SODIUM LAURYL SULFOACETATE

(CAS #1847-58-1)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: December 20, 2023

Expiration Date: December 20, 2028

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GreenScreen® Executive Summary for Sodium Lauryl Sulfoacetate (CAS #1847-58-1)

Sodium lauryl sulfoacetate, also known as sodium dodecyl sulfoacetate, is a sodium salt of a sulfoacetic acid ester with a 12-carbon alkyl alcohol. It functions as a cosmetic ingredient in personal care products (cleansing, foaming, and surfactant – cleansing agent).

Sodium lauryl sulfoacetate is a white solid at room temperature that is highly soluble in water. It is neither flammable nor reactive.

Sodium lauryl sulfoacetate was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes"). This score is based on the following hazard score:

- Benchmark 2f
    - Very High Group II Human Toxicity (eye irritation-IrE)

Data gaps (DG) exist for endocrine activity – E and neurotoxicity-repeated dose (Nr*). As outlined in GreenScreen® Guidance Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), sodium lauryl sulfoacetate meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gaps. In a worst-case scenario, if sodium lauryl sulfoacetate were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* tests for genotoxicity and *in silico* modeling for respiratory sensitization. The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties:

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

Type I (input data) uncertainties in sodium lauryl sulfoacetate's NAMs dataset include lack of validated test methods for respiratory sensitization. Sodium lauryl sulfoacetate's type II (extrapolation output) uncertainties include the limitations of *in vitro* genotoxicity assays to mimic *in vivo* metabolic conditions, inability of some *in silico* models to evaluate ionic substances and surfactants, and lack of defined applicability domains for OECD Toolbox when evaluation respiratory sensitization alerts. Some of sodium lauryl sulfoacetate's type II uncertainties were alleviated by the use of genotoxicity test batteries in combination with *in vivo* data, and ECHA's decision framework to evaluate respiratory sensitization.

GreenScreen® Hazard Summary Table for Sodium Lauryl Sulfoacetate

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F
						s	r*	s	r*	*	*								
L	**L**	*L*	*L*	DG	*M*	*M*	**L**	*L*	DG	*L*	*L*	*M*	**vH**	**H**	*H*	**L**	***vL***	*L*	*L*

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Chemical Assessment for Sodium Lauryl Sulfoacetate (CAS #1847-58-1)

Method Version: GreenScreen® Version 1.4
Assessment Type[1]: Certified
Assessor Type: Licensed GreenScreen® Profiler

GreenScreen® Assessment (v.1.4) Prepared By:
Name: Mouna Zachary, Ph.D.
Title: Senior Toxicologist
Organization: ToxServices LLC
Date: November 2, 2023

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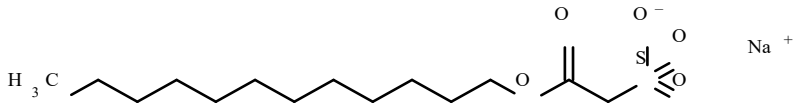
Name: Jennifer Rutkiewicz, Ph.D.
Title: Senior Toxicologist
Organization: ToxServices LLC
Date: December 20, 2023

Expiration Date: December 20, 2028[2]

Chemical Name: Sodium lauryl sulfoacetate

CAS Number: 1847-58-1

Chemical Structure(s):



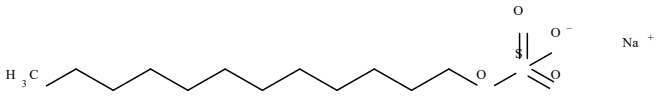
(PubChem 2023)

Also called: Acetic acid, sulfo-, 1-dodecyl ester, sodium salt; Acetic acid, sulfo-, dodecyl ester, S-sodium salt; Dodecyl sodium sulfoacetate; Dodecyl sulfoacetate S-sodium salt; Lathanol; Lathanol LAL; Lathanol-lal 70; Nacconol LAL; Sodium 2- (dodecyloxy)- 2- oxoethane- 1- sulphonate; Sodium 2-(dodecyloxy)-2-oxoethane-1-sulfonate; Sodium 2-(dodecyloxy)-2-oxoethane-1-sulphonate; Sodium lauryl sulfoacetate; Sulfoacetic acid 1-dodecyl ester, sodium salt; Sulfoacetic acid dodecyl ester S-sodium salt; Acetic acid, 2-sulfo-, dodecyl ester, sodium salt (1:1) (PubChem 2023).

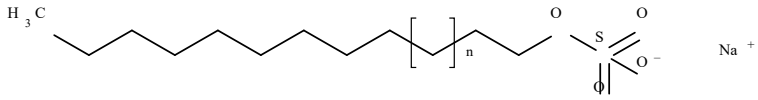
Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
Sodium lauryl sulfoacetate has relatively a complete toxicological dataset. However, some data gaps exist. Sodium lauryl sulfoacetate is an anionic surfactant that is the sodium salt of a sulfoacetic acid ester with a 12-carbon alkyl alcohol. Therefore, its structure is somewhat similar to those of alcohol/alkyl sulfates AS), which have been reviewed as a class by the Human & Environmental Risk Assessment (HERA) and the Organisation for Economic Cooperation and Development's (OECD) due to their structural similarities (HERA 2002, OECD 2007). Members of this chemical group are anionic surfactants consisting of a linear aliphatic hydrocarbon chain with a length between C8 and C18 and a polar sulfate or sulfonate group, neutralized with a counter ion such as sodium (Na+), potassium (K+), or ammonium (NH4 +). They can be single chemicals or mixtures and they have similar functional groups (aliphatic constituents) and physicochemical properties, and available data support similar metabolism and a similar order of toxicity (OECD 2007. HERA 2002). ToxServices considered data for

[1] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), or "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent).
[2] Assessments expire five years from the date of completion starting from January 1, 2019. An assessment expires three years from the date of completion if completed before January 1, 2019 (CPA 2018a).

related alkyl sulfates with similar carbon lengths to address the data gaps for the target chemical. These included sodium dodecyl sulfate (C12, CAS #151-21-3) and sulfuric acid, mono-C12-15-alkyl esters, sodium salts (CAS #68890-70-0). As these surrogates are sulfate esters rather than sulfoacetate esters like the target chemical, and have low maximum common substructure (MCS) Tanimoto coefficient[3] of 0.5 with the target chemical, ToxServices considered them to be weak surrogates and assigned low confidence to hazard scores based on data for these surrogates.



Surrogate: Sodium dodecyl sulfate (CAS #151-21-3)



Where n = 1-4

Surrogate: Sulfuric acid, mono-C12-15-alkyl esters, sodium salts (CAS #68890-70-0)

Identify Applications/Functional Uses (PubChem 2023, CIR 1987):

1. Cleansing, foaming, and surfactant – cleansing agent in cosmetics formulations.

Known Impurities[4]:
Sodium lauryl sulfoacetate may contain up to 18% sodium sulfate and sodium chloride as impurities (U.S. EPA 2004). The screen is performed on the theoretical pure substance.

GreenScreen® Summary Rating for Sodium Lauryl Sulfoacetate[5,6 7,8]: Sodium lauryl sulfoacetate was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes") (CPA 2018b). This score is based on the following hazard score combinations:
This score is based on the following hazard score:

- Benchmark 2f
    - Very High Group II Human Toxicity (eye irritation-IrE)

Data gaps (DG) exist for endocrine activity – E and neurotoxicity-repeated dose (Nr*). As outlined in GreenScreen® Guidance Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis) (CPA 2018b), sodium lauryl sulfoacetate meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gaps. In a worst-case scenario, if sodium lauryl sulfoacetate were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

[3] Determined using ChemMine's similarity workbench (https://chemminetools.ucr.edu/similarity/).
[4] Impurities of the chemical will be assessed at the product level instead of in this GreenScreen®.
[5] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.
[6] See Appendix A for a glossary of hazard endpoint acronyms.
[7] For inorganic chemicals only, see GreenScreen® Guidance v1.4 Section 12 (Inorganic Chemical Assessment Procedure).
[8] For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen® Guidance v1.4 Annex 2.

Figure 1: GreenScreen® Hazard Summary Table for Sodium Lauryl Sulfoacetate

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F
						s	r*	s	r*	*	*								
L	**L**	*L*	*L*	DG	*M*	*M*	**L**	*L*	DG	*L*	*L*	*M*	**vH**	**H**	*H*	**L**	***vL***	*L*	*L*

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

Environmental Transformation Products

Per GreenScreen® guidance (CPA 2018b), chemicals that degrade rapidly and completely (i.e., meet criteria for a Very Low for persistence) are not likely to form persistent biodegradation intermediates because the degradation intermediates will not persist long enough to be encountered after use or release of the parent chemical (i.e., relevant). As sodium lauryl sulfoacetate is readily biodegradable when tested experimentally, it is not expected to have relevant transformation products.

Introduction

Sodium lauryl sulfoacetate, also known as sodium dodecyl sulfoacetate, is a sodium salt of a sulfoacetic acid ester with a 12-carbon alkyl alcohol. It functions as a cosmetic ingredient in personal care products (cleansing, foaming, and surfactant – cleansing agent) (CIR 1987). ToxServices assessed sodium lauryl sulfoacetate against GreenScreen® Version 1.4 (CPA 2018b) following procedures outlined in ToxServices' SOPs (GreenScreen® Hazard Assessment) (ToxServices 2021).

U.S. EPA Safer Choice Program's Safer Chemical Ingredients List

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2023). It can be accessed at: http://www2.epa.gov/saferchoice/safer-ingredients. Chemicals on the SCIL have been assessed for compliance with the Safer Choice Standard and Criteria for Safer Chemical Ingredients (U.S. EPA 2015).

Sodium lauryl sulfoacetate is listed on the U.S. EPA SCIL as a surfactant with a Green Circle (Verified Low Concern).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen Benchmark™ 1 chemicals (CPA 2018b). Pharos (Pharos 2023) is an online list-searching tool that is used to screen chemicals against all of the lists in the List Translator electronically. ToxServices also checks the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b),[9] which are not considered GreenScreen® Specified Lists but are additional information sources, in conjunction with the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for sodium lauryl sulfoacetate can be found in Appendix C.

[9] DOT lists are not required lists for GreenScreen® List Translator v1.4. They are reference lists only.

- Sodium lauryl sulfoacetate is an LT-UNK chemical when screened using Pharos, and therefore a full GreenScreen® is required.
- Sodium lauryl sulfoacetate is not listed on the U.S. DOT list.
- Sodium lauryl sulfoacetate is listed on the following lists for multiple endpoints:
    - German FEA - Substances Hazardous to Waters - Class 1 – Low Hazard to Waters.
- Sodium lauryl sulfoacetate is not listed on any specified lists for single endpoints.

