File No: STD/1342

December 2009

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Dodecanoic acid, methyl-2-sulfoethyl ester, sodium salt (1:1)

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 the Environment, Water, Heritage and the Arts.

For the purposes of subsection 78(1) of the Act, this Full Public Report may be inspected at our NICNAS office by appointment only at 334-336 Illawarra Road, Marrickville NSW 2204.

This Full 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

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1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
A.S. Harrison & Co. Pty. Ltd. (ABN 89 000 030 437)
75 Old Pittwater Road
Brookvale, NSW 2100

NOTIFICATION CATEGORY
Standard: Chemical other than polymer (more than 1 tonne 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: acute oral toxicity, acute dermal toxicity, eye irritation, skin irritation, repeat dose toxicity, sensitisation and mutagenicity.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
Canada

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Iselux
Tauranol SLMI-85
Pureact SLMI-85
IAC 107

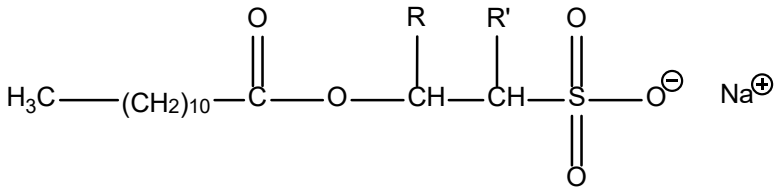
CAS NUMBER
928663-45-0

CHEMICAL NAME
Dodecanoic acid, methyl-2-sulfoethyl ester, sodium salt (1:1)

OTHER NAME(S)
INCI name: Sodium Lauroyl Methyl Isethionate

MOLECULAR FORMULA
$C_{15}H_{30}O_5S \cdot Na$

STRUCTURAL FORMULA



Where R and R' are either H or CH_3 and R is not equal to R'

MOLECULAR WEIGHT
344.44 g.mol^{-1}

ANALYTICAL DATA
Reference IR spectra were provided.

3. COMPOSITION

DEGREE OF PURITY 80-85%

NON HAZARDOUS IMPURITIES/RESIDUAL MONOMERS (>1% by weight)

Chemical Name	Dodecanoic acid		
CAS No.	143-07-7	*Weight %*	≤ 10
Chemical Name	Propanesulfonic acid, 1(or 2)-hydroxy-, sodium salt (1:1)		
CAS No.	869737-84-8	*Weight %*	≤ 10

ADDITIVES/ADJUVANTS None

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20°C AND 101.3 kPa: Waxy solid

Property	Value	Data Source/Justification
Melting Point	154.17°C	Measured
Boiling Point	Not determined	Decomposes at 310°C prior to boiling at both 10 kPa and atmospheric pressure.
Density	1099.6 kg/m^3 at 22°C	Measured
Vapour Pressure	Not determined	Decomposes at 310°C prior to boiling at both 10 kPa and atmospheric pressure.
Water Solubility	> 1000 g/L at 20°C	Measured
Hydrolysis as a Function of pH	Not determined	The notified chemical contains hydrolysable functionality, but hydrolysis is not expected to occur within the environmental pH range of 4-9.
Partition Coefficient (n-octanol/water)	Not determined	Cannot be measured due to the surfactant nature of the notified chemical.
Surface Tension	37.05 mN/m at 20°C	Measured
Adsorption/Desorption	Log K_{OC} < 1.3	Measured
Dissociation Constant	Not determined	The notified chemical is a sodium salt and is expected to be fully dissociated under ambient environmental

		conditions.
Particle Size	Not determined	Waxy solid
Flash Point	228ºC (closed cup)	MSDS
Flammability	Not highly flammable	Measured
Autoignition Temperature	> 400ºC	Measured
Explosive Properties	Not expected to be explosive	Estimated
Oxidising Properties	Not expected to be oxidising	Calculated

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

Reactivity
Decomposes at 310ºC, but expected to be stable under normal conditions of use.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will not be manufactured within Australia. The notified chemical will be imported in 90.7 kg fibre drums.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	50	70	80	90	100

PORT OF ENTRY
Sydney

TRANSPORTATION AND PACKAGING
The notified chemical and products containing it will be distributed by road. The final packaging will vary depending on the product but is expected to be plastic or glass in the 50-500 mL range.

USE
The notified chemical will be used as a component of personal care products. The notified chemical acts as a cleanser due to its surfactant properties and will be used at concentrations up to 50% in wash-off products and concentrations up to 17% in leave-on products.

The products that will contain the notified chemical are shampoos, conditioners, bath gels/foams, liquid soaps, face wash, shave foams/gels and secondary sunscreens.

OPERATION DESCRIPTION
After the notified chemical has been imported it will be sold to personal-care product manufacturers where it will be reformulated to produce a variety of cosmetic products. Details on how the notified chemical is to be used may vary depending on the company doing the reformulation and the type of product being produced.

