File No: LTD/1770

May 2020

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

3-Buten-2-one, 4-[(3*R*,6*R*)-2,2,3,6-tetramethylcyclohexyl]-, (3*E*)-*rel*-

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (the Act) and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by the Department of Health, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of Agriculture, Water and the Environment.

This Public Report is available for viewing and downloading from the NICNAS website or available on request, free of charge, by contacting NICNAS. For requests and enquiries please contact the NICNAS Administration Coordinator at:

Street Address:	Level 7, 260 Elizabeth Street, SURRY HILLS NSW 2010, AUSTRALIA.
Postal Address:	GPO Box 58, SYDNEY NSW 2001, AUSTRALIA.
TEL:	+ 61 2 8577 8800
FAX:	+ 61 2 8577 8888
Website:	www.nicnas.gov.au

Director
NICNAS

TABLE OF CONTENTS

SUMMARY

The following details will be published on our website:

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
LTD/1770	Firmenich Limited	3-Buten-2-one, 4-[(3*R*,6*R*)-2,2,3,6-tetramethylcyclohexyl]-, (3*E*)-*rel-*	No	≤ 1 tonne per annum	Fragrance ingredient

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification

Based on the available information, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia.

Human health risk assessment

Under the conditions of the occupational settings described, the notified chemical is not considered to pose an unreasonable risk to the health of workers.

When used in the proposed manner, the notified chemical is not considered to pose an unreasonable risk to public health.

Environmental risk assessment

On the basis of the maximum import volume of 1 tonne per annum, the notified chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical during reformulation:
  - Avoid contact with skin and eyes
  - Avoid inhaling aerosols or mists

- A person conducting a business or undertaking at a workplace should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical during reformulation:
  - Respiratory protection if aerosols or mists are expected to be generated

  Guidance in selection of personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

- A copy of the SDS should be easily accessible to employees.

- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)* as adopted for industrial chemicals in Australia, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation should be in operation.

Disposal

- Where reuse or recycling are not appropriate, dispose of the notified chemical in an environmentally sound manner in accordance with relevant Commonwealth, state, territory and local government legislation.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by physical containment, collection and subsequent safe disposal.

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

Therefore, the Director of NICNAS must be notified in writing within 28 days by the notifier, other importer or manufacturer:

(1) Under Section 64(1) of the Act; if
  - the importation volume exceeds one tonne per annum notified chemical;
  - the final use concentration of the notified chemical exceeds 0.08% in leave-on/rinse-off cosmetics, 0.7% in fine fragrances, 0.05% in household cleaning products or 0.5% in air fresheners.

or

(2) Under Section 64(2) of the Act; if
  - the function or use of the chemical has changed from a fragrance ingredient, or is likely to change significantly;
  - the amount of chemical being introduced has increased, or is likely to increase, significantly;
  - the chemical has begun to be manufactured in Australia;
  - additional information has become available to the person as to an adverse effect of the chemical on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

Safety Data Sheet
The SDS of the notified chemical provided by the notifier was reviewed by NICNAS. The accuracy of the information on the SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Firmenich Limited (ABN: 86 002 964 794)
73 Kenneth Road
BALGOWLAH NSW 2093

NOTIFICATION CATEGORY
Limited-small volume: Chemical other than polymer (1 tonne or less per year)

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: other names, analytical data, degree of purity, impurities and additives/adjuvants.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed for adsorption/desorption, dissociation constant, flammability, explosive properties and oxidising properties.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
NICNAS Permits

NOTIFICATION IN OTHER COUNTRIES
USA (1992), China (2013), Canada (2005), Japan (2008), EU (2008) and Switzerland (2009)

2. IDENTITY OF CHEMICAL

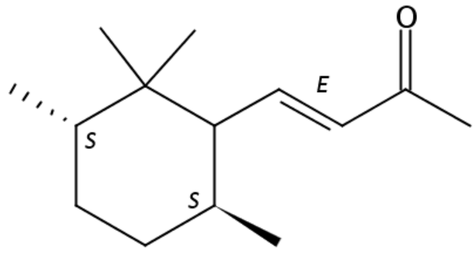
MARKETING NAME(S)
3-Buten-2-one, 4-[(3*R*,6*R*)-2,2,3,6-tetramethylcyclohexyl]-, (3*E*)-*rel*-

CAS NUMBER
762300-77-6

CHEMICAL NAME
3-Buten-2-one, 4-[(3*R*,6*R*)-2,2,3,6-tetramethylcyclohexyl]-, (3*E*)-*rel*-

MOLECULAR FORMULA
$C_{14}H_{24}O$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
208.34 g/mol

ANALYTICAL DATA
Reference NMR, IR, GC, GC-MS, UV spectra were provided.

3. COMPOSITION

DEGREE OF PURITY
> 90%

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 ºC AND 101.3 kPa: colourless to pale yellow liquid

Property	Value	Data Source/Justification
Melting Point/Freezing Point	-2 °C	Measured
Boiling Point	274 °C at 96.9 kPa	Measured
Density	917 kg/m^3 at 20 °C	Measured
Vapour Pressure	1.835×10^{-4} kPa at 25 °C	Measured
Water Solubility	4.196×10^{-3} g/L at 20 °C 4.144×10^{-3} g/L at 20 °C	Measured
Fat Solubility	Soluble in all proportions at 37 °C	Measured
Hydrolysis as a Function of pH	Hydrolytically stable	Measured
Partition Coefficient (n-octanol/water)	Isomer 1: log Pow = 4.498 at 25 °C Isomer 2: log Pow = 4.392 at 25 °C Isomer 3: log Pow = 4.369 at 25 °C	Measured
Adsorption/Desorption	log Koc = 3.69	Calculated by US EPI Suite
Flash Point	126-127 °C at 97 kPa	Measured
Flammability	Not determined	Not expected to be highly flammable based on flash point
Autoignition Temperature	> 220 °C	Measured
Explosive Properties	Not determined	Contains no functional groups that imply explosive properties
Oxidising Properties	Not determined	Contains no functional groups that imply oxidising properties

DISCUSSION OF PROPERTIES
For full details of tests on physical and chemical properties, refer to Appendix A.

Reactivity
The notified chemical is expected to be stable under normal conditions of use.

Physical hazard classification
Based on the submitted physico-chemical data depicted in the above table, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia.

The notified chemical has a flash point of 126 ºC which is greater than 93 °C. Based on *Australian Standard AS1940* definitions for combustible liquid, the notified chemical may be considered as a Class C2 combustible liquid if the chemical has a fire point below the boiling point.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be imported into Australia either in the neat form or as a component in fragrance formulations (≤ 2% concentration) or finished consumer products (≤ 0.7% concentration).

MAXIMUM INTRODUCTION VOLUME OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	≤ 1	≤ 1	≤ 1	≤ 1	≤ 1

PORT OF ENTRY
Sydney

TRANSPORTATION AND PACKAGING
The imported notified chemical or products containing it will be transported by road via truck to the notifier's warehouse or customers' facilities for storage or reformulation. Fragrance formulations containing the notified

chemical will be imported and distributed in tightly closed lacquered drums of varying sizes: 180, 100, 50, 25, 10 or 5 kg. End-use products will be packaged in containers suitable for retail sale.

