File No.: STD/1720

August 2020

AUSTRALIAN INDUSTRIAL CHEMICALS INTRODUCTION SCHEME (AICIS)

PUBLIC REPORT

2-Propen-1-aminium, *N,N,N*-tri-2-propen-1-yl-, chloride (1:1)

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals Act 2019* (the IC Act) and *Industrial Chemicals (General) Rules 2019* (the IC Rules) by following the *Industrial Chemicals (Consequential Amendments and Transitional Provisions) Act 2019* (the Transitional Act) and *Industrial Chemicals (Consequential Amendments and Transitional Provisions) Rules 2019* (the Transitional Rules). The legislations are Acts of the Commonwealth of Australia. The Australian Industrial Chemicals Introduction Scheme (AICIS) is administered by the Department of Health, and conducts the risk assessment for human health. 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 AICIS website. For enquiries please contact AICIS at:

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Executive Director
AICIS

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SUMMARY

The following details will be published on our website:

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
STD/1720	SNF (Australia) Pty Ltd	2-Propen-1-aminium, *N,N,N*-tri-2-propen-1-yl-, chloride (1:1)	Yes	≤ 40 tonnes per annum	Component of mining and construction sealant

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard Classification
Based on the available information, the assessed chemical is a hazardous chemical according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia. The hazard classification applicable to the assessed chemical is presented in the following table.

Hazard Classification	*Hazard Statement*
Skin sensitisation (Category 1)	H317 – May cause an allergic skin reaction

The environmental hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS) is presented below. Environmental classification under the GHS is not mandated in Australia and carries no legal status but is presented for information purposes.

Hazard Classification	*Hazard Statement*
Chronic (Category 1)	H411 – Toxic to aquatic life with long lasting effects

Human Health Risk Assessment
Provided that the recommended controls are being adhered to, under the conditions of the occupational settings described, the assessed chemical is not considered to pose an unreasonable risk to the health of workers.

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

Environmental Risk Assessment
On the basis of the PEC/PNEC ratio, the assessed chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

REGULATORY CONTROLS

Hazard Classification and Labelling

- The assessed chemical should be classified as follows:
  - Skin sensitisation (Category 1): H317 – May cause an allergic skin reaction

  The above should be used for products/mixtures containing the assessed chemical, if applicable, based on the concentration of the assessed chemical present.

Health Surveillance

- As the assessed chemical is a skin sensitiser, employers should carry out health surveillance for any worker who has been identified in the workplace risk assessment as having a significant risk of sensitisation.

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following engineering controls to minimise occupational exposure to the assessed chemicals during reformulation and end use processes:
  - Enclosed, automated processes, where possible
  - Local exhaust ventilation if aerosols are likely to be generated

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure to the assessed chemicals during reformulation and end processes:
  - Avoid contact with skin
  - Clean up spills promptly
  - Avoid inhalation of aerosols

- 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 assessed chemicals during reformulation and end processes:
  - Coveralls
  - Impervious gloves
  - Respiratory protection if inhalation exposure may occur

  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 assessed chemicals 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.

Storage

- The handling and storage of the assessed chemical should be in accordance with the Safe Work Australia Code of Practice for *Managing Risks of Hazardous Chemicals in the Workplace* (SWA, 2012) or relevant State or Territory Code of Practice.

Emergency procedures

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

Disposal

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

Regulatory Obligations

Specific Requirements to Provide Information
This risk assessment is based on the information available at the time of the application. The Executive Director may initiate an evaluation of the chemical based on changes in certain circumstances. Under section 101 of the IC Act the introducer of the assessed chemical has post-assessment regulatory obligations to provide information to AICIS when any of these circumstances change. These obligations apply even when the assessed chemical is listed on the Australian Inventory of Industrial Chemicals (the Inventory).

Therefore, the Executive Director of AICIS must be notified in writing within 20 working days by the applicant or other introducers if:

- the assessed chemical is included in products available to the public;
- the function or use of the chemical has changed from component of mining and construction sealant;
- 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 human health, or the environment.

The Executive Director will then decide whether an evaluation of the introduction is required.

Safety Data Sheet
The SDS of the product containing the assessed chemical provided by the applicant was reviewed by AICIS. The accuracy of the information on the SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND APPLICATION DETAILS

APPLICANT(S)
SNF (Australia) Pty Ltd (ABN: 32 050 056 267)
98 Broderick Road
LARA VIC 3212

APPLICATION CATEGORY
Standard: Chemical other than polymer (more than 1 tonne per year)

PROTECTED INFORMATION (SECTION 38 OF THE TRANSITIONAL ACT)
Data items and details exempt from publication include: analytical data, degree of purity, import volume, use details and site of reformulation.

VARIATION OF DATA REQUIREMENTS (SECTION 6 OF THE TRANSITIONAL RULES)
Schedule data requirements are varied for repeated dose toxicity.

PREVIOUS APPLICATION IN AUSTRALIA BY APPLICANT(S)
None

APPLICATION IN OTHER COUNTRIES
EU

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
FLOCRYL™ TAAC

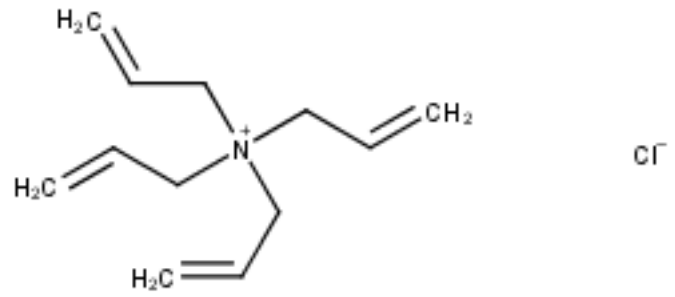
CAS NUMBER
13107-10-3

CHEMICAL NAME
2-Propen-1-aminium, *N,N,N*-tri-2-propen-1-yl-, chloride (1:1)

OTHER NAME(S)
2-Propen-1-aminium, *N,N,N*-tri-2-propenyl-, chloride (9CI)
Ammonium, tetraallyl-, chloride (8CI)
Tetraallylammonium chloride
TAAC

MOLECULAR FORMULA
$C_{12}H_{20}N.Cl$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
213.75 g/mol

ANALYTICAL DATA
Reference NMR and FTIR spectra were provided.