Reformulation
Reformulation will normally involve dissolving the notified chemical in hot water with other components in a jacketed vessel with agitation, before cooling to room temperature. The finished personal care product will then be transferred from the mixing vessel to a range of container types and sizes, the largest of which is expected to be 500 mL, using an automated filling line.

End use
There is potential for the finished products to be used in occupational settings, for example by beauticians or hairdressers using cosmetic products. Depending on the nature of the cosmetic product these could be applied 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

EXPOSURE DETAILS
The number and category of workers will vary depending on the nature of the customers' business. However, it is anticipated that typical practices by cosmetic manufacturers will include the use of adequate local ventilation, appropriate PPE, enclosed mixing vessel and filling areas as well as a high degree of process automation to protect workers. While the reformulation process will vary with the product and reformulation site, it is expected that at most sites local exhaust ventilation will be used.

Transport and warehouse workers will be exposed to the notified chemical only in the event of a spill due to an accident or leaking drum.
Reformulation
At customer reformulation facilities, exposure to the notified chemical (80-85% purity) or products (≤ 50% notified chemical) is possible during handling of the drums, cleaning and maintenance of the equipment. Skin, and eye contact (due to splashing) are likely to be the main routes of exposure. Inhalation exposure is likely to be negligible due to the expected low vapour pressure of the notified chemical and the use of local exhaust ventilation. Exposure is likely to be minimised by good personal hygiene practices (eg. washing hands after any contact, before breaks and meals, etc) and use of industrial standard PPE.

End use
Exposure of beauticians and hairdressers to the notified chemical at concentrations up to 50% could occur during final application of the cosmetic products to their clients. The main route of exposure is expected to be dermal, although ocular exposure to splashes is possible. PPE is not expected to be worn, however good hygiene practices are expected to be in place.

6.1.2. Public exposure
The general public will be repeatedly exposed to the notified chemical via a number of different consumer products (up to a maximum of 50% in wash off products and 17% in leave on products).

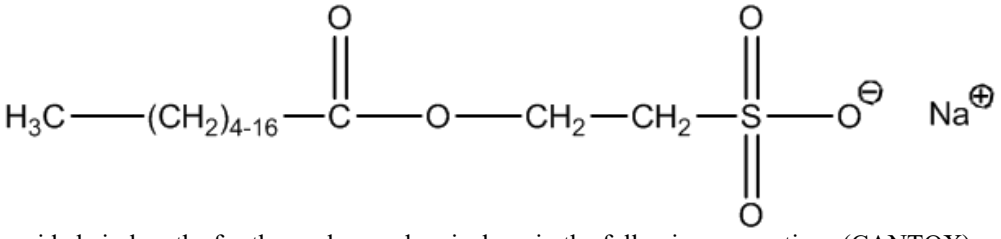
Use of moisturisers with secondary sunscreens is expected to give the highest single exposure because of the relatively large volumes of the products applied, and the "leave-on" nature of these products.

Public exposure from transport, storage and reformulation is considered to be negligible.

6.2. Human health effects assessment

The results from toxicological investigations conducted on the notified chemical and an analogue considered acceptable by NICNAS are summarised in the table below. Details of some of these studies can be found in Appendix B.

The structurally related analogue was the chemical SCI; CAS name: fatty acids, coco, 2-sulfoethyl esters, sodium salts; CAS number: 61789-32-0.



The fatty acid chain lengths for the analogue chemical are in the following proportions (CANTOX).

Chain length	C_6	C_8	C_{10}	C_{12}	C_{14}	C_{16}	C_{18}
% by weight	0-1	5-9	6-10	44-52	13-19	8-12	6-14.5

Endpoint	*Test substance*	*Result and Assessment Conclusion*	*Reference*
Rat, acute oral toxicity	SCI 47.5% concentration	oral LD50 > 5000 mg/kg bw test substance of low toxicity	Hazleton (1986a)
Rat, acute oral toxicity	SCI at 15% concentration	oral LD50 > 5000 mg/kg bw test substance of low toxicity	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Rat, acute oral toxicity	SCI at 20% concentration	oral LD50 6.4-8.0 g/kg bw test substance of low toxicity	IUCLID (2006)
Rabbit, skin irritation	SCI at 1 to 93.7% concentration	slight to moderate irritation	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Human, 14 Day Cumulative Irritation Test	notified chemical (concentration unknown)	moderately irritating under cumulative exposure	Essex (2007)
Rabbit, eye irritation	SCI 47.5% concentration	irritating	Hazleton (1986b)
Rabbit, eye irritation	SCI concentration from 2.5 to 24.5%	irritating	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Guinea pig, skin sensitisation – modified Buehler test.	SCI challenge concentration from 2 to 66%	no evidence of sensitisation	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Rat, repeat dose oral toxicity – 28 days.	SCI concentration from 0.1 to 1.0%	NOAEL > 1 g/kg bw/day	IUCLID (2006)
Rat, repeat dose dermal toxicity – 10 days.	SCI concentration from 10 to 60%	NOAEL > 4.35 g/kg bw/day	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Rat, repeat dose dermal toxicity – 28 days.	SCI concentration from 1 to 36%	NOAEL > 2.07 g/kg bw/day	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Mutagenicity – bacterial reverse mutation	SCI	non mutagenic	IUCLID (2006) J. Am. Coll. Toxicol. (1993)
Genotoxicity – in vitro Chinese hamster ovary cells	SCI	non genotoxic	IUCLID (2006) J. Am. Coll. Toxicol. (1993)

