File No: LTD/1578

June 2012

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-(C8-18 and C18-unsatd. acyl) derivs., inner salts (INCI name: Babassuamidopropyl Betaine)

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (Cwlth) (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 Ageing, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of Sustainability, Environment, Water, Population and Communities.

For the purposes of subsection 78(1) of the Act, this Public Report may be inspected at our NICNAS office by appointment only at Level 7, 260 Elizabeth Street, Surry Hills NSW 2010.

This Public Report is also 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:

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Director
NICNAS

TABLE OF CONTENTS

SUMMARY

The following details will be published in the NICNAS *Chemical Gazette:*

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS SUBSTANCE	INTRODUCTION VOLUME	USE
LTD/1578	Estee Lauder Pty Ltd	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-(C8-18 and C18-unsatd. acyl) derivs., inner salts (INCI name: Babassuamidopropyl Betaine)	Yes	≤1 tonnes per annum	Component of cosmetic products

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
As toxicity data were not provided, the notified chemical cannot be classified according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004). However, based on the information available, the notified chemical should be considered as though it is classified with at least the following risk phrase:

R36 Irritating to eyes

and

The classification of the notified chemical using the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS) (United Nations 2009) is presented below.

	Hazard category	*Hazard statement*
Serious Eye Damage/Eye Irritation	Category 2	Irritating to eyes
Environment	Acute 1	Very toxic to aquatic organisms
	Chronic 2	Toxic to aquatic organisms with long lasting effects

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 PEC/PNEC ratio and the assessed use pattern, the notified chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

REGULATORY CONTROLS
Hazard Classification and Labelling

- The Delegate (and/or the Advisory Committee on Chemicals Scheduling) should consider the notified chemical for listing on the SUSMP.

CONTROL MEASURES
Occupational Health and Safety

- No specific engineering controls, work practices or personal protective equipment are required for the safe use of the notified chemical itself. However, these should be selected on the basis of all ingredients in the formulation.

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

- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)] workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation must be in operation.

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

Public Health

- Consumer products containing the notified chemical at >5% concentration should be labelled with a warning against eye contact, and directions on first aid measures, should the product contact the eye (e.g. avoid contact with eyes, in case of contact with eyes, rinse immediately with plenty of water and seek medical advice).

- The following measures should be taken to minimise public exposure to the notified chemical:
  - the notified chemical should not be used in cosmetic products that are intended to be applied by spray;
  - the notified chemical should not be used in cosmetic products for the eyes.

Disposal

- The notified chemical should be disposed of to landfill. 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/polymer 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;
  - additional information becomes available on the sensitisation potential of the notified chemical;
  - the process for the manufacture of the notified chemical changes, such that the levels of 1,3-propanediamine, N,N-dimethyl- (DMAPA) or amidopropyl dimethylamine impurities increase from the levels specified in the notification;
  - the notified chemical is intended to be used in cosmetic products for eyes, or in products applied by spray;
  - the concentration of the notified chemical exceeds or is intended to exceed 2% in leave-on cosmetic products and 6% in rinse-off products.

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from a component of cosmetic products, or is likely to change 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.

Material Safety Data Sheet
The MSDS of the notified chemical and products containing the notified chemical provided by the notifier were reviewed by NICNAS. The accuracy of the information on the MSDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Estee Lauder Pty Ltd (ABN: 63 008 444 719)
165-175 Mitchell Road
Erskineville NSW 2043

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

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
No details are claimed exempt from publication.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: all physico-chemical endpoints.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None.

NOTIFICATION IN OTHER COUNTRIES
None.

