Australian Government
Department of Health and Aged Care
Australian Industrial Chemicals Introduction Scheme

Medium to long chain alkyl and alkene sulfonates

Evaluation statement (EVA00172)

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Draft

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AICIS evaluation statement (EVA00172)

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Medium to long chain alkyl and alkene sulfonates

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Reason for the evaluation

Evaluation Selection Analysis indicated a potential human health risk.

Parameters of evaluation

These chemicals are a group of medium to long chain alkyl and alkene sulfonic acids and their salts that are listed on the Australian Inventory of Industrial Chemicals (the Inventory).

This evaluation is a human health risk assessment of all identified industrial uses of the chemicals in Australia.

This group of chemicals belongs to a widely used class of anionic surfactants. These chemicals have been assessed as a group as they have similar use patterns and are expected to produce alkyl or alkene sulfonate anions at the pH of biological solutions. The cation components are not expected to contribute significantly to the toxicity of these chemicals.

The following chemicals will be referred to by alternative names in this evaluation:

- 1-Dodecanesulfonic acid, sodium salt (1:1) (CAS No. 2386-53-0) will be referred to as sodium 1-dodecanesulfonate
- 1-Octanesulfonic acid, sodium salt (1:1) (CAS No. 5324-84-5) will be referred to as sodium 1-octanesulfonate
- 1-Hexadecanesulfonic acid, sodium salt (1:1) (CAS No. 15015-81-3) will be referred to as sodium 1-hexadecanesulfonate
- Sulfonic acids, C_{13-18}-alkane hydroxy and C_{13-18}-alkene, sodium salts (CAS No. 68439-56-5) will be referred to as sodium C_{13-18} olefin sulfonate.

Several alkyl and alkene sulfonates have been assessed previously (NICNAS 2014; NICNAS 2015, NICNAS 2016). Except for sodium 1-octanesulfonate (CAS No. 5324-84-5) which has new data indicating corrosive effects which became available after the publication of the original report, these chemicals are not being evaluated as part of the evaluation as no significant new data are available. However, data on these chemicals have been used as read across to support conclusions on hazards and use.

Summary of evaluation

Summary of introduction, use and end use

There is limited information about the introduction, use and end use of these chemicals in Australia.

Based on international information for the chemicals and other alkane and alkene sulfonates, the chemicals in this evaluation are expected to be used as surfactants in cosmetic, domestic and commercial applications.

Some chemicals in this evaluation have reported use in personal care products (cosmetics). Information for other alkane and alkene sulfonates indicate likely use in hair care products (liquid), liquid hand soaps, liquid body soaps, skin-applied products (for personal cleanliness) and products diluted for bath use at concentrations up to 20%.

All chemicals in this evaluation are expected to be used as surfactants in domestic and commercial cleaning products. The typical end use concentrations are less than 5%, however, concentrations up to 30% have been reported. The product use category types include:

- laundry and dishwashing products,
- cleaning and furniture care products
- lubricants and greases.

Some chemicals in this evaluation have commercial and site-limited uses including in textile manufacturing, metal cleaning and functional use as an intermediate in the manufacture of chemicals.

Human health

Summary of health hazards

Limited health hazard data are available for these chemicals. The identified health hazards are based on available data for these chemicals, other alkane and alkene sulfonates and from read across to structurally similar medium to long chain alkyl sulfates.

Based on the limited available data, these chemicals:

- have low acute dermal toxicity
- are not considered to be skin sensitisers
- are not expected to cause serious systemic health effects following repeated exposure
- are not expected to cause specific adverse effects on fertility/sexual function and foetal development
- are not expected to have genotoxic potential
- are not expected to be carcinogenic.

For the unknown or variable composition, complex reaction products or biological materials (UVCBs) in this group, the severity of the health hazards outlined below will be dependent on the exact composition of the chemical.

Based on the limited available data from the chemicals in this evaluation and other alkyl and alkene sulfonates (median lethal dose (LD50) values typically between 500 and 2,000 mg/kg bw), most of the chemicals in this evaluation are expected to have moderate acute oral toxicity. Hazard classification is warranted unless experimental data indicates otherwise. Sodium 1-octanesulfonate has a reported LD50 of >5,000 mg/kg bw and does not require hazard classification. Although the available data on acute oral toxicity for the structurally similar alkyl sulfates indicates that the LD50 typically decreases with increasing alkyl chain lengths, no such trend could be identified for the alkyl and alkene sulfonates.

Based on available data including read across, the majority of chemicals in this group are irritating to skin with varying degrees of severity. The available data indicate that the severity of effects generally decreases with chain length and decreasing concentration. Sodium 1-octanesulfonate was reported to be corrosive to skin based on an in vitro assay (the Organisation for Economic Co-operation and Development (OECD) test guideline (TG) 437. Based on read across to structurally similar medium to long chain alkyl sulfates, the alkyl sulfonates with $<C_{12}$ alkyl chains are expected to be corrosive to skin. Animal data for other alkane and alkene sulfonates which have alkyl chains that are typically between C_{13} and C_{18} indicate that these chemicals are irritating to skin at various concentrations, but all signs of erythema and oedema were reversible. Effects sufficient to warrant classification have been observed in some studies. Limited observations of necrosis were reported for some UVCB alkyl sulfates containing mostly $\geq C_{12}$ alkyl chains, but most available studies indicate that these chemicals are irritating to skin. Therefore, most of the remaining chemicals in the group ($\geq C_{12}$) are expected to be irritating to skin but are not considered corrosive. Although the available data on skin irritation effects for the structurally similar alkyl sulfates indicates that alkyl sulfates with carbon chain between C_{16} and C_{18} are only slightly irritating to skin, no such trend could be identified for the alkyl and alkene sulfonates.

Based on available data including read across, the chemicals in this group are expected to cause serious eye damage. Sodium 1-octanesulfonate was reported to be damaging to eyes in an in vitro assay (OECD TG 437). Irreversible eye damage was reported in guideline animal studies for other alkyl and alkene sulfonates which have alkyl chains that are typically between C_{13} and C_{18}. Various alkyl sulfates with alkyl chains between C_{12} and C_{15} caused irreversible eye damage in rabbits. Although the available data on eye irritation effects for the structurally similar alkyl sulfates indicates that alkyl sulfates with carbon chain of C_{16} to C_{18} are only irritating to eyes, no such trend could be identified for the alkyl and alkene sulfonates.

In the absence of information on irritation or composition, alkanesulfonic acids, sodium salts (CAS No. 68608-15-1) is considered to be corrosive to skin and cause eye damage based on worst case assumptions on the composition of this chemical.

Based on the limited available data, chemicals in this group are not likely to cause serious systemic effects following repeated oral or dermal exposure. However, due to their skin irritating effects, they may compromise the integrity of the skin and increase dermal absorption of other chemicals present in product formulations.

Although no inhalation data are available, given the irritant properties of these chemicals, inhalation could lead to irritation or corrosion of the mucous membranes of the respiratory tract.

For further details of the health hazard information see **Supporting information**.

Hazard classifications relevant for worker health and safety

These chemicals satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) (UNECE 2017) for hazard classes relevant for work health and safety as follows. This does not consider classification of physical hazards and environmental hazards.

The proposed hazard classification is based on read across principles and available composition data. It should be used as a default for these chemicals. If empirical data become available for a specific chemical, this data may be used to amend the default classification for that chemical.

The following chemicals satisfy the criteria for classification according to the table below:

- 1-Hexanesulfonic acid, sodium salt (1:1) (CAS No. 2832-45-3)
- 1-Octanesulfonic acid (CAS No. 3944-72-7)
- 1-Octanesulfonic acid, sodium salt (1:1) (CAS No. 5324-84-5) (**except** for Acute toxicity)
- 1-Hexanesulfonic acid (CAS No. 13595-73-8)
- 1-Heptanesulfonic acid, sodium salt (1:1) (CAS No. 22767-50-6)
- Alkanesulfonic acids, sodium salts (CAS No. 68608-15-1).