Toxicokinetics, metabolism and distribution.
Based on the low molecular weight (344.44 $g.mol^{-1}$), the high water solubility (> 1000 g/L at 20°C) and the fact that it is an ionisable surfactant the notified chemical may be absorbed across biological membranes. In an *in vitro* study involving the analogue dodecanoic acid, 2-sulfoethyl ester, sodium salt (1:1) (CAS No. 7381-01-3) with human skin, an increasing rate of absorption was seen over time with a maximum rate of 30.1 ± 13.6 $\mu g/cm^2$ observed 48 hours after application (IUCLID, 2006). A further two *in vivo* studies in rats involving the analogue dodecanoic acid, 2-sulfoethyl ester, sodium salt (1:1) (CAS No. 7381-01-3) have been reported; in one of the experiments the level of absorption was measured 24 hours after exposure using ^{14}C isotope labelling which found absorption rates of between 0.1 to 0.3 $\mu g/cm^2$ (IUCLID, 2006). In the second experiment where the rats were exposed for 12 hours the absorption rate was found to plateau after 3 hours at a rate of 0.6 $\mu g/cm^2$ (IUCLID, 2006). Dodecanoic acid, 2-sulfoethyl ester, sodium salt (1:1) (CAS No. 7381-01-3) is a very good analogue of the notified chemical with the only difference in the two chemicals being one methyl group and therefore it is expected that the notified chemical would show similar rates of absorption.

Acute toxicity.
There are no acute toxicity studies available on the notified chemical. The analogue SCI is considered to be of low acute oral toxicity based on tests conducted in rats. Repeat dose dermal toxicity studies with the analogue SCI showed it was also of low acute dermal toxicity.

Irritation and Sensitisation.
Slight to moderate skin irritation was reported in a range of studies conducted with the analogue SCI on rabbits (J. Am. Coll. Toxicol. 1993). Slight skin irritation was reported in a test where the analogue SCI was tested at a

concentration of 1%, this test also involved a 30 min irradiation with the UV light on one of the test sites on the rabbit. No significant difference in irritation effects was noted between the irradiated and non-irradiated sites. There were two skin irritation studies conducted on SCI where the concentration was 5%, both studies used 24 hr applications and one showed slight irritation with the other showing moderate irritation. However, in the study which was found to be moderately irritating the irritation scores with the abraded skin were significantly higher than those seen in the non-abraded skin, with the effects seen in the non-abraded skin indicative of only slight irritation. A 24 hr semi-occluded application of the analogue SCI at a concentration of 15% showed moderate irritation. One further skin irritation study on SCI at a concentration of 93.7% also showed moderate irritation.

The analogue chemical SCI has been tested in a number of eye irritation studies where the concentration was from 2.5 to 47.5% (J. Am. Coll. Toxicol. 1993). The analogue SCI was found to be an eye irritant when applied to the eyes of 6 rabbits at a concentration of 47.5%. The next highest concentration where information is available on the analogue SCI is 24.5%, where corneal opacity was seen in 3/3 animals and conjunctival effects in 2 animals at the 24 hr observation with all symptoms clearing by day 14. In 2 different studies with SCI at a concentration of 15% it was found to be an irritant in one study where 0.1 mL of the test substance was placed in the eye, but only slightly irritating in the other study where a volume of 10 µL was used. At a concentration of 5% SCI was decribed as "minimally irritating" to rinsed eyes and "mildly irritating" to unrinsed eyes. At a concentration of 2.5% SCI was found to be slightly irritating to the eyes.

No evidence of sensitisation was noted in three studies on guinea pigs where the concentration of SCI ranged from 2 to 66%.