USE

The notified chemical will be used as a fragrance component in a variety of cosmetic and household products at typical final use concentrations of ≤ 0.08% in leave-on/rinse-off cosmetics, ≤ 0.7% in fine fragrances, ≤ 0.05% in household cleaning products, and ≤ 0.5% in air fresheners.

OPERATION DESCRIPTION

The reformulation procedures for incorporating the notified chemical into end-use products will likely vary depending on the nature of the cosmetic and personal care/household cleaning products formulated. This may involve both automated and manual processes including transferring and blending the notified chemical with other formulations. However, a typical blending operation will be highly automated and occur in a fully enclosed/contained environment, followed by automated filling using sealed delivery systems into containers of various sizes.

The end-use products containing the notified chemical may be used by consumers and professionals such as hairdressers, workers in beauty salons or cleaners. Depending on the nature of the product, these could be applied in a number of ways, such as by hand, using an applicator or sprayed.

6. HUMAN HEALTH IMPLICATIONS

6.1. Exposure Assessment

6.1.1. Occupational Exposure

CATEGORY OF WORKERS

Category of Worker	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transport and warehouse workers	unknown	unknown
Mixing	4	2
Drum handling	4	2
Drum cleaning/washing	4	2
Maintenance	4	2
Quality control	0.5	1
Packaging	4	2
Professional end users	not specified	not specified

EXPOSURE DETAILS

Transport and storage

Transport and storage workers may come into contact with the notified chemical in neat form or as a component of the imported preparations, only in the event of accidental rupture of containers. Incidental dermal or ocular exposure to the notified chemical may occur via during the clean-up of accidental spills.

Formulation of end use products

During reformulation, dermal, ocular and perhaps inhalation exposure (if aerosols or mists are formed) of workers to the notified chemical (at up to 100% concentration) may occur during weighing and transfer stages, equipment preparation, blending, quality control analysis and cleaning and maintenance of equipment. Inhalation exposure to vapours of the notified chemical is not expected given the low vapour pressure of the notified chemical. Exposure is expected to be minimised through the use of local exhaust ventilation, automated and enclosed systems, including sealed delivery systems and through the use of personal protective equipment (PPE) such as gloves, respirator, eye protection and protective clothing.

Beauty care and cleaning professionals

Exposure to the notified chemical in end-use products (at ≤ 0.7% concentration) may occur in professions where the services provided involve the application of cosmetic and personal care products to clients (e.g. hairdressers, workers in beauty salons) or in the cleaning industry. Such 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 products containing the notified chemical.

6.1.2. Public Exposure

There will be widespread and repeated exposure of the public to the notified chemical through the use of a variety of cosmetic and household products at various concentrations. The principal route of exposure will be dermal, while ocular and inhalation exposure is also possible, particularly if products are applied by spray.

Data on typical use patterns of product categories in which the notified chemical may be used are shown in the following tables (SCCS, 2012; Cadby *et al.*, 2002; ACI, 2010; Loretz *et al.,* 2006). For the purposes of the exposure assessment, Australian use patterns for the various product categories are assumed to be similar to those in Europe. In the absence of dermal absorption data, a dermal absorption (DA) of 100% was assumed for the notified chemical (ECHA, 2017). 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 notified chemical inhaled is 50%. A lifetime average female body weight (BW) of 64 kg (enHealth, 2012) was used for calculation purposes.

Cosmetic products (Dermal exposure)

Product type	**Amount** (mg/day)	**C** (%)	**RF** (unitless)	**Daily systemic exposure** (mg/kg bw/day)
Body lotion	7,820	0.08	1	0.0978
Face cream	1,540	0.08	1	0.0193
Hand cream	2,160	0.08	1	0.0270
Fragrances	750	0.7	1	0.0820
Deodorant (non-spray)	1,500	0.08	1	0.0188
Shampoo	10,460	0.08	0.01	0.0013
Hair conditioner	3,920	0.08	0.01	0.0005
Shower gel	18,670	0.08	0.01	0.0023
Hand wash soap	20,000	0.08	0.01	0.0025
Hair styling products	4,000	0.08	0.1	0.0050
Total				**0.2564**

C = concentration (%); RF = Retention Factor

Daily Systemic Exposure = (Amount × C × RF × dermal absorption)/body weight

Hair spray (inhalation exposure)

Product type	**Amount**	**C**	**Inhalation Rate**	**Exposure Duration (Zone 1)**	**Exposure Duration (Zone 2)**	**Fraction Inhaled**	**Volume (Zone 1)**	**Volume (Zone 2)**	**Daily systemic exposure**
	(g/day)	(%)	(m^3/day)	(min)	(min)	(%)	(m^3)	(m^3)	(mg/kg bw/day)
Hairspray	9.89	0.05	20	1	20	50	1	10	**0.0016**

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 1 [(amount × C × inhalation rate × exposure duration (zone 2) × fraction inhaled)/(volume (zone 2) × body weight)]

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	0.05	0.95	10	0.0017
Fabric softener	90	0.05	0.95	10	0.0007
Total					**0.0024**

Daily Systemic Exposure = (Amount × C × PR × PT)/body weight

Household products (Direct dermal exposure – from wearing clothes)

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	0.05	1,980	0.01	0.01	0.007	0.0000

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)
Dishwashing liquid	3	0.05	1,980	0.009	0.01	0.03	0.0001
All-purpose cleaner	1	0.05	1,980	1	0.01	0.007	0.0011
Total							**0.0012**

Daily Systemic Exposure = (Frequency × C × Contact area × Product Use Concentration × Film Thickness on skin × Time Scale factor × dermal absorption)/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 notified chemical. This would result in a combined internal dose of 0.2616 mg/kg bw/day. It is acknowledged that inhalation exposure to the notified chemical from use of other cosmetic and household products (in addition to hair spray) may occur. However it is considered that the combination of conservative hair spray inhalation exposure assessment parameters, (in particular assuming an airspace volume of 1 m^3 in zone 1), and the aggregate exposure form the use of the dermally applied products (which assumes a conservative 100% absorption rate), is sufficiently protective to cover additional inhalation exposure to the notified chemical from use of other spray cosmetic and household products with lower exposure factors (e.g. air fresheners).

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified chemical and an analogue are summarised in the following table. For full details of the studies, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	LD50 > 2000 mg/kg bw; low toxicity
Rat, acute dermal toxicity	LD50 > 2000 mg/kg bw; low toxicity
Skin Corrosion – *in vitro* EpiDerm^{TM} skin corrosion test	non-corrosive
Rabbit, skin irritation	slightly irritating
Rabbit, eye irritation	slightly irritating
Guinea pig, skin sensitisation – Magnusson and Kligman	no evidence of sensitisation
Rat, repeat dose oral toxicity – 90 days*	NOAEL = 30 mg/kg bw/day
Mutagenicity – bacterial reverse mutation	non mutagenic

* Analogue data

Toxicokinetics

No data on toxicokinetics for the notified chemical was provided. For dermal absorption, molecular weights below 100 g/mol are favourable for absorption and molecular weights above 500 g/mol do not favour absorption (ECHA, 2017). Dermal uptake is likely to be moderate to high if the water solubility is between 100-10,000 mg/L and the partition coefficient (log P) values between 1 and 4 (ECHA, 2017). Based on the low molecular weight (< 500 g/mol) and partition coefficient (log Pow = 4.369 – 4.498 at 25 °C) of the notified chemical, there is potential for the chemical to cross biological membranes.