Health hazards	Hazard category	Hazard statement
Acute toxicity	Acute Tox. 4	H302: Harmful if swallowed
Skin corrosion/irritation	Skin Corr. 1	H314: Causes severe skin burns and eye damage

Health hazards	Hazard category	Hazard statement
Serious eye damage/irritation	Eye Damage 1	H318: Causes serious eye damage

The following chemicals satisfy the criteria for classification according to the table below:

- 1-Dodecanesulfonic acid, sodium salt (1:1) (CAS No. 2386-53-0)
- 1-Pentadecanesulfonic acid, sodium salt (1:1) (CAS No. 5896-54-8)
- 1-Hexadecanesulfonic acid, sodium salt (1:1) (CAS No. 15015-81-3)
- Sulfonic acids, C_{13-18}-alkane hydroxy and C_{13-18}-alkene, sodium salts (CAS No. 68439-56-5)
- Sulfonic acids, C_{10-16}-alkane, sodium salts (CAS No. 68608-21-9)
- Sulfonic acids, C_{15-18}-alkane, sodium salts (CAS No. 68815-15-6)
- Alkanesulfonic acids, C_{13-18}-alkanesulfonic (CAS No. 91082-04-1)
- Sulfonic acids, C_{10-21}-alkane, sodium salts (CAS No. 91082-19-8)
- Sulfonic acids, C_{12-18}-*sec*-alkane, calcium salts (CAS No. 106233-07-2).

Health hazards	Hazard category	Hazard statement
Acute toxicity	Acute Tox. 4	H302: Harmful if swallowed
Skin corrosion/irritation	Skin Irrit. 2	H315: Causes skin irritation
Serious eye damage/irritation	Eye Damage 1	H318: Causes serious eye damage

Summary of health risk

Public

Based on the available use information, the public may be exposed to these chemicals by:

- direct application of products containing the chemicals to the skin and hair
- inhalation from domestic spray products if aerosolised
- incidental skin and eye contact with these chemicals during use of domestic products.

In addition, children may be exposed to these chemicals by accidentally ingesting liquid laundry detergent products.

The main route of exposure to these chemicals is expected to be via the skin. Incidental inhalation, ingestion and contact with the eyes may also occur.

The critical health effects for risk characterisation of these chemicals are skin corrosion or irritation and eye damage. Based on available use information, these chemicals are expected to be present in cosmetics at concentrations up to 20%, and in domestic cleaning and laundry products at concentrations up to 30%.

The hazard profile and risks of this group of chemicals are similar to a large number of surfactants that are extensively used in products, with severity of hazardous effects dependent on concentration and pH. The risks are reduced when products are formulated to be non-irritating via pH adjustment. Additionally, chemicals in this group are frequently formulated with related chemicals with similar toxicity including alcohol ethoxylates and alkyl

benzene sulfonates. Therefore, the risk may be impacted by the cumulative levels of surfactants. Any controls for these chemicals should be considered as part of a broader review of the management of surfactants in the *Poisons Standard* (SUSMP) (TGA 2025) (see **Proposed means for managing risk**).

Adverse effects have occurred in children accidentally exposed to similar chemicals from liquid laundry detergent capsules via ingestion, skin and eye contact. In 2013, an Australian Industry Guideline for Labelling & Packaging of Liquid Laundry Capsules was published by the industry. In 2015, the Australian Competition & Consumer Commission (ACCC) participated in a joint international campaign on liquid laundry detergent capsule about the potential risks associated with the use of capsules. The focus was to raise awareness of laundry capsule safety, including developing consistent safety information for parents and carers worldwide. Since 2019, the ACCC records have indicated that there has not been any reported complaints or incidents of adverse effects resulting from laundry capsule exposures.

Workers

During product formulation and packaging, dermal, ocular and inhalation exposure might occur, particularly where manual or open processes are used. These could include transfer and blending activities, quality control analysis, and cleaning and maintaining equipment. Worker exposure to these chemicals at lower concentrations could also occur while using formulated products containing these chemicals. The level and route of exposure will vary depending on the method of application and work practices employed. Good hygiene practices to minimise incidental oral exposure are expected to be in place.

Given the local health effects, these chemicals could pose a risk to workers. Control measures to minimise dermal, ocular and inhalation exposure are needed to manage the risk to workers (see **Proposed means for managing risk**).

Proposed means for managing risk

Public health

No specific regulatory controls are recommended for chemicals in this group as part of this evaluation. Any controls for these chemicals should be considered as part of a broader review of the management of surfactants in the *Poisons Standard* (SUSMP).

Workers

Recommendation to Safe Work Australia

It is recommended that Safe Work Australia (SWA) update the Hazardous Chemical Information System (HCIS) to include classifications relevant to work health and safety.

Information relating to safe introduction and use

The information in this statement including recommended hazard classifications, should be used by a person conducting a business or undertaking (PCBU) at a workplace (such as an employer) to determine the appropriate controls under the relevant jurisdiction Work Health and Safety laws.

Control measures that could be implemented to manage the risk arising from oral, dermal and inhalation exposure to these chemicals include, but are not limited to:

- using closed systems or isolating operations
- minimising manual processes and work tasks through automating processes
- adopting work procedures that minimise splashes and spills
- cleaning equipment and work areas regularly
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemicals.

Measures required to eliminate, or manage risk arising from storing, handling and using these hazardous chemicals depend on the physical form and how these chemicals are used.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

Model codes of practice, available from the Safe Work Australia website, provide information on how to manage the risks of hazardous chemicals in the workplace, prepare an SDS and label containers of hazardous chemicals. Your Work Health and Safety regulator should be contacted for information on Work Health and Safety laws and relevant Codes of Practice in your jurisdiction.

Conclusions

The Executive Director proposes to be satisfied that the identified risks to human health from the introduction and use of the industrial chemicals can be managed.

Note:

1. Obligations to report additional information about hazards under *Section 100* of the *Industrial Chemicals Act 2019* apply.
2. You should be aware of your obligations under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Supporting information

Grouping rationale

Chemicals in this group consist of medium to long chain alkane or alkene containing sulfonic acids and their sodium or calcium salts. Approximately half of the chemicals are discrete organic chemicals with alkyl chains of C_6 to C_{16} in length. The other half are unknown or variable composition, complex reaction products or biological materials (UVCBs), comprised of variable alkyl or alkenyl chains that are C_{10} to C_{21} in length (see **Chemical identity**).

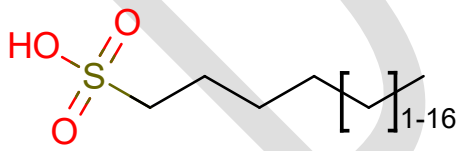
All chemicals in this group contain a hydrophobic aliphatic chain and a polar sulfonic acid group. The chemicals are anionic surfactants and are expected to have similar physicochemical and toxicological properties. The chemicals are expected to exist almost entirely as the alkyl and alkene sulfonate anion at the pH of biological solutions. The cation components are not expected to contribute significantly to the toxicity of these chemicals.

Several alkyl and alkene sulfonates have been assessed previously (NICNAS 2014; NICNAS 2015, NICNAS 2016). Sodium 1-octanesulfonate has been included in this evaluation as new data indicating corrosive effects has become available since the publication of the original report. Four chemicals (see **Introduction and use** section) have previously been published in evaluations for chemicals that are not expected to be commercially active in Australia. An evaluation of their hazards was not undertaken as part of this evaluation. These chemicals have been included to provide information regarding the hazards and potential risk if used.

Other previously assessed chemicals are not being evaluated as part of this evaluation as no significant new data are available. However, data on these chemicals has been used as read across to support conclusions on hazards and use.

