SODIUM LAURYL SULFATE AND C10-C16 ALKYL ALCOHOL SULFURIC ACID, SODIUM SALT

(CAS #151-21-3, 68585-47-7)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: April 15, 2021

Expiration Date: April 15, 2026

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TABLE OF CONTENTS

TABLE OF FIGURES

TABLE OF TABLES

GreenScreen® Executive Summary for Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #151-21-3, 68585-47-7)

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are sodium salts of alkyl alcohol sulfates. Sodium lauryl sulfate has a C12 carbon chain, C10-C16 alkyl alcohol sulfuric acid, sodium salt has a mixture of carbon chains with lengths of C10-C16, but mainly C12. Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt function primarily as ionic surfactants. Sodium lauryl sulfate also functions as a cleansing and foaming agent and denaturant in personal care and cosmetic products. It is also used as an emulsifier and surface-active agent in food manufacturing/processing, and the United States Food and Drug Administration (U.S. FDA) has permitted sodium lauryl sulfate as a direct and indirect food additive and as a packaging material for use during irradiation of prepackaged foods. Sodium lauryl sulfate is a white granular solid that has high water solubility and low volatility. It is non-reactive but is classified as a GHS Category 2 flammable solid.

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes"). This score is based on the following hazard score combinations:

- Benchmark 2f
    - Very High Ecotoxicity (acute aquatic toxicity-AA)
    - Very High Group II Human Health Hazard (acute toxicity-AT, eye irritation-IrE)

Data gaps (DG) exist for reproductive toxicity-R, endocrine activity-E, and neurotoxicity-Ns (single dose) and Nr* (repeated dose). As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt meet requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gaps. In a worst-case scenario, if sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a High score for the data gaps R or E, it would be categorized as a Benchmark 1 Chemical.

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* genotoxicity assays, *in vitro* and in silico endocrine activity assessments, and use of structural alerts to evaluate 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 sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt's NAMs dataset include no experimental data for endocrine activity and respiratory sensitization. Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt's Type II (extrapolation output) uncertainties include limitations in the applicability domains of the (Quantitative) Structure Activity Relationship ((Q)SAR) models applied in this assessment and exogenous metabolic systems used in *in vitro* genotoxicity tests that do not entirely mirror *in vivo* metabolism. Some of sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt's type II uncertainties were alleviated by the use of *in vitro* test batteries in combination of *in vivo* data.

GreenScreen® Hazard Summary Table for Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt

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**	DG	**L**	DG	*vH*	**M**	**L**	DG	DG	**L**	*L*	**H**	**vH**	**vH**	**H**	**vL**	**vL**	*L*	**M**

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 Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #151-21-3, 68585-47-7)

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

GreenScreen® Assessment (v.1.4) Prepared By:
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Title: Senior Toxicologist
Organization: ToxServices LLC
Date: March 22, 2021; April 15, 2021

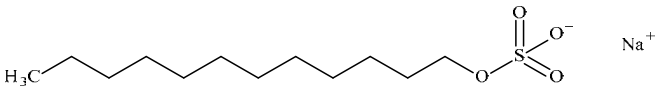
Quality Control Performed By:
Name: Bingxuan Wang, Ph.D., D.A.B.T.
Title: Senior Toxicologist
Organization: ToxServices LLC
Date: March 24, 2021; April 15, 2021

Expiration Date: April 15, 2026[2]

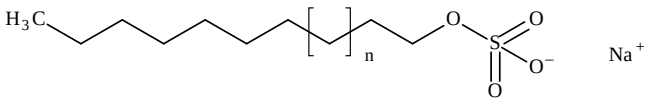
Chemical Name: Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt

CAS Number: 151-21-3, 68585-47-7

Chemical Structure(s):



Sodium Lauryl Sulfate



Where n = 1-7.

C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt

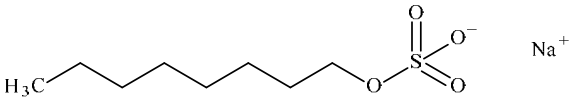
Also called:
Sodium Lauryl Sulfate:
Sodium dodecyl sulfate; Dodecyl alcohol, hydrogen sulfate, sodium salt; Dodecyl sodium sulfate; Dodecyl sulfate sodium; Dodecyl sulfate, sodium salt; EC 205-788-1; Lauryl sodium sulfate; Lauryl sulfate, sodium salt; Lauyl sodium sulfate; Monododecyl sodium sulfate; n-Dodecyl sulfate sodium; SLS; Sodium dodecyl sulphate; Sodium dodecylsulfate; Sodium lauryl sulphate; Sodium monododecyl sulfate; Sodium monolauryl sulfate; Sodium n-dodecyl sulfate; Sodiumlauryl ether sulfate; Sulfuric acid monododecyl ester sodium salt; Dodecyl sulfate sodium salt; Lauryl sulfate sodium salt; sodiumdodecylsulfate; Sodium Laurylsulfate; Laurylsulfuric Acid Sodium Salt; Dodecylsulfuric Acid Sodium Salt; dodecyl hydroxysulfonate, sodium salt; Lauryl sulfate sodium; sodiumlauryl sulfate; Sodium laurilsulfate; sodium dodecylsulphate; Sodium dedecyl sulfate; sodium n-dodecyl sulphate; lauryl sulphate sodium salt; dodecyl sulphate sodium salt; n-Dodecyl sulfate sodium salt; dodecyl

[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).