Acute toxicity

The notified chemical is of low acute oral and dermal toxicity based on studies conducted in rats.

Irritation

Based on the results in *an in vitro* EpiDerm^{TM} skin corrosion test, the notified chemical is considered to be non-corrosive.

The notified chemical was found to be slightly irritating to the skin and to eyes in studies conducted in rabbits.

Sensitisation

The notified chemical was not a skin sensitiser when tested in guinea pigs in a maximisation test (induction at 25% concentration (intradermal) and 100% concentration (topical) and challenge by topical administration at up to 100% concentration).

Repeated dose toxicity

No repeated dose toxicity data were submitted for the notified chemical. In a repeated dose oral (gavage) toxicity study an analogue chemical (3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, CAS No. 127-51-5) was administered to rats at 5, 30 and 500 mg/kg bw/day for 90 days (Politano *et al*., 2012). The systemic No

Observed Adverse Effect Level (NOAEL) was established as 30 mg/kg bw/day, based on statistically significant changes in blood chemistry parameters (reduced aspartate aminotransferase, and increased cholesterol, creatinine, and total protein) observed in both sexes at 500 mg/kg bw/day, statistically significant increases in liver and kidney weights observed in both sexes and in spleen weights observed in males at 500 mg/kg bw/day, adaptive hepatocyte enlargement observed in both sexes at 500 mg/kg bw/day, and thyroid and bone marrow histopathological changes observed in males at 500 mg/kg bw/day (Politano *et al*., 2012).

Mutagenicity
The notified chemical was negative in two bacterial reverse mutation assays.

Health hazard classification
Based on the available information, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia.

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety

Reformulation
Workers may experience dermal, ocular and perhaps inhalation exposure to the notified chemical at ≤ 100% concentration during reformulation. Given the notified chemical is a slight skin and eye irritant caution should be exercised when handling the notified chemical during reformulation processes. The use of local ventilation, enclosed/automated processes and PPE (i.e. protective clothing, safety glasses, impervious gloves and respiratory protection, if inhalation exposure may occur) are expected to minimise the potential for exposure.

Therefore, under the conditions of the occupational settings described, the risk to workers from use of the notified chemical is not considered to be unreasonable.

End-Use
Cleaners and beauty care professionals will handle the notified chemical at ≤ 0.7% concentration, similar to public use. Such professionals may use PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. Therefore, the risk to workers who use products containing the notified chemical is expected to be of a similar or lesser extent than consumers who use such products on a regular basis. For details of the public health risk assessment see section 6.3.2 below.

6.3.2. Public Health
Members of the public may experience repeated exposure to the notified chemical through the use of cosmetic and household products containing the notified chemical at ≤ 0.7% concentration. The main route of exposure is expected to be dermal and inhalation, with some potential for accidental ocular or oral exposure.

Eye and skin irritation
The notified chemical is a slight skin and eye irritant. However, risk of eye and skin irritation effects are not expected at the proposed low concentrations in end-use products (≤ 0.7%).

Repeated dose toxicity
The repeat dose toxicity potential was estimated by calculation of the margin of exposure (MoE) of the notified chemical using the worst case exposure scenario from use of multiple products as 0.2616 mg/kg bw/day (see Section 6.1.2). Using the NOAEL of 30 mg/kg bw/day derived from a 90-day repeated dose oral toxicity study on an analogue chemical, the margin of exposure (MOE) was estimated to be 114. A MOE value ≥ 100 is generally considered to be acceptable for taking into account intra- and inter-species differences.

When used in the proposed manner, the notified chemical is not considered to pose an unreasonable risk to public health.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE

The notified chemical will be imported into Australia either in finished consumer products, or in the neat form or as a component in fragrance formulations for reformulation into finished products. In general, the reformulation processes are expected to involve blending operations that will be highly automated and occur in an enclosed system, followed by automated filling of the finished products into end-use containers. According to the notifier, the liquid waste containing the notified chemical from reformulation equipment washing will be reused. Empty import containers containing residual notified chemical up to 0.1% of the import volume as estimated by the notifier, will either be recycled or disposed of through an approved waste management facility. Accidental spills of the notified chemical during import, transport, storage or reformulation are expected to be collected for disposal, in accordance with local government regulations.

RELEASE OF CHEMICAL FROM USE

The majority of the notified chemical are expected to be released to sewers across Australia as a result of its use in cosmetic and household products, which are washed off hair and skin of consumers as well as from cleaning activities.

RELEASE OF CHEMICAL FROM DISPOSAL

Empty end-use containers are disposed of through domestic garbage disposal and are expected to enter recycling facility or landfill.

7.1.2. Environmental Fate

The ready biodegradation test conducted on the notified chemical indicates that it is not readily biodegradable (no degradation over 28 days). However, the photolysis test conducted on the notified chemical reveals it underwent direct photodegradation with calculated half-lives in Australian natural waters ranged from 1 to 45 days. For details of the biodegradation and photodegradation studies, refer to Appendix C.

Following its use in cosmetic and household products, the majority of the notified chemical are expected to enter sewers across Australia. It is expected to be partly removed by partition to sludge at sewage treatment plant before releasing to surface waters. A small proportion of the notified chemical may be released to land when effluent is used for irrigation, or when sewage sludge is used for soil remediation. A minor amount of the notified chemical may also be disposed of to landfill as collected spills and empty container residues. In landfill, soil or sludge, the notified chemical is expected to have moderate mobility based on its calculated log Koc. The notified chemical in surface waters, soil, or landfill is expected to further photodegraded. The photodegradation products are expected to eventually transform into carbon dioxide and water.

7.1.3. Predicted Environmental Concentration (PEC)

A predicted environmental concentration (PEC) worst case scenario has been calculated. It was assumed that 100% of the annual import quantity of the notified chemical is released to the sewer from washing off hair and skin of consumers as well as from cleaning activities over 365 days/year, with no removal of the notified chemical by sewage treatment plant (STP) processes. The extent to which the notified chemical is removed from the effluent in STP processes based on the properties of the notified chemical has not been considered for the worst-case scenario.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	1,000	kg/year
Proportion expected to be released to sewer	100	%
Annual quantity of chemical released to sewer	1,000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release:	2.74	kg/day
Water use	200	L/person/day
Population of Australia (Millions)	24.386	million
Removal within STP	0%	

Daily effluent production:	4,877	ML
Dilution Factor – River	1	
Dilution Factor – Ocean	10	
PEC - River:	0.56	μg/L
PEC - Ocean:	0.06	μg/L

STP effluent re-use for irrigation occurs throughout Australia. The agricultural irrigation application rate is assumed to be 1000 L/m^2/year (10 ML/ha/year). The notified chemical in this volume is assumed to infiltrate and accumulate in the top 10 cm of soil (density 1500 kg/m^3). Using these assumptions, irrigation with a concentration of 0.562 μg/L may potentially result in a soil concentration of approximately 3.745 μg/kg. Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated irrigation, the concentration of notified chemical in the applied soil in 5 and 10 years may be approximately 18.73 μg/kg and 37.45 μg/kg, respectively.