Chemical identity

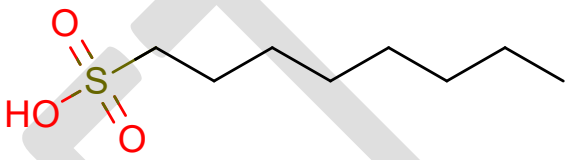
Most chemicals in this evaluation are linear or mostly linear primary alkane sulfonic acids (and their sodium salts) that conform to the following general structure:

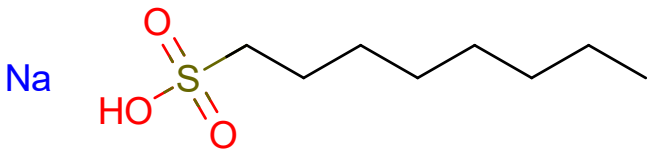


Of the chemicals conforming to this structure, 8 are discrete chemicals with defined alkyl chain lengths and 5 are UVCBs with variable alkyl chain lengths. The exceptions to this general structure are:

- sodium $C_{13\text{-}18}$ olefin sulfonate (CAS No. 68439-56-5), which is a UVCB that contains the sodium salt of an unsaturated alkene sulfonate, and a hydroxylated linear alkyl sulfonate with variable alkyl chains that are between C_{13} and C_{18}
- sulfonic acids, $C_{12\text{-}18}$-*sec*-alkane, calcium salts (CAS No. 106233-07-2), which is the calcium salt of a secondary alkane sulfonate where the sulfonic acid group is not at the end of the alkyl chain.

Information for 2 representative chemicals, an alkane sulfonic acid and the corresponding sodium salt, are presented below.

CAS number	3944-72-7
CAS name	1-Octanesulfonic acid
Molecular formula	$C_8H_{18}O_3S$
Associated names	Octane-1-sulfonate
Molecular weight (g/mol)	194.29
SMILES (canonical)	O=S(=O)(O)CCCCCCCC
Structural formula	

CAS number	5324-84-5
CAS name	1-Octanesulfonic acid, sodium salt (1:1)
Molecular formula*	$C_8H_{18}O_3S.Na$
Associated names	Sodium 1-octanesulfonate Sodium caprylyl sulfonate (INCI)
Molecular weight (g/mol)*	217.28
SMILES (canonical)*	[Na].O=S(=O)(O)CCCCCCCC
Representative structure*	

Additional chemical identity information

* This chemical is a salt and has been represented according to CAS nomenclature/identity conventions.

Relevant physical and chemical properties

Limited experimental data on the physical and chemical properties for these chemicals are available.

Sodium 1-octanesulfonate is a non-volatile white powder that forms micelles in water with a critical micelle concentration (CMC) of 9.836 g/L at 20°C and a surface tension of 44.93 mN/m at 25°C. The partition coefficient (logK_{ow}) was estimated to be <-2.25 at 20°C (REACH n.d.-a).

Based on the data for medium to long chain alkyl sulfates and sodium α-olefin sulfonates, chemicals in this group are expected to have low vapour pressures and high water solubility (OECD 2007). Therefore, the chemicals are not expected to be volatile. There is limited measured data on other physicochemical properties for these surfactants.

The CMC for various structurally similar sodium alkyl sulfates (chain lengths C_8–C_{16}) measured in water at 20°C were in the range 0.19–30.2 g/L, with shorter alkyl chains correlating to higher CMC (AICIS 2024a). The reported surface tensions of these sodium salts were in the range 35–55 mN/m at 20°C (OECD 2007).

Introduction and use

Australia

There is limited specific information about the introduction, use and end use of these chemicals in Australia.

Sodium 1-octanesulfonate was reported to have a use volume of <1,000 tonnes/year based on information previously provided to NICNAS under the 2006 Australian High Volume Industrial Chemicals List.

Based on available data, the following chemicals are not likely to be introduced for industrial use in Australia (AICIS 2023; AICIS 2024b):

- 1-Hexanesulfonic acid (CAS No. 13595-73-8)
- Sulfonic acids, $C_{15\text{-}18}$-alkane, sodium salts (CAS No. 68815-15-6)
- Alkanesulfonic acids, $C_{13\text{-}18}$-alkanesulfonic (CAS No. 91082-04-1)
- Sulfonic acids, $C_{12\text{-}18}$-*sec*-alkane, calcium salts (CAS No. 106233-07-2).

International

Limited specific data are available for the chemicals. Use information has been inferred from information for other alkane and alkene sulfonates including secondary alkyl sulfonates and α-olefin sulfonates.

Based on the available information, the chemicals are expected to be used as surfactants in cosmetic, domestic and commercial applications (OECD 2007).

In 2001, the total alkane sulfonate production in Europe was approximately 76,000 tonnes/year, with 63% of the alkane sulfonates used in household applications, 24% used in

industrial and institutional uses and the remaining 13% used in technical applications with limited environmental release (AISE and Cefic 2005).

Two of the chemicals in this group have identified cosmetic uses. Sodium 1-octanesulfonate is reported to have cosmetic use as a surfactant for cleansing in hair care products (EC n.d.; Personal Care Products Council n.d.; US EPA 2020). Sodium C_{13-18} olefin sulfonate is used in cosmetics including hair and bath products (Chemwatch n.d.). Use patterns are expected to be similar to other sodium α-olefin sulfonates. In 2013, sodium C_{14-16} olefin sulfonate had reported use in the United States of America (USA) in (Becker et al. 2023; CIR 2013):

- 247 rinse-off products, with maximum concentration of 19% in shampoos
- 9 leave-on products, with maximum concentration of 13.2% in personal care products
- 42 products diluted for (bath) use, with maximum reported concentration 10% in bubble bath products.

Other chemicals in this group may have cosmetic use in shampoos, hair conditioners, liquid soaps, cleansing, bath products and other personal care products due to their foaming and emulsifying properties at concentrations less than 20% (OECD 2007). However, no specific information on these other chemicals was identified.

Generally, all chemicals in this evaluation are anionic surfactants that are likely to be used in a variety of domestic and professional cleaning products. These include laundry products, detergents for dishwashing, hard surface cleaners, carpet cleaners dispersing agents and automotive cleaning products (DeLima Associates n.d.; OECD 2007; US EPA 2020). The typical concentrations of these chemicals in domestic and commercial cleaning products are between 3 and 5% and up to 30% (OECD 2007).

In the USA,1-octanesulfonic acid, sodium 1-octanesulfonate, sodium C_{13-18} olefin sulfonate and alkanesulfonic acids, sodium salts have reported uses in cleaning and washing agents, furniture care products and lubricants (Chemwatch n.d.; US EPA 2020). The reported concentrations of sodium 1-octanesulfonate in the USA domestic and commercial cleaning sprays is in the range 0.5–20%. However, the typical use concentrations are below 5% (DeLima Associates n.d.).

Secondary alkane sulfonates were reported to be used in Europe in 2002 at the following typical concentrations and product types (AISE and Cefic 2005):

- 8–10% (maximum 15%) in liquid laundry products
- 3.5–25% (maximum 29%) in liquid hand dishwashing products
- 0.2% in liquid machine dishwashing products
- 0.2–15% in liquid surface cleaning products
- 2–4% in spray surface cleaning products
- 0.7–3.4 % (maximum 4%) in toilet cleaning products.

Sodium α-olefin sulfonates have reported use in Canada in bathroom cleaning sprays at concentrations of 5% (Government of Canada 2017).

Chemicals in this group may also have commercial uses including (OECD 2007):

- textile and leather treatments
- metal cleaning, including in pickling baths
- steam jets for cleaning applications.

Alkanesulfonic acids, sodium salts (CAS No. 68608-15-1) has reported site-limited use as an intermediate (REACH n.d.-b). However, most of the chemicals in this group are not expected to be used as intermediates in manufacturing (OECD 2007).