Repeated Dose Toxicity
There was no repeated dose toxicity studies provided for the notified chemical. In a 28 day oral toxicity study using rats where SCI was incorporated in the food at concentrations of 0.1%, 0.3% and 1.0% w/w, which for the high dose group corresponded to approximately 1000 mg/kg bw/day, no significant toxicological effects related to treatment with the notified chemical were noted. In a 10 day dermal dose-range-finding study, irritation was seen at 40 and 60% concentrations with milder effects also seen at 20%. No significant adverse systemic effects were noted in the 10 day dermal study. In a 28 day dermal toxicity study in rats the analogue SCI was found to produce no significant treatment related changes at concentrations up to 36%.

Mutagenicity.
There is no available data on the mutagenic potential of the notified chemical. The analogues SCI was found to be negative in 2 bacterial reverse mutation assays, both in the presence and absence of metabolic activation. No statistically significant increases were seen in Chinese hamster ovary cells exposed to SCI.

Observations on Human Exposure.
In a 14 day cumulative irritation test using human volunteers the notified chemical (concentration not known) was found to show cumulative irritation from day 4 onwards.

A 4% aqueous solution of a gel cleanser containing 15% SCI was found to be non-irritating in a 48 hour patch test with 12 subjects (IUCLID 2006 and J. Am. Coll. Toxicol. 1993). In 6 modified soap chamber tests with the analogue SCI at a concentration of 8% it was found to be slightly irritating in 5 of the studies and irritating in the other (IUCLID 2006 and J. Am. Coll. Toxicol. 1993). In the 1 modified soap chamber test where SCI was found to be irritating it was noted that the cold and dry climatic conditions at the time might have aggravated the irritation. A 21 day cumulative irritation test on 35 subjects with SCI at a concentration of 0.1% produced only very slight signs of irritation (IUCLID 2006 and J. Am. Coll. Toxicol. 1993). A repeat application patch test (3 applications of 24 hours each) at concentrations of 0.2, 0.4 and 1.0% conducted with 10 volunteers produced slight irritation (IUCLID 2006 and J. Am. Coll. Toxicol. 1993). However, in a 14 day irritation study of a gel cleanser containing 15% SCI tests at 4 and 6% produced moderate to severe irritation (J. Am. Coll. Toxicol. 1993). The other ingredients in the gel cleanser were not specified and therefore it is not confirmed that SCI or other ingredients produced the irritant effects in this study.

Four human repeated insult patch tests (HRIPT) were conducted with personal washing bars containing 49.87% SCI at concentrations up to 8% (4% SCI) and no evidence of sensitisation was noted (J. Am. Coll. Toxicol. 1993). In another HRIPT 9 separate patches containing a skin cleanser with SCI at 17%, were applied to 96 test subjects over a period of 3 weeks during the induction phase (IUCLID 2006 and J. Am. Coll. Toxicol. 1993). After the challenge application 12 showed very slight signs of irritation and 2 had delayed mild to moderate erythema, which was not present in a follow up test on these 2 subjects. The test substance containing SCI at

17% was not sensitising. One further HRIPT with similar methods to the one mentioned above has been conducted using SCI (IUCLID 2006 and J. Am. Coll. Toxicol. 1993). The test material was applied as a 2% w/v solution using a product that contained 47.5% SCI and was found to have very low to nil potential for irritantion and sensitisation.

Health hazard classification
Based on the skin and eye irritation effects reported for the analogue chemical, the notified chemical is classified as hazardous according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004) with the following risk phrases:
Xi: R38 Irritating to the skin
Xi: R36 Irritating to eyes

6.3. Human health risk characterisation

6.3.1. Occupational health and safety
The greatest potential occupational exposure to the notified chemical is expected to be for hairdressers during the use of products containing the chemical at concentrations up to 50%.

Local effects
Irritation is the primary risk expected from the notified chemical to workers in occupational settings. The notified chemical was classified as a skin and eye irritant. The notifier has indicated that the notified chemical will be used in leave on products (secondary sunscreens) at concentrations of up to 17% and in wash off products (shave gels/foams, shampoo, conditioner etc) at concentrations up to 50%. The risk of skin and eye irritation in hairdressers cannot be ruled out at the proposed use concentrations and due to the repeated exposure experienced by these workers. Good hygiene practices, such as hand washing that may occur following application of the product is expected to reduce the risk of skin irritation by minimising the skin contact time. In addition, appropriate labelling of the product to warn against the possibility of irritation is expected to further lower the risk to hairdressers. In summary, the risk to hairdressers exposed to the notified chemical (up to 50%) is not considered to be unacceptable if appropriate labelling of the products is in place to warn against the possibility of skin and eye irritation.

Workers may be exposed to high concentrations of the notified chemical during reformulation of the imported raw chemical (80-85% purity). However, the use of engineering controls and PPE is expected to minimise the exposure during reformulation. Therefore the risk of significant irritation effects in these workers is not considered to be unacceptable.