7.2. Environmental Effects Assessment

No ecotoxicity data were submitted for this limited notification.

7.2.1. Predicted No-Effect Concentration

The Predicted No-Effect Concentration (PNEC) was not calculated as no ecotoxicity data were submitted.

7.3. Environmental Risk Assessment

The Risk Quotient (PEC/PNEC) was not calculated as no ecotoxicity data were submitted. On the basis of its degradability and the maximum import volume of 1 tonne per annum, the notified chemical is not considered to pose an unreasonable risk to the environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point/Freezing Point -2 ± 0.5 °C

Method	OECD TG 102 Melting Point/Melting Range
Remarks	Determined by observation of solidification of the liquid test substance
Test Facility	Firmenich (2004)

Boiling Point 274 ± 2 °C at 96.9 kPa

Method	OECD TG 103 Boiling Point
Remarks	Determined using boiling capillary tube containing a temperature sensor
Test Facility	Firmenich (2004)

Density 917 kg/m^3 at 20 °C

Method	OECD TG 109 Density of Liquids and Solids.
Remarks	Oscillating densitimeter method
Test Facility	Firmenich (2004)

Vapour Pressure 1.835×10^{-4} kPa at 25 °C

Method	OECD TG 104 Vapour Pressure
Remarks	Dynamic measurement method
Test Facility	Firmenich (1995)

Water Solubility Study 1 4.196 mg/L at 20 °C

Method	EEC Annex V, Directive 84/449/EEC A.6 Water Solubility.
Remarks	Flask Method
Test Facility	TLL (1992a)

Water Solubility Study 2 4.14 mg/L at 20 °C

Method	Directive 92/69/EEC A.6 Water Solubility.
Remarks	Flask Method
Test Facility	Firmenich (2007)

Fat Solubility Soluble in all proportions at 37 °C

Method	EEC Annex V, Directive 84/449/EEC A.7 Fat Solubility.
Remarks	Flask Method
Test Facility	TLL (1992a)

Hydrolysis as a Function of pH

Method	OECD TG 111 Hydrolysis as a Function of pH.

pH	*T (°C)*	$t_{1/2}$ *(year)*
2	40	> 1
5	40	> 1
7	40	> 1
8.5	40	> 1
12	40	> 1

Remarks	The test substance is hydrolytically stable.
Test Facility	Firmenich (2014)

Partition Coefficient (n-octanol/water)	Isomer 1: log Pow = 4.498 at 25 °C Isomer 2: log Pow = 4.392 at 25 °C Isomer 3: log Pow = 4.369 at 25 °C

Method	OECD TG 123 Partition Coefficient (n-octanol/water)
Remarks	Slow Stirring Method
Test Facility	Dr U Noack-Laboratorien (2015)

Flash Point	126 ± 2 °C at 97 kPa

Method	EC Council Regulation No 440/2008 A.9 Flash Point.
Remarks	Determined using a Rapid Flash Tester
Test Facility	Firmenich (2004)

Autoignition Temperature	> 220 °C

Method	EC Council Regulation No 440/2008 A.15 Auto-Ignition Temperature (Liquids and Gases)
Test Facility	Firmenich (2008)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE Notified chemical

METHOD Similar to OECD TG 401 Acute Oral Toxicity – Limit Test
Species/Strain Rat/Crl:CD(SD)BR
Vehicle Polyethylene glycol 400
Remarks - Method No significant protocol deviations

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
1	5 per sex	2000	0/10

LD50 > 2,000 mg/kg bw
Signs of Toxicity Signs of systemic toxicity including hunched posture and piloerection were noted on the day of dosing.
Effects in Organs No abnormalities were noted at necropsy.
Remarks - Results The animals showed expected body weight gain over the observation period.

CONCLUSION The notified chemical is of low toxicity via the oral route.

TEST FACILITY TLL (1992b)

B.2. Acute toxicity – dermal

TEST SUBSTANCE Notified chemical

METHOD Similar to OECD TG 402 Acute Dermal Toxicity – Limit Test
Species/Strain Rat/Crl:CD(SD)BR
Vehicle None
Type of dressing Semi-occlusive
Remarks - Method No significant protocol deviations

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
1	5 per sex	2000	0/10

LD50 > 2,000 mg/kg bw
Signs of Toxicity - Local Skin irritation of varying degree was noted at and around the application site in most animals.
Signs of Toxicity - Systemic Perinasal staining was noted on the day of dosing and slight piloerection were noted on day 5.
Effects in Organs Skin irritation effects were confirmed at necropsy. No other abnormalities were noted at necropsy.
Remarks - Results The animals showed expected body weight gain over the observation period.

CONCLUSION The notified chemical is of low toxicity via the dermal route.

TEST FACILITY TLL (1991a)

B.3. Skin Corrosion – *in vitro* EpiDerm^{TM} skin corrosion test

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 431 In vitro Skin Corrosion - Human Skin Model Test EpiDerm^{TM} Reconstructed Human Epidermis Model
Vehicle	None
Remarks - Method	No significant protocol deviations. The negative control was sterile distilled water and the positive control was 8.0 N Potassium hydroxide.

RESULTS

Test Material	*Mean OD$_{570}$ of Triplicate Tissues*		*Relative Mean Viability (%)*	
	3 min	*60 min*	*3 min*	*60 min*
Negative control	1.895	1.991	100	100
Test substance	2.299	2.303	121.3	115.7
Positive control	0.298	0.278	15.7	14

OD = optical density

Remarks - Results	Based on the mean tissue viability of ≥ 50% after 3 min exposure and ≥ 15% after 60 min exposure, the test substance is not predicted to be corrosive according to the test guidelines, using GHS criteria. Positive and negative controls performed as expected.
CONCLUSION	The notified chemical was considered non-corrosive to the skin under the conditions of the test.
TEST FACILITY	SPL (2005a)

B.4. Irritation – skin

TEST SUBSTANCE	Notified chemical
METHOD	Similar to OECD TG 404 Acute Dermal Irritation/Corrosion
Species/Strain	Rabbit/New Zealand White
Number of Animals	4
Vehicle	None
Observation Period	14 days
Type of Dressing	Semi-occlusive
Remarks - Method	No significant protocol deviations

RESULTS

Lesion	*Mean Score**				*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3	4			
Erythema/Eschar	1.7	2	2.3	2	3	> 14 days	1
Oedema	1.7	2	2.3	1.3	3	< 7 days	0

* Calculated on the basis of the scores at 24, 48, and 72 hours for EACH animals.

Remarks - Results	No mortality or signs of systemic toxicity were observed. Erythema and oedema were noted from 1 hour and 24 hours after dosing and persisted until the 72-hour observation. Oedema was absent in all animals and mild and moderate erythema remained in 2 animals at the 7-day observation. At the 14-day observation, 3 out 4 animals has fully recovered and mild erythema persisted in the remaining animal.

