File No: LTD/1692

March 2015

**NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)**

# PUBLIC REPORT

## Hexanedioic acid, polymer with 2,2-bis(hydroxymethyl)-1,3-propanediol, decanoate isooctadecanoate octanoate (INCI name: Pentaerythrityl Isostearate/Caprate/Caprylate/Adipate)

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

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

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


| | |
|---|---|
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**Director**
**NICNAS**

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# SUMMARY

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

| ASSESSMENT REFERENCE | APPLICANT(S) | CHEMICAL OR TRADE NAME | HAZARDOUS CHEMICAL | INTRODUCTION VOLUME | USE |
|---|---|---|---|---|---|
| LTD/1692 | Croda Australia and L'Oreal Australia Pty Ltd | Hexanedioic acid, polymer with 2,2-bis(hydroxymethyl)-1,3-propanediol, decanoate isooctadecanoate octanoate (INCI name: Pentaerythrityl Isostearate/Caprate/Caprylate/Adipate) | ND* | 7.5 tonnes per annum | Cosmetic ingredient |

*ND = not determined

# CONCLUSIONS AND REGULATORY OBLIGATIONS

**Hazard classification**
Based on the available information, the notified polymer is not recommended for classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals* (GHS), as adopted for industrial chemicals in Australia, or the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

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

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

**Environmental risk assessment**

On the basis of the assessed use pattern and expected low exposure to the aquatic environment, the notified polymer is not expected to pose an unreasonable risk to the environment.

**Recommendations**

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following engineering controls to minimise occupational exposure to the notified polymer during reformulation processes:
  - Enclosed, well-ventilated automated processes, where possible.

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure during handling of the notified polymer at a concentration of up to > 90% during reformulation:
  - Avoid contact with skin and eyes and 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 notified polymer during reformulation process:
  - Coveralls, impervious gloves, goggles

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

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

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

Disposal

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

Emergency procedures

- Spills or accidental release of the notified polymer should be handled by containment, physical 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 polymer is listed on the Australian Inventory of Chemical Substances (AICS).

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

(1) Under Section 64(1) of the Act; if
- the polymer has a number-average molecular weight of less than 1000;
- the concentration of the notified polymer is intended to exceed 50% in makeup products, 20% in rinse-off cosmetics, fragrance and deodorant products and 40% in other leave-on cosmetic products.

or

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

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

*(Material) Safety Data Sheet*
The (M)SDS of the notified polymer (and products containing the notified polymer) provided by the notifier was reviewed by NICNAS. The accuracy of the information on the (M)SDSs remains the responsibility of the applicant.

# ASSESSMENT DETAILS

## 1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Croda Australia (ABN: 34 088 345 457)
Suite 104, 447 Victoria St
Wetherill Park NSW 2164

L'Oreal Australia Pty Ltd (ABN: 40 004 191 673)
564 St Kilda Road
Melbourne VIC 3004

NOTIFICATION CATEGORY
Limited: Synthetic polymer with Mn ≥ 1,000 Da.

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: structural formulae, molecular weight, analytical data, degree of purity, polymer constituents, residual monomers, impurities, additives/adjuvants, use details, import volume and identity of manufacturer.

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

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
None

## 2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Supermol L
Supermol L-LQ-(RB)

CAS NUMBER
161308-02-7

CHEMICAL NAME
Hexanedioic acid, polymer with 2,2-bis(hydroxymethyl)-1,3-propanediol, decanoate isooctadecanoate octanoate

OTHER NAME(S)
Adipic acid, oligomeric reaction products with decanoic acid, isooctadecanoic acid, octanoic acid and pentaerythritol
Pentaerythrityl Isostearate/Caprate/Caprylate/Adipate (INCI name)

MOLECULAR FORMULA
$C_{18}\ H_{36}\ O_2$ . x $C_{10}\ H_{20}\ O_2$ . x $C_8\ H_{16}\ O_2$ . x $(C_6\ H_{10}\ O_4$ . $C_5\ H_{12}\ O_4)_x$

MOLECULAR WEIGHT
> 1,000 Da

ANALYTICAL DATA
Reference GPC, IR and UV spectra were provided.