Existing Australian regulatory controls

AICIS

No specific controls are currently available for these chemicals.

Public

No specific controls are currently available for these chemicals.

Workers

These chemicals are not listed on the HCIS (SWA n.d.).

No exposure standards are available for chemicals in this group in Australia.

International regulatory status

Exposure standards

No exposure standards were identified for chemicals in this group internationally.

Health hazard information

Health hazard data is available for sodium 1-octanesulfonate, which has been previously assessed by NICNAS (NICNAS 2016). As there is new in vitro data available for this chemical, it has been included in this group for evaluation. Limited hazard data was identified for the remaining chemicals, with the majority having no specific hazard data. For the UVCBs in this group, the severity of effects will be dependent on the exact composition of the chemical.

A number of alkane and alkene sulfonates have been previously assessed or are not listed on the Inventory. This includes secondary alkyl sulfonates and α-olefin sulfonates. Information on these other alkane and alkene sulfonates has been included in this report as read across to support hazard conclusions.

In this evaluation, the chemicals used as read across for hazard conclusions may be referred to using a common name or by their CAS number. For ease of reference, the CAS number, CAS name, alkyl chain length and common names used in the evaluation have been summarised in **Table 1**.

Table 1 – Alkane and alkene sulfonate chemicals used as read across in this evaluation

CAS number	CAS name	Alkyl chain length	Common name
68439-57-6	Sulfonic acids, C_{14-16}-alkane hydroxy and C_{14-16}-alkene, sodium salts	14–16	Sodium C_{14-16} olefin sulfonate
91082-14-3	Sulfonic acids, C_{15-18}-alkane hydroxy and C_{15-18}-alkene, sodium salts	15–18	Sodium C_{15-18} olefin sulfonate
93686-14-7	Sulfonic acids, C_{14}-alkane hydroxy and C_{14}-alkene, sodium salts	14	Sodium C_{14} olefin sulfonate
863609-89-6	Sulfonic acids, C_{14-18}-alkane hydroxy and C_{14-18}-alkene, sodium salts	14–18	Sodium C_{14-18} olefin sulfonate
Various	Various	14–17	SAS*

*Most of the data relates to the test substance which will be referred to as "SAS", which is a commercial mixture of multiple secondary alkane sulfonates. The linear alkyl chain (linearity > 98%) has typically 14 to 17 carbon units with an average of 15.9 carbon atoms (AISE and Cefic 2005; NICNAS 2014). SAS may be referred to by different CAS numbers and trade names in the available sources.

The health hazards of the alkyl and alkene sulfonates are expected to be similar to other anionic surfactants such as alkyl sulfates (OECD 2007). For both groups, the presence of the acidic sulfonate or sulfate group is expected to be the driver of local toxicological effects. Therefore, data from structurally similar medium to long chain alkyl sulfates was also used to support the hazard conclusions where appropriate. AICIS has previously assessed these alkyl sulfates and the trends established in that evaluation have been used to support the hazard conclusions for this evaluation (AICIS 2024a).

Toxicokinetics

There is limited data on the toxicokinetics of these chemicals.

Based on the available data, chemicals in this evaluation are expected to have similar absorption, distribution, metabolism and excretion characteristics. Their overall toxicokinetic profile is expected to be similar to alkyl sulfates.

Absorption

Alkane and alkene sulfonates are expected to be absorbed in the gastrointestinal tract based on studies in rats. Absorption may be reduced as the alkyl chain length increases (OECD 2007).

Dermal absorption of the alkane and alkene sulfonates is expected to be low. A dermal absorption of 0.2% of the applied dose was measured after application of ^{14}C-labelled sodium 1-dodecansulfonate to guinea pig skin. Similarly, 0.6% of an aqueous solution of ^{14}C-labelled C_{14} α-olefin sulfonate was absorbed through rat skin in 24 hours (OECD 2007).

With limited dermal absorption, it is not likely that these chemicals can be absorbed by the developing foetus via the placenta, or by the neonate via the breast milk (OECD 2007).

The structurally similar alkyl sulfates are well absorbed following oral administration with absorption through the skin expected to be limited (AICIS 2024a).

Distribution

The alkyl and alkene sulfonates in this group are expected to distribute mainly to the liver but may distribute to other organs depending on chain length.

In rats, ^{35}S-labelled sodium 1-dodecansulfonate was detected in the liver and kidneys 1 hour after oral administration. However, ^{35}S-labelled sodium 1-hexadecansulfonate was observed mainly in the stomach and gastrointestinal tract 2 hours after oral administration. After oral administration of a ^{14}C-labelled C_{14} hydroxy alkene sulfonate, blood concentrations peaked within 4 hours, and the chemical was detected in the gastrointestinal tract, kidneys and liver (OECD 2007).

Tissue disposition studies with a structurally similar alkyl sulfate in rats indicated that 36% of an intravenous dose reached the liver within 15 minutes, followed by the intestine, the kidney and the blood (AICIS 2024a).

Metabolism and excretion

Studies of the metabolism of sodium 1-dodecansulfonate and sodium 1-hexadecansulfonate indicate that the major metabolite of these chemicals is butyric acid 4-sulfonate. Most of the ingested compound is excreted via the urine with 85% and 60% recovery for the C_{12} and C_{16} alkane sulfonates, respectively. The majority of the remaining applied dose is excreted in the faeces (OECD 2007).

Based on comparison with alkyl sulfates (AICIS 2024a) it is expected that the major metabolite for even number chained alkyl sulfonates is butyric acid 4-sulfonate and for odd numbered chain would be propionic acid-3-sulfate. The major path of excretion is expected to be via the urine.

Acute toxicity

Oral

Limited data are available for these chemicals.

Based on the limited available data for chemicals in this evaluation and other alkyl and alkene sulfonates, most of the chemicals are expected to have moderate acute oral toxicity. Hazard classification is warranted for alkyl and alkene sulfonates unless experimental data indicates otherwise. For example, sodium 1-octanesulfonate is considered to have low acute oral toxicity based on the available guideline study and does not require hazard classification. The clinical signs of toxicity were often non-specific. However, necropsy of animals exposed to these chemicals indicated that most of these chemicals were irritating to the gastrointestinal tract. Although the available data on acute oral toxicity for the structurally similar alkyl sulfates indicates that the LD50 typically decreases with increasing alkyl chain lengths, no such trend could be identified for the alkyl and alkene sulfonates.

Chemicals in this evaluation

In an acute oral toxicity limit test conducted in accordance with US guideline 16 CFR 1500.3, Sprague Dawley (SD) rats (5/sex/dose) received a single dose of sodium 1-octanesulfonate at 5,000 mg/kg bw by oral gavage. No signs of clinical toxicity were observed and the LD50 was >5,000 mg/kg bw. No clinical signs of toxicity or abnormal findings were reported at necropsy (OECD 2007). Details on the concentration of the test substance are not available.

In a non-guideline acute oral toxicity study, male CF1 mice received a single dose of sulfonic acids, C_{15-18}-alkane, sodium salts (CAS no. 68815-15-6) at 60% concentration in water. The LD50 was 1,440 mg/kg bw (OECD 2007).

Other alkyl and alkene sulfonates – read across

The following LD50s for SAS in water were reported from acute oral toxicity studies conducted similarly to OECD TG 401:

- 500–2,000 mg/kg bw at 93% concentration
- 2,250 and 2,890 mg/kg bw in rats at 60% concentration (equivalent to 1,350 and 1,734 mg/kg bw of the active substance)
- 4,970 and 5,322 mg/kg bw in Wistar rats at 25% and 30% concentration (equivalent to 1,350 and 1,597 mg/kg bw of the active substance)
- 2,130 and 2,550 mg/kg bw in CD-1 mice at 60% concentration (equivalent to 1,350 and 1,530 mg/kg bw of the active substance).