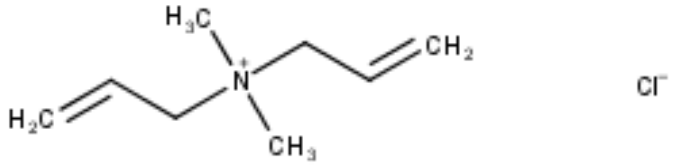
ANALOGUE PROVIDED FOR TOXICOLOGICAL DATA

CHEMICAL NAME
2-Propen-1-aminium, *N,N*-dimethyl-*N*-2-propen-1-yl-, chloride (1:1)

CAS NUMBER
7398-69-8

MOLECULAR FORMULA
$C_8H_{16}N.Cl$

STRUCTURAL FORMULA



JUSTIFICATION OF USE
The analogue chemical is used for repeated dose toxicity. This analogue is closely related to the assessed chemical, containing a quaternary ammonium and two allyl groups, instead of four allyl groups in the assessed chemical. There are two additional methyl groups in this analogue, compared to the assessed chemical. The analogue chemical is expected to have similar reactivity and physico-chemical properties to the assessed chemical, and is of lower molecular weight.

3. COMPOSITION

DEGREE OF PURITY
> 85%

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: dark brown mass (assessed chemical at > 85%); dark amber liquid (introduced form containing the assessed chemical at 40%)

Property	*Value*	*Data Source/Justification*
Melting Point	10 – 69 °C	Measured*
Boiling Point	Decomposes at > 140 °C	Measured*
Density	1,130 kg/m^3 at 23 °C	Measured*
Vapour Pressure	2 × 10^{-7} kPa at 25 °C	Measured*
Water Solubility	> 532 g/L at 20 °C	Measured*
Hydrolysis as a Function of pH	Not determined	-
Partition Coefficient (n-octanol/water)	log Pow = -2 to -1 at 20 °C	Estimated based on similar chemical structures
Surface Tension	72.4 mN/m	Measured*
Adsorption/Desorption	Not determined	Expected to sorb to soil due to cationic functionality
Dissociation Constant	Not determined	Chemical is a salt and is ionised under normal environmental conditions
Flash Point	122.4 °C at 101.3 kPa	Measured*
Pyrophoric Properties	Not pyrophoric	Measured*

Property	*Value*	*Data Source/Justification*
Autoignition Temperature	335 °C	Measured*
Explosive Properties	Not explosive	Measured*
Oxidising Properties	Not oxidising	Measured*

*Conducted on the test substance that contains the assessed chemical at > 85%.

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

Reactivity
The assessed chemical contains vinyl functional groups and, when mixed with other components of the sealant, are expected to undergo further polymerisation reactions to form a solid matrix. The reactions are intended by design as part of the use pattern.

Physical Hazard Classification
Based on the submitted physico-chemical data depicted in the above table, the assessed 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 assessed chemical has a flash point of 122.4 ºC which is greater than 93 °C. Based on *Australian Standard AS1940* definitions for combustible liquid, the assessed 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 ASSESSED CHEMICAL (100%) OVER NEXT 5 YEARS
The assessed chemical will not be manufactured in Australia. It will be imported at 40% concentration for reformulation into one part of a two-part sealing/grouting system for the mining and construction industry.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	15 – 20	15 – 20	15 – 30	15 – 40	15 – 40

PORT OF ENTRY
Melbourne

TRANSPORTATION AND PACKAGING
The assessed chemical at 40% concentration will be introduced to Australia by sea in 1000 kg IBCs and transported to the applicant's facilities for reformulation. After it has been reformulated into finished products containing the assessed chemical at ≤ 5% concentration, it will be transported in 1000 kg IBCs, 200 kg drums or 20 kg pails.

USE
The assessed chemical will be used as a component (at concentrations of ≤ 5%) of a two part industrial sealant/grout for mining and construction applications.

OPERATION DESCRIPTION

Reformulation
The assessed chemical will not be manufactured in Australia. The product containing the assessed chemical (at 40% concentration) will be reformulated with additional components, to form the finished end-use products at ≤ 5% concentration. At the reformulation sites, workers will open the imported containers and pump the solution through hoses into a blending vessel or an on-site holding tank, which will dose the solution into the blending vessel through fixed lines. Once other components are added, the blending vessel will be sealed, and contents will be mixed under general ventilation. Quality control (QA) staff will sample from the blending tank through a sampling port. After the quality control processes, the blended product (containing the assessed chemical at ≤ 5% concentration) will be pumped to an automated filling machine and filled into 1000 kg IBCs, 200 kg drums and 20 kg pails for distribution to customers.

End-use

When sealant containing the assessed chemical is typically used in construction to seal tunnel walls, workers will manually pour the two parts of the system into separate compartments of an injecting machine. The sealant will be used during the process of drilling holes into the concrete-lined tunnel wall. Purpose built injection ports will be inserted into the drill holes. A hose fitting will be screwed onto the port. The two-part sealant will be mixed *in situ* inside the injector and then injected under pressure behind the concrete wall through the port. When injection is completed, the hose coupling will be sealed off and removed from the port. The port will then be capped off and the sealant allowed to cure behind the concrete wall, sealing the wall from water permeation.

Usage for oil and gas wells will be similar to applications in tunnelling. A purpose-designed mixer/injector machine will be utilised at the injection well site. The sealant system is mixed within the injector machine at the on-site injector site, then injected into a well at the required depth, adjacent to the production well. The sealant will then penetrate the rock layer and seal around the production well shaft.

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	1-4	24
Reformulation workers	8	24
QA workers	0.5-2	24
Tunnelling workers	4-8	20 – 40
Oil and gas workers	4-8	5 – 10

EXPOSURE DETAILS

Transport and storage
Transport, storage and warehouse workers may come into contact with the assessed chemical at 40% concentration only in the event of accidental breaching of containers.

Reformulation
During reformulation, dermal, ocular and inhalation exposure of workers to the assessed chemical at up to 40% concentration may occur during handling of containers, during transfer stages, blending, quality control processes and cleaning and maintenance of equipment. It is expected that exposure will be minimised through the use of enclosed systems, and workers wearing personal protective equipment (PPE) such as coveralls, impermeable gloves, eye protection, and respirators if ventilation is inadequate. The potential for inhalation exposure would be reduced by the low vapour pressure of the assessed chemical, unless aerosols are generated during the reformulation process.

End-use
Exposure to the assessed chemical in end-use products (at ≤ 5% concentration) may occur for workers during the manual transfer of the sealants into the dispensing equipment. According to the applicant, appropriate PPE such as overalls, impervious gloves and eye protection is expected to be used by workers during end use, which would reduce the potential for exposure. Once the assessed chemical has been pumped into the required location and cured, it is not expected to be available for exposure.