Systemic effects
No toxicological data on the systemic effects from repeated exposure to the notified chemical are available. However, based on the data available for the analogue SCI systemic effects from repeated dermal or oral exposure to the notified chemical are not expected. Therefore the risk to workers from repeated exposure to the notified chemical would not be considered unacceptable.

6.3.2. Public health
The general public will be repeatedly exposed to the notified chemical via a number of different consumer products, applied to the skin at concentrations up to 17 % in leave on products and 50% in wash off products.

Local effects
The potential for skin and eye irritation when using the notified chemical is not considered to be unacceptable when used in leave on products at concentrations up to 17%.

Wash off products on the other hand will be used at concentrations up to 50% where the notified chemical is expected to be both a skin and eye irritant based on the results of tests conducted with the analogue SCI. However, the wash off nature of the products is expected to reduce the contact time with the eyes and skin and thus the potential for irritation. The risk of irritation may be minimised by the inclusion of appropriate labelling and directions for use to warn against the possibility of skin and eye irritation. When used in the proposed manner with appropriate safety information on the packaging, the risk to the public associated with eye and skin contact with the notified chemical at concentrations up to 50% in wash off products is not considered to be unacceptable.

Systemic effects
Based on the data available for the analogue SCI, systemic effects resulting from repeated dermal or oral exposure to the notified chemical are not expected and therefore, the risk to the public from repeated exposure to the notified chemical would not be considered unacceptable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1 Environmental Exposure

RELEASE OF CHEMICAL AT SITE
Release to the environment may occur in the unlikely event of an accident during transport or an accidental spill during handling. The notified chemical will be transported to Australia by ship in solid form in fibre drums. The notified chemical will be blended with other ingredients and packaged into plastic or glass consumer bottles (typically 50-500 mL). Spills of raw notified chemical are expected to be swept up, and if possible returned to the mixing vat. Contaminated raw notified chemical is expected to be disposed of to landfill. Release (<1%) from cleaning and maintenance operations of the blending and bottling equipment may occur, with rinsings being expected to be disposed of to sewer.

RELEASE OF CHEMICAL FROM USE
As the notified chemical is used in personal care products such as shampoos, facial cleansers and shower gels it is expected that effectively the entire annual volume will be released to sewer through consumer use. A small proportion (estimated to be ≤2%) may remain as residual within the end-use containers.

RELEASE OF CHEMICAL FROM DISPOSAL
It is expected that end use containers will be disposed of as domestic garbage and end up in landfill sites.

7.1.2 Environmental fate

A single ready biodegradability test report was submitted for an acceptable analogue of the notified chemical. The test report indicates that the acceptable analogue is readily biodegradable. Based on the result for the analogue, and considering the structure of the notified chemical, it is considered that the notified chemical is also readily biodegradable. For the details of the environmental fate study please refer to Appendix C.

The notified chemical is a biodegradable anionic surfactant and is therefore not expected to bioaccumulate.

7.1.3 Predicted Environmental Concentration (PEC)

Since most of the notified chemical will be washed into the sewer, under a worst case scenario, with no removal of the notified cheical in the sewage treatment plant, the resultant Predicted Environmental Concentration (PEC) in sewage inffluent on a nationwide basis is estimated as follows:

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	100,000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	100,000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release:	273.97	kg/day
Water use	200.0	L/person/day
Population of Australia (Millions)	21.161	million
Removal within STP	0%	
Daily effluent production:	4,232	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	64.74	µg/L
PEC - Ocean:	6.47	µg/L

7.2. Environmental effects assessment

No ecotoxicity data were submitted for the notified chemical. Three ecotoxicity studies were submitted for an acceptable analogue, as shown below. Details of these studies can be found in Appendix C.

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity (Acute - 96 h)	LC50 29.3 mg/L	Harmful to fish
Daphnia Toxicity (Acute – 48 h)	EC50 257.86 mg/L	Not harmful to aquatic invertebrates
Algal Toxicity (Acute – 96 h)	IC50 >1000 mg/L	Not harmful to algae

7.2.1 Predicted No-Effect Concentration

Based on the most sensitive endpoint for the analogue, the following PNEC has been derived using an assessment factor of 100.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
LC50 (Fish).	29.30	mg/L
Assessment Factor	100	
PNEC:	293.00	µg/L

7.3. Environmental risk assessment

Based on the PEC and PNEC, the Q values (Risk Quotient = PEC/PNEC) has been calculated as follows for river and ocean receiving environments.

Risk Assessment	***PEC µg/L***	***PNEC µg/L***	***Q***
Q - River:	64.74	293	0.221
Q - Ocean:	6.47	293	0.022

Based on the above Q values, the notified chemical is not considered to pose an unacceptable risk to aquatic ecosystems under a worst case scenario and with the proposed use pattern and volume. The risk to the environment is expected to be lower in reality due to the combined mitigating effects of biodegradation and removal within STPs.

