Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

4-Pentenal, 5-cyclohexyl-2,4-dimethyl-, (4*E*)-

Assessment statement

06 September 2021

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AICIS assessment statement

Chemical in this assessment

Name	CAS registry number
4-Pentenal, 5-cyclohexyl-2,4-dimethyl, (4*E*)-	1449104-34-0

Reason for the assessment

An application for an assessment certificate under section 31 of the *Industrial Chemicals Act 2019* (the Act).

Certificate Application type

Health and environment focus

Based on introduction, use and end use information described in the application, the exposure band of the introduction is 4 for human health (section 1, table item 6 of Schedule 1) and 3 for the environment (section 3, table item 3 of Schedule 1) of the *Industrial Chemicals (General) Rules 2019* (the Rules).

The assessed chemical has hazard characteristics in human health hazard band B (Schedule 1, clause 2) and environment hazard band C (Schedule 1, clause 4). In accordance with table item 5, section 28 and table item 7, section 29 of the Rules, the indicative human health risk for the proposed introduction is medium to high and the indicative environment risk for the proposed introduction is also medium to high.

Defined scope of assessment

The chemical has been assessed:

– as imported into Australia for up to 2.5 tonnes/annum;

– as introduced neat or as a component of liquid fragrance formulations at up to 5% concentration, for reformulation of end use cosmetic and household products and

– as imported in end use cosmetic and household products or formulated in Australia as a component in end use cosmetic and household products, at concentrations less than 1% in air fresheners (used as sprays, aerosols or candles), fine fragrances, cosmetics and household products, and up to 5% concentration in continuous action, electrical air fresheners.

Summary of assessment

Summary of introduction, use and end use

The assessed chemical will be imported into Australia either in the neat form or as a component of liquid fragrance formulations at up to 5% concentration, for reformulation into end use

cosmetic and household products, or as a component in formulated end use cosmetic and household products. The imported or reformulated end use products will contain the assessed chemical at less than 1% concentration in air fresheners (sprays, aerosols and candles), fine fragrances, cosmetics and household products, and up to 5% concentration in continuous action, electrical air fresheners.

The assessed chemical in neat form or as a component of liquid fragrance formulations at up to 5% concentration will be imported and distributed in tightly closed lacquered drums of varying sizes: 5 kg, 10 kg, 25 kg, 50 kg, 100 kg or 180 kg. Reformulation/re-packaging activity will not occur at the applicant's facility in Australia. The drums will be transported mainly by road to the warehouse for storage and later distributed to the formulators by road. Finished consumer products containing the assessed chemical at various concentrations will be packaged in containers suitable for retail sale.

Human health

Summary of health hazards

Based on the available data the assessed chemical is likely to be a skin sensitiser (see **Supporting information**) warranting hazard classification (see **Recommendations** section).

No inhalation toxicity data were provided on the assessed chemical.

The available toxicity data indicate that the assessed chemical:

- is likely to be of low acute oral toxicity;
- is slightly irritating to skin and eyes; and
- is not genotoxic.

Health hazard classification

Based on the available data, the assessed chemical warrants hazard classification for human health, according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS, United Nations 2017), as adopted for industrial chemicals in Australia.

Health hazards	Hazard category	Hazard statement
Skin sensitisation	Category 1B	H317: May cause an allergic skin reaction

The assessed chemical will not be used in cosmetics or household products in Australia at end use concentrations that warrant the above hazard classification, except in continuous action, electrical air fresheners.

Summary of health risk

Public

When introduced and used in the proposed manner, there will be widespread and repeated exposure of the public to the assessed chemical:

- at less than 1% concentration through the use of a wide range of cosmetic and household products containing the assessed chemical
- the principal route of exposure will be dermal, while ocular and inhalation exposures are also possible, particularly from air care products and from products applied by spray.