Hazard Statement and Occupational Control

Sodium lauryl sulfoacetate, is associated with several Globally Harmonized System of Classification and Labelling of Chemicals (GHS) hazard statements as shown in Table 1, identified by the majority of notifiers in the European Chemicals Agency (ECHA)'s classification and Labeling (C&L) inventory (ECHA 2023a).

Table 1: GHS H Statements for Sodium Lauryl Sulfoacetate (CAS #1847-58-1) (ECHA 2023a)

H Statement	H Statement Details
H302	Harmful if swallowed
H335	May cause respiratory irritation
H315	Causes skin irritation
H318	Causes serious eye damage

General personal protective equipment (PPE) recommendations are presented in Table 2, below. No occupational exposure limits (OELs) were identified.

Table 2: Occupational Exposure Limits and Recommended Personal Protective Equipment for Sodium Lauryl Sulfoacetate (CAS #1847-58-1)

Personal Protective Equipment (PPE)	Reference	Occupational Exposure Limits (OEL)	Reference
Protective eyeglasses, skin and body protection protective clothing and appropriate NIOSH approved respiratory protection when exposed to airborne dust	Cayman Chemical 2023	None identified	

Physicochemical Properties of Sodium Lauryl Sulfoacetate

Sodium lauryl sulfoacetate is a white solid at room temperature that is highly soluble in water (> 500 g/L). It has a low vapor pressure, indicating that it is not expected to volatilize under standard temperature and pressure. However, inhalation exposure to dust or aerosol particles is possible. The surrogate has calculated log K_{ow} value of -2.03 from its solubility in octanol (1.2 g/L) indicating that it not expected to bioaccumulate. *According to ECHA Guidance on regulatory compliant K_{ow} determination for surfactants (ECHA 2017), the calculated K_{ow} value based on the octanol and water solubilities is considered the most reliable method for surfactants while estimated values by EPI Suite™ are not appropriate as surfactants are outside the applicability domain of the program. Therefore, ToxServices did not weigh heavily on the estimated log Kow value for the target chemical that is reported in the United States Environmental Protection Agency's assessments (U.S. EPA 2007, 2009)*

Table 3: Physical and Chemical Properties of Sodium Lauryl Sulfoacetate (CAS #1847-58-1)		
Property	**Value**	**Reference**
Molecular formula	$C_{14}H_{27}O_5SNa$	PubChem 2023
SMILES Notation	CCCCCCCCCCCCOC(=O)CS(=O)(=O)[O-].[Na+]	PubChem 2023
Molecular weight	330.42 g/mol	PubChem 2023
Physical state	Solid	PubChem 2023, U.S. EPA 2007
Appearance	White powder	PubChem 2023
Melting point	163-175°C (decomposes)	U.S. EPA 2007
Boiling point	Decompose before boiling	U.S. EPA 2007
Vapor pressure	3.0×10^{-14} hPa at 25°C	U.S. EPA 2007
Water solubility	10,000 mg/L at 25°C	U.S. EPA 2007
Dissociation constant	Not identified	
Density/specific gravity	0.55	PubChem 2023
Partition coefficient	Log K_{ow} = 2.66 at 22°C (estimated) Log K_{ow} <= -2.03 at 20°C for the surrogate sodium dodecyl sulfate (CAS #151-21-3) (calculated from the solubilities of the test substance in water and 1-octanol)	U.S. EPA 2007, 2009 ECHA 2023b

Toxicokinetics

Very limited experimental toxicokinetics data were identified for sodium lauryl sulfoacetate. It is absorbed through the skin, based on a study in which guinea pigs were immersed in a 0.2% aqueous sodium lauryl sulfoacetate solution followed by analysis in blood (CIR 1987).

Data on the chemical class AS were available and are summarized briefly below:

- ECHA 2023b, OECD 2007, HERE 2002
    - *Absorption:*
        - *Oral:* AS were well absorbed when tested in rats, dogs and humans following oral exposure. An excretion of up to 98% of the dose administered (maximum for C12AS Na) was seen in the urine of treated animals. Based on that, the oral absorption for such compounds is assumed to be 100%.
        - *Dermal*: AS are expected to have low absorption following dermal exposure with a default assumption of 1% dermal absorption based on studies with isolated human skin and animal tests. As they are anionic surfactants, AS tend to bind to the skin surface. In animal studies, less than 0.4% of a 3 µmol dose of radio labeled sodium dodecyl sulfate was percutaneously absorbed in guinea pigs, based on recovery of the radiolabel in urine, feces, and expired air.
        - *Inhalation:* AS have low vapor pressure and therefore are not expected to be significantly volatile. However, they exist in powder form and hence finely divided powder or dust may enter the respiratory tract. Thus, absorption by inhalation is expected.
    - *Distribution:* Based on the results from the *in vivo* toxicity studies along with their relatively high water solubility, AS are distributed mainly to the liver.
    - *Metabolism:* Alkyl sulfates and alkane sulfonates are extensively metabolized in rats, dogs and humans to yield a sulfate ester as the final product of degradation. They are metabolized

by cytochrome P450-dependent ω-oxidation and subsequent ß-oxidation of the aliphatic fatty acids. End products of the oxidation are a C4 sulfate or sulfonate (even numbered chain lengths) and a C3 or C5 sulfate or sulfonate (odd numbered chain lengths).
    - *Elimination:* Urine excretion is the main route of elimination of AS and their metabolites.
- In summary and based on data for the chemical class (AS), oral absorption of sodium lauryl sulfoacetate is assumed to be high, as well as absorption by inhalation when the test substance is present as a finely divided powder or dust. Sodium lauryl sulfoacetate is expected to distribute mainly to the liver, and be metabolized to a smaller sulfate ester. The main excretion pathway is expected to be via urine.

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for carcinogenicity based on negative results in an oral carcinogenicity study conducted with the surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on reliable measured data for a weak surrogate.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA 2023b, OECD 2007
    - *Oral: Surrogate: Sulfuric acid, mono-C12-15-alkyl esters, sodium salts (CAS #68890-70-0)*: A pre-GLP combined chronic toxicity/carcinogenicity study conducted in a manner similar to OECD Guideline 453 (missing some examinations like urinalysis parameters) was performed with Colworth Wistar rats (45/sex/group) provided diets containing the test substance (30% active ingredient (a.i.) in water) at 0.015, 0.15, or 1.5% (contributing doses of 11, 113, and 1,125 mg/kg/day, respectively) for 2 years. Treatment did not increase the total number of tumors, the number of tumor-bearing rats, or the tumor incidence. While the total number of pancreatic tumors was increased in high dose males, this was due to a slight increase in both islet- and exocrine-type tumors. When analyzed separately, no statistically significant difference was detected between the treatment and control groups. The REACH dossier authors concluded that the surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts was not carcinogenic under the conditions of this test (Klimisch Score 2, reliable with restrictions).

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L
Sodium lauryl sulfoacetate was assigned a score of Low for mutagenicity/genotoxicity based on negative results in *in vitro* bacterial mutagenicity and chromosome aberration assays. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when negative data are available for both gene mutations and chromosome aberrations, and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on measured data of good quality for the target chemical.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.

- U.S. EPA 2004, 2007, 2009
    - *In vitro*: Negative results for mutagenicity were obtained in a non-GLP bacterial reverse mutation assay in which *Salmonella typhimurium* tester strains TA98, TA100, TA1535, TA1537, and TA1538, and *Saccharomyces cerevisiae* (D4) were exposed to 3% sodium lauryl sulfoacetate in a shampoo product at 0-1,000 µg/plate, with and without metabolic activation (Liver S9 mix). No increase in the mutation frequency was observed in the presence or absence of metabolic activation. Negative (dimethyl sulfoxide (DMSO) and positive controls (N-methyl,N-nitro,N-nitrosoguanidine, 9-aminoacridine, 2-nitrofluorene, 2-anthramine) were reported as valid (Klimisch score 2, reliable with restrictions).
    - *In vitro*: Negative results for mutagenicity were obtained in a non-GLP bacterial reverse mutation assay in which *S. typhimurium* tester strains TA98, TA100, TA1535, TA1537, and TA1538, and *S. cerevisiae* (D4) were exposed to 19 and 23% sodium lauryl sulfoacetate in a cleansing bar product at 0-1,000 µg/plate, with and without metabolic activation (Liver S9 mix). No increase in the mutation frequency was observed in the presence or absence of metabolic activation. Negative (water) and positive controls (N-methyl,N-nitro,N-nitrosoguanidine, 9-aminoacridine, 2-nitrofluorene, 2-anthramine) were reported as valid (Klimisch score 2, reliable with restrictions).
    - *In vitro*: In a GLP-compliant chromosome aberration study conducted according to OECD Guideline 473, human lymphocytes cells were treated with a commercial product containing 74.26% sodium lauryl sulfoacetate (trade name: Lathanol LAL) at concentrations of 50-500 µg/mL in the presence and absence of metabolic activation (Rat S9 mix). Cytotoxicity was observed at ≥ 200 µg/mL with metabolic activation and at ≥ 500 µg/mL without metabolic activation. There were no increases in the number of cells with chromosome aberrations and authors concluded that the test substance was not clastogenic. Vehicle and positive controls were reported as valid (Klimisch score 1, reliable without restriction).

Reproductive Toxicity (R) Score (H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for reproductive toxicity based on the lack of reproductive effects reported in an oral screening study at doses up to 1,000 mg/kg/day. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on a screening study that may not have examined all related endpoints.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
    - In a GLP-compliant reproductive/developmental toxicity screening test conducted according to OECD Guideline 421, male and female Crl:(WI) BR rats (10/sex/dose) were administered a commercial product containing approximately 73% sodium lauryl sulfoacetate (trade name: Lathanol LAL) at doses of 0, 40, 500, and 1,000 mg/kg/day in propylene glycol by gavage for two weeks prior to mating, during gestation, and up to postnatal day (PND) 3 (total of 42-46 days for females, and up until necropsy for males (approximately 39 days). Treatment caused effects in males and females at high dose, including a decrease in white blood cell counts (high dose males), decreased body weight gain (high dose males), and decreased food consumption (male and female – high dose). Treatment related macroscopic findings included thickening and irregular surface of the stomach, and microscopic findings included hyperplasia of the forestomach epithelium, lymphogranulocytic inflammation (increased white blood cells corresponding to increased white blood cell counts), and erosion

of the stomach for both male and female high dose groups. The study authors identified a NOAEL of 200 mg/kg/day and a LOAEL of 1,000 mg/kg/day for parental systemic toxicity based on pathology finding in the stomach. In terms of reproductive toxicity, there were no treatment related effects on reproductive parameters measured in this study including the male number paired with, mating date, confirmation of pregnancy, delivery day, or numbers of corpora lutea and implantations. Additionally, there were no test-material-related microscopic changes reported in the testes or epididymides of adult male rats or in the ovaries of adult female rats. Therefore, the authors reported the reproductive NOAEL of 1,000 mg/kg/day for this study, the highest dose tested (Klimisch score 1, reliable without restriction).