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Mackam BB-30 (containing 30% notified chemical)

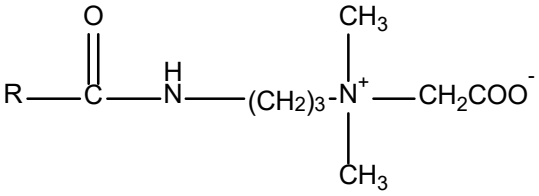
CAS NUMBER
147170-44-3

CHEMICAL NAME
1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-(C8-18 and C18-unsatd. acyl) derivs., inner salts

OTHER NAME(S)
Babassuamidopropyl Betaine (INCI name)

MOLECULAR FORMULA
Unspecified

STRUCTURAL FORMULA



R = derived from fatty acids of babassu oil
A typical distribution of the fatty acids in babassu oil is C8:0 (4-8%), C10:0 (4-8%), C12:0 (44-47%), C14:0 (15-20%), C16:0 (6-9%), C18:0 (3-5%), C18:1 (10-12%), C18:2 (1-3%) (CIR, 2010).

MOLECULAR WEIGHT
316-426 Da

ANALYTICAL DATA
Reference IR spectrum was provided.

3. COMPOSITION

DEGREE OF PURITY UVCB substance

IDENTIFIED IMPURITIES
(as manufactured, i.e., contained in Mackam BB-30 containing notified chemical at 30%)

Chemical Name	1,3-Propanediamine, N,N-dimethyl- (DMAPA)		
CAS No.	109-55-7	*Weight %*	<0.001%
Hazardous Properties	Xn; R22 C; R34 R43 Conc. ≥25%: C; R34; R22; R43; ≥10% Conc. <25%: C; R34; R43; ≥5% Conc. <10%: Xi; R36/38; R43; ≥1% Conc. <5%: Xi; R43.		
Chemical Name	Acetic acid, 2-hydroxy-		
CAS No.	79-14-1	*Weight %*	<0.5%
Hazardous Properties	C; R34 Xn; R20/22; Xi; R37 Conc. ≥25%: C; R34; R20/22; R37; ≥20% Conc. <25%: Xi; R36/37/38; ≥10% Conc. <20%: Xi; R36/38.		
Chemical Name	Acetic acid, 2-chloro-, sodium salt (1:1)		
CAS No.	3926-62-3	*Weight %*	<0.005%
Hazardous Properties	T; R25 Xi; R38 Conc. ≥25%: T; R25; R38; ≥20% Conc. <25%: Xn; R22; R38; ≥3% Conc. <20%: Xn; R22.		
Chemical Name	Acetic acid, 2,2-dichloro-, sodium salt (1:1)		
CAS No.	2156-56-1	*Weight %*	<0.007%
Chemical Name	Amidopropyl dimethylamines		
CAS No.	Various	*Weight %*	<0.35%
Chemical Name	1,2,3-Propanetriol		
CAS No.	56-81-5	*Weight %*	2.2%
Chemical Name	Sodium chloride		
CAS No.	7647-14-5	*Weight %*	<5.5%

ADDITIVES/ADJUVANTS None

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 ºC AND 101.3 kPa: pale yellow liquid*

Property	Value	Data Source/Justification
Boiling Point*	100 ºC	MSDS
Density*	1046 kg/m^3	MSDS
Vapour Pressure	6.63 x 10^{-3} kPa at 25 ºC	Estimated – modified grain method (US EPA, 2009) for the 12:0 derivative
Water Solubility	10 - 50 g/L at 20 °C	Analogue chemical (IUCLID, 2000)**. Based on structural features, the notified chemical is expected to be dispersible in water.
Hydrolysis as a Function of pH	Not determined	The notified chemical contains functional groups that are expected to hydrolyse slowly in the environmental pH range (4-9) at ambient temperature
Partition Coefficient (n-octanol/water)	Not determined	Expected to partition to the interface between octanol and water based on its surfactant properties
Adsorption/Desorption	Not determined	Expected to adsorb to sludge and sediment based on its surfactant properties
Dissociation Constant	Not determined	Expected to be ionised in the environment
Flash Point	Not determined	Manufactured as an aqueous solution
Flammability	Not determined	Manufactured as an aqueous solution
Autoignition Temperature	Not determined	Manufactured as an aqueous solution
Explosive Properties	Not determined	Contains no functional groups that imply explosive properties
Oxidising Properties	Not determined	Contains no functional groups that imply oxidative properties

*Aqueous solution containing the notified polymer at 30% concentration.
**See Section 6.2 for a discussion of the analogue chemical.