The assessed chemical is a skin sensitiser, but given the proposed low use concentrations (at less than 1% concentration in air fresheners (sprays, aerosols and candles), fine fragrances, cosmetics and household products), skin sensitisation effects are not expected.

While continuous action, electrical air fresheners will contain the assessed chemical at up to 5% concentration, as minimal dermal exposure is expected from these air fresheners, skin sensitisation effects are not expected.

No inhalation toxicity data are provided for the assessed chemical. However, the half-life of the assessed chemical in air is calculated to be 1.04 hours based on reactions with hydroxyl radicals (see Environmental fate section under **Supporting information**). In the event of release to the atmosphere, the assessed chemical is not expected to persist in the atmospheric compartment. Therefore, use at 5% concentration in continuous flow air fresheners is not expected to cause significant inhalation exposure to the assessed chemical to cause unreasonable risk.

The repeated dose toxicity potential of the assessed chemical was estimated by calculating the margin of exposure (MoE), using the worst case exposure scenario from use of multiple products simultaneously by an individual. The total daily systemic exposure was estimated as 2.40 mg/kg bw/day (see Human exposure section under **Supporting information**). Using a No Observed Adverse Effect Level (NOAEL) of 300 mg/kg bw/day for the assessed chemical (derived from a repeated dose oral toxicity study in rats on an analogue chemical), the MoE was estimated to be 125. A MoE value greater than or equal to 100 is considered acceptable to account for intra- and inter-species differences.

When introduced in accordance with the terms of the assessment certificate, the assessed chemical is not considered to pose an unreasonable risk to the public.

Workers

Workers may experience exposure to the assessed chemical in its neat form or at up to 5% concentration during weighing and transfer stages, blending, quality control analysis and cleaning and maintenance of equipment, particularly where manual or open processes are used. Exposure to the assessed chemical in end use products (at less than 1% concentration) may occur in professions where the services provided involve the application of cosmetic and personal care products to clients (e.g. hairdressers and workers in beauty salons) or the use of household products in the cleaning industry.

Workers may experience an allergic skin reaction if exposed to the assessed chemical at higher concentrations during end use product formulation activities. Specific risk management measures (see **Recommendations** section) are required to manage the risks to workers.

The frequency and extent of exposure of workers applying products to clients is similar to public exposure or lower if PPE is used.

Environment

Summary of environmental hazard characteristics

According to domestic environmental hazard thresholds and based on the available data, the assessed chemical is:

- Not Persistent (not P)
- Not Bioaccumulative (not B)
- Toxic (T)

Environmental hazard classification

Three acute endpoints were available. The aquatic acute classification was determined from the lowest acute endpoint (algae) and was determined to be Acute Category 1. One chronic endpoint was available (algae). Therefore, the aquatic chronic hazard was determined using both the chronic and acute data and the most stringent outcome was adopted. The most stringent outcome was based on the chronic data taking into account that the substance is rapidly degradable. Therefore, the overall long-term classification is Chronic Category 3 (United Nations, 2017).

Environmental Hazard	Hazard Category	Hazard Statement
Acute Aquatic	Category 1	H400: Very toxic to aquatic life
Chronic Aquatic	Category 3	H412: Harmful to aquatic life with long lasting effects

Summary of environmental risk

Based on the end use as a fragrance in cosmetics and other consumer products, the majority of the assessed chemical is expected to be released into sewage treatment plants (STPs). The calculated aquatic environmental risk quotient for the assessed uses of the chemical is less than or equal to 0.017.

Therefore, there are no identified risks to the environment that require specific risk management measures, if the assessed chemical is introduced in accordance with the terms of the assessment certificate.

Conclusions

The conclusions of this assessment are based on the information described in this assessment statement. Obligations to report additional information about hazards under section 100 of the *Industrial Chemicals Act 2019* apply.

The Executive Director is satisfied that when the assessed chemical is introduced and used in accordance with the terms of the assessment certificate, the human health and environment risks can be managed. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory. The proposed means for managing the risks identified during this assessment are set out in the **Recommendations** section.