6.1.2. Public Exposure
The assessed chemical is intended only for use in construction applications such as industrial tunnelling and at mining sites. Public exposure to the assessed chemical or its breakdown products is not expected, unless accidental release of the assessed chemical to the public occurs during transport.

6.2. Human Health Effects Assessment
The results from toxicological investigations conducted on a formulation containing the assessed chemical are summarised in the following table. For details of the studies, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*
Acute oral toxicity – rat*	LD50 > 2,000 mg/kg bw for the test substance
Acute dermal toxicity – rat*	LD50 > 2,000 mg/kg bw for the test substance
Skin irritation – rabbit*	test substance is non-irritating
Eye irritation – rabbit*	test substance is slightly irritating
Skin sensitisation – guinea pig, maximisation test*	test substance shows evidence of sensitisation
Mutagenicity – bacterial reverse mutation	non mutagenic
Genotoxicity – *in vitro* chromosome aberration test	non genotoxic

*Tests were carried out on a solution of the assessed chemical in which the concentration is not known, but has been estimated at 35%.

In addition, the following studies were conducted using an analogue chemical:

Endpoint	*Result and Assessment Conclusion*
Repeat dose oral toxicity – rat, 28 days	NOAEL > 500 mg/kg bw/day
Repeat dose oral toxicity – rat, 90 days	not established
Repeat dose oral toxicity – dog, 90 days	not established

Toxicokinetics, Metabolism and Distribution
No information on toxicokinetics of the assessed chemical was provided. The high water solubility (> 532 g/L at 20 °C) and low partition coefficient (log Pow < -1) of the assessed chemical is expected to limit its potential for dermal absorption.

Acute Toxicity
A solution of the assessed chemical was found to have low acute oral and dermal toxicity in rats. Based on the estimated concentration tested (35%), the potential for acute toxicity for the neat chemical cannot be ruled out. No information is available on acute inhalation toxicity.

Irritation and Sensitisation
Based on studies conducted in rabbits, a solution of the assessed chemical (estimated at 35%) was considered to be non-irritating to the skin and eyes. The potential for irritation effects at 100% cannot be ruled out.

A solution of the assessed chemical (estimated at 35%) gave positive results in a guinea pig skin sensitisation test, with skin reactions observed in the challenge phase in 60% of the animals induced with the solution topically. Based on this information, the assessed chemical should be considered as a skin sensitiser. Due to the unknown concentration of the solution tested, the exact potency of the assessed chemical as a skin sensitiser cannot be estimated.

Repeated Dose Toxicity
A 28-day repeat dose study was conducted in rats, with an analogue chemical administered through the oral route at dose levels of 0, 25, 100 and 500 mg/kg bw/day. The No Observed Adverse Effect Level (NOAEL) was established as 500 mg/kg bw/day, the highest dose tested, for both males and females in this study.

Two 90-day repeat dose toxicity feeding studies that are pre-OECD guidelines and non-GLP were also provided on the analogue chemical. Dose levels up to 1,200 mg/kg bw/day in rats and up to 800 mg/kg bw/day in dogs were tested. In the study conducted on rats, 1/20 high dose males died due to congestion in the intestines and 1/20 females died from acute cystitis. Rats in the mid and high dose group showed a decrease in body weight gain, and males in the high dose group and females in the mid and high dose groups showed a reduction in terminal body weight. Several animals in the low and mid dose group showed incidences of haematuria at the six weeks observation point, although no other adverse effects were observed. In the study conducted in dogs, a reduction in body weight gain was observed in all treatment groups of males (24.4%, 13.4%, 26.7% reduction respectively) and high dose females (5.9%), The males of the high dose group showed a statistically significant reduction of terminal body weight compared to the control group. A statistically significant reduction of absolute heart weight was observed in the high dose males, but with no associated histological changes. A No Observed Adverse Effect Level (NOAEL) was not established for these two studies on rats and dogs.

Mutagenicity/Genotoxicity
The assessed chemical was not mutagenic in a bacterial reverse mutation study and was not considered to be clastogenic in a chromosome aberration test.

Health Hazard Classification
Based on the available information, the assessed chemical is a hazardous chemical according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia. The hazard classification applicable to the assessed chemical is presented in the following table.

Hazard Classification	*Hazard Statement*
Skin sensitisation (Category 1)	H317 – May cause an allergic skin reaction

6.3. Human Health Risk Characterisation
Based on the information available, the primary hazard of the assessed chemical is its skin sensitisation potential, for which potency has not been determined. Acute or repeated dose toxicity and irritation cannot be ruled out at high concentrations

6.3.1. Occupational Health and Safety

Reformulation
During reformulation, workers may come into contact with the assessed chemical at up to 40% concentration during transfer, maintenance, and cleaning operations. Control measures indicated on the SDS for the assessed chemical include use of adequate general ventilation and suitable PPE such as coveralls, impervious gloves and safety glasses, to minimise worker exposure.

End-use
During end-use, professional workers carrying out mining work and construction work such as tunnelling may come into contact with the assessed chemical at ≤ 5% concentration during loading and cleaning of equipment used to apply the products containing the assessed chemical. Other processes are automated and are not expected to lead to exposure. Exposure and risk would be mitigated by use of control measures such as the PPE stated by the applicant. Once the product containing the assessed chemical has been pumped into the required location and cured, it is not expected to be available for exposure.

Provided that the recommended controls are being adhered to, under the conditions of the occupational settings described, the assessed chemical is not considered to pose an unreasonable risk to the health of workers.

6.3.2. Public Health
Products containing the assessed chemical will not be available to the public. The assessed chemical is intended only for use in industrial uses, and public exposure to the assessed chemical is not expected.

When used in the proposed manner, the assessed 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 assessed chemical is not manufactured in Australia. Some release may occur from accidental spills during the reformulation into the product. The applicant estimates that this may account for up to 0.5% of the import volume of the assessed chemical. Any accidental spills are to be collected and disposed of by licensed waste contractors. Release may also occur from the flushing of equipment lines and tanks which are to be recycled where possible. Where recycling is not possible, the wash water will be collected and treated in an on-site wastewater treatment plant. The applicant estimates that up to 0.2% of the import volume of the assessed chemical may be disposed of in this way.

RELEASE OF CHEMICAL FROM USE
The assessed chemical is expected to be cured and cross-linked into the sealant matrix during its use as grout for mining and construction applications. Accidental release of the assessed chemical may occur during the connection and disconnection of containers to the equipment. The applicant estimates that this may account for up to 0.1% of the import volume of the assessed chemical.