Clinical signs of toxicity included coat bristling, ataxia, sedation, squatting posture and diarrhoea (AISE and Cefic 2005; REACH n.d.-c).

In acute oral toxicity studies conducted in accordance with or similarly to OECD TG 401 with sodium C_{14-16} olefin sulfonate:

- Wistar rats received a single dose of the chemical at 25% concentration in water. The LD50 was 578 mg/kg bw (OECD 2007)
- Wistar rats received a single dose of the chemical at 34.1% concentration in water. The LD50 was 1,379 mg/kg bw (REACH n.d.-d)
- Wistar rats received a single dose of the chemical at 35% concentration in water. The LD50 was 6,314 mg/kg bw (equivalent to 2,210 mg/kg bw) (REACH n.d.-d)
- SD rats received a single dose of the chemical at 37% concentration in water. The LD50 was 2,220 mg/kg bw (OECD 2007).

Some clinical signs of toxicity reported in these studies. These included piloerection, hunched posture, muscle spasms, hypothermia, irregular breathing and lethargy (OECD 2007; REACH n.d.-d).

In a non-guideline study, male CF1 mice received a single dose of the sodium salts of the sodium C_{15-18} olefin sulfonate at 38% concentration in water by oral gavage. The LD50 was 1,368 mg/kg bw (OECD 2007).

Alkyl sulfates – read across

The available data on acute oral toxicity for alkyl sulfates indicates that the LD50 typically decreases with increasing alkyl chain lengths. Most of the data on acute oral toxicity is available for UVCBs containing alkyl chains with greater than 10 carbon atoms. Reported oral LD50 values in rats were (AICIS 2024a; NICNAS 2013):

- 500–2,000 mg/kg bw for sodium C_{12-14} alkyl sulfate
- 1,000–2,000 mg/kg bw for C_{12} and C_{10-16} alkyl sulfates
- 977–1,427 mg/kg bw for sodium lauryl sulfate
- >2,000 mg/kg bw for C_{12-15}, C_{12-16} and C_{12-18} alkyl sulfates
- >3,000 mg/kg bw for C_{14}, C_{16} and C_{18} alkyl sulfates
- >5,000 mg/kg bw for C_{14-18} and C_{16-18} alkyl sulfates.

The counter ion does not appear to substantially influence the severity of acute oral toxicity. Clinical signs observed were piloerection, lethargy, decreased motor activity and decreased respiratory rate. At necropsy the major findings were signs of irritation in the gastrointestinal tract and pallor in inner organs (OECD 2007).

Dermal

No data are available for these chemicals.

Based on the low dermal absorption of alkyl and alkene sulfonates and read across data from other alkyl and alkene sulfonates and structurally similar alkyl sulfates the chemicals in this group are expected to have low acute dermal toxicity.

Other alkyl and alkene sulfonates – read across

In subacute studies of dermal toxicity with SAS, no adverse effects were observed (AISE and Celic 2005).

Sodium C_{14-16} olefin sulfonate at 36.9% concentration was reported to have low dermal toxicity, with a reported LD50 > 6,000 mg/kg bw (equivalent to 2,214 mg/kg bw of the active substance) in rats in a guideline acute dermal toxicity study (NICNAS 2015; OECD 2007; REACH n.d.-d).

Alkyl sulfates – read across

In guideline OECD TG 402 studies in rats LD50 values > 2000 mg/kg bw/day were reported for C_8 and C_{10-16} alkyl sulfates. Lower LD50 values have been reported for some chemicals but the reliability of these studies could not be determined and was not sufficient to warrant classification (AICIS 2024a).

Inhalation

No data are available for these chemicals.

Corrosion/Irritation

Skin irritation

Based on the available data these chemicals are irritating to skin with varying degrees of severity. The available data indicate that the severity of effects generally decreases with chain length and decreasing concentration. Although the available data on skin irritation for the structurally similar alkyl sulfates indicates that C_{16}–C_{18} alkyl sulfates are only slightly irritating to skin, no such trend could be identified for the alkyl and alkene sulfonates.

A guideline in vitro study indicates that sodium 1-octanesulfonate is corrosive to skin. Based on the weight of evidence of available data including read across information from structurally similar alkyl sulfates, the following discrete chemicals in this group with $<C_{12}$ alkyl chains are expected to be corrosive to skin, warranting hazard classification:

- 1-Hexanesulfonic acid, sodium salt (1:1) (CAS No. 2832-45-3)
- 1-Octanesulfonic acid (CAS No. 3944-72-7)
- 1-Octanesulfonic acid, sodium salt (1:1) (CAS No. 5324-84-5)

- 1-Hexanesulfonic acid (CAS No. 13595-73-8)
- 1-Heptanesulfonic acid, sodium salt (1:1) (CAS No. 22767-50-6).

Although variable results have been observed in multiple studies with secondary alkane sulfonates (typically $C_{14–17}$) and α-olefin sulfonates ($C_{14–18}$), irritant effects sufficient to warrant classification have been observed. In the absence of data, classification is also warranted for all discrete chemicals and UVCBs that typically contain ≥C_{12} alkyl chains (but not if the composition indicates that there is more than 5% of ≤C_{10} alkyl chains):

- 1-Dodecanesulfonic acid, sodium salt (1:1) (CAS No. 2386-53-0)
- 1-Pentadecanesulfonic acid, sodium salt (1:1) (CAS No. 5896-54-8)
- 1-Hexadecanesulfonic acid, sodium salt (1:1) (CAS No. 15015-81-3)
- Sulfonic acids, C_{13-18}-alkane hydroxy and C_{13-18}-alkene, sodium salts (CAS No. 68439-56-5)
- Sulfonic acids, C_{10-16}-alkane, sodium salts (CAS No. 68608-21-9)
- Sulfonic acids, C_{15-18}-alkane, sodium salts (CAS No. 68815-15-6)
- Alkanesulfonic acids, C_{13-18}-alkanesulfonic (CAS No. 91082-04-1)
- Sulfonic acids, C_{10-21}-alkane, sodium salts (CAS No. 91082-19-8)
- Sulfonic acids, C_{12-18}-*sec*-alkane, calcium salts (CAS No. 106233-07-2).

In the absence of information on the composition, alkanesulfonic acids, sodium salts (CAS No. 68608-15-1) is considered to be corrosive to skin based on a worst case assumption, unless data on composition or irritation are available.

Chemicals in this evaluation

In a GLP compliant in vitro skin corrosion assay conducted in accordance with OECD TG 431, sodium 1-octanesulfonate was applied to reconstructed human epidermis (EpiSkin™) for 3 and 60 minutes. The mean tissue viability was 87.9 and 4.2 after 3 and 60 minutes, respectively. These results warrant a UN GHS skin corrosive category 1B/1C hazard classification based on the test method prediction model criteria (≥35% after 3 min exposure AND <35% after 60 minute exposure) (REACH n.d.-a).

Other alkyl and alkene sulfonates – read across

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 male New Zealand white (NZW) rabbits were treated with SAS (93% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 0.7, 1,1 for erythema and 0, 0.3, 1.3, for oedema (maximum score of 4). All effects were reversible (REACH n.d.-c).

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 male NZW rabbits were treated with SAS (93% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 0.7, 2, 0.3 for erythema and 0.3, 0.3, 0.3, for oedema (maximum score of 4). All effects were reversible (REACH n.d.-c).

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 male NZW rabbits were treated with SAS (93% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 0.3, 0.3, 1, for oedema (maximum score of 4). Signs of erythema were observed in all animals at 24 hours and in 1

animal at 48 and 72 hours. No erythema scores were not reported. All effects were reversible (REACH n.d.-c).

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 male NZW rabbits were treated with SAS (60% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 3.67, 3, 3.67 for erythema and 2.33, 2.67, 2.33, for oedema (maximum score of 4). All effects were reversible (REACH n.d.-c).