Recommendations

Workers

Recommendation to Safe Work Australia

- It is recommended that Safe Work Australia (SWA) update the *Hazardous Chemical Information System* (HCIS) to include the classification relevant to work health and safety (see **Health hazard classification**).

Advice to industry

- The following control measures should be implemented to manage the risk arising from exposure to the assessed chemical during formulation activities:
    - Use of engineering controls such as
        - Enclosed and automated processes if possible
        - Adequate workplace ventilation to avoid accumulation of vapours, mists or aerosols
    - Use of safe work practices to
        - Avoid contact with skin
        - Avoid inhalation of vapours, mists or aerosols
    - Workers should wear the following personal protective equipment (PPE)
        - Impervious gloves
        - Respiratory protection where local ventilation may be inadequate
        - Protective clothing
- As the assessed chemical is a skin sensitiser, employers should carry out health surveillance for any worker who has been identified in the workplace risk assessment as having a significant risk of skin sensitisation.
- The storage of the assessed chemical should be in accordance with the Safe Work Australia *Code of Practice for Managing Risks of Hazardous Chemicals in the Workplace* (SWA, 2012) or relevant State or Territory Code of Practice.

Environment

No specific recommendations for safe use of the assessed chemical are required when the assessed chemical is introduced in accordance with the terms of the assessment certificate.

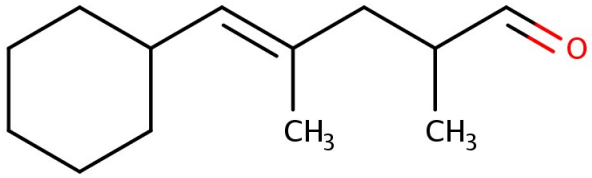
Supporting information

Chemical identity

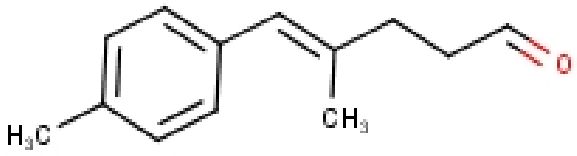
The assessed chemical is a racemic mixture with a degree of purity > 80% (greater than 80%). The two enantiomers are individually identified as follows:

Chemical Name (Enantiomer)	4-Pentenal, 5-cyclohexyl-2,4-dimethyl, (2*R*,4*E*)-
Chemical Name (Enantiomer)	4-Pentenal, 5-cyclohexyl-2,4-dimethyl, (2*S*,4*E*)-

Other Chemical Identity Information

Synonyms	(4*E*)-5-Cyclohexyl-2,4-dimethylpent-4-enal (IUPAC name)
Structural formula	
Molecular formula	$C_{13}H_{22}O$
Molecular weight (g/mol)	194.31
SMILES	O=CC(C)CC(=CC1CCCCC1)C

Analogue Chemical Identity Information

Chemical Name	4-Pentenal, 4-methyl-5-(4-methylphenyl)-, (4*E*)-
CAS Number	1226911-69-8
Structural formula	

Chemical Name	4-Pentenal, 4-methyl-5-(4-methylphenyl)-, (4*E*)-
Molecular formula	$C_{13}H_{16}O$
Molecular weight (g/mol)	188.27
SMILES	O=CCCC(=CC1=CC=C(C=C1)C)C

Relevant physical and chemical properties

All measured values are based on the studies provided on the assessed chemical and conducted according to OECD test guidelines.