RELEASE OF CHEMICAL FROM DISPOSAL

The assessed chemical is expected to be disposed of primarily to landfill at the end of its useful life. The applicant estimates that up to 0.1% of the import volume of the assessed chemical is expected to remain as residues in empty product containers. These containers are expected to be either recycled or disposed of to domestic landfill.

7.1.2. Environmental Fate

During its use in industrial mining grout/sealants, the assessed chemical is expected to be cured and cross-linked into the sealant matrix where it is not expected to be bioavailable. The sealant matrix containing the reacted assessed chemical is expected to eventually degrade in-situ. Some of the assessed chemical may remain in the end use and bulk containers, which are either recycled or disposed of to landfill.

The assessed chemical is not readily biodegradable (0% after 28 days). For details of the biodegradation study, refer to Appendix C. The assessed chemical is not expected to bioaccumulate due to its low log Pow (log Pow = -2 to -1). In landfill, the assessed chemical is expected to degrade into water and oxides of carbon and nitrogen. The applicant expects some of the assessed chemical to be released to sewer from reformulation sites and disposal. The total is estimated as 1% of the import volume.

7.1.3. Predicted Environmental Concentration (PEC)

The use pattern will result in a portion of the assessed chemical being washed into the sewer. The predicted environmental concentration (PEC) has been calculated assuming the realistic worst-case scenario with 1% release of the assessed chemical into sewer systems nationwide over 260 working days per annum. The extent to which the assessed chemical is removed from the effluent in STP processes based on the properties of the assessed chemical has not been considered for this scenario, and therefore no removal of the assessed chemical during sewage treatment processes, is assumed. The PEC in sewage effluent on a nationwide basis is estimated as follows:

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	40,000	kg/year
Proportion expected to be released to sewer	1%	
Annual quantity of chemical released to sewer	400	kg/year
Days per year where release occurs	260	days/year
Daily chemical release:	1.54	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:	0.32	µg/L
PEC - Ocean:	0.03	µg/L

Partitioning to biosolids in STPs Australia-wide may result in the assessed chemical being present in biosolids. However, the estimated concentration is considered negligible.

7.2. Environmental Effects Assessment

The results from ecotoxicological investigations conducted on the assessed chemical are summarised in the table below. Details of these studies can be found in Appendix C.

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	EC50 = 11 mg/L	Harmful to fish
Daphnia Toxicity	EC50 = 80 mg/L	Harmful to aquatic invertebrates
Algal Toxicity	EC50 = 8.6 mg/L NOEC = 5 mg/L	Toxic to algal growth
Fish Early Life Stage Toxicity	NOEC > 100 mg/L	Not harmful to early life stage fish
Earthworm Toxicity	NOEC > 5000	Not harmful to earthworms

Based on the above ecotoxicological endpoints for the assessed chemical, the assessed chemical is expected to be toxic to algal growth and harmful to fish and aquatic invertebrates. Therefore, the assessed chemical is classified as 'H401 – Toxic to aquatic life' according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)* (United Nations, 2009). The assessed chemical is not readily biodegradable but is not expected

to bioaccumulate. Therefore, the assessed chemical is formally classified under the GHS for its long-term hazard as H411 – Toxic to aquatic life with long lasting effects.

7.2.1. Predicted No-Effect Concentration

A Predicted No-Effect Concentration (PNEC) was calculated based on the acute endpoint for algae (EC50 = 8.6 mg/L) using an assessment factor of 50, as three acute and one chronic toxicity values were available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
EC50 (Alga).	8.6	mg/L
Assessment Factor	50	
Mitigation Factor	1	
PNEC:	172	µg/L

7.3. Environmental Risk Assessment

Risk Assessment	***PEC µg/L***	***PNEC µg/L***	***Q***
Q - River:	0.32	172	< 0.01
Q - Ocean:	0.03	172	< 0.01

The risk quotient for the aquatic environment (Q = PEC/PNEC) has been calculated based on the worst-case assumption of 1% release into the waterways with no removal in STPs. As the Q value is significantly less than 1, the assessed chemical is unlikely to reach ecotoxicologically significant concentrations. A PEC/PNEC ratio for soil was not calculated as the concentration in soil is considered negligible and the assessed chemical is not harmful to earthworms. Accordingly the risk to the terrestrial environment is not considered unreasonable. Therefore, on the basis of the PEC/PNEC ratio, the assessed chemical is not considered to pose an unreasonable risk to the environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point/Freezing Point 10 – 69 °C

Method	OECD TG 102 Melting Point/Melting Range (1997)
Remarks	Differential scanning calorimetry (DSC) was used. The melting point was given as a range because the first signs of melting was observed at 10 °C, and all solid material had melted by 69 °C.
Test Facility	Solvias (2003a)

Boiling Point Decomposed at > 140 °C

Method	OECD TG 103 Boiling Point (1997)
Remarks	Both a melting point apparatus and DSC were used. Signs of decomposition was observed at 140 °C and peaked at 184 °C.
Test Facility	Solvias (2003b)

Density 1,130 kg/m^3 at 23 °C

Method	OECD TG 109 Density of Liquids and Solids (1997)
Remarks	A pycnometer was used.
Test Facility	Solvias (2003c)

Vapour Pressure 2×10^{-7} kPa at 25 °C

Method	OECD TG 104 Vapour Pressure (1997)
Remarks	Calculated using MPBPWIN program. Alternatively, the thermogravimetry method was used and a value of 1.5×10^{-7} kPa at 25 °C was measured.
Test Facility	Solvias (2003d)

Water Solubility ≥ 532 g/L at 20 °C

Method	OECD TG 105 Water Solubility
Remarks	Flask Method/Column Elution Method
Test Facility	Solvias (2003e)

Partition Coefficient (n-octanol/water) log Pow = -2 to -1 at 20 °C

Method	OECD TG 117 Partition Coefficient (n-octanol/water).
Remarks	Partition coefficient could not be determined for the assessed chemical using the Flask Method. The Log Pow value is an estimation based on literature evaluations on several structurally similar chemicals.
Test Facility	Solvias (2003f)

Surface Tension 72.4 mN/m at 20 °C

Method	OECD TG 115 Surface Tension of Aqueous Solutions (1995)
Remarks	Concentration: 1 g/L
Test Facility	Solvias (2003g)

Flash Point 122.4 °C at 101.3 kPa

Method	EC Council Directive 92/69/EEC A.9 Flash Point (1992)
Remarks	Pensky-Martens test method was used.
Test Facility	Safety and Security (2003a)