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 64.735 µg/L may potentially result in a soil concentration of approximately 4.316×10^{-1} mg/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 2.158 mg/kg and 4.316 mg/kg, respectively.

8. CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
Based on the available data for the analogue chemical, the notified chemical is classified as hazardous according to the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)] with the following risk phrases:

- Xi: R38 Irritating to the skin
- Xi: R36 Irritating to eyes

and

As a comparison only, the classification of the notified chemical using the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS) (United Nations 2003) is presented below. This system is not mandated in Australia and carries no legal status but is presented for information purposes.

	Hazard category	***Hazard statement***
Skin irritation	Category 2	Causes skin irritation
Eye irritation	Category 2A	Causes serious eye irritation
Environment	Acute Category 3	Harmful to aquatic life

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

When used in the proposed manner with appropriate safety information on the packaging, the notified chemical is not considered to pose an unacceptable risk to public health.

Environmental risk assessment
On the basis of the PEC/PNEC ratio and the reported use pattern, the notified chemical is not expected to pose a risk to the environment.

Recommendations

REGULATORY CONTROLS
Hazard Classification and Labelling

- Safe Work Australia should consider the following health hazard classification for the notified chemical:
  - Xi: R38 Irritating to the skin
  - Xi: R36 Irritating to eyes

- Use the following risk phrases for products/mixtures containing the notified chemical:
  - Conc ≥ 20%: R36; R38

Material Safety Data Sheet

- The MSDS provided by the notifier should be amended as follows:
  - Include the risk phrase R36 Irritating to eyes for products containing ≥ 20% of the notified chemical
  - Include the risk phrase R38 Irritating to the skin for products containing ≥ 20% of the notified chemical
  - Include appropriate safety phrases.

CONTROL MEASURES
Occupational Health and Safety

- Employers should implement the following engineering controls to minimise occupational exposure to the notified chemical during reformulation:
  - Automated processes
  - Local exhaust ventilation

- Employers should implement the following safe work practices to minimise occupational exposure during reformulation of the notified chemical:
  - Avoid contact with skin and eyes

- Employers in hair salons should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical as introduced:
  - Good hygiene practices should be maintained
  - Avoid eye contact

- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical during reformulation:
  - impervious gloves
  - safety glasses
  - protective clothing

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

- 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.

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 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(2) of the Act; if
  - the function or use of the chemical has changed from a component of personal care products at concentrations up to 50% for wash-off products and concentrations up to 17% for leave-on products, or is likely to change significantly;

- the amount of chemical being introduced has increased from 100 tonnes, 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.

No additional secondary notification conditions are stipulated.

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

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point 154.17ºC

Method	Not specified
Remarks	The melting point was determined using a Fisher-Johns melting point apparatus with a 0-160ºC thermometer.
Test Facility	Innospec (2008a)

Boiling Point Not determined

Method	Not specified
Remarks	Decomposes at 310ºC prior to boiling at both 10 kPa and atmospheric pressure. The test sample was analysed by DSC using a TA Instruments DSC 2010 instrument and a pinhole crucible with a nitrogen purge.
Test Facility	Innospec (2009a)

Density 1099.6 kg/m^3 at 22ºC

Method	OECD TG 109 Density of Liquids and Solids.
Remarks	The density was determined using the hydrostatic balance method.
Test Facility	Innospec (2007a)

Vapour Pressure Not determined

Method	Not specified
Remarks	Decomposes at 310ºC prior to boiling at both 10 kPa and atmospheric pressure. The test sample was analysed by DSC using a TA Instruments DSC 2010 instrument and a pinhole crucible with a nitrogen purge.
Test Facility	Innospec (2009a)

Water Solubility >1000 g/L at 20ºC

Method	OECD TG 105 Water Solubility.
Remarks	Flask Method. Approximately 7.5 g of purified notified chemical was added to 3 mL of water. Following heating, cooling and agitation, a homogenous semi-transparent viscous liquid was produced (pH ~5.5).
Test Facility	Innospec (2007b)

Hydrolysis as a Function of pH

Remarks	The notified chemical contains hydrolysable functionality, but hydrolysis is not expected to occur within the environmental pH range of 4-9.

Partition Coefficient (n-octanol/water) Not determined

Remarks	Cannot be measured due to the surfactant nature of the notified chemical.
Test Facility	Innospec (2008d)

Surface Tension 37.05 mN/m at 20ºC

Method	Not specified
Remarks	Concentration: 0.9604 g/L The test sample was analysed using a CSC-DeNouy interfacial tensiometer.
Test Facility	Innospec (2008b)

Adsorption/Desorption – screening test

log K_{oc} <1.3 at 25°C

Method OECD TG 121 Adsorption - Desorption Using HPLC.
Remarks An upper limit for the soil adsorption constant of the notified chemical was derived based on its more rapid elution from a standard HPLC column that the reference compound, acetamide (Log K_{OC} = 1.3).
Test Facility Huntingdon Life Sciences (2009)

Dissociation Constant Not determined

Remarks The notified chemical is a sodium salt and is expected to be fully dissociated under ambient environmental conditions.

