment report on ‘Chemicals with limited data availability that are used in fragrances’ to be considered for Tier III assessment. Similar targeted consultation with industry will help to address the areas of uncertainty for the other chemicals in this group.

Environmental Hazard Classification

Insufficient data are presented in this assessment to classify the aquatic hazards of the chemicals in this group according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (UNECE, 2009).

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