Physical form	Colourless liquid
Melting point	< -20 °C
Boiling point	260.1 °C
Density	905 kg/m^3 at 20 °C
Vapour pressure	0.750 Pa at 20°C and 0.987 Pa at 25°C
Water solubility	8.94 mg/L at 20°C
Flash point	112 °C
Auto flammability	220 °C
Hydrolysis as a function of pH	Not determined
Ionisable in the environment?	No
Acid dissociation constant (pKa)	N/A
Octanol-water partition coefficient (log K_{ow})	4.39 at 22 °C
Adsorption coefficient (log Koc)	3.68 at 30 °C

Human exposure

Workers

Reformulation

Typically, reformulation processes may incorporate blending operations that are highly automated and occur in a fully enclosed/contained environment, followed by automated filling using sealed delivery systems into containers of various sizes. Dermal, ocular and inhalation exposure (if aerosols or mists are formed) of workers to the assessed chemical in its neat form or at up to 5% concentration is possible during weighing and transfer stages, blending, quality control analysis, packaging and cleaning, and during maintenance of equipment. However, the exposure is expected to be minimised through the use of mechanical ventilation and/or enclosed systems, and through the use of PPE such as protective clothing, eye protection, impervious gloves and appropriate respiratory protection.

Professional End Use

Exposure to the assessed chemical in end use products at less than 1% concentration may occur in professions where the services provided involve the application of cosmetic and personal care products to clients (e.g. hairdressers and workers in beauty salons) or the use of household products in the cleaning industry. These products, depending on their nature, could be applied in a number of ways, such as by hand, using an applicator or sprayed. The principal route of exposure will be dermal and inhalation (for air care products), while ocular exposure is also possible. Professionals may use PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. If PPE is used, exposure of such workers is expected to be of a similar or lesser extent than that experienced by consumers using the end use products containing less than 1% of the assessed chemical.

Public

There will be widespread and repeated exposure of the public to the chemical at up to 5% concentration through the use of a wide range of cosmetic and household products. The principal route of exposure will be dermal, while ocular and/or inhalation exposures are also possible, particularly if the products are applied by spray or when used in air fresheners.

Data on typical use patterns of products (SCCS 2012; Cadby et al. 2002; ACI 2010; Loretz et al. 2006) in which the assessed chemical may be used are shown in the following tables. For the purposes of exposure assessment, Australian use patterns for the various product categories are assumed to be similar to those in Europe. Given the low molecular weight (194.31 g/mol) and the partition coefficient (log Pow = 4.39 at 22 °C) of the assessed chemical, there is potential for it to cross biological membranes, including the skin. A dermal absorption (DA) rate of 100% was therefore used along with a lifetime average female body weight (BW) of 70 kg (enHealth 2012) for calculation purposes. For the inhalation exposure assessment, a 2-zone approach was used (Steiling et al. 2014; Rothe et al. 2011; Earnest Jr. 2009). An adult inhalation rate of 20 m^3/day (enHealth 2012) was used and it was conservatively assumed that the fraction of the assessed chemical inhaled is 50%.

The following tables provide information on exposure estimates obtained using the above parameters.

Cosmetic products (dermal exposure)

Product type	**Amount** (mg/day)	**C** (%)	**RF**(unitless)	**Daily systemic exposure** (mg/kg bw/day)
Body lotion	7820	1	1	1.2219
Face cream	1540	1	1	0.2406
Hand cream	2160	1	1	0.3375
Fine fragrances	750	1	1	0.1172
Deodorant	1500	1	1	0.2344
Shampoo	10460	1	0.01	0.0163
Conditioner	3920	1	0.01	0.0061
Shower gel	18670	1	0.01	0.0292
Hand soap	20000	1	0.01	0.0313
Hair styling products	4000	1	0.1	0.0625
Total				**2.2970**

C = maximum intended concentration of assessed chemical; RF = retention factor
Daily systemic exposure = (Amount × C × RF × DA)/BW

Household products (Indirect dermal exposure – from wearing clothes)

Product type	**Amount** (g/use)	**C** (%)	**Product Retained (PR)** (%)	**Percent Transfer (PT)** (%)	**Daily systemic exposure** (mg/kg bw/day)
Laundry liquid	230	1	0.95	10	0.0341
Fabric softener	90	1	0.95	10	0.0134
Total					**0.0475**