Flammability – Pyrophoric properties Not pyrophoric

Method	EC Council Directive 92/69/EEC A.13 Pyrophoric Properties of Solids and Liquids
Remarks	Did not ignite or char in contact with air.
Test Facility	Safety and Security (2003b)

Autoignition Temperature 335 °C

Method	EC Council Directive 92/69/EEC A.15 Auto-Ignition Temperature (Liquids and Gases)
Remarks	An electrically heated ignition vessel was used.
Test Facility	Safety and Security (2003c)

Explosive Properties Not explosive

Method	EC Council Directive 92/69/EEC A.14 Explosive Properties.
Remarks	Tested for thermal and mechanical (shock) sensitivity. Mechanical (friction) sensitivity was not tested, as not considered suitable for a liquid such as the assessed chemical.
Test Facility	Safety and Security (2003d)

Oxidizing Properties Not oxidising

Method	Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria. Part III, section 34. United Nations, 1995 EC Council Directive 92/69/EEC A.21 Oxidizing Properties (draft) (Liquids)
Remarks	Tested as a mixture with fibrous cellulose. The criteria for a positive result, for spontaneous ignition or lower comparative time for rise in pressure, were not met.
Test Facility	Safety and Security (2003e)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute Oral Toxicity – Rat

TEST SUBSTANCE	Assessed chemical (concentration not known, estimated 35%)
METHOD	OECD TG 401 Acute Oral Toxicity – Limit Test (1987)
Species/Strain	Rat/Crl:CD (SD)
Vehicle	Water
Remarks – Method	GLP Compliance Statement. No significant protocol deviations. A range-finding study was conducted at dose levels of 500, 1,000, and 2000 mg/kg bw of the test substance.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw)*	*Mortality*
1	5 F, 5 M	2,000	0/10

LD50	> 2,000 mg/kg bw
Signs of Toxicity	No signs of systemic toxicity were noted. All animals showed expected body weight gain over the observation period.
Effects in Organs	Enlarged submandibular lymph nodes was found in one male and pelvic dilation of one kidney was found in one female. These observations were not considered by the study authors to have toxicological significance.
Remarks – Results	The test report did not indicate that dosage was adjusted to account for concentration.
CONCLUSION	The test substance is of low acute toxicity via the oral route.
TEST FACILITY	Toxicol (1994a)

B.2. Acute Dermal Toxicity – Rat

TEST SUBSTANCE	Assessed chemical (concentration not known, estimated at 35%)
METHOD	OECD TG 402 Acute Dermal Toxicity – Limit Test (1987)
Species/Strain	Rat/Crl:CD (SD)
Vehicle	None. The assessed chemical was applied undiluted.
Type of dressing	Occlusive.
Remarks – Method	GLP Compliance Statement. No significant protocol deviations. A range-finding study was conducted at dose levels of 500, 1,000, and 2000 mg/kg bw of the test substance.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw)*	*Mortality*
1	5 F, 5 M	2,000	0/10

LD50	> 2,000 mg/kg bw
Signs of Toxicity – Local	A scab on the right ventral inguinal region of the skin on one male was observed.
Signs of Toxicity – Systemic	No signs of systemic toxicity were noted. All animals showed expected body weight gain over the observation period.
Effects in Organs	Enlarged submandibular lymph nodes were observed in one male (both nodes) and one female (left node). Distended uterus was seen on two

	female rats. These observations were not considered by the study authors to have toxicological significance.
Remarks – Results	The test report did not indicate that dosage was adjusted to account for concentration.
CONCLUSION	The test substance is of low acute toxicity via the dermal route.
TEST FACILITY	Toxicol (1994b)

B.3. Skin Irritation – Rabbit

TEST SUBSTANCE	Assessed chemical (concentration not known, estimated 35%)
METHOD	OECD TG 404 Acute Dermal Irritation/Corrosion (1992)
Species/Strain	Rabbit/New Zealand White
Number of Animals	3
Vehicle	None. The assessed chemical was applied undiluted.
Observation Period	3 days
Type of Dressing	Semi-occlusive
Remarks – Method	GLP Compliance Statement. No significant protocol deviations.

RESULTS

Remarks – Results	No signs of irritation was observed on any animal throughout the observation period. The test report did not indicate that dosage was adjusted to account for concentration.
CONCLUSION	The test substance is non-irritating to the skin.
TEST FACILITY	Toxicol (1994c)

B.4. Eye Irritation – Rabbit

TEST SUBSTANCE	Assessed chemical (concentration not known, estimated 35%)
METHOD	OECD TG 405 Acute Eye Irritation/Corrosion (1987)
Species/Strain	Rabbit/New Zealand White
Number of Animals	3
Observation Period	3 days
Remarks – Method	GLP Compliance Statement. No significant protocol deviations.

RESULTS

Lesion	*Mean Score* Animal No.*			*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3			
Conjunctiva – Redness	0	0	0	0	n/a	0
Conjunctiva – Chemosis	0	0	0	0	n/a	0
Conjunctiva – Discharge	0	0	0.33	1	< 48 hours	0
Corneal Opacity	0	0	0	0	n/a	0
Iridial Inflammation	0	0	0	0	n/a	0

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

Remarks – Results	One animal showed slight discharge from the treated eye at the 24 hour examination, which did not persist. No other signs of irritation was observed on any animal throughout the entire observation period. The test

report did not indicate that dosage was adjusted to account for concentration.

CONCLUSION The test substance is slightly irritating to the eye.

TEST FACILITY Toxicol (1994d)

B.5. Skin Sensitisation – Guinea Pig Maximisation Test

TEST SUBSTANCE Assessed chemical (concentration not known, estimated 35%)

METHOD OECD TG 406 Skin Sensitisation – Guinea Pig Maximisation Test

Species/Strain Guinea pig/Dunkin-Hartley Albino

PRELIMINARY STUDY Maximum non-irritating concentration: 100%
Intradermal: 1%, 5%, 10%, 25%, 50%, and 100%
Topical: 12.5%, 25%, 50%, and 100%

MAIN STUDY

Number of Animals Test Group: 20 F Control Group: 10 F

Vehicle Water

Positive Control Not conducted in parallel with the test substance, but had been conducted previously in the test laboratory using mercaptobenzothiazole (MBT).

INDUCTION PHASE Induction concentration:
Intradermal: 10%
Topical: 100%

Signs of Irritation After topical induction (but not intradermal induction), the tested animals showed a marked increase in irritation levels compared to the vehicle treated controls. This result may have been influenced by the dermal application of 10% sodium lauryl sulfate in light paraffin, for the purpose of causing local irritation.