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for developmental toxicity based on the lack of developmental effects reported in an oral screening study at doses up to 1,000 mg/kg/day. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on a screening study that may not have examined all related endpoints.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
  - In the previously described GLP-compliant reproductive/developmental toxicity screening test conducted according to OECD Guideline 421, male and female Crl:(WI) BR rats (10/sex/dose) were administered a commercial product containing approximately 73% sodium lauryl sulfoacetate (trade name: Lathanol LAL) at doses of 0, 40, 500, and 1,000 mg/kg/day in propylene glycol by gavage for two weeks prior to mating, during gestation, and up to PND 3 (total of 42-46 days for females, and up until necropsy for males (approximately 39 days). Litters were evaluated for number and sex of pups, stillbirths, live births, postnatal mortality, presence of gross anomalies, weight gain, physical or behavioral abnormalities, and external examinations. There were no treatment related effects on any of these evaluated parameters. Authors assigned NOAEL of 1,000 mg/kg/day for developmental toxicity under the conditions of this study (Klimisch score 1, reliable without restriction).

Endocrine Activity (E) Score (H, M, or L): DG
Sodium lauryl sulfoacetate was assigned a score of Data Gap for endocrine activity due to lack of sufficient data. A subchronic oral study in rats reported epithelial whorls in the thyroids of female at 750 mg/kg/day, but this study did not include hormone analysis, and the relevance of the pathological change is unclear.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

- U.S. EPA 2004, 2007, 2009
    - In the GLP-compliant subchronic repeated dose toxicity study conducted in a manner similar to OECD Guideline 408 that is described in detail below for the systemic toxicity (repeated dose) endpoint, male and female CD (SD) BR rats (20/sex/group) were administered 0, 75, 250, and 750 mg/kg/day of sodium lauryl sulfoacetate (73.8% purity) in distilled water by gavage for 90 days. Epithelial whorls were observed in the thyroid of top dose females.

Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. See GreenScreen® Guidance v1.4, Annex 2 for more details.

Acute Mammalian Toxicity (AT) (Group II) Score (vH, H, M, or L): *M*

Sodium lauryl sulfoacetate was assigned a score of Moderate for acute toxicity based on a dermal LD_{50} value of < 1,280 mg/kg in male rabbits. GreenScreen® criteria classify chemicals as a Moderate hazard for acute toxicity when the most conservative dermal LD_{50} values are >1,000 – 2,000 mg/kg and they are classified as GHS Category 4 acute toxicants for any route of exposure (CPA 2018b). The confidence in the score is low as insufficient details were provided to confirm that the dermal LD_{50} does not fall in the range for a High.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
    - *Oral*: LD_{50} (Sprague-Dawley rats) > 2,000 mg/kg for a test substance containing 64-85% active ingredient (sodium lauryl sulfoacetate) (GLP-compliant, OECD Guideline 401) (Klimisch score 1, reliable without restriction). *The adjusted LD_{50} for 100% active ingredient would be > 1,280-1,680 mg/kg*[10].
    - *Dermal*: LD_{50} (New Zealand White rabbits) > 2,000 mg/kg in females and < 2,000 mg/kg in males for a test substance containing 64-85% active ingredient (GLP-compliant, OECD Guideline 402) (Klimisch score 1, reliable without restriction). *The adjusted LD_{50} for 100% active ingredient would be < 1,280-1,680 mg/kg in males.*

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-single) (Group II) Score (vH, H, M, or L): *M*

Sodium lauryl sulfoacetate was assigned a score of Moderate for systemic toxicity (single dose) based on ToxServices classifying it to GHS Category 3 for respiratory irritation, as skin and eye irritation data indicate that it is corrosive to the eyes and irritating to the skin, and therefore it is most likely to be also irritating to the respiratory tract. GreenScreen® criteria classify chemicals as a Moderate hazard for systemic toxicity (single dose) when they are classified as GHS Category 3 specific target organ toxicants following single exposures for respiratory tract irritation (CPA 2018b). The confidence in the score is low due to lack of acute inhalation toxicity studies on the target chemical or a surrogate.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
    - *Oral*: In a GLP-compliant acute oral toxicity study conducted according to OECD Guideline

[10] LD_{50} for sodium lauryl sulfoacetate (active ingredient) = (LD_{50} the trade name x purity %) / 100 = (2,000 mg/kg x 64) / 100 = 1,280 mg/kg

401, male and female Sprague-Dawley rats (5/sex/dose) received a commercial product containing 64-85% sodium lauryl sulfoacetate moistened with distilled water at a single dose of 2,000 mg/kg via gavage. An observation period of 14 days followed. Animals exhibited clinical signs of toxicity such as loose stool, hypoactivity and prostration on day 1. Necropsy of dead animals (1 male and 1 female) revealed distended stomach and intestines with gas and fluid and red colored small intestine in the female. There were no treatment related effects on body weight. The study authors identified an oral LD_{50} of > 2,000 mg/kg (Klimisch score 1, reliable without restriction).

- *Dermal:* In a GLP-compliant acute dermal toxicity study conducted according to OECD Guideline 402, New Zealand White rabbits (5/sex/dose) were dermally administered a commercial product containing 64-85% sodium lauryl sulfoacetate moistened with distilled water at a single dose of 2,000 mg/kg under occluded conditions for 24 hours and were observed for 14 days. Treatment caused mortality (three males and one female). Clinical signs of toxicity were limited to dermal irritation which was characterized as erythema (until day 7-8), oedema (until day 9-11), eschar, and coriaceousness (leathery texture) (until day 11-14) and formation of scar tissue. Necropsy of dead animals showed severe tissue damage and necrosis of the skin at the application site. The study authors identified a dermal LD_{50} of < 2,000 mg/kg in males (Klimisch score 1, reliable without restriction).

- In summary, treatment-related effects identified in the single oral and dermal exposure studies included potentially neurological signs of toxicity and dermal irritation at the site of application (dermal toxicity studies only). The potentially neurological signs of toxicity are discussed under the neurotoxicity section below. As sodium lauryl sulfoacetate is irritating to skin and eyes when tested at concentrations of 64% and above (see the corresponding sections below), it is expected to be also irritating to the respiratory tract. Therefore, ToxServices classified sodium lauryl sulfoacetate as a GHS Category 3 specific target organ toxicant following single exposures for respiratory irritation. This corresponds to a GreenScreen® score of Moderate. The confidence level of the score is reduced due to lack of an acute inhalation toxicity study.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-repeat) (Group II*) Score (H, M, or L): L

Sodium lauryl sulfoacetate was assigned a score of Low for systemic toxicity (repeated dose) based on an oral NOAEL of 250 mg/kg/day in a 90-day study in rats, which is above the d GHS guidance cut-off value of 100 mg/kg/day (oral) for Category 2. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when animal studies identify oral LOAELs of > 100 mg/kg/day in 90-day studies, and when they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on measured data of high quality for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
  - In a GLP-compliant dose range-finding 28-day oral study, male and female CD rats (5/sex/group) were administered sodium lauryl sulfoacetate (73.8% purity) at doses of 0, 50, 200, and 800 mg/kg/day by gavage. The concentrations as measured were 98-108% of nominal concentrations. The animals were evaluated for clinical signs of toxicity, food and water consumption, body weight gain, hematology, clinical chemistry, organ weight, gross pathology, and histopathology. No mortality was observed. Treatment caused poor coat condition in mid-dose females and high-dose males, and post-dose salivation for all high dose animals. Males at the high dose group had increased absolute and relative liver weights

while females at the same dose group had increased relative kidney and brain weights. Macroscopic findings included raised black foci on the non-glandular mucosa of the stomach in one high dose male. The study authors identified a systemic toxicity NOAEL of 200 mg/kg/day and a LOAEL of 800 mg/kg/day based on organ weight changes and macroscopic findings in the stomach (Klimisch score 2, reliable with restrictions). *The LOAEL of 800 mg/kg/day is above the duration-adjusted GHS guideline value for Category 2 of 30-300 mg/kg/day for a 28-day study (UN 2023). However, the NOAEL of 200 mg/kg/day is within the GHS Category 2 guidance values. Therefore, there is insufficient information to conclude that adverse effects do not occur at 300 mg/kg/day.*

- In a GLP-compliant subchronic repeated dose toxicity study conducted in a manner similar to OECD Guideline 408, male and female CD (SD) BR rats (20/sex/group) were administered 0, 75, 250, and 750 mg/kg/day of sodium lauryl sulfoacetate (73.8% purity) in distilled water by gavage for 90 days. The animals were evaluated for clinical signs of toxicity, food and water consumption, body weight gain, hematology, clinical chemistry, organ weight, gross pathology, and histopathology. Treatment related effects included a decrease in white blood cell counts (high dose males), increased blood urea levels (females, all doses), and increased absolute and relative liver weights (top dose females). Histopathology findings included treatment-related effects in the stomach consistent with mucosal irritation for both males and females at 250 mg/kg/day and above. Furthermore, epithelial whorls were observed in the thyroid of top dose females. The study authors identified a systemic toxicity NOAEL of 75 mg/kg/day and a LOAEL of 250 mg/kg/day based on the histological changes in the stomach mucosa (Klimisch score 1, reliable without restriction). *As sodium lauryl sulfoacetate is a surfactant with corrosive/irritating properties, ToxServices considered the changes observed in the stomach as a local response to the repeated gavage with a corrosive substance. Thus, for GHS classification purposes, ToxServices considered effects other than gastrointestinal irritation (GI). Based on this, ToxServices assigned a systemic toxicity NOAEL of 250 mg/kg/day for this study based on clinical chemistry changes and liver weight changes. The NOAEL of 250 mg/kg/day is above the GHS Guidance oral threshold of 100 mg/kg/day in a 90-day study. Therefore, sodium lauryl sulfoacetate is not classified for systemic toxicity following oral repeated exposure per GHS.*

Neurotoxicity (single dose, N-single) (Group II) Score (vH, H, M, or L): *L*

Sodium lauryl sulfoacetate was assigned a score of Low for neurotoxicity (single dose) based on the lack of neurotoxic effects in acute oral and dermal toxicity studies in rats and rabbits. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (single dose) when adequate negative data are available, and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on studies with limited neurotoxicity examination.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
  - *Oral*: In the previously described GLP-compliant acute oral toxicity study conducted according to OECD Guideline 401, male and female Sprague-Dawley rats (5/sex/dose) received a commercial product containing 64-85% sodium lauryl sulfoacetate moistened with distilled water at a single dose of 2,000 mg/kg via gavage. An observation period of 14 days followed. Animals exhibited clinical signs of neurotoxicity such as hypoactivity and prostration (one animal) on day 1 which disappeared by the end of the observation period.