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 male NZW rabbits were treated SAS (30% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 3, 2.7, 3 for erythema and 1.3, 1.7, 1 for oedema (maximum score of 4). All effects were reversible (REACH n.d.-c).

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 NZW rabbits were treated with sodium C_{14-16} olefin sulfonate (95% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 2, 2, 2 for erythema and 1.3, 0, 1.7 for oedema (maximum score of 4). All effects were reversible (REACH n.d.-d).

In a GLP compliant skin irritation study conducted in accordance with OECD TG 404, 3 NZW rabbits were treated with sodium C_{14-16} olefin sulfonate (40% concentration) for 4 hours under semi-occlusive conditions. Observations were recorded at 24, 48, 72 hours and 7 days after patch removal. The following mean scores for individual animals were reported: 2.3, 2, 0.3 for erythema and 0.3, 1.7, 0 for oedema (maximum score of 4). All effects were reversible (OECD 2007; REACH n.d.-d).

In a non-GLP compliant skin irritation study conducted similarly to OECD TG 404, 3 NZW rabbits were treated with sodium C_{14-16} olefin sulfonate (at 37% concentration) for 24 hours under occlusive conditions. Observations were recorded at 24, 48 and 72 hours after patch removal. The following mean scores for individual animals were reported: 3, 3, 3 for erythema and 3, 3, 2.5 for oedema (maximum score of 4). 3 additional animals were exposed to the same chemical at 5% concentration and exhibited similar signs of erthyema and oedema (REACH n.d.-d).

In a series of non-guideline Draize tests, the structurally similar chemical sodium C_{14-18} olefin sulfonate was considered to be very slightly irritating to guinea pig skin at 5–15% concentration (OECD 2007).

Alkyl sulfates – read across

Structurally similar C_8 and C_{10} alkyl sulfates caused irreversible destruction of skin tissues after 4-hour exposures in rabbits. The corrosive nature of these chemicals is also supported by in vitro data. Limited observations of necrosis were reported for alkyl sulfates containing carbon chains of C_{12} to C_{15}, however the majority of available studies indicate that these chemicals are moderate to severe irritants to skin. Alkyl sulfates with alkyl chains that are in the range C_{16} to C_{18} are slightly irritating to skin in rabbits (AICIS 2024a; NICNAS 2013; OECD 2007).

Eye irritation

Based on the weight of evidence of available data including read across information ,the chemicals in this evaluation are expected to cause serious eye damage, warranting hazard classification. Although the available data on eye irritation for the structurally similar alkyl sulfates with alkyl chains in the range C_{16} to C_{18} indicates that they are only irritating to eyes, no such trend could be identified for the alkyl and alkene sulfonates.

In the absence of information on composition, alkanesulfonic acids, sodium salts (CAS No. 68608-15-1) is considered to cause eye damage based on a worst case assumption, unless data on composition or irritation are available.

Chemicals in this evaluation

In a GLP compliant ex vivo eye corrosivity/irritation study conducted according to OECD TG 437, sodium 1-octanesulfonate (20% w/w) was applied to 3 bovine corneae per group. The mean in vitro irritancy score (IVIS) was 208.5. Based on the criteria of the assay (IVIS >55 is regarded as serious eye damage), the chemical was considered to cause severe eye damage (REACH n.d.-a).

Other alkyl and alkene sulfonates – read across

In a GLP compliant eye irritation study conducted similarly to OECD TG 405, SAS (15% concentration) was instilled into 1 eye each of 3 NZW rabbits. The eyes were observed at 24, 48 and 72 hours and up to 21 days after exposure. Mean scores for animal 1 were: corneal opacity 1/4, iritis 0/2, conjunctival redness 1.67/3 and chemosis 0/4. Mean scores for animal 2 were: corneal opacity 1/4, iritis 0/2, conjunctival redness 2/3 and chemosis 0.67/4. Mean scores for animal 3 were: corneal opacity 1/4, iritis 0/2, conjunctival redness 2/3 and chemosis 0.33/4. Most signs of irritation resolved within 21 days. One animal exhibited diffuse areas of opacity on day 21 that were less severe than earlier in the study and with no other indicators of persisting eye damage (REACH n.d.-c).

In a GLP compliant eye irritation study conducted similarly to OECD TG 405, SAS (30% concentration) was instilled into 1 eye each of 3 NZW rabbits. The eyes were washed out after 24 hours and observed at 24, 48 and 72 hours. In one animal, the following mean scores were recorded: corneal opacity 0.67/4, iritis 0/2, conjunctival redness 2/3 and chemosis 1.33/4. No signs of eye irritation were observed in the other animals with mean scores of 0 for all parameters. All signs of irritation in the first animal resolved within 7 days (REACH n.d.-c). In this study, a low volume of the chemical (0.01 mL) was used, which may affect the severity of results.

In a GLP compliant eye irritation study conducted similarly to OECD TG 405, SAS (30% concentration) was instilled into 1 eye of 1 NZW rabbit. The eyes were washed out after 24 hours and observed at 24, 48 and 72 hours and 7 days. The following scores were reported: corneal opacity 1–3/4, iritis 0–1/2, conjunctival redness 2–3/3 and chemosis >2/4. Signs of eye irritation were not reversible within 7 days. At 7 days, a clear vascularisation in eye of the rabbit was observed (REACH n.d.-c).

In a non-GLP compliant eye irritation study conducted according to OECD TG 405, SAS (60% concentration) was instilled into 1 eye each of 3 white Russian rabbits. The eyes were observed at 24, 48 and 72 hours and up to 21 days. The following mean scores were recorded: corneal opacity 1.33/4, iritis 0.89/2, conjunctival redness 3/3 and chemosis 1.22/4. Signs of chemosis resolved completely within 14 days. However, signs of corneal opacity, iritis and conjunctival redness persisted through all 21 days of the study (REACH n.d.-c).

In guideline studies, sodium C_{14-16} olefin sulfonate was reported to cause effects on the eye that persisted for 21 days when applied at concentrations between 30% and 90% to rabbit eyes (NICNAS 2015; REACH n.d.-d).

In Draize tests, the sodium C_{10-18} (even-numbered) α-olefin sulfonates caused slight but reversible irritation to rabbit eyes when tested at 1 and 5% concentrations (OECD 2007).

Alkyl sulfates - read across

No eye irritation data is available for alkyl sulfates with alkyl chains less than 12 carbons in length. It is expected that these chemicals cause eye damage as they are corrosive (AICIS 2024a).

Various alkyl sulfates with carbon chains between 12 and 15 carbon atoms in length caused irreversible eye damage in rabbits. However, a C_{16-18} alkyl sulfate (CAS No. 68955-20-4) was, at most, irritating to rabbit eyes in guideline studies, potentially indicative of a lower potential for irreversible effects on the eyes with increasing alkyl chain length (AICIS 2024a; NICNAS 2013; OECD 2007).

Respiratory irritation

While these chemicals are not expected to be volatile, their corrosion and/or irritant properties indicates that inhalation or aerosols containing them may lead to irritation or corrosion of the mucous membranes of the respiratory tract.

Observation in humans

Limited data are available for alkyl and alkene sulfonates. SAS (60 % concentration) was tested for skin irritation in 15 test human volunteers with healthy skin. The volunteers were dermally exposed in an open patch test for 15 minutes. Very slight itching was reported in two test volunteers, whereas the remaining 13 volunteers had no adverse effects (NICNAS 2014).

In skin irritation studies in humans, structurally similar alkyl sulfates are reported to be moderate to strong skin irritants at concentrations of 10% or greater and slightly irritating at 1% (AICIS 2024a).

Sensitisation

Skin sensitisation

Limited data are available for these chemicals.

A single case of allergic contact conjunctivitis was reported in humans from a detergent product containing sodium 1-dodecanoate. However, based on the weight of evidence from read across information, these chemicals are not expected to be skin sensitisers.