CHALLENGE PHASE

1st Challenge Topical: 100%

2nd Challenge None

Remarks – Method GLP Compliance Statement.
No significant protocol deviations.

No dermal effects were reported in the topical rangefinder studies. In the intradermal range finding studies, effects were seen from Day 2, when grey focus with eschar formation and area of ulceration was observed on animals treated at 100%, grey focus with surrounding erythema was observed on animals treated at 50% and 25%, and all doses at 10% or less showed erythema formation. On Days 3-6, depressed eschar was found on animals treated at 100%, 50% and 25%, and erythema was observed at lower doses.

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after Challenge*	
		24 h	*48 h*
Test Group	100%	10/20	12/20
Negative Control Group	100%	0/10	0/10

Remarks – Results A positive response was observed in 60% of animals by the 48 hour observation period. No responses were seen in any of the control animals, when challenged with the test substance or vehicle.

The test report did not indicate that dosage was adjusted to account for concentration.

CONCLUSION	There was evidence of reactions indicative of skin sensitisation to the test substance under the conditions of the test.
TEST FACILITY	Toxicol (1994e)

B.6. Repeat Dose Oral Toxicity – Rat

TEST SUBSTANCE	Analogue chemical
METHOD	OECD TG 407 Repeated Dose 28-day Oral Toxicity Study in Rodents (1995) EC Directive 96/54/EC B.7 Repeated Dose (28 Days) Toxicity (Oral)
Species/Strain	Rat/Crl:CD (SD)
Route of Administration	Oral – gavage/diet/drinking water
Exposure Information	Total exposure days: 28 days Dose regimen: 7 days per week Post-exposure observation period: 14 days
Vehicle	Water
Remarks – Method	GLP Certificate. The dose levels were selected at the request of the sponsor based on available toxicological data. Analysis of the analogue chemical showed that it was present at 63% in the liquid. However dosage was adjusted to account for this concentration, with a correction factor of 1.59. Statistical significance was recorded only at $P < 0.01$ for some parameters.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw/day)*	*Mortality*
Control	5 F, 5 M	0	0/10
Low Dose	5F, 5 M	25	0/10
Mid Dose	5F, 5 M	100	0/10
High Dose	5F, 5 M	500	0/10
Control Recovery	5F, 5 M	0	0/10
High Dose Recovery	5F, 5 M	500	0/10

Mortality and Time to Death

There were no unscheduled deaths for the duration of this study.

Clinical Observations

There were no treatment-related effects on clinical signs, limb strength, spontaneous motility, or food consumption for animals at all doses. Faeces of all animals were within normal consistency throughout the experimental period.

Laboratory Findings – Clinical Chemistry, Haematology, Urinalysis

No test substance-related changes were reported for haematology or clinical chemistry parameters.

Effects in Organs

No test substance-related changes in the relative and absolute organ weights were noted for the organs of all treated animals. One male in the low dose group showed an increased lobular pattern in the liver, and one male in the high dose recovery group showed a reduced testes and epididymides size, that was reflected in lower organ weights and histological changes. These changes were considered by the study author to be incidental.

Remarks – Results

All animals showed expected body weight gain over the total duration of the study.

CONCLUSION

The No Observed (Adverse) Effect Level (NOAEL) was established as > 500 mg/kg bw/day in this study, based on the highest dose tested.

TEST FACILITY LPT (2008)

B.7. Repeat Dose Oral Toxicity – Rat

TEST SUBSTANCE Analogue chemical

METHOD Similar to OECD TG 408 Repeated Dose 90-Day Oral Toxicity Study in Rodents

Species/Strain	Rat/Sprague Dawley
Route of Administration	Oral – diet
Exposure Information	Total exposure days: 90 days Dose regimen: 7 days per week Post-exposure observation period: None
Vehicle	Not specified
Remarks – Method	No GLP Compliance Statement. Non-standard method that is similar but pre-dates the OECD TG. The analogue chemical was supplied at 60%, however dosage was adjusted to account for concentration. The study also tested the polymer of the analogue chemical at dose levels of 2,500 mg/kg bw/day. Only the results for the analogue chemical are reported.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw/day)*	*Mortality*
Control	20 F, 20 M	0	0/40
Low Dose	20 F, 20 M	75	0/40
Mid Dose	20 F, 20 M	300	0/40
High Dose	20 F, 20 M	1,200	2/40

Mortality and Time to Death

One male animal in the high dose group died on Day 29 and the necropsy revealed moderate congestion in the intestines. One female animal in the high dose group died on Day 44 and the necropsy revealed that acute cystitis was the cause of death. All other animals survived for the duration of the study.

Clinical Observations

The animals in the mid and high dose groups showed a dose-dependent reduction in mean body weight gain, compared to the controls. Males showed an 8.9% and 9.8% reduction and females showed a 7.1% and 13.7% reduction, at the mid and high doses respectively. The males in the high dose group and females in the mid and high dose groups also showed a statistically significantly lower terminal body weight (7.2%, 7.3 and 7.3% respectively) compared to the control group. Food consumption was generally unchanged, with the exception that the females in the high dose group showed a slight reduction.

Laboratory Findings – Clinical Chemistry, Haematology, Urinalysis

There were no statistically significant treatment-related changes in the various clinical chemistry and blood parameters in animals from any of the dose groups. Two animals in the low dose group and three in the mid dose group displayed haematuria at six weeks, but this effect was not observed subsequently.

Effects in Organs

There were no statistically significant changes in the mean organ weights of treated animals, compared to the control group mean organ weights.

Remarks – Results

A NOAEL was not established by the study authors.

TEST FACILITY Pharmacopathics (1976a)

B.8. Repeat Dose Oral Toxicity – Dog

TEST SUBSTANCE	Analogue chemical
METHOD	Similar to OECD TG 409 Repeated Dose 90-Day Oral Toxicity Study in Non-Rodents
Species/Strain	Dog/beagle
Route of Administration	Oral – diet
Exposure Information	Total exposure days: 90 days Dose regimen: 7 days per week Post-exposure observation period: None
Vehicle	Not specified
Remarks – Method	No GLP Compliance Statement. Non-standard method that is similar to but pre-dates the OECD TG. Limited haematological and clinical chemistry parameters were tested. The analogue chemical was supplied at 60%, however dosage was adjusted to account for concentration. The study also used the polymer of the analogue chemical at dose levels of 1,250 mg/kg bw/day. Only the results for the analogue chemical are reported.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw/day)*	*Mortality*
Control	4 F, 4 M	0	0/8
Low Dose	4 F, 4 M	50	0/8
Mid Dose	4 F, 4 M	200	0/8
High Dose	4 F, 4 M	800	0/8

Mortality and Time to Death

There were no unscheduled deaths for the duration of this study.