DISCUSSION OF PROPERTIES
Reactivity
The notified chemical is expected to be stable under normal conditions.

Dangerous Goods classification
Based on the submitted physical-chemical data in the above table the notified chemical is not classified according to the Australian Dangerous Goods Code (NTC, 2007). However, the data above do not address all Dangerous Goods endpoints. Therefore, consideration of all endpoints should be undertaken before a final decision on the Dangerous Goods classification is made by the introducer of the chemical.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be imported in finished cosmetic products at up to 6% 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 by wharf

IDENTITY OF RECIPIENTS

Estee Lauder Pty Ltd

TRANSPORTATION AND PACKAGING
The products containing the notified chemical (at up to 6% concentration) will be imported in containers suitable for retail sale (e.g. 250 mL). These will be packaged in cardboard cartons. The cartons will be distributed within Australia by road.

USE
The notified chemical will be used as a component of rinse-off (at up to 6%) and leave-on cosmetic products (at up to 2% concentration).

OPERATION DESCRIPTION
The notified chemical will be imported as a component of finished cosmetic products. Reformulation will not take place in Australia.

The finished products containing the notified chemical will be used by consumers and professionals (such as workers in beauty salons). Application of products could be by hand or through the use of an applicator.

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 storage	4	12
Store persons	4	12
Salon workers	unspecified	unspecified

EXPOSURE DETAILS
Transportation and storage workers may only be exposed to the notified chemical as a component of end-use products (at up to 6% concentration) in the unlikely event of an accident.

Exposure to the notified chemical in end-use products may occur in professions where the services provided involve the application of cosmetic and personal care products to clients (e.g. workers in beauty salons). Such professionals may use some personal protective equipment (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 (at up to 6% concentration) through the use of the rinse-off and leave-on cosmetic products. The principal route of exposure will be dermal, although ocular and inhalation exposure is also possible.

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified chemical are summarised in the table below. Details of this study can be found in Appendix A.

Endpoint	*Result and Assessment Conclusion*
Human, skin sensitisation (RIPT) (0.6%)	No evidence of sensitisation

Much of the discussion below regarding the health effects of the notified chemical, is based on information that was provided for a structurally similar analogue of the notified chemical, cocamidopropyl betaine (CAPB; CAS No. 61789-40-0; CIR, 2010). CAPB is considered to be a suitable analogue for the notified chemical, as the only difference between the chemicals is the oil source from which the fatty acids are derived (i.e. coconut oil for CAPB, and babassu oil for the notified chemical). As shown in the table below, the fatty acid compositions

of these chemicals are very similar, with both chemicals predominantly composed of C12 fatty acids.

Fatty acid	*Analogue chemical (CAPB) (%)*	*Notified chemical (%)*
C6:0	0.008-1.2	0
C8:0	3.4-15	4-8
C10:0	3.2-15	4-8
C12:0	41-51.3	44-47
C14:0	13-23	15-20
C16:0	4.2-18	6-9
C18:0	1.6-4.7	3-5
C18:1	3.4-12	10-12
C18:2	0.9-3.7	1-3
C20:0	1.03	0

Toxicokinetics, metabolism and distribution.
Absorption of the notified chemical across dermal and gastrointestinal membranes is possible based on the relatively low molecular weight of the notified chemical (<500 Da) and given that it is a surfactant (EC, 2003).

Acute toxicity.
Acute oral toxicity studies in rats and mice indicated that the LD50 values of the analogue chemical (at 30-35.61% concentration) ranged from >1800 mg/kg bw (male rats) up to >5000 mg/kg bw, with mortalities noted in most studies (CIR, 2010). Of note is an acute oral toxicity study conducted in Sprague-Dawley rats (5/sex) at a single dose of 1800 mg/kg bw (formulation containing 35.61% analogue chemical), where no males but all five females died (ACC, 2001; CIR, 2010). Overall, the data suggests that mortality occurs following oral administration of the analogue chemical and that it may be an acute oral toxicant. Therefore, based on these data the notified chemical may be harmful if swallowed.