## 3. COMPOSITION

DEGREE OF PURITY
> 90%

## 4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: Amber/yellow liquid

| Property | Value | Data Source/Justification |
|---|---|---|
| Melting Point/Freezing Point | Not determined | The Polymer is liquid at ambient temperature |
| Boiling Point | > 200 °C | Statement by notifier |
| Density | 0.981 at 25°C | Statement by notifier |
| Vapour Pressure | Not determined | Expected to be low on the basis of the high molecular weight (>1000). |
| Water Solubility | 1.28 x $10^{-35}$ g/L | Calculated using WSKOW v1.42 (US EPA, 2011). |
| Hydrolysis as a Function of pH | $t_{½}$ = 16.78 and 1.68 minutes at pH 7 and 8 respectively. | Calculated using HYDROWIN v2.00 (US EPA, 2011). |
| Partition Coefficient (n-octanol/water) | log Kow = 31.87 | Calculated using KOWWIN v1.68 (US EPA, 2011). |
| Adsorption/Desorption | log $K_{oc}$ = 17.96 | Calculated using KOCWIN v2.00 (US EPA, 2011). |
| Dissociation Constant | Not determined | No dissociable functionality. |
| Flash Point | > 100 °C (open cup) | (M)SDS |
| Autoignition Temperature | Not determined | Expected to be high on the basis of the flash point. |
| Explosive Properties | Not determined | Contains no functional groups that would imply explosive properties. |
| Oxidising Properties | Not determined | Contains no functional groups that would imply oxidising properties. |

DISCUSSION OF PROPERTIES
*Reactivity*
The notified polymer is expected to be stable under normal conditions of use.

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

## 5. IDENTITY AND EVALUATION OF ANALOGUES

**Analogue 1**
CHEMICAL NAME
Fatty acids, $C_{16-18}$ and $C_{18}$-hydroxy, polymers with adipic acid, decanoic acid, isostearic acid, octanoic acid, pentaerythritol and stearic acid

CAS NUMBER
130353-58-1

OTHER NAME(S)
Pentaerythrityl Stearate/Caprate/Caprylate/Adipate (INCI name)

MOLECULAR WEIGHT
Unspecified

**Analogue 2**
CHEMICAL NAME
Isooctadecanoic acid, 1,1'-[2,2-bis[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl] ester

CAS NUMBER
62125-22-8

OTHER NAME(S)
Pentaerythrityl Tetraisostearate (INCI name)

MOLECULAR WEIGHT
1202 Da

**Analogue 3**
CHEMICAL NAME
Carboxylic acids, $C_{5-9}$, tetraesters with pentaerythritol

CAS NUMBER
67762-53-2

OTHER NAME(S)
Pentaerythrityl Tetra $C_{5-9}$ Acid Esters (INCI name)

MOLECULAR WEIGHT
585 Da

**Analogue 4**
CHEMICAL NAME
Pentaerythritol esters of isooctanoic acid and C8-10 fatty acids

CAS NUMBER
Not known.

MOLECULAR WEIGHT
697 Da

The analogues are deemed suitable to inform the hazard profile of the notified polymer, due to structural and physico-chemical properties similarities.

## 6. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified polymer will be imported into Australia in formulated finished cosmetic products and as the polymer itself for reformulation.

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

| *Year* | *1* | *2* | *3* | *4* | *5* |
|---|---|---|---|---|---|
| *Tonnes (Croda)* | 2.5 | 2.5 | 2.5 | 2.5 | 2.5 |
| *Tonnes (L'Oreal)* | 5 | 5 | 5 | 5 | 5 |

PORT OF ENTRY
Melbourne and Sydney.

TRANSPORTATION AND PACKAGING
The notified polymer in its neat form will be imported to Australia by sea and transported by rail or road from the port of entry to the customer's storage facility in 50 kg plastic containers. Products containing the notified polymer, also imported to Australia by sea, will be packed in bottles and tubes (sizes up to 500mL made mainly from HDPE) as follows: dozens inside a shipper, with multiple shippers per pallet and multiple pallets per shipping container. The containers will be taken from the wharf in Melbourne and/or Sydney and transported to the appropriate central distribution centres and delivered to major retailer warehouses.