Clinical Observations

All treated male animals showed a reduction of mean body weight gain compared to the control group. The low, mid and high dose groups showed a 24.4%, 13.4%, 26.7% reduction respectively. High dose females showed a 5.9% reduction in mean weight gain, compared to the control mean, but comparable or higher weight gain than the control group was reported for other dose groups. The males of the high dose group showed a statistically significant lower mean terminal body weight, compared to the control group. Food consumption was mostly comparable to the control animals in all dose groups.

Laboratory Findings – Clinical Chemistry, Haematology, Urinalysis

There were no treatment-related changes in the various clinical chemistry, blood parameters and urine parameters in animals from any of the dose groups at the end of the treatment period. Several parameters showed isolated statistically significantly changes, but were not considered to have toxicologically relevance.

Effects in Organs

Two dogs from the low and mid dose groups were found to have hypoplastic testes, but these effects were considered by the study authors to be congenital rather than treatment-related. A statistically significant reduction of absolute heart weight was observed in high dose males, but with no associated histological changes, and a lower liver weight was observed in low dose males. There were no other statistically significant differences in the organ weights of the animals in the control group and animals from any of the dose groups.

Remarks – Results

A NOAEL was not established by the study authors.

TEST FACILITY Pharmacopathics (1976b)

B.9. Genotoxicity – Bacteria

TEST SUBSTANCE	Assessed chemical at 35.2% concentration
METHOD	OECD TG 471 Bacterial Reverse Mutation Test (1997) EC Council Regulation No 440/2008 B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria Plate incorporation procedure (test 1)/Pre incubation procedure (test 2)
Species/Strain	*Salmonella typhimurium*: TA1535, TA1537, TA98, TA100 *Escherichia coli*: WP2uvrA
Metabolic Activation System	S9-Mix from phenobarbital /β-naphthoflavone induced rat liver
Concentration Range in Main Test	a) With metabolic activation: 100 – 15,000 µg/plate b) Without metabolic activation: 100 – 15,000 µg/plate
Vehicle	Water
Remarks – Method	GLP Certificate. Pre incubation test was only conducted on *E.coli*: WP2uvrA. The maximum dose of 15,000 µg/plate was selected to account for the purity of the test substance. Vehicle and positive controls were run concurrently with the test substance.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	-	> 15,000	Negative	Negative
Test 2	-	> 15,000	Negative	Negative
Present				
Test 1	-	> 15,000	Negative	Negative
Test 2	-	> 15,000	Negative	Negative

Remarks – Results	A slight cytoxicity was observed as small decreases in the number of revertants in the 15,000 µg/plate for the plate test, and 7500 and 15,000 µg/plate for the pre incubation test. No significant increases in the frequency of revertant colonies were observed for any of the bacterial strains, at any test concentration, either with or without metabolic activation. The positive and vehicle controls gave satisfactory responses confirming the validity of the test system.
CONCLUSION	The test substance was not mutagenic to bacteria under the conditions of the test.
TEST FACILITY	BASF (2011)

B.10. Genotoxicity – *In Vitro* Mammalian Chromosome Aberration Test

TEST SUBSTANCE	Assessed chemical at 87.8% concentration
METHOD	OECD TG 473 *In vitro* Mammalian Chromosome Aberration Test (1997) EC Directive 2000/32/EC B.10 Mutagenicity – *In vitro* Mammalian Chromosome Aberration Test
Species/Strain	Human peripheral blood cells
Cell Type/Cell Line	Lymphocytes
Metabolic Activation System	S9 mix from Aroclor-1254 induced rat liver
Vehicle	Culture medium

Remarks – Method GLP Certificate

A vehicle control and two positive controls (mitomycin C in the absence of S9, cyclophosphamide in the presence of S9) were run concurrently with the assessed chemical.

In the tests without S9, the levels that could be analysed were limited at higher concentrations by an aggregate that did not allow cells to spread on the slide for analysis.

Metabolic Activation	*Test Substance Concentration (µg/mL)*	*Exposure Period*	*Harvest Time*
Absent			
Test 1	39.06, 78.13, 156.3, 312.5, 625*, 1250*, 2500*, 5000	3 hours	20 hours
Test 2	156.3, 312.5*, 625*, 1250*, 2500, 3750	20 hours	20 hours
Test 3	156.3, 312.5, 625, 1250*, 2500, 3750	44 hours	44 hours
Present			
Test 1	39.06, 78.13, 156.3, 312.5, 625, 1250*, 2500*, 5000*	3 hours	20 hours
Test 2	312.5, 625, 1250, 2500*, 3750*, 5000*	3 hours	20 hours
Test 3	312.5, 625, 1250, 2500, 3750, 5000*	3 hours	44 hours

*Cultures selected for metaphase analysis

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/mL) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	-	> 2,500	≥ 5,000	Negative
Test 2	-	> 1,250	≥ 2,500	Negative
Test 3	-	≥ 2,500	Negative	Negative
Present				
Test 1	-	> 5,000	Negative	Negative
Test 2	-	> 5,000	Negative	Negative
Test 3	-	> 5,000	Negative	Negative

Remarks – Results The test substance did not cause any dose related or statistically significant increase in the number of cells with structural chromosome aberrations in either the absence or presence of metabolic activation when tested up to the highest concentration.

The positive and vehicle controls gave satisfactory responses confirming the validity of the test system.

CONCLUSION The test substance was not clastogenic to human lymphocytes treated *in vitro* under the conditions of the test.

TEST FACILITY CIT (2003)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready Biodegradability

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 301 F Ready Biodegradability: Manometric Respirometry Test
Inoculum	Activated sludge
Exposure Period	28 days
Auxiliary Solvent	None
Analytical Monitoring	Biochemical Oxygen Demand (BOD)
Remarks – Method	Sodium benzoate was used as a reference substance. A toxicity control was also conducted.