An acute dermal toxicity study in rats was conducted using 2000 mg/kg bw of a 31% formulation of the analogue chemical (CIR, 2010). Irritation was observed, but there were no clinical signs of systemic toxicity or mortalities. The lack of effects in this study suggests that the notified chemical is likely to be of low acute dermal toxicity.

Irritation.
The notified chemical has a quaternary ammonium functional group, which is a structural alert for corrosion (Hulzebos *et al*., 2005 and Tsakovska *et al.*, 2007).

Numerous skin irritation studies, conducted with formulations containing 7.5-30% analogue chemical, indicated that the analogue has irritant properties. The studies were, in-general, conducted under occlusive conditions, with exposure times of up to 24 hours (7.5-10%) (CIR, 2010). Based on the information available, the notified chemical is likely to be a skin irritant.

Eye irritation studies with the analogue chemical showed that corrosive and necrotic effects occurred at 30% whereas less severe effects were observed at lower concentrations of 2.3-10% (CIR, 2010). The notifier has classified the notified chemical with the risk phrase R36: Irritating to eyes, however, based on studies conducted on the analogue, the notified chemical may be a severe eye irritant.

Sensitisation.
The notified chemical has a quaternary ammonium functional group, which is a structural alert for sensitisation (Barratt *et al*., 1994).

Conflicting results have been obtained with the analogue chemical in animal studies. Positive results were reported in an LLNA study (an EC_3 value was not reported) (CIR, 2010). In addition, positive results were obtained in two guinea pig maximisation studies conducted by a single laboratory, the first at 3% induction and 3% challenge, and the second at 0.15% induction and 0.015% challenge (CIR, 2010). However, there was no sensitisation in a guinea pig maximisation test when the analogue chemical was tested at 6% induction and 1% challenge (CIR, 2010). In addition, no sensitisation was observed in another test in guinea pigs at 0.75% induction and 0.02% challenge.

No evidence of sensitisation was reported in a HRIPT on a formulation containing the notified chemical at 0.6% concentration (a 10% dilution of a ~6% formulation) with 110 volunteers. In HRIPT studies on

formulations containing the analogue chemical, no evidence of sensitisation was reported at concentrations of 1.87% (88 subjects), 0.93% (93 subjects), 0.3% (100 subjects), 1.5-3.0% (141 subjects), 6.0% (210 subjects), 0.018% (27 subjects) (CIR, 2010). However, positive results were observed in provocative studies conducted on formulations containing the analogue chemical (at 0.3-1% concentration), conducted in subjects diagnosed with various forms of contact dermatitis, suggesting that the analogue may cause reactions in sensitive individuals (CIR, 2010).

The CIR study authors note that sensitisation effects of the analogue chemical (and related compounds) are most likely due to the impurities, including DMAPA and amidopropyl dimethylamines, however, they do not exclude the possibility of the analogue causing the sensitisation. The potential for skin sensitisation, due to the presence of the above impurities in the notified chemical, will be limited by their reported low concentration (<10 ppm DMAPA and <0.35% amidopropyl dimethylamines).

In summary, a definitive conclusion cannot be made on the skin sensitisation potential of the notified chemical. The available information suggests that skin sensitisation is possible. Although there are some inconsistencies in the results reported for studies conducted on the analogue chemical, the scientific data points towards the positive findings being caused by impurities, in particular DMAPA and amidopropyl dimethylamines, which are present in the notified chemical at low concentrations.

Repeated Dose Toxicity.
There are no repeat dose toxicity data on the notified chemical. In a 28-day repeated dose oral toxicity study, rats were administered a 30.6% solution of the analogue chemical at 0, 100, 500 or 1000 mg/kg bw/day. Inflammation of the non-glandular stomach was noted in animals of the high-dose group, although this effect was attributed to the irritant properties of the test material. Mortality was also observed in this study at all treatment levels but there was no dose-response relationship (CIR, 2010).