Necropsy of dead animals (1 male and 1 female) revealed distended stomach and intestines with gas and fluid and red colored small intestine in the female (Klimisch score 1, reliable without restriction). *While hunched posture and prostration have been observed in this study, they are likely the result of general discomfort reactions to bolus dosing of a corrosive test substance rather than specific neurotoxic signs. Therefore, ToxServices did not consider the effects to warrant classification.*

- *Dermal:* In a GLP-compliant acute dermal toxicity study conducted according to OECD Guideline 402, New Zealand White rabbits (5/sex/dose) were dermally administered a commercial product containing 64-85% sodium lauryl sulfoacetate moistened with distilled water at a single dose of 2,000 mg/kg under occluded conditions for 24 hours and were observed for 14 days. Treatment caused mortality (three males and one female). There were no clinical signs of neurotoxicity (Klimisch score 1, reliable without restriction). *Clinical signs of neurotoxicity often evaluated in animal studies include: drowsiness, narcosis, reduced alertness, loss of reflexes, lack of coordination, irritability, fatigue, impaired memory function, deficits in perception and coordination, reaction time, or sleepiness, lethargy, and ataxia. If these effects are not transient in nature, then they shall be considered to support classification for Category 1 or 2 specific target organ toxicity single exposure. As animals in this study did not show any of these signs, ToxServices concluded that sodium lauryl sulfoacetate was not neurotoxic in this study.*

Neurotoxicity (repeated dose, N-repeated) (Group II*) Score (H, M, or L): DG
Sodium lauryl sulfoacetate was assigned a score of Data Gap due to lack of data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- No data were identified.

Skin Sensitization (SnS) (Group II*) Score (H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for skin sensitization based on a conclusion from the Cosmetic Ingredient Review (CIR) Expert Panel, as no skin reactions were seen in human and animal assays on cosmetic formulations containing the target chemical at concentrations up to 2%, supported by negative results in a mouse local lymph node assay with the surrogate. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate negative data are available and the substance is not GHS classified (CPA 2018b). The confidence in the score is low because the human studies only tested up to 2% and the animal study is on a weak surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- CIR 1987
  - In a guinea pig maximization test, a product containing 2.1% sodium lauryl sulfoacetate was neither irritating nor sensitizing to the skin.
  - Human repeat insult patch tests (HRIPTs) indicate that sodium lauryl sulfoacetate at 0.18% to 0.7% in aqueous solution is a mild to strong dermal irritant with repeated use, but it is not a sensitizer.
  - Products diluted to contain a0.7% to 0.75% sodium lauryl sulfoacetate were non-phototoxic to guinea pig skin. Overall, sodium lauryl sulfoacetate is a moderate skin and eye irritant and is not a dermal sensitizer.

- ECHA 2023b
    - *Surrogate: Sodium dodecyl sulfate (CAS #151-21-3):* A local lymph node assay (LLNA) (GLP status not specified) conducted in a manner similar to OECD Guideline 429 (3 instead of 4 animals/group, limited details on test substance) was performed with mice (3/group, strain and sex not specified) administered topical applications of 5%, 10%, or 25% sodium dodecyl sulfate (purity not specified) in DMSO on three consecutive days, or intradermal injections of 0.05%, 0.5%, or 5% Sodium dodecyl sulfate in saline followed five day later with topical applications of 5% Sodium dodecyl sulfate in 50% DMSO on three consecutive days. For the topical application exposures only, the stimulation indices (SIs) were 0.73, 1.61, and 1.13 for the 5%, 10%, or 25% solutions, respectively. For the intradermal injection followed by topical application exposures, the SIs were 1.58, 1.93, and 1.48 for the 0.05%, 0.5%, and 5% solutions, respectively. As none of the SIs exceeded 3, the REACH dossier authors concluded that sodium dodecyl sulfate was not sensitizing to the skin under the tested conditions (Klimisch Score 2, reliable with restrictions).

Respiratory Sensitization (SnR) (Group II*) Score (H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for respiratory sensitization based on the lack of dermal sensitization potential according to the ECHA guidance (2017). GreenScreen® criteria classify chemicals as a Low hazard for respiratory sensitization when they are not GHS classified (CPA 2018b). Confidence in the score is low as this evaluation does not include non-immunologic mechanisms of respiratory sensitization, and no specific data are available for respiratory sensitization.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2023
    - Sodium lauryl sulfoacetate does not contain any structural alerts for respiratory sensitization (Appendix D).
- Based on the weight of evidence and guidance from ECHA regarding assessment of respiratory sensitization potential, a score of Low were assigned. The guidance from ECHA states that the mechanisms leading to respiratory sensitization are essentially similar to those leading to skin sensitization (ECHA 2017). ECHA recommended that if a chemical is not a dermal sensitizer based on high quality data, it is unlikely to be a respiratory sensitizer. ECHA also noted that this rationale does not cover respiratory hypersensitivity caused by non-immunological mechanisms, for which human experience is the main evidence of activity (ECHA 2017). As sodium lauryl sulfoacetate was not sensitizing to the skin (see skin sensitization section above), and a literature search did not find any human evidence of respiratory sensitization by sodium lauryl sulfoacetate, and as sodium lauryl sulfoacetate does not contain any structural alerts for respiratory sensitization (OECD 2023), sodium lauryl sulfoacetate is not expected to be a respiratory sensitizer.

Skin Irritation/Corrosivity (IrS) (Group II) Score (vH, H, M, or L): *M*
Sodium lauryl sulfoacetate was assigned a score of Moderate for skin irritation/corrosivity based on causing mild irritation when tested in rabbits, classifying it to GHS Category 3. GreenScreen® criteria classify chemicals as a Moderate hazard for skin irritation when they are classified to GHS Category 3 (CPA 2018b). The confidence in the score is low due to lack of measured data on the neat chemical (100%) as the available data were on commercial products contain up to 85% the target chemical.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.

- U.S. EPA 2004
    - In a GLP-compliant skin irritation key study conducted according to OECD Guideline 404, 0.5 g of a commercial product containing 64-85% sodium lauryl sulfoacetate (trade name: Lathanol LAL) moistened with distilled water was dermally administered to the clipped skin of six male New Zealand White rabbits for 4 hours under occlusive conditions. Animals were monitored for 14 days. Treatment caused mild irritation with the mean erythema and edema scores at 24, 48, and 72 hours of 1.5 (individual scores of 1.0, 0, 1.6, 2.0, 2.0, 2.6) and 0.3 (individual scores of 0, 0, 0.3, 0.3, 0.3, 1.3). The effects were fully reversible within 7 days. The authors concluded that sodium lauryl sulfoacetate is moderately irritating to the skin under the test conditions (Klimisch score 1, reliable without restriction). *According to GHS Criteria, chemicals that are Category 3 (mild irritant) should have a mean value between 1.5 and 2.3 for erythema/edema in at least 2 of 3 tested animals at 24, 48, and 72 hours or, if reactions are delayed, on 3 consecutive days after the onset of skin reactions. As the erythema scores at 24, 48, and 72 hours were > 1.5 (score of 2) in at least two animals, ToxServices classified sodium lauryl sulfoacetate to GHS Category 3.*
    - Additional skin irritation studies were reported in Appendix A for sodium lauryl sulfoacetate. These studies have a Klimisch score of 3 (not reliable) due to the limited information concerning test conditions and/or experimental methods. Therefore, ToxServices did not consider them in this assessment in the presence of a high quality key study.

Eye Irritation/Corrosivity (IrE) (Group II) Score (vH, H, M, or L): vH
Sodium lauryl sulfoacetate was assigned a score of Very High for eye irritation/corrosivity based on ToxServices classifying it to GHS Category 1 as irreversible effects to the eyes were observed in an *in vivo* study. GreenScreen® criteria classify chemicals as a Very High hazard for eye irritation/corrosivity when they are corrosive and classified to GHS Category 1 (CPA 2018b). The confidence in the score is high as it is based on measured data of good quality for the target chemical.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
    - In a GLP-compliant ocular irritation test conducted according to OECD Guideline 405 study, 0.1 mL of a commercial product containing 64-85% sodium lauryl sulfoacetate (trade name: Lathanol LAL) was instilled in the eyes of six female New Zealand white rabbits without washing. Animals were monitored for 21 days. Treatment caused corneal and conjunctival reactions with severe discharge, which persisted for 21 days. The 24/48/72 hours mean values were 1/4 for cornea opacity, 0.3 for iris, 2/3 for conjunctivae and 1.5/5 for chemosis. Effects on iris, and chemosis were still observed in 1 animal after 21 days while corneal and conjunctival reactions were seen in 2 animals after 21 days. Based on this, authors concluded that the test substance is moderately irritating to the eye (Klimisch score 1, reliable without restriction). *According to GHS Criteria, chemicals that are Category 1 (serious eye damage / irreversible effects on the eye) should produce in at least one animal effects on the cornea, iris, or conjunctiva, that are not expected to reverse or have not fully reversed within an observation period of normally 21 days. Therefore, ToxServices classified sodium lauryl sulfoacetate to eye irritation Category 1 based on irreversible effects to the eyes observed in this study.*
- CIR 1987
    - Products containing sodium lauryl sulfoacetate were minimal to slight irritants to rabbit eyes

at concentrations of 0.35% and 3%.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): H
Sodium lauryl sulfoacetate was assigned a score of High for acute aquatic toxicity based on measured acute aquatic toxicity values as low as 4.2 mg/L across all three trophic levels. GreenScreen® criteria classify chemicals as a High hazard for acute aquatic toxicity when acute aquatic toxicity values are > 1 to 10 mg/L (CPA 2018b). The confidence in the score is high as it is based on reliable measured data for the target chemical for all three trophic levels.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004, 2007, 2009
  - 96-hour LC_{50} (*Danio rerio*, fish) = 4.2 mg/L active ingredient (nominal); test substance is Lathanol LAL powder (purity 70.2%) (GLP-compliant, OECD Guideline 203) (Klimisch score of 1, reliable without restriction).
  - 48-hour EC_{50} (*Daphnia magna*, water flea) = 5.9 mg/L active ingredient; test substance is Lathanol LAL powder (purity 74.26%) (OECD Guideline 202, GLP) (Klimisch 1, reliable without restriction).
  - 72-hour EC_{50} (*Selenastrum capricornutum*, green algae) = 6.8 mg/L for growth rate and 1.9 mg/L for biomass active ingredient; test substance is Lathanol LAL powder (purity 74.26%) (OECD Guideline 201, GLP) (Klimisch 1, reliable without restriction).