C = maximum intended concentration of assessed chemical
Daily systemic exposure = (Amount × C × PR × PT × DA)/BW

Household products (Direct dermal exposure)

Product type	**Frequency** (use/day)	**C** (%)	**Contact area** (cm^2)	**Product use C** (g/cm^3)	**Film thickness** (cm)	**Time scale factor**	**Daily systemic exposure** (mg/kg bw/day)
Laundry liquid	1.43	1	1980	0.01	0.01	0.007	0.0003
Dishwashing liquid	3	1	1980	0.009	0.01	0.03	0.0025
All-purpose cleaner	1	1	1980	1	0.01	0.007	0.0217
Total							**0.0245**

C = maximum intended concentration of assessed chemical
Daily systemic exposure = (Frequency × C × Contact area × Product Use Concentration × Film Thickness on skin × Time Scale Factor × DA)/BW

Hair spray (inhalation exposure)

Product type	**Amount** (g/day)	**C** (%)	**Inhalation Rate** (m^3/day)	**Exposure duration (Zone 1)** (min)	**Exposure duration (Zone 2)** (min)	**Fraction Inhaled** (%)	**Volume (Zone 1)** (m^3)	**Volume (Zone 2)** (m^3)	**Daily systemic exposure** (mg/kg bw/day)
Hairspray	9.89	1	20	1	20	50	1	10	**0.0322**

C = maximum intended concentration of assessed chemical
Total daily systemic exposure = Daily systemic exposure in Zone 1 [(amount × C × inhalation rate × exposure duration (zone 1) × fraction inhaled)/(volume (zone 1) × body weight)] + Daily systemic exposure in Zone 2 [(amount × C × inhalation rate × exposure duration (zone 2) × fraction inhaled)/(volume (zone 2) × body weight)]

The worst case scenario estimation using these assumptions is for a person who is a simultaneous user of all products listed in the above tables that contain the assessed chemical at the maximum intended concentrations specified by the applicant in various product types. This would result in a combined internal dose of 2.40 mg/kg bw/day for the assessed chemical. It is acknowledged that inhalation exposure to the assessed chemical from use of other cosmetic and household products (in addition to hair spray) may occur. However, the

combination of the conservative hair spray inhalation exposure assessment parameters used and the aggregate exposure from use of the dermally applied products (using a conservative 100% dermal absorption rate), are sufficiently protective to cover additional inhalation exposure to the assessed chemical from the use of other spray cosmetic and household products containing it with low exposure (e.g. air fresheners).

Health hazard information

Acute toxicity

Based on an acute oral toxicology study of the assessed chemical (OECD TG 420), the assessed chemical is likely to be of low acute toxicity to rats via the oral route (LD50 > 2000 mg/kg bw).

No acute dermal or inhalation toxicity data are available for the assessed chemical.

Corrosion/Irritation

Skin irritation

The assessed chemical was determined not to be irritating to the skin in an *in vitro* skin irritation test using the EpiSkin™ reconstructed human epidermis tissue model (EpiSkin™ Small Model) (OECD TG 439). The relative mean viability of the test item-treated tissues was 86.9% after the 15 minute exposure period (followed by 42 hours post-exposure incubation period). Under the conditions of this study and according to the test guideline, the test substance was not considered to be irritating to the skin for classification using the GHS criteria.

The assessed chemical was further tested using an *in vivo* skin irritation test in rabbits (OECD TG 404). A single 4-hour, semi occluded application of the test substance to the intact skin of two rabbits, produced very slight to well-defined erythema and very slight to slight oedema. Treated skin sites appeared normal at the 7-Day observation and no other skin reactions were noted. Under the conditions of this study, the assessed chemical is a slight skin irritant but does not require classification for skin irritation according to the GHS criteria.