Other alkyl and alkene sulfonates – read across

In a non-GLP compliant guinea pig maximisation test (GPMT) conducted according to OECD TG 406, intradermal induction was performed on 10 male guinea pigs using 5% SAS (60% concentration) in Freund's Complete Adjuvant (FCA). The animals were challenged twice

with 5% SAS (60% concentration) in water. After challenge, no reactions were reported in the animals (AISE and Cefic 2005; NICNAS 2014).

In a non-GLP compliant maximisation test conducted similarly to OECD TG 406, intradermal induction was performed on 20 male guinea pigs using 5% SAS (60% concentration) in FCA and topical induction after 1 week with 5% SAS (60% concentration) in water. The animals were challenged with 5% SAS (60% concentration) in water. After challenge, no reactions were reported in the animals (AISE and Cefic 2005).

In a GPMT conducted according to OECD TG 406, intradermal induction was performed on 10 male guinea pigs using 0.1% of sodium C_{14} olefin sulfonate (CAS No. 93686-14-7) and topical induction with 18.12% of the chemical. The animals were challenged with 1% and 5% of the chemical. After challenge, no reactions were reported in the animals (OECD 2007).

In a GPMT, intradermal induction was performed on 10 female Dunkin-Hartley guinea pigs with 100% sodium C_{14-16} olefin sulfonate (38% concentration) and topical induction with 100% sodium C_{14-16} olefin sulfonate. In one animal, irritation and exudation was reported at the injection site. The animals were challenged with 12.5% and 25% sodium AOS. After challenge, no reactions were reported in the animals (CIR 2013).

In a GPMT, topical induction under occlusive conditions was performed on male Hartley guinea pigs with 50% sodium C_{14-16} olefin sulfonate (39% concentration). The animals were challenged with 50% sodium C_{14-16} olefin sulfonate. Signs of oedema were observed in the animals during induction and challenge, and the severity of reaction was generally weaker after challenge. In one animal there was a slightly positive oedema response after challenge. The chemical was determined to be non-sensitising in this study (CIR 2013).

In a GPMT, intradermal induction was performed on 10 male albino guinea pigs with 3.75% sodium C_{14-16} olefin sulfonate (15% concentration) and topical induction with 3.75% sodium C_{14-16} olefin sulfonate. The animals were challenged with 1.63% sodium AOS. The chemical was determined to be non-sensitising in this study (CIR 2013).

In a GPMT, intradermal induction was performed on guinea pigs with 3.75% sodium C_{14-16} olefin sulfonate (36.9% concentration) and topical induction with 3.75% sodium C_{14-16} olefin sulfonate. The animals were challenged with 3.75% sodium AOS topically under occlusion. The chemical was determined to be non-sensitising in this study (CIR 2013).

In a GPMT, intradermal induction was performed on 15 guinea pigs with a 1:1:1 mixture of a magnesium C_{14}, C_{16} and C_{18} olefin sulfonate at 0.5% and topical induction with 2% of the same mixture. The animals were then challenged with 0.1% of the same mixture. The mixture was determined to be non-sensitising (OECD 2007).

Alkyl sulfates – read across

The structurally similar medium and long chain alkyl sulfates are not considered to be skin sensitisers based on negative results from animal studies (AICIS 2024a; OECD 2007).

Observation in humans

One case of allergic contact conjunctivitis from synthetic detergents containing sodium 1-dodecanesulfonate tested at 0.1% was reported (OECD 2007).

While there are infrequent reports of contact sensitisation to the structurally similar chemical sodium lauryl sulfate, the incidence is sufficiently low that this chemical is not considered a sensitiser (NICNAS 2013).

There was no evidence of skin sensitisation for sodium C_{14-16} olefin sulfonate at a concentration of 4% in an occlusive Draize test with 88 human volunteers (NICNAS 2015; OECD 2007).

In silico

Discrete chemicals in this group have no structural alerts for protein binding based on the mechanistic profiling functionality of OECD QSAR Application Toolbox (OECD n.d.) and the knowledge based expert system Deductive Estimation of Risk from Existing Knowledge (DEREK) Nexus version 6.0.1 (Lhasa Limited n.d.).

Repeat dose toxicity

Oral

Based on the limited data available for sodium 1-octanesulfonate and the read across information from other alkane and alkene sulfonates, the chemicals in this evaluation are not expected to cause serious systemic health effects following repeated oral exposure.

Chemicals in this evaluation

In a non-GLP compliant 13 week study conducted similarly to OECD TG 408, Carworth Farm 'E' strain rats (12/sex/dose) were administered sodium 1-octanesulfonate (86% concentration) in their diet at 40, 200, 1,000 or 5,000 ppm, equivalent to approximately 3, 17, 86 and 430 mg/kg bw/day, respectively. No treatment-related effects were observed in urinalysis, haematology, clinical chemistry, organ weights, gross pathology and histopathology parameters at any dose level compared to control animals. A no observed adverse effect level (NOAEL) of 5,000 ppm in diet (equivalent to 430 mg/kg bw/day) was established in this study (REACH n.d.-a).

Other alkane and alkene sulfonates – read across

In a non-GLP compliant oral repeated dose study, SD rats (30/sex/dose) were administered SAS (60% concentration) in diet at approximately 62.5, 200 or 1,000 mg/kg bw/day for 52 weeks. Reduced body weight gain was observed in the highest dose group. No other treatment-related adverse effects were reported. The NOAEL in this study was 200 mg/kg bw/day (AISE and Cefic 2005; NICNAS 2014).

In a 2 year oral repeated dose toxicity study, SD CFY rats (50/sex/dose) were administered sodium C_{14-16} olefin sulfonate in diet at 0, 1,000, 2,500 or 5,000 ppm, equivalent to 0, 39, 96 and 195 mg/kg bw/day for females, and 0, 57, 132 and 259 mg/kg bw/day for males, respectively. Significant reduced body weight gain was reported in both sexes between 14 and 26 weeks in the highest dose group. No other treatment-related adverse effects were reported. The NOAEL in this study was 2,500 ppm (equivalent to 96 mg/kg bw/day for females and 132 mg/kg bw/day for males) (NICNAS 2015; OECD 2007).

A NOAEL of 200 mg/kg bw/day was established in a 90 day oral toxicity study in rats fed sodium C_{14-16} olefin sulfonate, based on slight increases in the relative liver weight ratio in

animals receiving 1000 mg/kg bw/day (highest dose tested). In a separate 91 day oral toxicity study, there were no treatment-related effects in rats exposed to sodium C_{14-16} olefin sulfonate (34% concentration) at doses up to 500 mg/kg bw/day (NICNAS 2015).

In an oral repeated dose toxicity study, Wistar rats (10/sex/dose) were treated with sodium C_{14} olefin sulfonate (CAS No. 93686-14-7) via gavage at 0, 100, 250 or 500 mg/kg bw/day for 26 weeks. Increased mortality and decreased body weight gain was reported at the highest dose. Increased level of serum glutamic oxaloacetic transaminase (GOT), glutamate-pyruvate transaminase (GPT) and alkaline phosphatase (ALP) and adrenal weights was observed at this dose. The NOAEL was determined to be 100 mg/kg bw/day (OECD 2007).

Dermal

Based on the read across information from other alkane and alkene sulfonates, the chemicals in this evaluation are not expected to cause serious systemic health effects following repeated dermal exposure.

In a subacute dermal repeated dose study, female CD-1 mice (25/dose) were administered up to 32% w/v SAS (60% concentration) by dermal application for 5 weeks. Encrustation, skin thickening, erythema and skin sloughing were observed at the treated skin sites in all mice within 2–7 days of treatment at 16 and 32% w/v. Increased absolute and relative spleen weights was reported in mice at 32% w/v. However, this was considered a secondary response due to skin inflammation caused by the irritating properties of SAS. An NOAEL was determined to be 8% w/v (OECD 2007).