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *H*
Sodium lauryl sulfoacetate was assigned a score of High for chronic aquatic toxicity based on a measured NOEC value of 0.86 mg/L in algae. GreenScreen® criteria classify chemicals as a High hazard for chronic aquatic toxicity when the most conservative chronic aquatic toxicity value is > 0.1 to 1.0 mg/L (CPA 2018b). The confidence in the score is low due to lack of measured data in daphnia and fish.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004
  - 72-hour NOEC (*S. capricornutum*, green algae) = 0.86 mg/L test substance is Lathanol LAL powder (purity 74.26%) (OECD Guideline 201, GLP) (Klimisch 1, reliable without restriction).

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): L
Sodium lauryl sulfoacetate was assigned a score of Low for persistence based on meeting the GHS rapid degradation criteria when tested according to OPPTS Guideline Number 835.3120 (Sealed Vessel Carbon Dioxide Production Test) and on soil, sediment, or water being judged to be the dominant environmental compartment by expert opinion. GreenScreen® criteria classify chemicals as a Low hazard for persistence when they meet the rapid degradation criteria under GHS, and they primarily partition to soil, water or sediment (CPA 2018b). The confidence in the score is high as it is based on measured data of high quality for the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2004
  - In a GLP-compliant ready biodegradability test conducted according to OECD Guideline 301B (CO2 Evolution), activated domestic sludge was exposed to a commercial product containing 72% sodium lauryl sulfoacetate (trade name: Lathanol LAL powder) at 33 mg/L for 28 days. The test substance achieved a degradation rate of 51-62% after 28 days. The positive control (sodium acetate) performed as expected. Authors concluded that Lathanol LAL powder is not readily biodegradable under the test conditions (Klimisch Score 1, reliable without restriction).
  - In another GLP-compliant test conducted according to OPPTS Guideline Number 835.3120 (Sealed Vessel Carbon Dioxide Production Test), non-adapted activated domestic sludge was exposed to a commercial product containing 69.66% sodium lauryl sulfoacetate (trade name: Lathanol LAL powder) at 10 mg/L for 28 days. The test substance degraded at 57.7% after 10-days and at 70.2% after 28 days. The positive control (sodium benzoate) performed as expected. Authors concluded that Lathanol LAL powder is readily biodegradable under the test conditions (Klimisch Score 1, reliable without restriction).
- U.S. EPA 2007
  - Sodium lauryl sulfoacetate is readily biodegradable when tested in two tests (as summarized by U.S. EPA (2009) and described briefly below) and therefore it is expected to have a low persistence potential.
  - Sodium lauryl sulfoacetate achieved a degradation rate of 56% in the modified Sturm method using activated sludge as inoculum. In another test, using activated sludge from a wastewater treatment plant as inoculum, 70% of sodium lauryl sulfoacetate had degraded after 28 days.
- U.S. EPA 2009
  - Although sodium lauryl sulfoacetate is reported as readily not biodegradable in two biodegradation tests (51–62% degradation rate in 28 days and 38–66% in 28 days), the U.S. EPA stated it is expected to have a low persistence potential. No further details were provided on the tests.
- Based on the weight of evidence, a score of Low was assigned. Biodegradation studies with a commercial product containing approximately 70% sodium lauryl sulfoacetate indicate that it will undergo biodegradation, but the rate varied in different studies. The tested compound reached > 70% degradation in 28 days in one study conducted according to OPPTS Guideline Number 835.3120 at the starting concentration of 10 mg/L, but it did not meet the criteria in another test (OECD 301B) at the starting concentration of 33 mg/L. According to the OECD guidance, positive results in ready biodegradability tests are considered valid regardless of negative results, when the scientific quality of the positive study is appropriate (OECD 2001). Therefore, ToxServices relied on the OPPTS Guideline Number 835.3120 study that reported 70.2% degradation in 28 days to classify sodium lauryl sulfoacetate as rapidly degradable and assign a score of Low for this endpoint. Due to its surface-active properties, sodium lauryl sulfoacetate is outside the applicability domain of the EPI Suite™ and therefore modeling could not be performed to determine environmental distribution. However, the high-water solubility and low vapor pressure indicates that sodium lauryl sulfoacetate is unlikely to partition mainly to the air.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vL*

Sodium lauryl sulfoacetate was assigned a score of Very Low for bioaccumulation based on measured BCFs ≤ 73 for alkyl sulfates with ≤ C16 alkyl chains. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when BCF/BAF values are ≤ 100 and log K_{ow} values are ≤ 4 (CPA 2018b). The confidence in the score is low as it is based on measured data for weak surrogates.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2007, 2009
  - Sodium lauryl sulfoacetate is expected to have a low bioaccumulation potential based on its estimated log K_{ow} value of 2.66 by EPI Suite™ v 3.20. *As explained previously, sodium lauryl sulfoacetate is outside the applicability domain of the EPI Suite™ as it is a surfactant. Therefore, ToxServices did not weigh heavily on the estimated log K_{ow} to assign a score for this endpoint.*
- ECHA 2023b
  - *Surrogate: Sodium dodecyl sulfate (CAS #151-21-3):* A non-GLP-compliant bioaccumulation test was performed with carp (*Cyprinus carpio*) exposed to sodium dodecyl sulfate (purity not specified) at 0.5 mg/L for 72 hours. The BCF was calculated as ~ 4. No further details were provided (Klimisch Score 2, reliable with restrictions).
  - *Surrogate: Sodium dodecyl sulfate (CAS #151-21-3):* A non-GLP-compliant bioaccumulation test was performed with carp (*C. carpio*) exposed to radiolabeled Sodium dodecyl sulfate (purity not specified) at 0.85 mg/L for up to 24 hours following by up to 48 hours in clean water. Maximum BCFs were identified after 8 hours during the exposure period, with the highest BCF of 19 identified in the gall bladder. After the exposure period, the test material continued to concentrate in the gall bladder, with a BCF of 82 identified after the 48 hours depuration period. The BCFs decreased in all other tissues examined (gills, blood, skin surface, hepatopancreas, kidney, brain, and muscle) (Klimisch Score 2, reliable with restrictions).
  - *Surrogate: Sodium dodecyl sulfate (CAS #151-21-3):* A non-GLP-compliant bioaccumulation test was performed with goldfish (*C. auratus*) exposed to ^{14}C or ^{35}S-radiolabeled sodium dodecyl sulfate (purity not specified) at 50 mg/L for 24 hours. The test material concentration in the gall bladder and, to a lesser extent, in the liver and gut. The BCF was calculated as 1.5 (Klimisch Score 2, reliable with restrictions).
  - *Surrogate: Sodium dodecyl sulfate (CAS #151-21-3):* A non-GLP-compliant bioaccumulation test was performed with carp (*C. carpio*) exposed to sodium dodecyl sulfate (purity not specified) at an unspecified concentration for 120 hours. The BCFs were 3.9-5.3. No further details were provided (Klimisch Score 2, reliable with restrictions).
  - *Surrogate: Sodium dodecyl sulfate (CAS #151-21-3):* A non-GLP-compliant bioaccumulation test was performed with carp (*C. carpio*) exposed to ^{35}S-radiolabeled sodium dodecyl sulfate (purity not specified) at 0.25 mg/L for 24 hours. The BCF was calculated as 2.1 (Klimisch Score 2, reliable with restrictions).
- OECD 2007
  - *Surrogate: Members of the AS Category*: Alkyl sulfates with ≤ C16 alkyl chains have BCFs ≤ 73 and their bioaccumulation potential is expected to be low.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for reactivity based on its NFPA and HMIS rating of 0 for instability supported by lack of functional groups associated with explosive or oxidizing properties. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when they are not GHS classified for any of the reactivity sub-endpoints (CPA 2018b). The confidence in the score is low due to lack of measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- Cayman Chemical 2023
  - A safety data sheet for sodium lauryl sulfoacetate states that it has a physical/reactivity hazard of 0 from HMIS ("Materials that are normally stable, even under fire conditions, and will not react with water, polymerize, decompose, condense, or self-react. Non-explosives (e.g., helium)") [11] and NFPA ("Normally stable, even under fire exposure conditions, and is not reactive with water") [12].
- No measured data were identified. Therefore, screening procedures for explosivity were used here to estimate the reactivity property of sodium lauryl sulfoacetate. These procedures are listed in the GHS (UN 2023).
  - Based on its structure, sodium lauryl sulfoacetate is not considered explosive or self-reactive due to lack of functional groups associated with explosive or self-reactive properties (See Appendix E).
  - Based on the structure of its structure, sodium lauryl sulfoacetate is not considered to have oxidizing properties as it does not contain any structural groups known to be correlated with a tendency to react exothermally with combustible materials. Specifically, organic substances which contain oxygen, fluorine, or chlorine where these elements are chemically bonded only to carbon or hydrogen, classification as an oxidizing liquid need not be applied. Therefore, as sodium lauryl sulfoacetate does not have chlorine or fluorine, classification is not warranted.

Flammability (F) Score (vH, H, M, or L): *L*
Sodium lauryl sulfoacetate was assigned a score of Low for flammability based on its NFPA and HMIS flammability rating of 0. GreenScreen® criteria classify chemicals as a Low hazard for flammability when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low due to lack of measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- Cayman Chemical 2023
  - A safety data sheet for sodium lauryl sulfoacetate states that it is not flammable and it has a flammability rating of 0 from HMIS and NFPA; which correspond to "Materials that will not burn and are not considered flammable or combustible under OSHA's Hazard Communication Standard.