CONCLUSION	The notified chemical is slightly irritating to the skin.
TEST FACILITY	TLL (1992c)

B.5. Irritation – eye

TEST SUBSTANCE	Notified chemical
METHOD	Similar to OECD TG 405 Acute Eye Irritation/Corrosion
Species/Strain	Rabbit/New Zealand White
Number of Animals	4
Observation Period	72 hours
Remarks - Method	No significant protocol deviations

RESULTS

Lesion	*Mean Score**				*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3	4			
Conjunctiva: redness	0	0.3	0	0	2	< 48 hours	0
Conjunctiva: chemosis	0	0	0	0	2	-	0
Conjunctiva: discharge	0	0	0	0	2	-	0
Corneal opacity	0	0	0	0	-	-	0
Iridial inflammation	0	0	0	0	-	-	0

* Calculated on the basis of the scores at 24, 48, and 72 hours for EACH animals.

Remarks - Results	Mild to moderate conjunctival redness, chemosis and discharge were observed after dosing and only mild redness were noted in 1 animal at the 24-hour observation.
CONCLUSION	The notified chemical is slightly irritating to the eye.
TEST FACILITY	TLL (1992d)

B.6. Skin sensitisation – guinea pig, maximisation test

TEST SUBSTANCE	Notified chemical
METHOD	Similar to OECD TG 406 Skin Sensitisation – Magnusson and Kligman
Species/Strain	Guinea pig/Dunkin-Hartley
PRELIMINARY STUDY	Intradermal: 25% (the highest concentration that caused an acceptable local response) Topical: 100% (maximum non-irritating concentration)
MAIN STUDY	
Number of Animals	Test Group: 20 Control Group: 10
Vehicle	Ethanol
Positive control	Not conducted in parallel with the test substance, but had been conducted previously in the test laboratory using 1-chloro-2,4-dinitrobenzene.
INDUCTION PHASE	Induction Concentration: intradermal: 25% topical: 100%
Signs of Irritation	Not reported
CHALLENGE PHASE	
challenge	topical: 50% and 100%
Remarks - Method	No significant protocol deviations

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after Challenge*	
		24 h	*48 h*
Test Group	50% or 100%	0/20	0/20
Control Group	50% or 100%	0/10	0/10

Remarks - Results	No signs of irritation were observed after challenge in control and test animals.
CONCLUSION	There was no evidence of reactions indicative of skin sensitisation to the notified chemical under the conditions of the test.
TEST FACILITY	TLL (1992e)

B.7. Genotoxicity – bacteria

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 471 Bacterial Reverse Mutation Test Plate incorporation procedure
Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100, TA102
Metabolic Activation System	S9 fraction from phenobarbital/β-naphthoflavone induced rat liver
Concentration Range in Main Test	a) With metabolic activation: 50 – 5000 µg/plate b) Without metabolic activation: 50 – 5000 µg/plate
Vehicle	Dimethylsulphoxide
Remarks - Method	No significant protocol deviations. The dose selection for the main tests was based on the toxicity observed in a preliminary test carried out at 0.15 – 5000 µg/plate using TA100. Positive controls: With metabolic activation: 2-aminoanthracene (TA1535, TA1537, TA100); benzo(a)pyrene (TA98); 1,8-dihydroxyanthraquinone (TA102) Without metabolic activation: N-ethyl-N'-nitro-N-nitrosoguanidine (TA1535, TA100); 9-aminoacridine (TA1537); mitomycin C (TA102); 4-nitroquinoline-1-oxide (TA98)

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	> 5000	> 5000	≥ 5000	negative
Test 2		> 5000	≥ 5000	negative
Present				
Test 1	> 5000	≥5000	≥ 5000	negative
Test 2		≥ 5000	≥ 5000	negative

Remarks - Results	No significant increases in the frequency of revertant colonies were observed for any of the bacterial strains, with any dose of the test substance, either with or without metabolic activation. The positive and negative controls gave a satisfactory response confirming the validity of the test system.
CONCLUSION	The notified chemical was not mutagenic to bacteria under the conditions of the test.
TEST FACILITY	SPL (2005b)

B.8. Genotoxicity – bacteria

TEST SUBSTANCE Notified chemical

METHOD OECD TG 471 Bacterial Reverse Mutation Test.
Plate incorporation procedure

Species/Strain *S. typhimurium*: TA1535, TA1537, TA98, TA100
Metabolic Activation System S9 fraction from phenobarbital/β-naphthoflavone induced rat liver
Concentration Range in Main Test a) With metabolic activation: 0.064 – 40 µg/plate
b) Without metabolic activation: 0.32 – 200 µg/plate
Vehicle Dimethylsulphoxide
Remarks - Method No significant protocol deviations. The dose selection for the main tests was based on the toxicity observed in a preliminary test carried out at 1.6 – 5000 µg/plate using TA98.

Positive controls:
With metabolic activation: 2-aminoanthracene
Without metabolic activation: sodium azide (TA1535, TA100); 9-aminoacridine (TA1537); 2-nitrofluorene (TA98)

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	≥ 40	≥ 40	> 40	negative
Test 2		≥ 40	> 40	negative
Present				
Test 1	≥ 200	≥ 200	> 200	negative
Test 2		≥ 200	> 200	negative

Remarks - Results No significant increases in the frequency of revertant colonies were observed for any of the bacterial strains, with any dose of the test substance, either with or without metabolic activation.

The positive and negative controls gave a satisfactory response confirming the validity of the test system.

CONCLUSION The notified chemical was not mutagenic to bacteria under the conditions of the test.

TEST FACILITY TLL (1991b)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready biodegradability

TEST SUBSTANCE	Notified chemical
METHOD	ISO Guidelines No. 14593 Ready Biodegradability CO_2 in Sealed Vessels (similar to OECD TG 301 B)
Inoculum	Activated sludge from a domestic sewage treatment plant
Exposure Period	28 days
Auxiliary Solvent	None
Analytical Monitoring	Dissolved Organic Carbon and Inorganic Carbon by TOC
Remarks - Method	No major deviations from the test guidelines were reported. The test substance was directly added to the test medium in the test vessels. A toxicity control was run.

RESULTS

Test substance		*Sodium benzoate*	
Day	*% Degradation*	*Day*	*% Degradation*
2	1	2	77
10	-1	10	77
20	-4	20	86
28	0	28	91

Remarks - Results	All validity criteria for the test were satisfied. The toxicity control exceeded 25% biodegradation after 14 days showing that toxicity was not a factor inhibiting the biodegradability of the test substance. The degree of degradation of the test substance after 28 days was 0%.
CONCLUSION	The test substance is not readily biodegradable.
TEST FACILITY	Safepharm (2005)

C.1.2. Photodegradation

Laboratory photodegradation studies are conducted in pure water. However, natural water can contain clay, silt, and organic matter such as algae, soluble coloured organic compounds, and plankton. Additionally to be relevant to Australia, any extrapolation from the laboratory study must also account for the composition of Australian waters and the intensity and frequency of sunlight. The notifier has extrapolated the half-lives of between 2.7 and 7.8 hours from the photodegradation study in pure water (below) using comparisons of photodegradation rates of the notified chemical in reconstituted or natural water and modelling (Emberger & Lin, Lin 2017).

The photodegradation study included a test using reconstituted natural water (RNW). It was conducted using 9.15 mg/L of natural organic matter (NOM) using a conversion of 1.72 (Pribyl 2010) for organic carbon, and is relevant to Australian conditions which have NOM of between 2 and 10 mg/L (Bolto et al., 2007). In both pure water and RNW the notified chemical could not be detected after 4 hours, demonstrating that rates of degradation in both media are similar.