Flammability Not highly flammable

Method EC Directive 92/69/EEC A.10 Flammability (Solids).
Remarks No significant protocol deviations. GLP compliant.
Test Facility Chilworth (2008)

Autoignition Temperature > 400°C

Method EC Directive 92/69/EEC A.16 Relative Self-Ignition Temperature for Solids.
Remarks No significant protocol deviations. GLP compliant.
Test Facility Chilworth (2008)

Explosive Properties Not expected to be explosive

Method EC Directive 92/69/EEC A.14 Explosive Properties.
Remarks No significant protocol deviations. GLP compliant.
Test Facility Chilworth (2008)

Oxidizing Properties Not expected to be oxidising

Method EC Directive 92/69/EEC A.17 Oxidizing Properties (Solids).
Remarks No significant protocol deviations. GLP compliant.
Test Facility Chilworth (2008)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE: SCI (47.5% concentration in a syndet bar)

METHOD: Not specified
Generally equivalent to OECD TG 401 Acute Oral Toxicity.
Species/Strain: Rat/Sprague-Dawley
Vehicle: Distilled water
Remarks - Method: The rats were dosed by gavage.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
I	5 per sex	5000	0/10

LD50: > 5000 mg/kg bw
Signs of Toxicity: Symptoms consisted of diarrhoea, red-stained face, possible respiratory congestion, excessive salivation, hypoactivity and a yellow-stained genital area. All symptoms had cleared within 48 hours.
Effects in Organs: The rat's organs were not examined.
Remarks - Results: Body weight gains were as expected.

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

TEST FACILITY: Hazleton (1986a)

B.2. 14-Day Cumulative Skin irritation – human volunteers

TEST SUBSTANCE: Notified chemical (concentration unknown)

METHOD: No approved test method
Study Design: 14 different test substances were measured including the notified chemical, distilled water (negative control) and sodium lauryl sulphate (positive control at 0.5%). Approximately 0.1-0.15 g of the test substances were applied to an occlusive patch that measured 2 by 2 cm. The patches were placed on the back of the test subjects and changed once per day for 14 consecutive days apart from Sundays. If a score of 3 or 4 occurred with any test article then further patch testing at the test site was terminated and the attained score was assigned to that site for the subsequent scheduled test days.
Study Group: 22 Human test subjects (1 male, 21 female) were used with ages ranging from 28 to 70 years. Two subjects (1 per sex) did not complete the test for reasons unrelated to the study.
Vehicle: Unknown
Remarks - Method: The irritation reactions were marked using a 6 point scale as follows:
0 = no reaction
0.5 = barely perceptible (minimal, faint, uniform or spotty erythema)
1 = mild (pink, uniform erythema covering most of the contact site)
2 = moderate (pink-red erythema visibly uniform in entire contact site)
3 = marked (bright red erythema with/without petechiae or papules)
4 = severe (deep red erythema with/without visculation or weeping)

RESULTS

Days	1	2	3	4	5	6	7	8	9	10	11	12	13	14	total
Score†	0.5	4	6	18.5*	18.5	29	32	34	32.5	39	45*	45	48	48	400

† Combined score for the notified chemical for all 20 subjects for that day.
* Scores were not recorded on Sundays so the following days score was assigned.

Remarks - Results

15 Out of 20 test subjects treated with the notified chemical were assigned a score of 3.
The combined total for all 20 subjects over the 14 days for the positive control was 673.5 and for the negative control was 117.5.

CONCLUSION

A 14-day cumulative irritation test was conducted using the notified chemical (concentration unknown) under occlusive dressing. The notified chemical was irritating under the conditions of the test.

TEST FACILITY

Essex (2007)

B.3. Irritation – eye

TEST SUBSTANCE

SCI (47.5% concentration in a syndet bar)

METHOD

Not specified

Species/Strain: Rabbit/New Zealand White
Number of Animals: 6
Observation Period: 7 days
Remarks - Method: Sodium fluorescein was used to aid in the assessment of the eyes.
Scoring was based on the Draize scale.
The test method differed from OECD TG 405 Acute Eye Irritation/Corrosion in that observations were not continued beyond 7 days despite ocular lesions being present.