USE
The notified polymer will be used in a wide range of cosmetic products applied on skin and by spray, up to a concentration of 50%. The concentration of the notified polymer in individual cosmetic products is exempt information.

OPERATION DESCRIPTION

*Reformulation*
When reformulated in Australia, the notified polymer will be blended into end-use consumer products at customer sites. Procedures will vary depending on the nature of the cosmetic product being formulated. Both manual and automated steps will be involved. For example, a chemist will sample the notified polymer manually, a compounder will weigh an appropriate amount of the notified polymer into a container then add the amount directly into a flame proof mixing tank, and periodic sampling for quality control purposes will also be carried out during the reformulation process. Automated processes may include mixing and filling of end-use containers with products. These processes are typically carried out in a closed system with adequate ventilation.

*End-use*
Finished cosmetic products containing the notified polymer at up to 50% concentration will be used by consumers and by professionals such as hairdressers and beauticians. Depending on the nature of the product, the method of application could be varied – by hand, using an applicator or sprayed.

## 7. HUMAN HEALTH IMPLICATIONS

### 7.1. Exposure Assessment

#### 7.1.1. Occupational Exposure

CATEGORY OF WORKERS

| *Category of Worker* | *Exposure Duration (hours/day)* | *Exposure Frequency (days/year)* |
|---|---|---|
| Transport and storage / warehousing | 4 | 25 |
| Professional compounder / process operator | 8 | 25 |
| Chemist / QC | 3 | 12 |
| Packers (dispensing & capping) | 8 | 25 |
| Waste management | 1 | 40 |
| Hairdressers / Beauticians | 1 | 100 |

EXPOSURE DETAILS
*Transport and storage*
Transport and storage workers may come in contact with the notified polymer either in neat form or at various concentrations in cosmetic products (up to 50%), only in the event of accidental rupture of containers.

*Reformulation*
During reformulation into cosmetic products, dermal, ocular and inhalation exposure of workers (up to >90% concentrations) may occur when handling the notified polymer or products containing it. Exposure is expected to be minimised through the use of local exhaust ventilation and/or automated/enclosed systems as well as through the use of personal protective equipment (PPE) such as coveralls, safety glasses and impervious gloves.

The notifier stated that workers will be required to wear the following PPE: gloves, eye protection, and protective clothing. Full-face protection will be used when there is potential for direct exposure to aerosols and splashes. Respirator will be used if ventilation is inadequate.

Exposure to the notified polymer in end-use products (up to 50% concentration) may occur in professions that involve the use of cosmetic/personal care products (hair dressers and beauty salon workers). Depending on the types of products and method of application, dermal, inhalation and incidental ocular exposure may occur.

#### 7.1.2. Public Exposure

There will be widespread and repeated exposure of the public to the notified polymer (up to 50% concentration) through the use of cosmetic products. The principal route of exposure would be dermal, while ocular and inhalation exposures are also possible, particularly if products are applied by spray. Accidental ingestion of products containing the notified polymer is also possible from use of lip products.

A combined internal dose of 10.1 mg/kg bw/day was estimated using data on typical use patterns of cosmetic product categories in which the notified polymer may be used at up to 50% concentration (SCCS, 2010; Cadby

*et al*, 2002; SDA, 2005; specific use details of the notified polymer are considered exempt information). This estimation assumed a worst case scenario and is for a person who is a simultaneous user of a selection of cosmetic products that may contain the notified polymer.

### 7.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified polymer and suitable analogues are summarised in the following table. Refer to the Appendix for details of the studies.

| *Endpoint* | *Result and Assessment Conclusion* |
|---|---|
| Rat, acute oral toxicity (analogue 2) | LD50 > 10,000 mg/kg bw |
| Skin irritation (in vitro) (notified polymer) | non-irritating |
| Rabbit, skin irritation (analogue 2) | slightly irritating |
| Eye irritation (in vitro) (5, 10 & 15% notified polymer) | non-irritating |
| Rabbit, eye irritation (analogue 2) | slightly irritating |
| Human, skin sensitisation – RIPT (40% notified polymer) | no evidence of sensitisation |

*Toxicokinetics, metabolism and distribution.*
No toxicokinetic data were submitted for the notified polymer. Based on the high molecular weight (> 1,000 Da), the estimated very low water solubility ($1.28 \times 10^{-35}$ g/L) and high calculated partition coefficient (log Kow = 31.87) dermal absorption of the notified polymer is expected to be very low. A value of 10% was assumed for the purpose of the risk assessment (ECHA 2012). The dermal bioavailability for analogue 3, which has a significantly lower molecular weight compared to the notified polymer, was reported to be 2 – 6% (CIR 2012).