Eye irritation

The Bovine Corneal Opacity and Permeability (BCOP) test method (OECD TG 437) was performed to determine the eye irritating potential of the assessed chemical in isolated bovine corneas *in vitro*. The undiluted test item was tested through topical application to corneas for 10 minutes and post-exposure incubation period of 120 minutes. The test item resulted in a mean *in vitro* irritancy score (IVIS) of 0.2 after 10 minutes of treatment, which was < 3.0 (less than 3.0) in the prediction model; IVIS was 2.0 in the negative control and 38.8 in the positive control. Therefore, under the conditions of this study and according to the TG, the assessed chemical does not require classification according to the GHS criteria.

The assessed chemical was further tested for eye irritation using two rabbits (OECD TG 405). A single application of the test substance produced no corneal or iridial effects. Moderate conjunctival irritation was noted in treated eyes 1 hour after treatment with minimal conjunctival irritation noted at the 24 and 48 hour observations. Both treated eyes appeared normal at 72 hours following treatment. Under the conditions of this study, the assessed chemical is a slight eye irritant but does not require classification according to the GHS criteria.

Sensitisation

Skin sensitisation

The skin sensitisation potential of the assessed chemical was assessed using a local lymph node assay (LLNA) in mice (OECD TG 429). The mice were treated by daily application of 25 µL of the test substance at concentrations of 25%, 10% or 5% (v/v), to the dorsal surface of each ear for three consecutive days.

There were no deaths or signs of systemic toxicity, and body weights were comparable to controls. A stimulation index (SI) of 4 was noted at the 25% (v/v) test substance concentration, with a dose response (SIs of 1.5% and 1.9% at 5% and 10% (v/v) test substance concentration, respectively). The concentration of test item expected to cause a 3-fold increase in ^{3}HTdR incorporation (EC3 value) was calculated (by linear interpolation) to be 17.9%. The SI for the positive control was 7.6, indicating appropriate performance of the assay.

The assessed chemical is a skin sensitiser, requiring classification for Skin Sensitisation (Cat 1B: H317: May cause an allergic skin reaction).

Repeat dose toxicity

Oral

Repeated dose toxicity information was not submitted for the assessed chemical. However, the applicant submitted a repeated dose toxicity study of an analogue chemical, which was appropriate for read across to the assessed chemical.

In a range finding study, the test substance was administered by gavage to three groups (3 animals/sex/group), for up to seven consecutive days, at dose levels of 250, 500, and 1000/750 mg/kg bw/day. Two males treated with 1000 mg/kg bw/day died in this study. Gastric inflammation and sloughing of the stomach lining was noted in the two dead animals. However, following the dose level reduction to 750 mg/kg bw/day, there was no further deterioration in the condition of the surviving animal from this treatment group. Animals treated at 250 and 500 mg/kg bw/day showed dose tolerance.

The repeated dose toxicity study was performed to examine the systemic toxic potential of the analogue chemical in rats (OECD TG 407). In this study, three treatment groups and a control group was formed (5 animals/sex/group), which received the test substance by oral gavage daily at doses of 0 (control), 30, 300 and 750 mg/kg bw/day for 28 days.

Clinical findings were confined to transient episodes of increased salivation which developed during the first week of treatment in animals at 300 and 750 mg/kg bw/day and persisted (sporadically) through to Day 28. As the test substance has been confirmed to cause an irritant dermal response, such observations were considered by the study authors to be related to the oral administration of an unpleasant tasting or slightly irritant formulation rather than systemic toxicity.

There were no deaths during the course of this study and there were also no treatment-related changes in behavioural parameters, functional performance tests, sensory reactivity assessment, body weight, food consumption, haematology or blood chemistry. No macroscopic abnormalities were identified in any animal at terminal necropsy. Although males treated with 750 mg/kg bw/day showed statistically significantly elevated liver and kidney weights, these increases were minimal when expressed as percentages; 0.72% (kidney

weights) and 4.46% (liver weights), compared to the control group. Furthermore, there were no supporting microscopic findings detected to suggest treatment-related hepatic changes and individual kidney weights in the animals given 750 mg/kg bw/day were within the historical ranges.