[11] https://www.bgsu.edu/content/dam/BGSU/envhs/documents/Hazard-Communication/HMIS-Labeling-Information.pdf
[12] https://www.nfpa.org/News-and-Research/Publications-and-media/Blogs-Landing-Page/NFPA-Today/Blog-Posts/2021/11/05/Hazardous-Materials-Identification

Use of New Approach Methodologies (NAMs)[13] in the Assessment, Including Uncertainty Analyses of Input and Output

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* tests for genotoxicity and *in silico* modeling for respiratory sensitization. NAMs are non-animal alternatives that can be used alone or in combination to provide information for safety assessment (Madden et al. 2020). At present, there is not a uniformly accepted framework on how to report and apply individual NAMs (U.S. EPA 2020, OECD 2020). The expanded application of NAMs greatly amplifies the need to communicate uncertainties associated with their use. As defined by EFSA (2018), uncertainty is "a general term referring to all types of limitations in available knowledge that affect the range and probability of possible answers to an assessment question." The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties (OECD 2020):

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

As shown in Table 4, Type I (input data) uncertainties in sodium lauryl sulfoacetate's NAMs dataset include lack of validated test methods for respiratory sensitization. Sodium lauryl sulfoacetate's type II (extrapolation output) uncertainties include the limitations of *in vitro* genotoxicity assays to mimic *in vivo* metabolic conditions, inability of some *in silico* models to evaluate ionic substances and surfactants, and lack of defined applicability domains for OECD Toolbox when evaluation respiratory sensitization alerts. Some of sodium lauryl sulfoacetate's type II uncertainties were alleviated by the use of genotoxicity test batteries in combination with *in vivo* data, and ECHA's decision framework to evaluate respiratory sensitization.

Table 4: Summary of NAMs Used in the GreenScreen® Assessment, Including Uncertainty Analyses

Uncertainty Analyses (OECD 2020)	
Type I Uncertainty: Data/Model Input	**Genotoxicity:** No Type I uncertainty is identified on using the *in vitro* genotoxicity as they are considered relevant (appropriate for the evaluation of the corresponding hazards as recommended in the OECD Guideline), reliable (they have Klimisch scoring of 2 or 1) and adequate (validated methods). **Respiratory sensitization**: No experimental data are available and there are no validated test methods.
Type II Uncertainty: Extrapolation Output	**Genotoxicity:** The bacterial reverse mutation assay (as defined in OECD Guideline 471) only tests point-mutation inducing activity in non-mammalian cells, and the exogenous metabolic activation system does not entirely mimic *in vivo* conditions[14]. The *in vitro* chromosome aberration assay (OECD Guideline 473) does not measure aneuploidy and it only measures structural chromosomal

[13] NAMs refers to any non-animal technology, methodology, approach, or combination thereof that inform chemical hazard and risk assessments. NAMs include *in silico*/computational tools, *in vitro* biological profiling (e.g., cell cultures, 2,3-D organotypic culture systems, genomics/transcriptomics, organs on a chip), and frameworks (i.e., adverse outcome pathways (AOPs), defined approaches (DA), integrated approaches to testing and assessment (IATA).

[14] https://www.oecd-ilibrary.org/docserver/9789264071247-en.pdf?expires=1614097593&id=id&accname=guest&checksum=89925F80B9F4BD2FFC6E90F94A0EE427

	aberrations. The exogenous metabolic activation system does not entirely mirror *in vivo* metabolism[15]. **Respiratory sensitization**: The OECD Toolbox only identifies structural alerts, and does not define applicability domains. Additionally, the ECHA guidance (2017), on which the use of OECD Toolbox structural alerts is based, does not evaluate non-immunologic mechanisms for respiratory sensitization.	
Endpoint	**NAMs Data Available and Evaluated? (Y/N)**	**Types of NAMs Data (*in silico* modeling/*in vitro* biological profiling/frameworks)**
Carcinogenicity	N	
Mutagenicity	Y	*In vitro* data: Bacterial reverse mutation assay/ *in vitro* chromosome aberration assay
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	N	
Acute mammalian toxicity	N	
Single exposure systemic toxicity	N	
Repeated exposure systemic toxicity	N	
Single exposure neurotoxicity	N	
Repeated exposure neurotoxicity	N	
Skin sensitization	N	
Respiratory sensitization	Y	*In silico* modeling: OECD Toolbox structural alerts
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	
Chronic aquatic toxicity	N	
Persistence	N	Modeling is not feasible as surfactants are outside the applicability domain of EPI Suite™
Bioaccumulation	N	Modeling is not feasible as surfactants are outside the applicability domain of EPI Suite™

[15] https://www.oecd-ilibrary.org/docserver/9789264264649-en.pdf?expires=1614098015&id=id&accname=guest&checksum=6A4F9CE52EA974F5A74793DD54D54352

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Madden, J.C., S.J. Enoch, A. Paini, and M.T.D. Cronin. 2020. A review of *in silico* tools as alternatives to animal testing: principles, resources, and applications. *Alt. Lab. Animals.* 1-27. Available: https://journals.sagepub.com/doi/pdf/10.1177/0261192920965977

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APPENDIX A: Hazard Classification Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for Sodium Lauryl Sulfoacetate (CAS #1847-58-1)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	Sodium Lauryl Sulfoacetate	1847-58-1	*L*	**L**	*L*	*L*	DG	*M*	*M*	**L**	*L*	DG	*L*	*L*	*M*	**vH**	**H**	***H***	**L**	*vL*	*L*	*L*

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	No	No		
2	No	No	No	No	No	Yes	No
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Sodium Lauryl Sulfoacetate	2

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

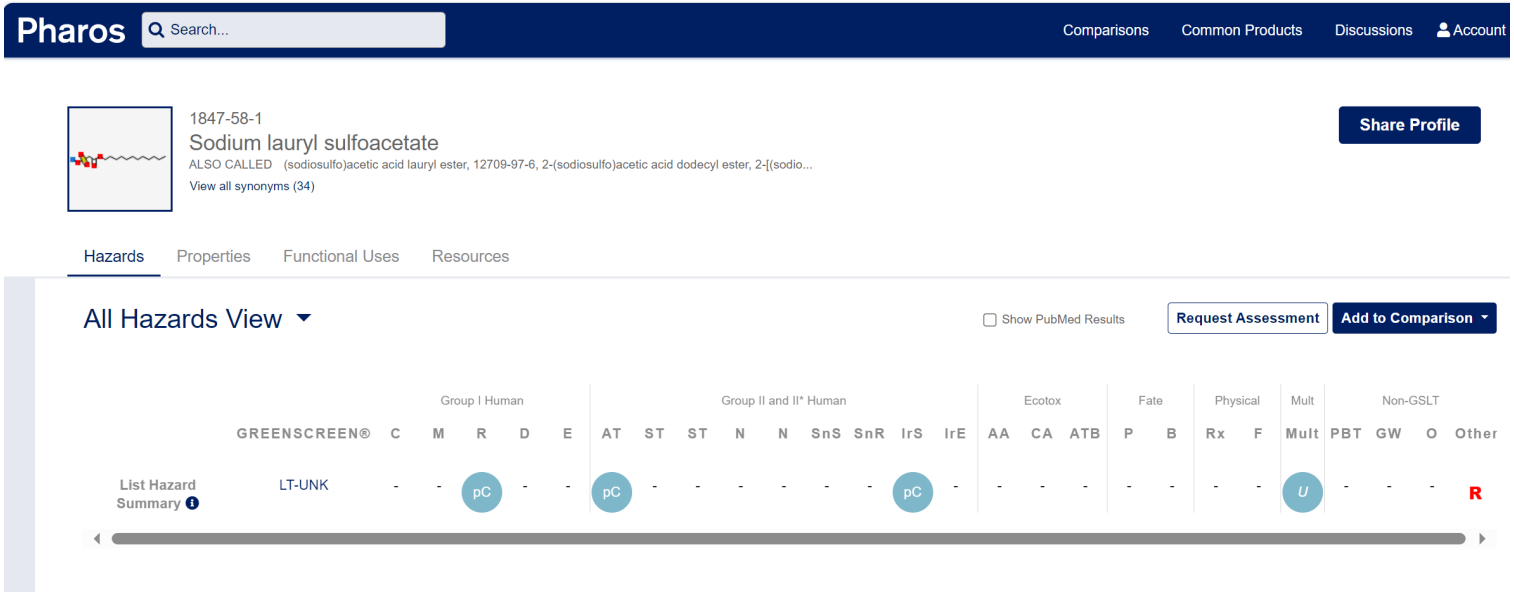
Chemical Name	Final GreenScreen® Benchmark Score
Sodium Lauryl Sulfoacetate	2

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for Sodium Lauryl Sulfoacetate (CAS #1847-58-1)



Hazard Lists

Download Lists

ENDPOINT	HAZARD LEVEL	GREENSCREEN®	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Reproductive Toxicity	pC	NoGS	DK-EPA - Danish Advisory List	Repr. 2; H361 - Suspected of damaging fertility or the unborn child (modeled)	
Acute Mammalian Toxicity	pC	NoGS	DK-EPA - Danish Advisory List	Acute Tox. 4 - Harmful if swallowed (modeled)	
Skin Irritation/Corrosivity	pC	NoGS	DK-EPA - Danish Advisory List	Skin Irrit. 2 - Causes skin irritation (modeled)	
Human and/or Aquatic toxicity and/or Persistence and/or Bioaccumulation	U	LT-UNK	German FEA - Substances Hazardous to Waters	Class 1 - Low Hazard to Waters	

Restricted Substance Lists (1)

- TSCA Chemical Substance Inventory (Active-Inactive): TSCA Chemical Substance Inventory - Active

Positive Lists (3)

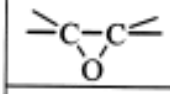
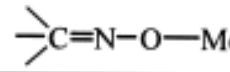
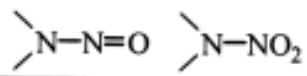
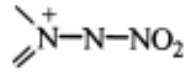
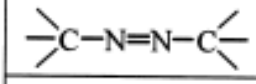
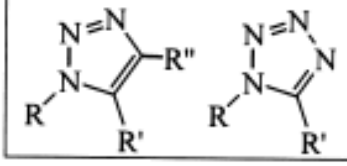
- Cosmetic Ingredient Review (CIR): Safe as Used
- Inventory of Existing Cosmetic Ingredients in China (IECIC 2021): Cosmetic Ingredients
- US EPA - DfE Safer Chemicals Ingredients list (SCIL): Surfactants - Green Circle (Verified Low Concern)

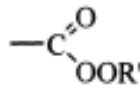
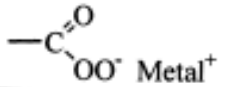
Discussions

No discussions have been posted yet.