*Acute toxicity.*
Acute toxicity information on the notified polymer was not provided. The notified polymer is of high molecular weight and is unlikely to readily cross biological membranes. Information on analogues 2 and 3 (CIR 2012) also support an expected low acute toxicity for the notified polymer.

*Irritation and sensitisation.*
Skin and eye irritancy potential of the notified polymer was assessed as very low in the *in vitro* MatTek EpiDerm skin model and in an *in vitro* Hen's Egg Test on Chorio-Allantoic-Membrane (HET-CAM) respectively. Analogue 2 was found to be slightly irritating to the skin and the eye when tested on rabbits. Analogue 1 was also reported to have low skin and eye irritation (CPT 1995, Biogir 1991a, Biogir 1991b).

The notified polymer was not irritating or sensitising to the skin at 40% concentration in a human repeat insult patch test (HRIPT) with 97 subjects. The notified polymer has no structural alerts for sensitisation.

*Repeated dose toxicity.*
No repeat dose toxicity studies on the notified polymer were provided. Use of the OECD QSAR Toolbox indicates that the monomers of the notified polymer show little or no toxicity at the proposed use concentrations in cosmetics (up to 50%) for the notified polymer.

Analogue 4 is reported in a US EPA Hazard Characterisation Document (US EPA 2010) to have been tested in rats (Crl:CD BR 5/sex/dose) via oral gavage for 28 days at 0, 100, 500 and 1000 mg/kg bw/day. There were no clear treatment-related effects on clinical signs, body weight, food consumption, functional observation battery, motor activity, clinical laboratory parameters, gross necropsy, organ weights or histopathological observations. The NOAEL was established at 1,000 mg/kg bw/day (highest dose tested).

A 90-day dermal toxicity study on Analogue 3 is reported in cosmetic ingredient review for pentaerythrityl tetraesters (CIR 2012). According to the report, the test substance was applied at concentrations of 0, 800 and 2,000 mg/kg bw to clipped back of Sprague Dawley rats (n=10/sex) for 5 day/week for 13 weeks. The area was not covered but collars were used to prevent grooming of the area. Males in the high dose group weighed 10% less than the control group and 7% less than those in the low dose group at the end of the study. No effects on the body weights occurred in females. No other signs of systemic toxicity were reported. There was minimal skin irritation; flanking with slight erythema was observed in both treatment groups. Microscopic examination of the skin revealed very minor epidermal hyperplasia and chronic inflammation of the dermis. The NOAEL was reported to be 2,000 mg/kg bw/day.

*Mutagenicity/Genotoxicity.*
No mutagenicity/genotoxicity studies were reported for the notified polymer. Bacterial reverse mutation assays carried out on analogue 3 and analogue 4 found the chemicals to be non-toxic and non-mutagenic at up to the

highest test concentration of 5,000 µg/plate. An *in vitro* chromosome aberration test carried out on analogue 4 using Chinese Hamster Ovary cells was reported to be negative. *In vivo* micronucleus assays on analogue 3 and analogue 4 in rats showed no evidence of genotoxicity (CIR 2012, US EPA 2010).

*Toxicity for reproduction.*
No reproduction toxicity studies were reported for the notified polymer. A reproduction/developmental toxicity study is reported for analogue 4 (US EPA 2010). As per the report, pregnant female Crl:CD BR VAF/Plus strain rats (25/group) were administered the test substance by oral gavage at 0, 100, 500 or 1,000 mg/kg bw/day on days 6 to 15 of gestation. There were no treatment related mortalities, clinical signs or effects on maternal body weight, uterine weight, food consumption or gross pathology. No treatment-related effects were observed on implantation parameters, mean foetal body weight, mean skeletal ossification sites or number of total or individual variations and malformations. A NOAEL of 1,000 mg/kg bw/day was reported.