The notifier recalculated the quantum yield obtained in the photodegradation study, due to the baseline of the UV spectrum not being perfectly at zero and trace impurities in PNA, which should have been recrystallised twice for optimal results. The recalculated value was 0.51.

The recalculated quantum yield was verified by comparing the degradation of the notified chemical in pure water (in duplicate) at Princeton New Jersey (40.3°N; 74.7°W) on 21/7/2017 and 27/10/2017 on clear days. An additional factor of 2 was included to account for the geometric differences between surface water and quartz (Mill et al., 1982). The calculated half-lives were 0.38 and 1.14 hours, respectively and compared with the measured values of 0.40 and 1.15 hours respectively.

The half-lives were calculated for water containing 2.5, 5, 7.5 and 10 mg/L DOC, at three latitudes 10 °S, 25 °S and 40°S at 1 and 5 m depths which is representative of a shallow and deep lake (Fee et al., 1996). The intensity of the sunlight was obtained from Bird and Hulstrom, (1981) model, obtained from (https://www2.pvlighthouse.com.au/calculators/solar%20spectrum%20calculator/solar%20spectrum%20calculator.aspx). The effects of the DOC and depth of water on the attenuation of light was accounted for by correlating the DOC with the diffuse attenuation coefficient K_{d}, according to Morris et al, (1995). The notifier did not include effects from turbidity on Kd. However, this was found to be acceptable for several reasons.

Firstly Australian waters under base flow conditions are not significantly more turbid than natural waters found in many industrialised countries (Henderson, Liu & Baldwin 2013, Cugley, Shukla & Sarneckis 2002, Mawhinney & Muschal, 2015, Bartley et al., 2012, Waters & Packet 2007, Yu, Zhang & Lemckert c 2015, Abril et al., 2002, Pawlowski et al., 2012 and Vilizzi 2012, USGS 2017-2018 and Voichick & Topping 2012). Therefore the correlation between Kd and organic carbon as proposed by Morris et al., (1995) would also be valid for Australian waters. Secondly turbidity is a bulk property of natural water's propensity to scatter and absorb light rather than transmit it in straight lines and is related to the of the amount of suspended and dissolved particles in solution (Dunlop, McGregor & Horrigan 2005). This lack of distinction between absorption and scattering means that the effects of turbidity on the rate degradation of a chemical are not well correlated. This is because only absorption of light results in a reduction in the energy available for photolysis, while scattering is elastic with no reduction in the energy of the photon (Zheng, Dickey & Chang 2002). Scattering may even extend the path length of the photon's travel through water which can increase the rate of degradation. Thirdly most measurements of turbidity are conducted in the visible of near infrared spectrum (USEPA 1993; Oregon Department of Environmental Quality 2014, Lake Superior streams 2018, Flint River Watershed Coalition 2011, Rasmussen et al., 2009), whilst most photodegradation occurs from the absorption of light in the near UV part of the spectrum (Banwell 1983 pp 234-237, Smith, Baker & Fahy 1983).

The degradation rates of the notified chemical were further modified by considering the number of sunny days in Australia. This was averaged from Bureau of Meteorology data from all capital cities in Australia and 14 major regional towns. A percentage of sunshine was determined by adding all sunny days and half of the partly sunny days for each location and dividing by the number of days in a year. The percentage was then averaged for all of Australia. The overall methodology is considered a reasonable estimate of the half-lives of the notified chemical relevant to Australian conditions and are presented below (Table 1).

Table 1: Estimated photodegradation half-lives (day) of the notified chemical in Australian natural waters

[DOC] (mgC/L)	***2.5***	***5***	***7.5***	***10***	***2.5***	***5***	***7.5***	***10***
10° S	1.3	3.0	4.9	6.9	6.3	15	24	35
25° S	1.4	3.2	5.3	7.6	6.9	16	27	38
40° S	1.7	3.9	6.4	9.1	8.2	19	32	45

A reasonable worst-case value of 45 days was calculated demonstrating the notified chemical is not likely to be persistent.

TEST SUBSTANCE	Notified Chemical
METHOD	OECD TG 316 Direct photolysis U.S. EPA OPPTS 835.2210 TG Direct photolysis
Light source and Spectrum	Atlas Suntest XLS+ solar simulator equipped with 1700 W xenon arc lamps, working at wavelengths from 290 to 800 nm.
Relative Intensity	765 W/m^{2} at 25 °C
Spectrum of Test Substance	290 to 390 nm
Exposure Period	0.25, 0.5, 0.75, 1, 2, 4, 6, 8, 10 and 25 h
Remarks – Method	No major deviations from the test guidelines were reported. A preliminary test was conducted at 0.2, 1 and 10 mg/L of notified chemical. Based on the results of the preliminary test, solutions containing ~ 2 mg/L of the notified chemical were prepared according to the guidelines and photodegradation experiments were conducted in special quartz test tubes under simulated sunlight. Dark controls and test solutions in reconstituted natural water (RNW) were also run. The RNW contained 5.32 mg C/L. Additional test solutions containing ~ 10 mg/L were prepared for the investigation of degradation products. A

photodegradation screening test was performed to see whether it was a considerable process. Simultaneous photodegradation of the notified chemical and the actinometer 4-Nitroanisole [para-nitroanisole (PNA)] was conducted to determine the direct photodegradation quantum yield of the notified chemical. The degradation products were analysed by gas chromatography -mass spectrometry (GC-MS) and ultra-high performance liquid chromatography - high resolution mass spectrometry (UHPLC-HRMS) analyses.

RESULTS

The calculated half-lives in clear water under Australian geographical conditions are between 2.7 and 7.8 hours.

Remarks - Results

The rates of degradation of the notified chemical at various concentrations in the preliminary test were similar, demonstrating that the rate of degradation is independent of the concentration in the range of 0.1 - 10 mg/L. There was no degradation of the notified chemical or PNA in the dark controls. A λmax, (the wavelength at which the maximum light is absorbed) for the notified chemical could not be established, but absorbance increased, with decreasing wavelength for wavelengths between 390 and 290 nm. Photoisomerization of the notified chemical yielded the corresponding Z isomers and Norrish Type II cleavage of the notified chemical led to the formation of four isomers of 4-(2,2,3,6-tetramethylcyclohexylidene)butan-2-one. These volatile compounds, detected by GC-MS, only represented a portion of the total degradation products. Their concentrations in the test solutions initially increased and then began to decrease due to further degradation into non-volatile compounds. Non-volatile photodegradation products of the notified chemical were found to be numerous and more polar than the notified chemical by UHPLC-HRMS analysis. They were likely formed through photo-induced oxidation. These photooxidation products underwent further direct and indirect photodegradation. These processes are expected to continue to transform the entire set of degradation products into smaller and more polar compounds and eventually into carbon dioxide and water. Although there were some differences in the proportions of the degradation products in the RNW test, the degradation pathway is similar to that of the test in pure water.

The notified chemical could not be detected after 4 hours, and the half-life of the notified chemical was calculated as 0.18 ± 0.005 hours in pure water. The half-life in RNW was not calculated but the notified chemical could also not be detected after 4 hours, demonstrating rapid degradation.

The quantum yield (the proportion of absorbed photons, which lead to a degradation reaction in comparison with the total of absorbed photons) for the notified chemical was calculated as 0.0969. From the quantum yield an estimate of the photodegradation rate of the notified chemical in sunlit surface water as a function of latitude and season was made using (Equation 1).