RESULTS

Lesion	*Mean Score**	*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
Conjunctiva: redness	2.3	3	> 7 days	3
Conjunctiva: chemosis	2.7	4	> 7 days	3
Conjunctiva: discharge	1.6	3	> 7 days	2
Corneal opacity	1.1	2	> 7 days	2
Iridial inflammation	0.8	1	> 7 days	1

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

Remarks - Results

Despite there still being effects present at the end of 7 days no further observations were recorded. It is therefore not possible to tell if all ocular lesions would be resolved within a 21 day period but all of the symptoms had reduced from the maximum values and in 2 animals no symptoms were present at day 7.

CONCLUSION

The notified chemical is irritating to the eye.

TEST FACILITY

Hazleton (1986b)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready biodegradability

TEST SUBSTANCE	Acceptable Analogue
METHOD	OECD TG 301 B Ready Biodegradability: CO_2 Evolution Test.
Inoculum	Activated Sewage Sludge
Exposure Period	28 d
Auxiliary Solvent	None reported
Analytical Monitoring	None
Remarks - Method	Characterisation and stability information for the test substance was not provided and mixture analysis was not performed.

RESULTS

Test substance		*Aniline*	
Day	*% Degradation*	*Day*	*% Degradation*
2	15.22	2	-0.15
4	35.62	4	6.74
6	48.19	6	30.91
8	57.08	8	48.24
12	69.34	12	67.93
19	81.44	19	77.22
26	88.75	26	81.32
28	90.40	28	82.50

Remarks - Results	The test substance met the 10-day window criterion. All other test validity criteria were satisfied.
CONCLUSION	The notified chemical is classified as being ready biodegradable.
TEST FACILITY	Stillmeadow Inc (2007a)

C.2. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE	Acceptable Analogue
METHOD	OPPTS 850.1075 Acute Toxicity Test – Static.
Species	Fathead Minnow (*Pimephales promelas*)
Exposure Period	96 h
Auxiliary Solvent	None reported
Water Hardness	Not reported
Analytical Monitoring	None
Remarks – Method	Characterisation and stability information was not provided and mixture analysis was not performed.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*6 h*	*24 h*	*48 h*	*72 h*	*96 h*
0	-	30	0	0	0	0	0
0.1	-	30	0	0	0	0	0
1.0	-	30	0	0	0	0	0
10	-	30	1	1	1	1	1
100	-	30	30	30	30	30	30
1000	-	30	30	30	30	30	30

LC50	29.3 mg/L at 96 hours (95% C.I. 25.2 – 34.1 mg/L)
NOEC	10 mg/L at 96 hours
Remarks – Results	Physical abnormalities were noted only in the 100 and 1000 mg/L concentrations. The digestive contents were expelled through the anus and the eyes were ruptured. All test validity criteria were satisfied.

CONCLUSION The notified chemical is harmful to fish.

TEST FACILITY Stillmeadow Inc (2005a)

C.2.2. Acute toxicity to aquatic invertebrates

TEST SUBSTANCE Acceptable Analogue

METHOD OPPTS 850.1010 48-Hour Static Acute Toxicity Test to *Daphnia magna*.

Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	None reported
Water Hardness	Not reported
Analytical Monitoring	None
Remarks - Method	Characterisation and stability information was not provided and mixture analysis was not performed.

RESULTS

Concentration mg/L		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual*		*24 h*	*48 h*
0	-	30	0	0
0.1	-	30	1	1
1.0	-	30	1	1
10	-	30	0	1
100	-	30	1	3
1000	-	30	30	30

EC50	257.86 mg/L at 48 hours (95% C.I. 194.351-341.83 mg/L)
NOEC	10 mg/L at 48 hours
Remarks - Results	All test validity criteria were satisfied.

CONCLUSION The notified chemical is not harmful to aquatic invertebrates.

TEST FACILITY Stillmeadow Inc (2005b)

C.2.3. Algal growth inhibition test

TEST SUBSTANCE	Acceptable Analogue
METHOD	OPPTS 850.5400 96 hour Growth Inhibition to the Freshwater Algae *Selenastrum capricornutum*
Species	*Selenastrum capricornutum*
Exposure Period	96 hours
Concentration Range	Nominal: 0, 0.1, 1.0, 10, 100 and 1000 mg/L
Auxiliary Solvent	None reported
Water Hardness	Not reported
Analytical Monitoring	None
Remarks - Method	Characterisation and stability information was not provided and mixture analysis was not performed.

RESULTS

Growth Rate	
IC50	*NOEC*
mg/L at 96 h	*mg/L*
>1000	<0.1

Remarks - Results	The cell densities after 24 hours in all test mixtures were lower that for the controls. In the case of the 10, 100 and 1000 mg/L mixtures, no measurable cell densities were recorded after 24 hours. However after 48 hours all test mixtures had comparable cell densities in the range 1.1-1.3×10^6 cells/mL. All test validity criteria were satisfied.
CONCLUSION	The notified chemical is not harmful to algae
TEST FACILITY	Stillmeadow Inc (2005c)

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