***Health hazard classification***
Based on the available information, the notified polymer is not recommended for classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia, or the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

### 7.3. Human Health Risk Characterisation

#### 7.3.1. Occupational Health and Safety

*Transport and Reformulation*
Workers may experience dermal and accidental ocular exposure to the notified polymer (at up to >90% concentration) during transport and formulation processes. This exposure may occur during handling of the containers, cleaning and/or maintenance of the equipment. At these facilities, exposure may also extend to compounders and laboratory staff involved in the formulation of the end products containing the notified polymer and the sampling and quality control testing of these products. The notifier has stated that processes will include use of enclosed, automated processes. The use of PPE (impervious gloves, safety glasses and coveralls) should further minimise the potential for exposure.

Therefore, under the expected scenarios for transport and reformulation, the risk to workers from use of the notified polymer is not considered to be unreasonable.

*End-use*
Workers involved in professions where the services provided involve the application of cosmetic products to clients (e.g. hairdressers or beauty salon workers), may be exposed to the notified polymer during their application of products to salon clients. Such professionals may use PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. The risk to these workers is expected to be of a similar or lesser extent than that experienced by consumers using products containing the notified polymer on a regular basis (for details of the public health risk assessment, see Section 6.3.2.).

Based on the information available, the risk to workers associated with use of the notified polymer at ≤ 50% concentration in cosmetic products is not considered to be unreasonable.

#### 7.3.2. Public Health

Members of the public may be repeatedly exposed to the notified polymer during the use of cosmetic products at up to 50% concentration. Based on available information on the notified polymer and analogues, it is expected to have low acute toxicity and low irritation and no sensitisation potential. The available data did not raise concern for genotoxicity or reprotoxicity.

The repeated dose toxicity potential was estimated by calculation of the margin of exposure (MOE) of the notified polymer using the worst case exposure scenario from the use of multiple products of 10.1 mg/kg bw/day (see Section 6.1.2.). Using the NOAEL in the oral repeated dose toxicity study reported for analogue 4 (1,000 mg/kg bw/day) in the calculation of the MOE, the MOE was estimated to be 99. A MOE value greater than or equal to 100 is considered acceptable to account for intra- and inter-species differences. As, the NOAEL of 1,000 mg/kg bw/day is considered to be conservative since it was based on the highest dose tested, and the systemic toxicity of analogue 4 is expected to be higher than that of the notified polymer due to smaller molecular weight and greater bioavailability, the calculated MOE is considered to be acceptable. Therefore the

risk to the public from use of the notified polymer at up to 50% in cosmetic products is not considered to be unreasonable.

## 8. ENVIRONMENTAL IMPLICATIONS

### 8.1. Environmental Exposure & Fate Assessment

#### 8.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE

The notified polymer will not be manufactured in Australia. It will be imported as a component of finished cosmetic products (e.g. lipsticks) or reformulated into cosmetic products at customer sites in Australia. There is unlikely to be any significant release of the notified polymer to the environment from storage and transport, except in the case of accidental spills. Accidental spills are expected to be contained and disposed of to landfill.

RELEASE OF CHEMICAL FROM USE

The notified polymer is a component in finished cosmetic products. The formulated product will be applied to the skin and will either be ingested, wiped off by tissues and disposed of to domestic garbage, or washed off the body and ultimately released to sewer.

RELEASE OF CHEMICAL FROM DISPOSAL

Expired waste and residue of the notified polymer in the empty containers (3%) is likely either to share the fate of the container and be disposed of to landfill, or to be washed to sewer when containers are rinsed before recycling.

#### 8.1.2. Environmental Fate

The majority of the notified polymer will be disposed of to the sewer and, as it is a high molecular weight non-ionic polymer, it is estimated to be removed by up to 90% in sewage treatment plants by partitioning to sediment and sludge (Boethling & Nabholz, 1997). The notified polymer that partitions to sludge will be removed with the sludge for disposal to landfill or used in soil remediation. Hence, it is not anticipated to be significantly bioavailable to aquatic organisms. In the aquatic environment it is unlikely to bioaccumulate based on its high molecular weight and low water solubility. In landfill it is expected to degrade biotically and abiotically to form water and oxides of carbon.