Equation 1

$$k_{dir} = \phi \sum_{\lambda} \epsilon_{\lambda} L_{\lambda}$$

The value for E_{λ} in W/m^2, was generated using SMARTS model developed by the US Department of Energy, Office of Energy Efficiency and Renewable Energy (http://www.nrel.gov/rredc/smarts/).

The half-lives were calculated using the well-known equation

(Equation 2).

Equation 2

$$t_{1/2} = \frac{ln2}{k_{dir}}$$

The values at various latitudes and seasons are presented below.

Table 2: Direct photodegradation half-lives (hours) of the notified chemical estimated as a function of season and latitude

	Summer				**Winter**			
Latitude	10°S	20°S	30°S	40°S	10°S	20°S	30°S	40°S
Half-life (hr)	2.8	2.7	2.7	2.8	3.4	4.1	5.3	7.8

CONCLUSION
Degradation of the notified chemical is rapid in clear water even during winter at 40°S with a half-life of 7.8 hours.

TEST FACILITY
Firmenich (2017)

BIBLIOGRAPHY

Abril G., Nogueira M., Etcheber H., Cabec¸adas G., Lemaire E. and Brogueira M. J. (2002) Behaviour of Organic Carbon in Nine Contrasting European Estuaries Estuarine, Coastal and Shelf Science 54, 241–262, available online at http://www.idealibrary.com

ACI (2010) Consumer Product Ingredient Safety, Exposure and risk screening methods for consumer product ingredients, 2nd Edition, American Cleaning Institute, Washington DC.

Banwell C.N. (1983) Fundamentals in Molecular Spectroscopy 3rd Ed., McGraw Hill International (UK) LTD. ISBN 0-07-084139-X

Bartley R., Speirs W. J., Ellis T. W., and Waters D. K. (2012) A review of sediment and nutrient concentration data from Australia for use in catchment water quality models Marine Pollution Bulletin 65 101–116.

Bird, R. E., & Hulstrom, R. L., 1981. Simplified Clear Sky Model for Direct and Diffuse Insolation on Horizontal Surfaces, Technical Report No. SERI/TR-642-761, Golden, CO: Solar Energy Research Institute.

Bolto B., Dixon D. Eldridge R. King S. (2007) Removal of Natural Organic Matter from Drinking Water, Research Report No 7 CSIRO Molecular Science CRC for Water Quality and Treatment 2007.

Cadby, PA., Troy, WR., Vey, MGH. (2002) Consumer Exposure to Fragrance Ingredients: Providing Estimates for Safety Evaluation. Regulatory Toxicology and Pharmacology, 36:246-52.

Cugley, J. Shukla C. & Sarneckis K. (2002) Environment Protection Agency South Australia ISBN 1 876562 18 8 January

Dr U Noack-Laboratorien (2015) [Notified Chemical]: Partition Coefficient (n-Octanol/Water), Slow Stirring Method (Study No. COE16119, March, 2015). Sarstedt, Germany, Dr U Noack-Laboratorien (Unpublished report submitted by the notifier).

Dunlop J., McGregor G., and Horrigan N., 2005 Potential impacts of salinity and turbidity in riverine ecosystems Characterisation of impacts and a discussion of regional target setting for riverine ecosystems in Queensland The State of Queensland ISBN 1 74172 078 8 QNRM 05523

Earnest, C.W., Jr. (2009) A Two-Zone Model to Predict Inhalation Exposure to Toxic Chemicals in Cleaning Products, MScEng thesis, The University of Texas at Austin.

ECHA (2017) Guidance on Information Requirements and Chemical Safety Assessment Chapter R.7c: Endpoint specific guidance, June 2017, version 3.0. European Chemicals Agency, https://echa.europa.eu/documents/10162/13632/information_requirements_r7c_en.pdf

Emberger M. & Lin J 2017, Photodegradation of [Notified Chemical] in the Aquatic Environment. Submitted to NICNAS (unpublished).

enHealth (2012) Australian Exposure Factor Guide, companion document to: Environmental Health Risk Assessment: Guidelines for assessing human health risks from environmental hazards, EnHealth, Commonwealth of Australia.

Fee, E. J., Hecky, R. E., Kasian, S. E. M., Cruikshank ,D. R., 1996. Effects of lake size, water clarity, and climatic variability on mixing depths in Canadian Shield lakes. Limnol. Oceanogr., 41(5), 912-920.

Firmenich (1995) [Notified Chemical]: Vapour Pressure (Study No. 1966(E)-FRF, August, 1995). La Plaine, Switzerland, Firmenich SA (Unpublished report submitted by the notifier).

Firmenich (2004) [Notified Chemical]: Determination of General Physico-Chemical Properties: Melting/Freezing Temperature, Boiling Temperature, Relative Density and Flash Point (Study No. E026-10.2004, November, 2004). La Plaine, Geneva, Switzerland, Firmenich SA (Unpublished report submitted by the notifier).

Firmenich (2007) [Notified Chemical]: Determination of General Physico-Chemical Properties: Water Solubility (Study No. E065-08.2007, October, 2007). La Plaine, Geneva, Switzerland, Firmenich SA (Unpublished report submitted by the notifier).

Firmenich (2008) [Notified Chemical]: Autoignition Temperature (Study No. 103551-DMR, July, 2008). La Plaine, Geneva, Switzerland, Firmenich SA (Unpublished report submitted by the notifier).

Firmenich (2014) Stability Test of [Notified Chemical] (March, 2014). La Plaine, Geneva, Switzerland, Firmenich SA (Unpublished report submitted by the notifier).

Firmenich (2017) Photodegradation of [Notified Chemical] in the Aquatic Environment and Supplemental Information. Princeton, USA, Firmenich USA (Unpublished report submitted by the notifier).

Flint River Watershed Coalition (2011) Flint River GREEN Notebook www.FlintRiver.org

Henderson, B., Liu Y., and Baldwin D. (2013) Trends in physical and chemical aspects of water quality in the Murray-Darling Basin 1978-2012. CSIRO Water for a Healthy Country Flagship, Australia.

Lake Superior Streams (2018) Turbidity & TSS accessed http://www.lakesuperiorstreams.org/understanding/param_turbidity.html 15 August 2018

Lin J. 2017 Photodegradation of [Notified Chemical] in the aquatic environment: supplemental information to support the PBT assessment, FIRMENICH, Inc. 27 November 2017 (unpublished).

Loretz, L., Api, A.M., Barraj, L., Burdick, J. Davis, D.A., Dressler, W., Gilberti, E., Jarrett, G., Mann, S., Pan, Y.H.L., Re, T., Renskers, K., Scrafford, C., Vater, S. (2006) Exposure data for personal care products: Hairspray, spray perfume, liquid foundation, shampoo, body wash, and solid antiperspirant, Food and Chemcal Toxicology 44:2008-2018.

Mawhinney, W. & Muschal, M. (2015). Assessment of Murray-Darling Basin Plan water quality targets in New South Wales; 2007 to 2012. New South Wales Department of Primary Industries, Water, Sydney. ISBN 978-1-74256-792-1

Miller G. C. & Zepp R. G. (1979) Effects of Suspended Sediments on Photolysis Rates of Dissolved Pollutants Environmental Research Laboratory. U.S. Environmental Protection Agency. Athens. GA U.S.A. Water Research Vol. 13, pp 453 - 459 Pergamon Press Ltd Printed in Great Britain.