In another 28-day repeated dose oral toxicity study, rats were administered a solution containing the analogue chemical (concentration not stated) at 0, 250, 500 or 1000 mg/kg bw/day. The NOEL was reported as 500 mg/kg bw/day, which appears to be based on non-systemic irritant effects on the non-glandular stomach. No mortalities were observed (CIR, 2010).

In a 90-day repeated dose oral toxicity study, rats were administered a solution containing the analogue chemical (concentration not stated) at 0, 250, 500 or 1000 mg/kg bw/day. There were no mortalities and the noted effects are isolated to the stomach region and appear to be irritant in nature. The NOEL established by the study authors was 250 mg/kg bw/day, based on these effects (CIR, 2010).

Mutagenicity.
The analogue chemical was not mutagenic in numerous bacterial reverse mutation assays. Negative results were also obtained for the analogue chemical in a mouse lymphoma test and a micronucleus test in mice (CIR, 2010).

Carcinogenicity.
No signs of carcinogenicity were noted in a 20 month dermal study in mice (3 applications/week) for a hair dye formulation containing the analogue chemical at a concentration of 0.09% (CIR, 2010).

The formation of nitrosamines is possible. Secondary amides (and the identified impurities) may serve as substrates for N-nitrosation, therefore formulation with N-nitrosating agents should be avoided (CIR, 2010).

Health hazard classification
As toxicity data were not provided, the notified chemical cannot be classified according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004). However, based on the information available, the notified chemical should be considered as though it is classified with at least the following risk phrase:

R36 Irritating to eyes

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety
Workers involved in professions where the services provided involve the application of cosmetic products to clients (e.g. hairdressers and beauty salon workers) may be exposed to the notified chemical (at up to 6% concentration). The risk to these workers is expected to be of a similar or lesser extent than that experienced

by consumers using products containing the notified chemical (for details of the public health risk assessment, see Section 6.3.2.).

Based on the information available, the risk to workers associated with use of the notified chemical at up to 6% concentration in rinse-off cosmetic products and 2% concentration in leave-on products, is not considered to be unreasonable.

6.3.2. Public Health

The general public will be repeatedly exposed to the notified chemical (at up to 6% concentration) through the use of rinse-off and leave-on cosmetic products.

Local effects.

At the proposed use concentration, skin irritancy effects are not expected. However, the potential for eye irritancy is of concern, particularly with rinse-off products (up to 6% notified chemical). As the notified chemical cannot be used in cosmetic products for the eyes, ocular exposure is only expected to occur in the unlikely event of an accident. In addition, due to the reduced contact time likely associated with rinse-off products and the likely dilution of products with water at the time of eye contact, the extent of irritation should be reduced. The potential for eye irritation may be further minimised by the inclusion of appropriate labelling and directions for use to warn against eye contact. Therefore, the risk to the public from possible slight eye irritancy of products containing the notified chemical at up to 6% is not considered to be unreasonable.

Based on the information available, there is concern for potential skin sensitisation following contact with the notified chemical. However, given that available scientific information indicates that the observed sensitisation effects of similar chemicals are likely due to the presence of impurities, and the concentration of these impurities in the notified chemical is very low, sensitisation is not expected from use of the notified chemical at the proposed usage concentrations of up to 6%.

Systemic toxicity.

The repeated dose toxicity effects of the notified chemical have not been determined. However, based on studies conducted on an analogue chemical, systemic toxicity is not expected.

Based on the information available, the risk to the public associated with use of the notified chemical at up to 6% concentration in rinse-off cosmetic products and up to 2% concentration in leave-on products, is not considered to be unreasonable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE

The notified chemical will be manufactured overseas and imported in finished cosmetic hair and skin products. Release of the notified chemical to the environment is unlikely except in the event of a transport accident or an accidental spill during handling. Accidental spills of formulated products containing the notified chemical are expected to be physically contained and then absorbed into absorbent powder if necessary. The chemical will be collected into sealed containers and finally disposed of to landfill.