#### 8.1.3. Predicted Environmental Concentration (PEC)

The predicted environmental concentration (PEC) has been calculated assuming a worst case scenario of 100% release of the notified polymer into sewer systems nationwide and no removal from STPs.

| ***Predicted Environmental Concentration (PEC) for the Aquatic Compartment*** | | |
|---|---|---|
| Total Annual Import/Manufactured Volume | 7,500 | kg/year |
| Proportion expected to be released to sewer | 100% | |
| Annual quantity of polymer released to sewer | 7,500 | kg/year |
| Days per year where release occurs | 365 | days/year |
| Daily polymer release: | 20.55 | kg/day |
| Water use | 200 | L/person/day |
| Population of Australia (Millions) | 22.613 | million |
| Removal within STP | 0% | |
| Daily effluent production: | 4,523 | ML |
| Dilution Factor - River | 1.0 | |
| Dilution Factor - Ocean | 10.0 | |
| PEC - River: | 4.54 | µg/L |
| PEC - Ocean: | 0.45 | µg/L |

STP effluent re-use for irrigation occurs throughout Australia. The agricultural irrigation application rate is assumed to be 1000 L/$m^2$/year (10 ML/ha/year). The notified polymer 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 4.54 µg/L may potentially result in a soil concentration of approximately 30.29 µg/kg.

Assuming accumulation of the notified polymer in soil for 5 and 10 years under repeated irrigation, the concentration of notified polymer in the applied soil in 5 and 10 years may be approximately 151 µg/kg and 302.9 µg/kg, respectively.

### 8.2. Environmental Effects Assessment

No ecotoxicity data were submitted. High molecular weight chemicals without significant ionic functionality are of low concern to the aquatic environment. Due to its low solubility and likelihood for adsorption to sludge and sediment, the notified polymer is not expected to be present in water at concentrations that are hazardous to aquatic organisms.

#### 8.2.1. Predicted No-Effect Concentration

A predicted no-effect concentration (PNEC) was not calculated since no ecotoxicity data were available for the notified polymer.

### 8.3. Environmental Risk Assessment

The majority of notified polymer disposed of to the sewer is expected to be removed by partitioning to sludge and sediment during sewage treatment plant processes. As a result, it is not likely to be present in ecotoxicologically significant concentrations in the aquatic environment. In the aquatic environment it is unlikely to bioaccumulate based on its high molecular weight and low water solubility. Therefore, the notified polymer is not expected to pose an unreasonable risk to the environment on the basis of the assessed use pattern.

# APPENDIX: TOXICOLOGICAL INVESTIGATIONS

## 1. Acute toxicity – oral

TEST SUBSTANCE: Analogue 2

METHOD: Similar to OECD TG 401 Acute Oral Toxicity.
- Species/Strain: Rat/CD
- Vehicle: Vegetable oil
- Remarks - Method: A single group of rats were exposed to the test substance by oral gavage. The rats were observed for signs of toxicity immediately after administration, 4 h after dosing and then daily for 14 days.

RESULTS

| *Group* | *Number and Sex of Animals* | *Dose mg/kg bw* | *Mortality* |
|---|---|---|---|
| 1 | 5 F & 5 M | 10,000 | 0/10 |

- LD50: > 10,000 mg/kg bw
- Signs of Toxicity: All the rats were hypoactive at the 4 h observation period. No signs of toxicity were observed after that till the end of the study period.
- Effects in Organs: No histopathological studies were conducted
- Remarks - Results: None

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

TEST FACILITY: TLL (1981a)

## 2. Irritation – skin

TEST SUBSTANCE: Analogue 2

METHOD: Similar to OECD TG 404 Acute Dermal Irritation/Corrosion.
- Species/Strain: Rabbit/New Zealand White
- Number of Animals: Six
- Vehicle: None
- Observation Period: 48 hours
- Type of Dressing: Occlusive
- Remarks - Method: The method varied from that of OECD TG 404. Each rabbit was tested for irritancy potential of the test substance at 2 different sites. One site was lightly abraded with a needle to damage the stratum corneum. 0.5ml of the test substance was applied to each site and left for 24 h. The sites were evaluated 1 h and 48 h after patch removal.