Mill, T. et al., 1982. Laboratory Protocols for Evaluating the Fate of Organic Chemicals in Air and Water. EPA Report No. 600/3–82–022.

Morris D. P., Zagarese H., Williamson C. E., Balseiro E. G., Hargreaves B. R., Modenutti B., Moeller R. and Queimalinos C. (1995) The attenuation of solar UV radiation in lakes and the role of dissolved organic carbon Limnol. Oceanogr. 40(8), 1995, 1381-1391, by the American Society of Limnology and Oceanography, Inc.

Oregon Department of Environmental Quality (2014) Turbidity Technical Review Summary of Sources, Effects, and Issues Related to Revising the Statewide Water Quality Standard for Turbidity Last Updated: By: Aron Borok 24 April 2014.

Pawlowski S. , Jatzek2 J., Brauer T., Hempel K. and Maisch R. 2012 34 years of investigation in the Rhine River at Ludwigshafen, Germany – trends in Rhine fish populations Environmental Sciences Europe, 24:28 Page 2 of 8 available http://www.enveurope.com/content/24/1/28.

Politano, V.T., Lapczynski, A.A., Ritacco, G., Api,A.M. (2012) Ninety-Day Toxicity Study of Alpha-Iso-Methylionone in Rats, International Journal of Toxicology 31(6): 595-601.

Pribyl D. W. 2010 A critical review of the conventional SOC to SOM conversion factor Department of Soil, Water, Climate, University of Minnesota, United States Geoderma 156 (2010) 75–83.

Rasmussen, P.P., Gray, J.R., Glysson, G.D., and Ziegler, A.C., (2009) Guidelines and procedures for computing time-series suspended-sediment concentrations and loads from in-stream turbidity-sensor and streamflow data: U.S. Geological Survey Techniques and Methods, book 3, chap. C4, 52 p. ISBN 978-1–4113–2410–7RESEARCH Open Access.

R. C. Smith, K. S. Baker, and J. B. Fahy 1983 United States Environmental Protection Agency EPA-600/S3-83-060 Sept. Effects of Suspended Sediments on Penetration of Solar Radiation into Natural Waters.

Rothe, H., Fautz, R., Gerber, E., Neumann, L., Rettinger, K., Schuh, W., Gronewold, C. (2011) Special aspects of cosmetic spray evaluations: Principles on inhalation risk assessment, Toxicology Letters 205 (2011) 97-104.

Safepharm (2005) [Notified Chemical]: Assessment of Ready Biodegradability CO_2 in Sealed Vessels (Study no. 161/466, February, 2005). Derby, UK, Safepharm Laboratories Limited (Unpublished report submitted by the notifier).

SCCS (2012) Notes of Guidance for testing of Cosmetic Ingredients and Their Safety Evaluation (8th revision) European Commission - Scientific Committee on Consumer Safety.

SPL (2005a) [Notified Chemical] Determination of Corrosivity Potential in the Epiderm^{TM} Human Skin Model (Study No. 161/467, February, 2005). Shardlow, Derbyshire, UK, Safepharm Laboratories Limited (Unpublished report submitted by the notifier).

SPL (2005b) [Notified Chemical] Reverse Mutation Assay "Ames Test" Using *Salmonella typhimurium* (Study No. 161/468, February, 2005). Shardlow, Derbyshire, UK, Safepharm Laboratories Limited (Unpublished report submitted by the notifier).

Steiling, W., Bascompta, M., Carthew, P., Catalano, G., Corea, N., D'Haese, A., Jackson, P., Kromidas, L., Meurice, P., Rothe, H., Singal, M. (2014) Principle considerations for the risk assessment of sprayed consumer products, Toxicology Letters 227:41-49.

TLL (1991a) [Notified Chemical] Acute Dermal Toxicity Study in the Rat (Study No. A/D/31645, October, 1991). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

TLL (1991b) [Notified Chemical] Bacterial Reverse Mutation Assay (Study No. M/AMES/31646, September, 1991). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

TLL (1992a) Determination of General Physico-Chemical Parameters on [Notified Chemical]: Water Solubility, Fat Solubility (Study No. N/M/32663, May, 1992). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

TLL (1992b) [Notified Chemical] Acute Oral Toxicity Study in the Rat (Study No. A/O/31644, April, 1992). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

TLL (1992c) [Notified Chemical] Acute Dermal Irritation/Corrosion Study (Study No. A/S/31641, February, 1992). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

TLL (1992d) [Notified Chemical] Acute Eye Irritation Study (Study No. A/E/31642, April, 1992). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

TLL (1992e) [Notified Chemical] Guinea-Pig Maximisation Test (Study No. A/M/31643, January, 1992). Ledbury, Herefordshire, England, Toxicol Laboratories Limited (Unpublished report submitted by the notifier).

United Nations (2009) Globally Harmonised System of Classification and Labelling of Chemicals (GHS), 3rd revised edition. United Nations Economic Commission for Europe (UN/ECE), <http://www.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html>.

US EPA (1993) U.S. Environmental Protection Agency Method 180.1 Determination of Turbidity by Nephelometry Edited by O'Dell J. W. Inorganic Chemistry Branch Chemistry Research Division Revision 2.0 August 2013 Environmental Monitoring Systems Laboratory Office of Research and Development Cincinnati, Ohio.

US EPA (2012) Estimation Programs Interface (EPI) SuiteTM for Microsoft® Windows, v 4.1. United States Environmental Protection Agency. Washington DC, USA.

USGS (2017-2018) accessed https://waterdata.usgs.gov/nwis/uv?referred_module=qw&search_criteria=search_site_no&submitted_form=introduction.

Vilizzi L. (2012) The common carp, Cyprinus carpio, in the Mediterranean region: origin, distribution, economic benefits, impacts and management Murray-Darling Freshwater Research Centre, La Trobe University, Wodonga, Vic, Australia Fisheries Management and Ecology, Vol 19, 93–110.

Voichick, N., and Topping, D.J, 2014, Extending the turbidity record—making additional use of continuous data from turbidity, acoustic-Doppler, and laser diffraction instruments and suspended-sediment samples in the Colorado River in Grand Canyon: U.S. Geological Survey Scientific Investigations Report 2014–5097, 31 p., http://dx.doi.org/10.3133/sir20145097.

Waters D. & Packett R. (2007) Sediment and nutrient generation rates for Queensland rural catchments – an event monitoring program to improve water quality modelling Wilson, A.L., Dehaan, R.L., Watts, R.J., Page, K.J., Bowmer, K.H., & Curtis, A. Proceedings of the 5th Australian Stream Management Conference. Australian rivers: making a difference. Charles Sturt University, Thurgoona, New South Wales 2007.

Yu Y., Hong Z & Lemckert C. (c 2015) Salinity and turbidity distributions in the Brisbane River estuary, Australia.

Zheng X., Dickey T. & Chang G. (2002) Variability of the downwelling diffuse attenuation coefficient with consideration of inelastic scattering Applied Optics October 2002 Optical Society of America.