RESULTS

Test Substance		*Sodium Benzoate*		*Toxicity control*	
Day	*% Degradation*	*Day*	*% Degradation*	*Day*	*% Degradation*
2	0*	2	49	2	17
4	0*	4	65	4	22
12	0*	12	84	12	31
22	0*	22	88	22	32
28	0*	28	92	28	33

*Negative degradation values were corrected to 0

Remarks – Results	All validity criteria were met. The difference in extremes of the measured degradation of the test item was <10% between replicates, the oxygen uptake in the inoculum blank was 14 mg O_2/L and the pH was maintained between 7.5 and 8.5. The degradation of the reference substance was based on measurements from a single test vessel, due to a leak in the duplicate test vessel. This is not expected to have significantly affected the outcome of the study. The toxicity test reached 33% degradation and therefore the test substance is not considered toxic to the inoculum.
CONCLUSION	The test substance is not readily biodegradable
TEST FACILITY	Solvias (2003h)

C.2. Ecotoxicological Investigations

C.2.1. Acute Toxicity to Fish

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 203 Fish, Acute Toxicity Test – static
Species	*Danio rerio* (zebrafish)
Exposure Period	96 hours
Auxiliary Solvent	None
Water Hardness	160 mg $CaCO_3$/L
Analytical Monitoring	Ion exchange chromatography
Remarks – Method	Based on a range finding study, test concentrations (detailed below) were prepared from dilution of a stock solution.

RESULTS

Concentration (mg/L)		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*4 h*	*24 h*	*48 h*	*72 h*	*96 h*
Control	-	7	0	0	0	0	0
1.7	< LOQ	7	0	0	0	0	0
4.7	< LOQ	7	0	0	0	0	0
13	11	7	0	1	1	2	2
36	31	7	0	2	7	7	7
100	106	7	0	7	7	7	7

LC50	11 mg/L at 96 hours
NOEC (or LOEC)	4.7 mg/L at 96 hours
Remarks – Results	All validity criteria were met. The dissolved oxygen content was maintained at > 60% of the air saturation value and the concentration of the test substance was analysed. LC50 values were calculated based on the measured test concentrations.
CONCLUSION	Test substance is harmful to fish
TEST FACILITY	Solvias (2003i)

C.2.2. Acute Toxicity to Aquatic Invertebrates

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 202 Daphnia sp. Acute Immobilisation Test and Reproduction Test – Static
Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	None
Analytical Monitoring	Ion exchange chromatography
Remarks – Method	Based on a range finding study, test concentrations (detailed below) were prepared from dilution of a stock solution. A reference substance (potassium dichromate) was run prior to the definitive study as part of a quarterly quality assurance program.

RESULTS

Concentration (mg/L)		*Number of D. magna*	*Number Immobilised*	
Nominal	*Measured**		*24 h*	*48 h*
Control	-	20	1	1

20	17	20	1	1
30	24	20	0	0
45	39	20	0	0
68	60.5	20	0	2
102	103	20	0	9

*Arithmetic mean of initial and end concentrations

LC50	80 mg/L at 48 hours
NOEC (or LOEC)	39 mg/L at 48 hours
Remarks – Results	EC50 was calculated based on nominal concentrations of the test substance. All validity criteria were met. Dissolved oxygen was maintained at > 3 mg/L, pH was maintained between 8.0 and 8.5 and temperature was maintained between 19.5 and 20.1°C. The 24 h EC50 of the reference substance was 0.9 mg/L (within the expected range).
CONCLUSION	The test substance is harmful to aquatic invertebrates.
TEST FACILITY	Solvias (2003j)

C.2.3. Algal Growth Inhibition Test

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 201 Alga, Growth Inhibition Test (1984)
Species	*Pseudokirchneriella subcapitata*
Exposure Period	72 hours
Concentration Range	Nominal: 0.4 - 100 mg/L Actual: mg/L
Auxiliary Solvent	None
Analytical Monitoring	Ion exchange chromatography
Remarks – Method	Based on a range finding study, test concentrations were prepared from dilution of a stock solution.

RESULTS

Growth rate		*Biomass*	
ErC50 (mg/L)	*NOEC (mg/L)*	*EbC50 (mg/L)*	*NOEC (mg/L)*
9.6	5	4.0	1.2

Remarks – Results	All validity criteria (OECD TG 201 1984) were met. The control cell density increased by a factor >16.
CONCLUSION	Test substance is toxic to algal growth
TEST FACILITY	Solvias (2003k)

C.2.4. Fish Early Life-Stage Toxicity Test

TEST SUBSTANCE	Solution containing the assessed chemical at 40% concentration
METHOD	OECD TG 212 Fish, Short-term Toxicity Test on Embryo and Sac-fry Stages – Semi-static
Species	*Brachydanio rerio* (zebrafish)
Exposure Period	9 Days
Auxiliary Solvent	None
Water Hardness	125 mg $CaCO_3$/L
Analytical Monitoring	LC-MS/MS
Remarks – Method	As per OECD test guidelines. No deviations were noted.

RESULTS

Nominal concentration test substance (mg/L)	Number exposed	Number hatched	Number surviving on Day 9	Mean total length (mm)
Control	60	57	57	4.2 ± 0.2
11	60	58	58	4.2 ± 0.1
25	60	57	57	4.2 ± 0.1
52	60	52	52	4.3 ± 0.1
114	60	56	56	4.2 ± 0.1
250	60	56	56	4.1 ± 0.1

NOEC >100 mg/L at 9 Days
LOEC >100 mg/L at 9 Days
Remarks – Results 250 mg/L test substance is equivalent to 100 mg/L of the assessed chemical. All validity criteria were met, dissolved oxygen was maintained at >60%, water temperature was maintained at 25°C ± 1°C. In the control group 95% of the embryos hatched and 100% survival rate post hatching was achieved.

CONCLUSION The test substance is not harmful to the early life-stage of fish.

TEST FACILITY Harlan (2009)

C.2.5. Acute Toxicity to Earthworms

TEST SUBSTANCE Assessed chemical

METHOD OECD TG 207 Earthworm, Acute Toxicity Tests
Species *Eisenia foetida*
Duration 14 days
Concentration range 470 – 5000 mg/kg (dry wt.)
Remarks – Method No range finding test was conducted, five concentrations of the assessed chemical were prepared by dissolving it in deionised water and adding directly to soil which was then divided up into the test vessels.

RESULTS

Nominal Concentration (mg/kg dry weight)	*Total number of test earthworms*	*Exposure duration*	
		7 d *Cumulative mortality (%)*	*14 d* *Cumulative mortality (%)*
Control	40	0	0
470	40	0	0
860	40	0	0
1540	40	0	0
2780	40	0	0
5000	40	0	10

Remarks – Results The validity criterion was met.
CONCLUSION The assessed chemical is not harmful to earthworms.

TEST FACILITY Solvias (2003l)

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