RESULTS

| *Lesion* | *Mean Score** | | | | | | *Maximum Value* | *Maximum Duration of Any Effect* | *Maximum Value at End of Observation Period* |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | | | |
| *Erythema/Eschar* | 0.50 | 1.00 | 0.00 | 1.00 | 0.50 | 1.00 | 1 | 48 h | 1 |
| *Oedema* | 0.00 | 0.25 | 0.00 | 0.00 | 0.00 | 0.25 | 1 | 24 h | 0 |

* Calculated on the basis of the scores for abraded and unabraded skin at 1 h and 48 hours for EACH animal.

- Remarks - Results: Desquamation of the skin was observed in one rabbit at 48 h on the abraded site.

| | |
|---|---|
| CONCLUSION | The analogue chemical is slightly irritating to the skin. |
| TEST FACILITY | TLL (1981b) |

**3. Irritation – skin (in vitro)**

| | |
|---|---|
| TEST SUBSTANCE | Notified polymer |
| METHOD | The MatTek Corporation EpiDerm™ Skin Model *In vitro* Toxicity Test. |
| Vehicle | |
| Remarks - Method | MatTek Epiderm tissue samples were treated with the test substance (100 µL) and negative control for 1, 4 and 24 h exposure times. The identity of the negative control was not given. Each treatment was conducted in duplicate. Following treatment, the viability of the tissues was determined after a 3-hour exposure to MTT and conversion to formazin derivative, and the absorbance of each sample was measured at 570 nm. With the absorbance of the negative control defined as 100%, the percent absorbance of the test substance was determined. The mean percent viability was used to calculate the $ET_{50}$ (the time at which the EpiDerm tissue viability was reduced 50% compared to control tissues). |

RESULTS

| *Test material concentration* | *Test material incubation time* | *Relative mean Viability (%)* |
|---|---|---|
| 100% | 1 h | 92 |
| 100% | 4.5 h | 98 |
| 100% | 20 h | 92 |

| | |
|---|---|
| Remarks - Results | The test substance elicited an $ET_{50}$ greater than 24 h. |
| CONCLUSION | The notified polymer was predicted to be non-irritating to the skin under the conditions of the test. |
| TEST FACILITY | CPT (2005a) |

**4. Irritation – eye**

| | |
|---|---|
| TEST SUBSTANCE | Analogue 2 |
| METHOD | Similar to the OECD TG 405 Acute Eye Irritation/Corrosion guidelines. |
| Species/Strain | Rabbit/New Zealand White |
| Number of Animals | Six |
| Observation Period | 72 hours |
| Remarks - Method | 0.1ml of undiluted test substance was instilled into one eye of each of the test animals. The other eye served as a control. The eyes were not washed after instillation of the test substance. The eyes were examined at 24 h, 48 h and 72 h after instillation for damage or irritation to the cornea, iris and conjunctiva. |

RESULTS

| *Lesion* | *Mean Score** | | | | | | *Maximum Value* | *Maximum Duration of Any Effect* | *Maximum Value at End of Observation Period* |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | | | |
| *Conjunctiva: redness* | 0.33 | 0.33 | 0.66 | 0.33 | 1.33 | 0.33 | 2 | 48 h | 0 |
| *Conjunctiva: chemosis* | 0.00 | 0.00 | 0.00 | 0.00 | 0.66 | 0.3 | 1 | 48 h | 0 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| *Conjunctiva: discharge* | 0.00 | 0.33 | 1.00 | 0.33 | 1.33 | 0.66 | 2 | 48 h | 0 |
| *Corneal opacity* | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0 | --- | 0 |
| *Iridial inflammation* | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0 | --- | 0 |

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

CONCLUSION The analogue chemical is slightly irritating to the eye.

TEST FACILITY TLL (1981c)

**5. Irritation – eye (in vitro)**

TEST SUBSTANCE Notified polymer

METHOD The Hen's Egg Test – Utilizing the Chorioallantoic Membrane (HET-CAM) Test. Modification of that described by Kemper and Luepke (1986).