RELEASE OF CHEMICAL FROM USE

As the notified chemical will be used in rinse-off and leave-on cosmetic products, it is expected that effectively the entire annual import volume will be released to sewer through consumer use. A small proportion may remain as residues within the end-use containers.

RELEASE OF CHEMICAL FROM DISPOSAL

Expired wastes and residue of the notified chemical in the empty containers are likely either to share the fate of the container and be disposed of to landfill, or to be washed to sewer when containers are rinsed before recycling.

7.1.2. Environmental Fate

The notified chemical is expected to be readily biodegradable based on a ready biodegradability study submitted for an acceptable analogue. The majority of the notified chemical is expected to be released to the sewerage system. In waste water treatment processes in sewage treatment plants (STPs), a high proportion of the notified chemical is expected to be removed from influent due to its expected sorption to sludge and sediment and rapid biodegradation. The notified chemical that partitions to sludge will be removed for disposal to landfill or used on land for soil remediation. In soil, the notified chemical is expected to be degraded by abiotic and biotic processes to form water and oxides of carbon and nitrogen.

If released to surface waters in treated effluent, the notified chemical is expected to partition to suspended solids and organic matter and is anticipated to rapidly biodegrade. Based on its surface activity, the notified chemical is not expected to bioaccumulate.

For the details of the environmental fate study please refer to Appendix B.

7.1.3. Predicted Environmental Concentration (PEC)

A worst case PEC for discharge of the notified chemical to surface waters has been calculated assuming that all of the imported quantity of the chemical is discharged to sewers nationwide and that no removal occurs in sewage treatment plants. The details of the calculation are as follows:

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)	22.613	million
Removal within STP	0%	
Daily effluent production:	4,232	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.61	µg□L
PEC - Ocean:	0.061	µg/L

The notified chemical is readily biodegradable and is expected to adsorb to sludge, thus, its removal from sewage treatment plants (STPs) is expected. However, for the worst case scenario, it is assumed that the notified chemical is not removed from influent and is released with STP effluent. 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 0.606 µg/L may potentially result in a soil concentration of approximately 4.039 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 20.19 µg/kg and 40.39 µg/kg, respectively. However, given the expected degradation and sorptive qualities of the notified chemical, these values should be considered as theoretical maximum concentrations only.

7.2. Environmental Effects Assessment

Ecotoxicity results were provided for an acceptable analogue of the notified chemical in a reliable, internationally peer reviewed data set (IUCLID, 2000). The endpoints are summarised in the table below.

Endpoint; Guideline	*Species*	*Result*	*Assessment Conclusion*
Acute			
Fish Toxicity (96 h); Directive 84/44/9/EEC C.2	*Brachydanio rerio*	LC50 = 1 – 10 mg/L	Toxic
Daphnia Toxicity (48 h); OECD TG 202	*Daphnia magna*	EC50 = 6.5 mg/L	Toxic

Algal Toxicity (96 h); OECD TG 201	*Scenedesmus subspicatus*	E_rC50 = 0.55 mg/L	Very Toxic
Chronic			
Daphnia Toxicity (21 days); OECD TG 202	*Daphnia magna*	NOEC = 0.9 mg/L	Harmful with long lasting effects
Algal Toxicity (96 h); OECD TG 201	*Scenedesmus subspicatus*	E_rC0 = 0.09 mg/L	Toxic with long lasting effects
Bacterial Toxicity (30 min); OECD TG 209	*Pseudomonas putida*	EC0 > 3,000 mg/L	Not Harmful

Under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS; United Nations, 2009) the notified chemical is classified as acutely toxic to fish and aquatic invertebrates and very toxic to algae. Based on the acute toxicity to algae the notified chemical is formally classified under the GHS as "Acute category 1; Very toxic to aquatic life". Based on the chronic toxicity to algae and expected rapid biodegradability, the notified chemical is formally classified as "Chronic category 2; Toxic to aquatic life with long lasting effects".