Explosivity – Full List

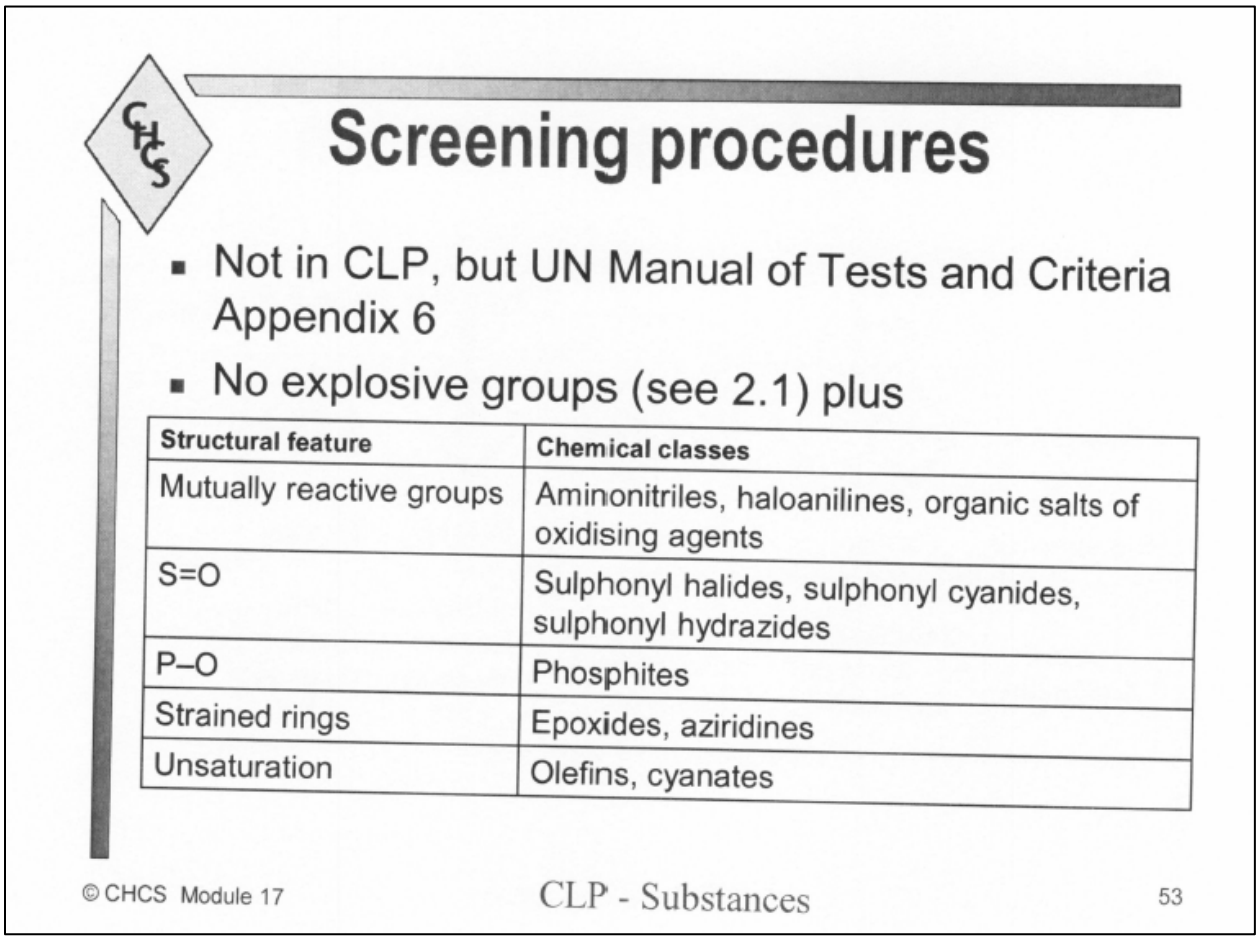
Table R.7.1-28 Chemical groups associated with explosive properties

Chemical group	Chemical Class
-C≡C- -C≡C-Metal -C≡C-Halogen	Acetylenic Compounds Metal Acetylides Haloacetylene Derivatives
	Diazo Compounds
-N=O -NO_2	Nitroso and Nitro Compounds,
R-O-N=O R-O-NO_2	Acyl or Alkyl Nitrites and Nitrates
	1,2-Epoxides
	Metal Fulminates or *aci*-Nitro Salts
	N-Metal Derivatives (especially heavy metals)
	N-Nitroso and N-Nitro Compounds
	N-Azolium Nitroimidates
	Azo Compounds
Ar-N=N-O-Ar	Arene Diazoates
$(ArN=N)_2O$, $(ArN=N)_2S$	Bis-Arenediazo Oxides and Sulfides
RN=N-NR'R''	Triazines
	High-nitrogen Compounds: e.g. Triazoles, Tetrazoles

Chemical group	Chemical Class
[1] ROOR', [2] 	Peroxy Compounds: [1] Alkyl hydroperoxides (R'=H), Peroxides (R'=organic); [2] Peroxo acids (R'=H), Peroxyesters (R'=organic)
[1] ROOMetal, [2] 	Metal peroxides, Peroxoacids salts
$-N_3$	Azides e.g. PbN_6, CH_3N_3
$^{-}O-C-N_2^{+}$	Arenediazonium oxides i.e. inner diazonium salts in which the counter ion is an oxide
Ar-N=N-S- Ar-N=N-S-Ar	Diazonium sulfides and derivatives, Arenediazo Aryl Sulfides
XO_n	Halogen Oxide: e.g. percholrates, bromates, etc
NX_3 e.g. $NC1_3$, $RNC1_2$	N-Halogen Compounds

Adapted from Bretherick (Bretherick's Handbook of Reactive Chemical Hazards 6th Ed., 1999. Butterworths, London)

Self-Reactive Substances

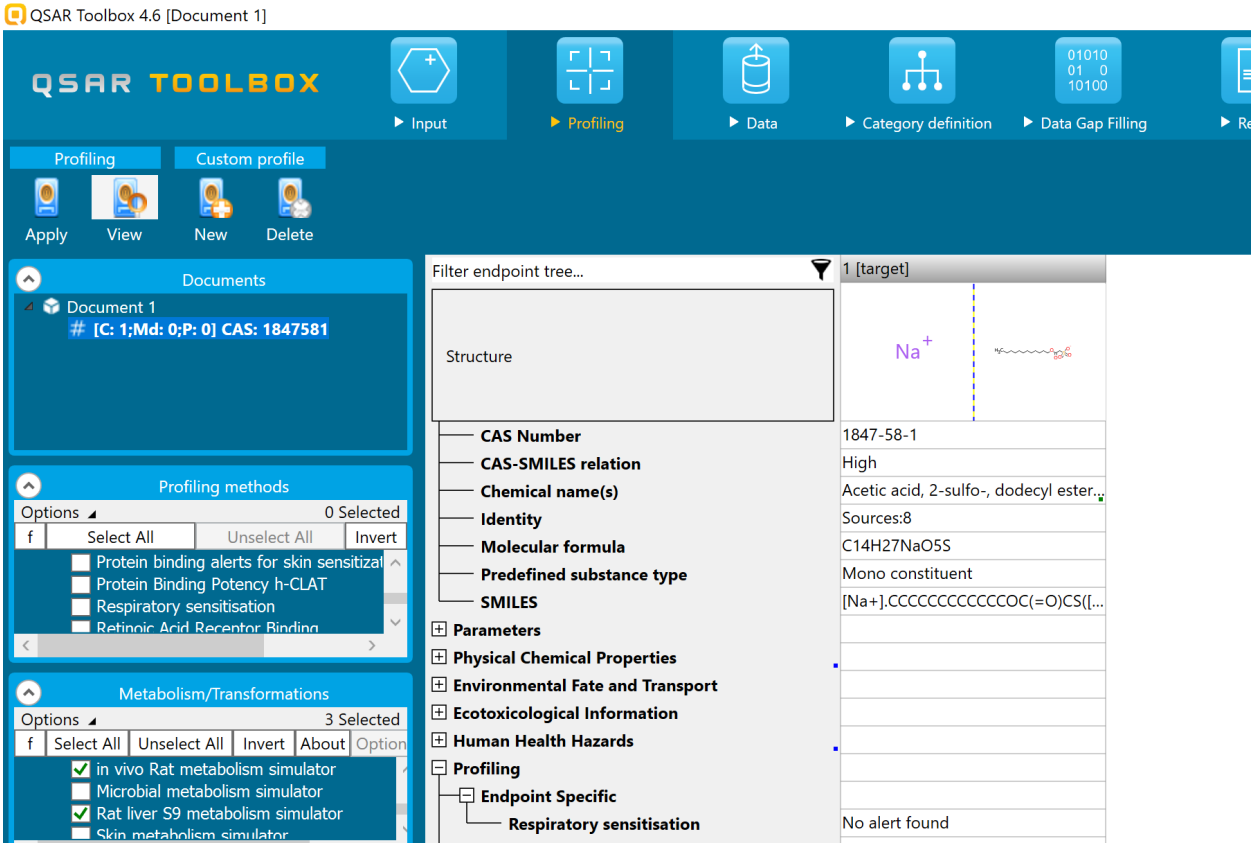


Screening procedures

- Not in CLP, but UN Manual of Tests and Criteria Appendix 6
- No explosive groups (see 2.1) plus