Species/Strain Moyer's chicken eggs

Vehicle Corn oil

Remarks - Method The eggs were fertilised and incubated for the test substance, negative and positive controls readings taken at 0.5, 2 and 5 mins. The eggs were incubated at 37°C and a relative humidity of 60–70% in an automatic, rotating incubator for 9 days. On day 10, the shell over the air sac of each egg was removed. The inner egg membrane sack was wetted with physiological saline for approximately 2–5 minutes and then the inner egg membrane was removed carefully to reveal the CAM. A 300 µL solution of the test substance (undiluted) was applied to each CAM with 5 mL of physiological saline. All CAM's were observed immediately prior to test substance administration and at 30 seconds, 2 and 5 minutes after exposure to the test article. The reactions of the CAM, the blood vessels, including the capillaries, and the albumin were examined and the following scores for irritant effects were applied as described below:

| | *Scores at time (min)* | | |
|---|---|---|---|
| *Effect* | 0.5 | 2 | 5 |
| Hyperemia | 5 | 3 | 1 |
| Minimal Hemorrhage ("Feathering") | 7 | 5 | 3 |
| Hemorrhage (Obvious leakage) | 9 | 7 | 5 |
| Coagulation and/or thrombosis | 11 | 9 | 7 |

Each reaction type can be recorded only once for each CAM, therefore the maximum score per CAM is 32. The mean score was determined for all CAMs similarly tested.

Scoring is according to severity and time needed for the effect to occur. The earlier a symptom is recorded the higher the numerical value is assigned to it. The order of the severity of the endpoints is as follows: Coagulation and/or thrombosis > haemorrhage > minimal haemorrhage > hyperemia.

The notified polymer was tested at 5%, 10% and 15% concentrations in corn oil. The duration of application with the test substance and vehicle was 20 seconds. No positive control was used.

RESULTS

| *Test substance* | *Total scores of quadruplicate samples* | | | Average |
|---|---|---|---|---|
| | 0.5 min | 2 min | 5 min | |
| *Vehicle control* | 0 | 3 | 2 | 1.25 |
| *5%* | 0 | 0 | 4 | 1 |
| *10%* | 0 | 0 | 3 | 0.75 |
| *15%* | 0 | 3 | 2 | 1.25 |

Remarks - Results: Hyperemia was observed at 5 minutes in all the CAMs exposed to 5% of test substance and in 3 of 4 CAMs exposed to 10% of test substance.
Hyperemia was observed in 1 CAM at 2 minutes and 2 CAMs at 5 minutes when exposed to test substance at 15% concentration.

CONCLUSION: Under the conditions of the test the notified polymer is predicted to be non-irritating to the eye.

TEST FACILITY: CPT (2005b)

**6. Skin sensitisation – human volunteers**

TEST SUBSTANCE: Notified polymer (40%)

METHOD: Repeated insult patch test with challenge – in-house method

Study Design: Induction Procedure: 20 µg of the test substance was applied to the infrascapular area of the back, either to the right or left of the midline. This procedure was performed Mondays, Wednesdays and Fridays for three consecutive weeks until 9 applications of the test article had been made. Subjects removed the patches 48 hours (for patches applied on Mondays and Wednesdays) or 72 hours (for patches applied on Fridays) after each application.
Rest Period: 10-15 days
Challenge Procedure: conducted on the sixth week of the study and applied on virgin sites. The patches were removed after 48 h, and sites were scored at patch removal and 48 h after patch removal.

Study Group: 75 F, 30 M; age range 18-70 years

Vehicle: Petrolatum

Remarks - Method: Occluded. The test substance was spread on a 8 mm Finn Chamber.

RESULTS

Remarks - Results: 97/105 enrolled subjects successfully completed the test procedure. Two serious adverse effects occurred: one subject had a mild stroke and another had moderate headaches and depression both required hospitalisation; neither of the adverse effects observed were considered treatment related. The other six subjects were lost to follow up (3) and withdrew voluntarily (3).
There was no skin reactivity observed at any time during the course of the study.

CONCLUSION: The test substance was non-irritating and non-sensitising under the conditions of the test.

TEST FACILITY: TKL (2005)

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