Treatment related histopathological renal changes, characterised by minimal or mild basophilic epithelium in the collecting tubules, were identified in all the males and four females at 750 mg/kg bw/day and in four males and one female at 300 mg/kg bw/day. Associated single cell necrosis of collecting tubules (minimal) was noted in only one male at 750 mg/kg bw/day. No treatment-related changes were seen in animals exposed to 30 mg/kg bw/day. While it is possible that the necrosis identified in only one high dose male may be a result of biological variability, as this was a degenerative tissue change, necrosis cannot be wholly excluded.

Mild to minimal mitoses observed in animals at 300 mg/kg bw/day (1/5 in males; 0/5 females) and 750 mg/kg bw/day (4/5 in males; 2/5 in females) were stated to be adaptive responses to a slightly irritant test substance by the study authors. Considering the low incidence of this observation in animals at 300 mg/kg bw/day with no other related adverse effects, 300 mg/kg bw/day is considered to be the NOAEL.

Genotoxicity

A study was performed to evaluate the potential of the assessed chemical to cause point mutations in a bacterial reverse mutation assay using *Salmonella typhimurium* strains TA98, TA100, TA1535 and TA1537 and *Escherichia coli* strain WP2uvrA- in both the presence and absence of S9-mix (OECD TG 471). No significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, with any dose of the test substance, either with or without metabolic activation (S9-mix) between 0.015 and 1500 µg/plate, depending on bacterial strain type and presence or absence of S9-mix. Under the conditions of this study, the assessed chemical was considered to be non-mutagenic in the presence and absence of metabolic activation.

Another study was performed to assess the potential of the assessed chemical to cause chromosomal aberrations in cultured mammalian cells (human lymphocytes) (OECD TG 473). The selection of the maximum dose level (240 µg/mL and 120 µg/mL for the 4(20)-hour exposure groups and the continuous exposure group, respectively) was confounded by the fact that the onset of toxicity and the lowest precipitating parameters coincided. All the positive control chemicals induced a demonstrable positive response ($p \leq 0.01$) and confirmed the validity and sensitivity of the assay and the integrity of the S9-mix.

Even though the dose level selected could be considered excessively toxic, the test item did not induce any statistically significant increases in the frequency of cells with chromosomal aberrations, using a dose range that included a dose level that either induced or exceeded 55±5% mitotic inhibition. Under the conditions of this study, the assessed chemical was considered to be non-clastogenic to human lymphocytes *in vitro*.

Environmental exposure

Significant releases of the assessed chemical to the environment are not expected during reformulation, transport or storage. Based on the assessed use as a fragrance in various consumer products, the majority of the assessed chemical is expected to be released to sewers.

Environmental fate

The assessed chemical is readily biodegradable (64% degradation over 28 days, OECD TG 301 D) and is therefore not persistent. The chemical has a low bioconcentration factor (BCF = 4.5) estimated by QSAR modelling. This value is supported by literature data which indicate that aldehydes are expected to metabolise in fish and mammals and therefore reduce their potential for bioconcentration (Nilsson et al, 1988; Parker et al., 1990; Pan et al., 2014). The biotransformation products are expected to be more polar than the parent chemical and will therefore be easily excreted. Therefore, the assessed chemical is considered to be not bioaccumulative.

A majority of the assessed chemical will be disposed of into STPs and released to the environment with effluent from STPs. A proportion of assessed chemical may be applied to land when biosolids are applied to agricultural soils, or disposed of to landfill as waste. The assessed chemical residues in landfill and soils are expected to have slight mobility based on its estimated soil adsorption coefficient (log Koc = 3.68). In the aquatic and soil compartments, the assessed chemical is expected to ultimately degrade through biotic and abiotic processes to form water and oxides of carbon.