Genotoxicity

Based on the available data for sodium 1-octanesulfonate and the read across information from other alkyl and alkene sulfonates, these chemicals are not expected to have genotoxic potential. Structurally similar alkyl sulfates are not considered to have genotoxic potential (AICIS 2024a).

In vitro

Chemicals in this evaluation

Negative results were reported for sodium 1-octanesulfonate in the following genotoxicity studies (REACH n.d.-a):

- a bacterial reverse mutation assay (OECD TG 471) in *Salmonella typhimurium* strains TA 98, TA 100, TA 102, TA 1535 and TA 1537, with and without metabolic activation (S9) at concentrations up to 5,000 µg/plate
- a chromosome aberration assay (OECD TG 473) in human lymphocytes with and without metabolic activation (S9) at concentrations up to 2,500 µg/mL
- a mammalian gene mutation assay (OECD TG 476) in the mouse lymphoma L5178Y cells with and without metabolic activation (S9) at concentrations up to 80 µg/mL.

Other alkyl and alkene sulfonates – read across

Negative results were reported for SAS (30% concentration) in a bacterial reverse mutation assay (OECD TG 471) in *S. typhimurium* strains TA 98, TA 100, TA 1535 and TA 1537, with

and without metabolic activation (S9) at concentrations up to 5 µL/plate (AISE and Cefic 2005).

In a mammalian cell gene mutation assay conducted according to OECD TG 476, SAS (93% concentration) was non-mutagenic in the hypoxanthine-guanine-phosphoribosyl-transferase (HPRT) locus assay using Chinese Hamster V79 cells (NICNAS 2014).

Negative results were reported for sodium $C_{14\text{-}16}$ olefin sulfonate and sodium C_{14} olefin sulfonate (CAS No. 93686-14-7) in (OECD 2007):

- a bacterial reverse mutation assay (OECD TG 471) in *S. typhimurium* strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538 and *Escherichia coli* WP2uvrA, with and without metabolic activation (S9) at concentrations up to 10,000 µg/plate
- a chromosome aberration assay (OECD TG 473) in Chinese hamster V79 or CHL cells, with and without metabolic activation (S9) at concentrations up to 250 µg/mL.

In vivo

In 2 non-guideline mammalian erythrocyte micronucleus tests, CD1 or NMRI mice (5/sex/dose) were administered SAS (60% concentration) by gavage for 2 days. There were no significant increases in the incidence of micronuclei in polychromatic erythrocytes at concentrations up to 1,200 mg/kg bw/day, indicating a lack of clastogenic activity (AISE and Cefic 2005).

In silico

The discrete chemicals in this group have no structural alerts for Ames mutagenicity based on the mechanistic profiling functionality of the OECD QSAR Toolbox v4.5 (OECD n.d.), and the knowledge based expert system DEREK Nexus version 6.0.1 (Lhasa Limited n.d.). These chemicals are predicted to be in vitro Ames negative by the OASIS–TIMES (Optimised Approach based on Structural Indices Set–Tissue Metabolism Simulator; version 2.31), with model Ames Mutagenicity S9 activated v18.18 (OASIS LMC n.d.).

Carcinogenicity

No data are available for these chemicals.

Based on the read across information from other alkane and alkene sulfonates, chemicals in this group are not expected to have carcinogenic potential. Structurally similar alkyl sulfates are not considered to have carcinogenic potential (AICIS 2024a).

In a 2 year carcinogenicity study, CD rats (50/sex/dose) received SAS (60% concentration) in their diet at 0.08, 0.4 or 2% (w/w) (equivalent to 40, 200 or 1,000 mg/kg bw/day). Reduced body weight gain was observed in both males (0 to 52 weeks) and females (0 to 12 weeks) at 2% (w/w). No treatment-related clinical signs, or incidences of non-neoplastic and neoplastic histopathological findings were reported (AISE and Cefic 2005; NICNAS 2014).

In a 2 year dermal carcinogenicity study, CD-1 mice (100 sex/dose) were topically exposed to SAS (60% concentration) in water at concentrations up to 1% w/v for 80 weeks and observed for a further 24 weeks. No treatment-related clinical signs, or incidences of non-neoplastic and neoplastic histopathological findings were reported (AISE and Cefic 2005; NICNAS 2014).

In a 2 year carcinogenic study, SD CFY rats (50/sex/dose) were administered sodium C_{14-16} olefin sulfonate in diet at 0, 1,000, 2,500 and 5,000 ppm (equivalent to 0, 39, 96 and 195 mg/kg bw/day for males and 0, 57, 132 and 259 mg/kg bw/day for females, respectively). Mortalities were reported in all groups including the control group. Decreased food intake in females (0 to 52 weeks) and decreased body weight gain (14 to 26 weeks) in both sexes was observed. Increased incidences of pancreatic islet cell tumours (male), adrenal tumours (male) and thyroid tumour (female) were reported at 57 and 132 mg/kg bw/day doses, while the incidences at the highest dose were comparable with the control group. These incidences were within the historical control data. No adverse clinical, haematological or clinical chemistry effects and no adverse histopathological findings were reported (NICNAS 2015; OECD 2007).

There were no increases in tumours reported in a 24–27 week carcinogenicity study in Wistar rats exposed to sodium C_{14-16} olefin sulfonate in the diet at doses up to 500 mg/kg bw/day (NICNAS 2015).

In a 2 year dermal carcinogenicity study, 1 mL/kg bw/day of 10% sodium C_{14-16} olefin sulfonate in deionised water (calculated 100 mg/kg bw/day) was applied to the clipped dorsal surface of Long-Evans rats (50/sex/dose) twice per week. Relative kidney weights were significantly decreased in dosed males. Mortality, mean body weights, food consumption, haematology, urinalysis, and post-mortem observations were comparable to the control group. No carcinogenic effects were reported in the study (NICNAS 2015; OECD 2007).

No significant treatment-related toxicity or lesions were reported in a 92 week dermal exposure study in Swiss Webster mice treated with sodium C_{14-16} olefin sulfonate at concentrations up to 25% (NICNAS 2015).

Reproductive and development toxicity

No data are available for these chemicals.

Based on the weight of evidence of read across data from other alkane and alkene sulfonates, the chemicals are not expected to cause specific adverse effects on fertility or development following oral exposure. No concerns for reproductive or developmental toxicity were identified for alkyl sulfates (AICIS 2024a).

In a 2 generation reproductive toxicity study, Charles River CD rats were administered SAS (60% concentration) in the diet at concentrations of 1,000, 3,000 and 10,000 ppm from 60 days prior to mating and throughout 3 successive pregnancies. The only adverse effect in any generation was a slight, but not statistically significant, reduction in body weight in males in the high dose group. There were no signs of reproductive or developmental toxicity in any generation during the study. Therefore, the NOAEL for reproductive and developmental toxicity in the study was 10,000 ppm (approximately equivalent to 500 mg/kg bw/day (AISE and Cefic 2005).

In studies with sodium C_{14-16} olefin sulfonate including two generation studies in rats, mice and rabbits, there was no evidence of specific reproductive or developmental toxicity, with all adverse effects occurring in the presence of maternal toxicity (NICNAS 2015).

In various oral reproductive and developmental toxicity studies in rats, mice and rabbits with structurally similar alkyl sulfates with carbon chain between C_{12} and C_{18} in length, there were limited observations of effects on the offspring at doses
≥ 500 mg/kg bw/day. Some reported adverse effects included decreased mean foetal body weights, increased incidences of stillbirths and increased incidences of skeletal defects and

abnormalities. However, all adverse effects in the offspring occurred in the presence of maternal toxicity, therefore, alkyl sulfates are not considered to cause specific reproductive or developmental toxicity (OECD 2007).

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