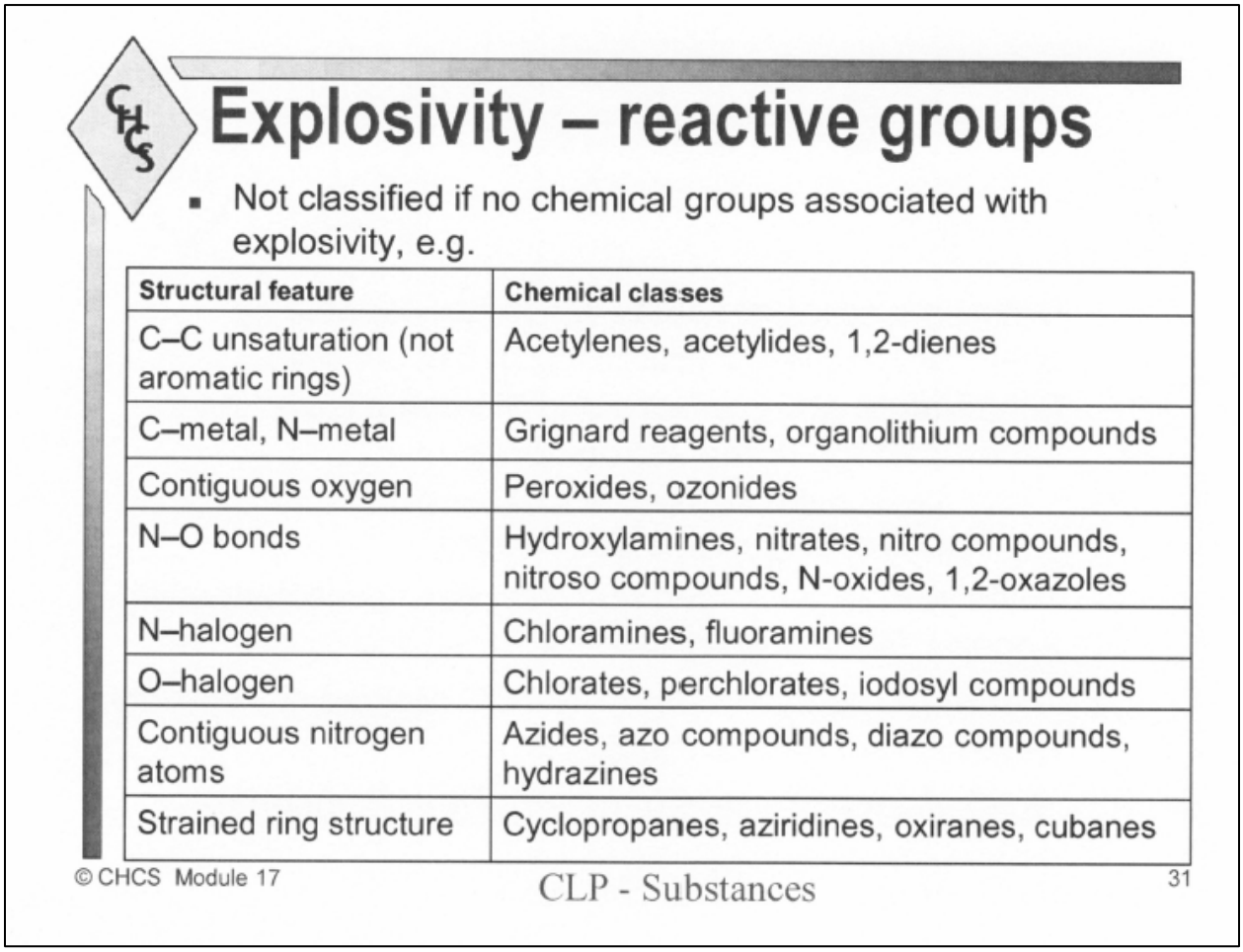
Structural feature	Chemical classes
Mutually reactive groups	Aminonitriles, haloanilines, organic salts of oxidising agents
S=O	Sulphonyl halides, sulphonyl cyanides, sulphonyl hydrazides
P–O	Phosphites
Strained rings	Epoxides, aziridines
Unsaturation	Olefins, cyanates

APPENDIX D: OECD Toolbox Respiratory Sensitization Results for Sodium Lauryl Sulfoacetate (CAS #1847-58-1)



APPENDIX E: Known Structural Alerts for Reactivity

Explosivity – Abbreviated List



Explosivity – reactive groups

- Not classified if no chemical groups associated with explosivity, e.g.

Structural feature	Chemical classes
C–C unsaturation (not aromatic rings)	Acetylenes, acetylides, 1,2-dienes
C–metal, N–metal	Grignard reagents, organolithium compounds
Contiguous oxygen	Peroxides, ozonides
N–O bonds	Hydroxylamines, nitrates, nitro compounds, nitroso compounds, N-oxides, 1,2-oxazoles
N–halogen	Chloramines, fluoramines
O–halogen	Chlorates, perchlorates, iodosyl compounds
Contiguous nitrogen atoms	Azides, azo compounds, diazo compounds, hydrazines
Strained ring structure	Cyclopropanes, aziridines, oxiranes, cubanes

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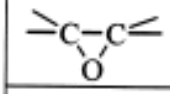
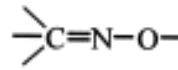
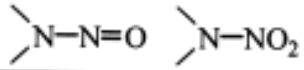
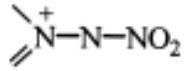
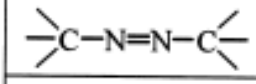
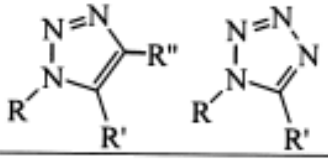
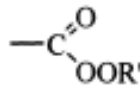
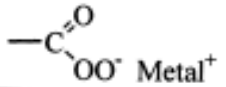
Explosivity – Full List

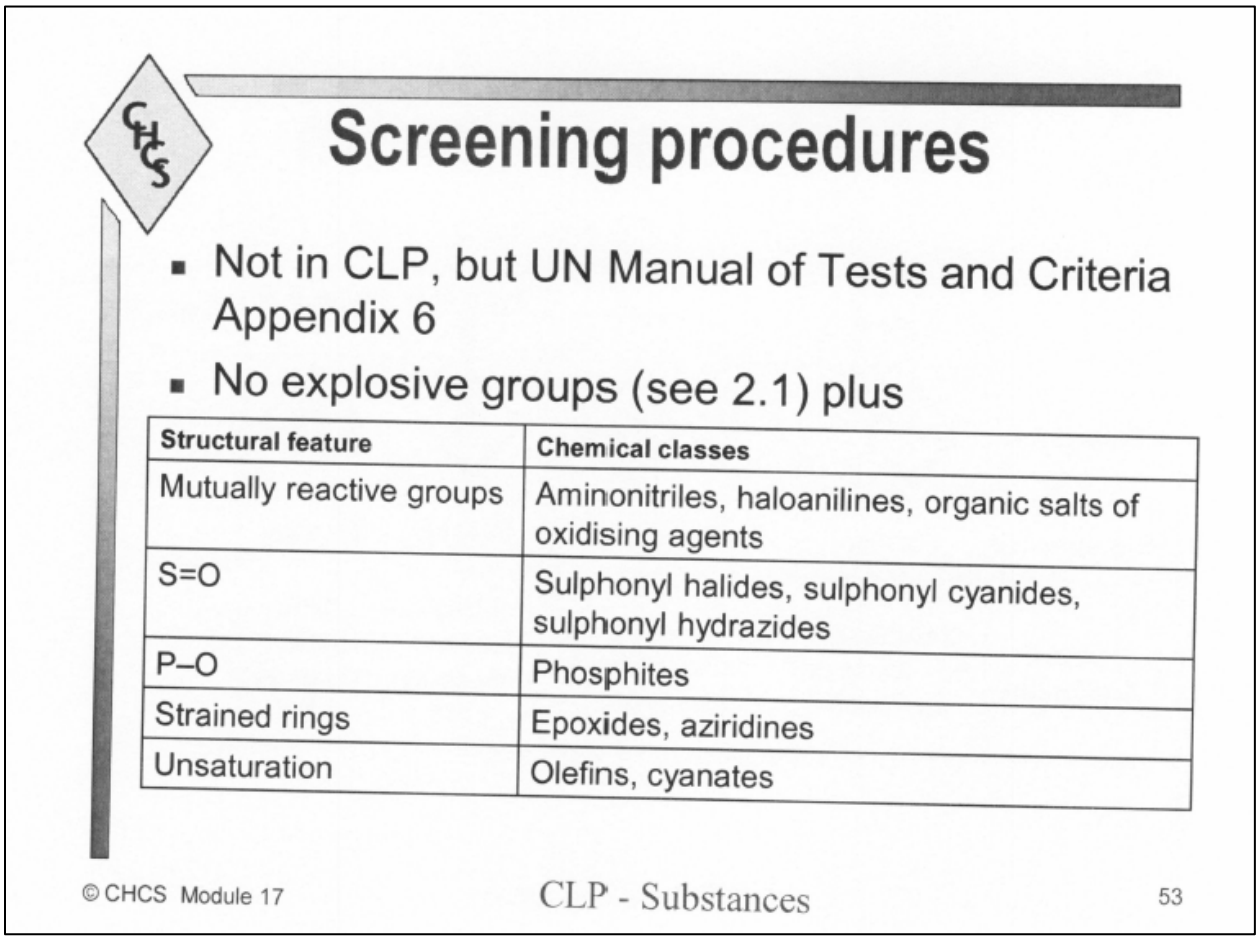
Table R.7.1-28 Chemical groups associated with explosive properties

Chemical group	Chemical Class
-C≡C- -C≡C-Metal -C≡C-Halogen	Acetylenic Compounds Metal Acetylides Haloacetylene Derivatives
	Diazo Compounds
-N=O -NO_2	Nitroso and Nitro Compounds,
R-O-N=O R-O-NO_2	Acyl or Alkyl Nitrites and Nitrates
	1,2-Epoxides
	Metal Fulminates or *aci*-Nitro Salts
	N-Metal Derivatives (especially heavy metals)
	N-Nitroso and N-Nitro Compounds
	N-Azolium Nitroimidates
	Azo Compounds
Ar-N=N-O-Ar	Arene Diazoates
$(ArN=N)_2O$, $(ArN=N)_2S$	Bis-Arenediazo Oxides and Sulfides
RN=N-NR'R''	Triazines
	High-nitrogen Compounds: e.g. Triazoles, Tetrazoles

Chemical group	Chemical Class
[1] ROOR', [2] 	Peroxy Compounds: [1] Alkyl hydroperoxides (R'=H), Peroxides (R'=organic); [2] Peroxo acids (R'=H), Peroxyesters (R'=organic)
[1] ROOMetal, [2] 	Metal peroxides, Peroxoacids salts
$-N_3$	Azides e.g. PbN_6, CH_3N_3
$^{-}O-C-N_2^{+}$	Arenediazonium oxides i.e. inner diazonium salts in which the counter ion is an oxide
Ar-N=N-S- Ar-N=N-S-Ar	Diazonium sulfides and derivatives, Arenediazo Aryl Sulfides
XO_n	Halogen Oxide: e.g. percholrates, bromates, etc
NX_3 e.g. $NC1_3$, $RNC1_2$	N-Halogen Compounds

Adapted from Bretherick (Bretherick's Handbook of Reactive Chemical Hazards 6th Ed., 1999. Butterworths, London)

Self-Reactive Substances



APPENDIX F: Change in Benchmark Score

Table 5 provides a summary of changes to the GreenScreen® Benchmark™ for sodium lauryl sulfoacetate. This is a new assessment.

Table 5: Change in GreenScreen® Benchmark™ for Sodium lauryl sulfoacetate

Date	GreenScreen® Benchmark™	GreenScreen® Version	Comment
November 20, 2023	BM-2	v. 1.4	New GreenScreen® assessment

Licensed GreenScreen® Profilers

Sodium Lauryl Sulfoacetate GreenScreen® Evaluation (v1.4) Prepared by:

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Sodium Lauryl Sulfoacetate GreenScreen® Evaluation (v1.4) QC'd by:

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