The assessed chemical is moderately volatile (vapour pressure 0.987 Pa at 25 °C) and may volatilise to air during use or STP processes. The half-life of the assessed chemical in air is calculated to be 1.04 hours based on reactions with hydroxyl radicals (AOPWIN v1.92; US EPA, 2012). Therefore, in the event of release to atmosphere, the assessed chemical is not expected to persist in the atmospheric compartment.

Predicted environmental concentration (PEC)

The predicted environmental concentrations (PEC) in water (receiving environments) have been calculated based on 100% release of the assessed chemical (from the introduction volume) into sewer systems nationwide over 365 days per annum. The extent to which the assessed chemical is removed from the effluent in STP processes is based on its physico-chemical properties and its tested biodegradability, modelled by SimpleTreat 3.0 (Struijs, 1996) and is estimated to be 90%. Therefore 10% of the total introduction volume is estimated to be released to the aquatic environment. The calculation of the PEC is detailed in the table below:

Total Annual Import Volume	2500	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	2500	kg/year
Days per year where release occurs	365	days/year
Daily chemical release	6.85	kg/day
Water use	200.0	L/person/day
Population of Australia	24.386	million
Removal within STP	90%	mitigation
Daily effluent production	4877	ML

Total Annual Import Volume	2500	kg/year
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River	0.14	µg/L
PEC - Ocean	0.014	µg/L

Partitioning to biosolids in STPs Australia-wide may result in an average biosolids concentration of 2.25 mg/kg (dry wt). Biosolids are applied to agricultural soils, with an assumed average rate of 10 t/ha/year. Assuming a soil bulk density of 1500 kg/m^3 and a soil-mixing zone of 10 cm, the concentration of the assessed chemical may approximate 0.015 mg/kg in applied soil. This assumes that degradation of the assessed chemical occurs in the soil within 1 year from application. Assuming accumulation of the assessed chemical in soil for 5 and 10 years under repeated biosolids application, the concentration of assessed chemical in the applied soil in 5 and 10 years may approximate 0.075 mg/kg and 0.15 mg/kg, respectively.

Environmental effects

Effects on Aquatic Life

Acute toxicity

The results from the supplied ecotoxicological studies conducted on the assessed chemical are summarised in the table below.

Taxon	Endpoint	Method
Fish	96 h LC50 = 2.62 mg/L	OECD TG 203
Invertebrate	48 h EC50 = 0.977 mg/L	OECD TG 202
Algae	72 h ErC50 = 0.811 mg/L	OECD TG 201
Algae	72 h NOEC = 0.264 mg/L	OECD TG 201

The assessed chemical is acutely toxic to fish and acutely very toxic to aquatic invertebrates and algae. The most sensitive taxonomic group is algae.

Predicted no-effect concentration (PNEC)

A Predicted No-Effect Concentration (PNEC) was calculated based on the above acute endpoint for algae using an assessment factor of 100 as three acute trophic endpoints are available. The resulting PNEC is 8.11 µg/L.

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemical according to domestic environmental hazard thresholds is presented below:

Persistence

Not Persistent (Not P). Based on the ready biodegradability study and half-life < 60 days in environmental water, the assessed chemical is categorised as Not Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on modelling and literature data the chemical has a low potential for bioaccumulation and is categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on the available acute and chronic ecotoxicity values below 1 mg/L, the assessed chemical is categorised as Toxic.

Environmental risk characterisation

The risk quotient (RQ = PEC/PNEC) for the assessed chemical is calculated to be 0.017 for riverine compartments and less than 0.01 for marine compartments. The risk quotient for discharge of treated effluents containing the assessed chemical to the aquatic environment indicates that the assessed chemical is unlikely to reach ecotoxicologically significant concentrations based on its annual importation quantity. The assessed chemical is rapidly biodegradable and is expected to have a low potential for bioaccumulation. Therefore, the assessed chemical is unlikely to pose significant risk to aquatic life based on its assessed use pattern as a fragrance in cosmetics and other consumer products.

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