7.2.1. Predicted No-Effect Concentration

The endpoint from the most sensitive species from the results of the ecotoxicological studies summarised above was used to calculate the Predicted No-Effect Concentration (PNEC). An assessment factor of 50 was used as chronic toxicity endpoints are available for the effects of an acceptable analogue of the notified chemical on aquatic species from two trophic levels.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
96 h E_rC0 (alga)	0.09	mg/L
Assessment Factor	50	
PNEC:	1.8	µg/L

7.3. Environmental Risk Assessment

Risk Assessment	PEC µg/L	PNEC µg/L	Q
Q - River	0.61	1.8	0.339
Q - Ocean	0.061	1.8	0.034

The risk quotient (Q = PEC/PNEC) for aquatic exposure is calculated to be <1 based on the above calculated PEC and PNEC values. The calculated risk quotient is an upper limit since it is likely that a substantial amount of notified chemical will rapidly biodegrade in the environment. Moreover, the notified chemical is not expected to bioaccumulate nor be persistent in the environment. The Q value of <1 indicates the notified chemical is not expected to pose an unreasonable risk to the aquatic environment based on the assessed use pattern.

APPENDIX A: TOXICOLOGICAL INVESTIGATIONS

A.1. Skin sensitisation – human volunteers

TEST SUBSTANCE	Notified chemical (6% concentration in shampoo formulation)
METHOD	Human repeat insult patch test (HRIPT)
Study Design	Induction Procedure: Nine 24 hour applications of a 0.150 mL 10% aqueous dilution of the test material infused in a 2×2 cm semi occluded patch. Patches were applied on Mondays, Wednesdays and Fridays each week to the same site. Patches were removed by technicians, with the exception of patches applied on Fridays, which were removed by the participants. Rest Period: 9 days. Challenge Procedure: The test material was applied as per the induction phase to the original site and a separate naïve site. The subjects were examined for skin reactions at 24 and 48 hours after test material administration.
Study Group	75 females (20-76 years) and 35 males (18-69 years).
Vehicle	Test material administered as a 10% aqueous dilution (equivalent to test concentration of 0.6%)
Remarks - Method	Six subjects dropped out of the study with no reasons reported (prior to challenge). In a follow-up phase, the subjects were given the opportunity to report any dermal signs for two weeks following completion of the study.
RESULTS	
Remarks - Results	No adverse skin reactions were noted in the subjects at induction or challenge, or during the follow up phase.
CONCLUSION	The test substance was non-sensitising under the conditions of the test.
TEST FACILITY	Product Investigations (2003)

APPENDIX B: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

B.1. Environmental Fate

B.1.1. Ready biodegradability

TEST SUBSTANCE	Analogue of the notified chemical (26 – 30% w/w)
METHOD	OECD 310 Ready Biodegradability – CO_2 in sealed vessels (Headspace test)
Inoculum	Activated sludge from a domestic wastewater treatment plant
Exposure Period	28 days
Auxiliary Solvent	None reported
Analytical Monitoring	CO_2 analysis
Remarks - Method	No significant protocol deviations were reported. The test substance was tested at 20 mg/L organic carbon and 22 ± 2 °C. A reference substance (sodium benzoate, 20 mg C/L) and inhibition control (test substance and reference substance at the same concentrations as inoculated test medium) were run in parallel.

RESULTS

Test substance		*Sodium Benzoate*	
Day	*% Degradation*	*Day*	*% Degradation*
4	39.64	4	78.19
7	52.47	7	93.39
14	83.68	14	96.77
28	84.08	28	96.92

Remarks - Results	No significant deviations from test guidelines were reported and all validity criteria were satisfied. The mean cumulative net CO_2 evolved from the inhibition control was 90.77% after 28 days indicating the test substance was not toxic to the inoculum. The reference substance reached the pass level '10 day window' criterion and thus confirmed the suitability of the inoculum and test conditions. The test substance reached the pass level for biodegradation within the 10 day window.
CONCLUSION	The test substance, and by inference the notified chemical, is readily biodegradable
TEST FACILITY	Laboratório de Meio Ambiente (2010)

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