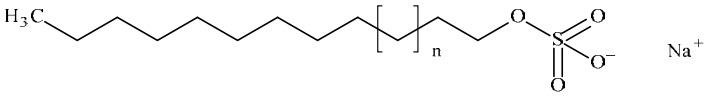
sulfuric acid sodium salt; Dodecyl sulphuric acid sodium salt; Dodecyl sulfuric acid ester sodium salt; 12768-45-5; SDS (ChemIDplus 2021a, PubChem 2021a)

C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt:
(C10-C16) Alkylalcohol sulfuric acid, sodium salt; (C10-C16)Alkylalcohol sulfuric acid, sodium salt; C10-C16 Alkyl alcohol sulfuric acid sodium salt; EINECS 271-557-7; Sulfuric acid, mono-C10-16-alkyl esters, sodium salts; sodium; methane; tridecyl sulfate; sodium;methane; tridecyl sulfate (ChemIDplus 2021b, PubChem 2021b)

Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
ToxServices identified data gaps for sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt. Therefore, Toxservices included data for related alkyl alcohol sulfuric acid, sodium salts, some of which are constituents of C10-C16 alkyl alcohol sulfuric acid, sodium salt, and potassium, ammonium, and magnesium salts of C10-C16 alkyl alcohol sulfuric acid to address these data gaps. ToxServices does not expect the potassium, ammonium, or magensium cations to have greater toxicity that the sodium cation.

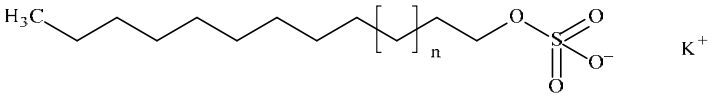


Surrogate: Sodium Octyl Sulphate (CAS #142-31-4)



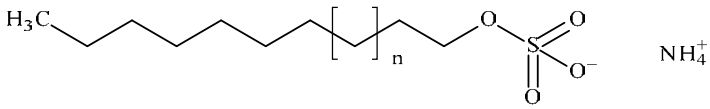
Where n = 1 or 2

Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Sodium Salts (CAS #91783-23-2)



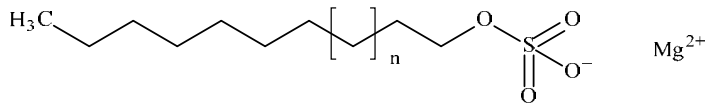
Where n = 1 or 2

Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Potassium Salts (CAS #91783-22-1)



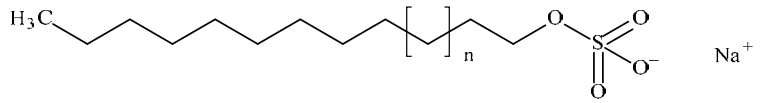
Where n = 1-7.

Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Ammonium Salts (CAS #68081-96-9)



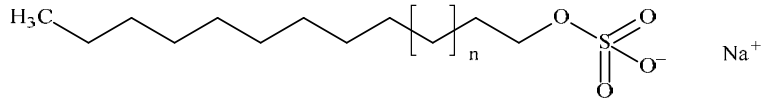
Where n = 1-7.

Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Magnesium Salts (CAS #68081-97-0)



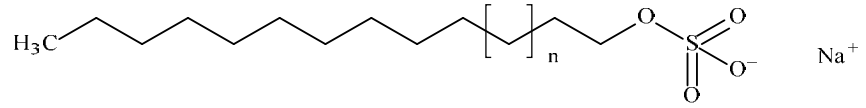
Where n = 1-3

Surrogate: Sulfuric Acid, Mono-C12-14-Alkyl Esters, Sodium Salts (CAS #85586-07-8)



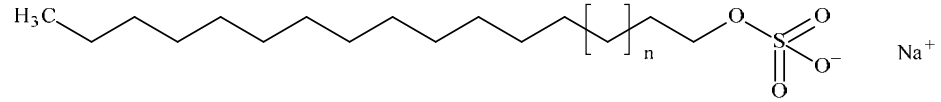
Where n = 1-4

Surrogate: Sulfuric Acid, Mono-C12-15-Alkyl Esters, Sodium Salts (CAS #68890-70-0)



Where n = 1-3

Surrogate: Sulfuric Acid, Mono-C13-15-Alkyl Esters, Sodium Salts (CAS #86014-79-1)



Where n = 1-3

Surrogate: Sulfuric Acid, Mono-C16-18-Alkyl Esters, Sodium Salts (CAS #68955-20-4)

Identify Applications/Functional Uses (OECD 2009, EC 2021, U.S. FDA 2021**):**
1. Ionic surfactant.
2. Cleansing and foaming agent, denaturant, and surfactant (emulsifying and/or cleansing) in cosmetics. and personal care products.
3. Emulsifier and surface-active agent in food manufacturing/processing.

Known Impurities[3]:
Commercial alkyl sulfate products containing sodium sulfate and residual alcohols (OECD 2009). The screen is performed on the theoretical pure substance.

[3] Impurities of the chemical will be assessed at the product level instead of in this GreenScreen®.

GreenScreen® Summary Rating for Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt[4,5 6,7]**:** Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were 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:

- Benchmark 2f
  - Very High Ecotoxicity (acute aquatic toxicity-AA)
  - Very High Group II Human Health Hazard (acute toxicity-AT, single dose neurotoxicity-Ns, eye irritation-IrE)

Data gaps (DG) exist for reproductive toxicity-R, endocrine activity-E, and neurotoxicity-Ns (single dose) and Nr* (repeated dose). As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt meet requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gaps. In a worst-case scenario, if sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a High score for the data gaps R or E, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Summary Table for Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt

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**	DG	**L**	DG	*vH*	**M**	**L**	DG	DG	**L**	*L*	**H**	**vH**	**vH**	**H**	**vL**	**vL**	*L*	**M**

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 sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are readily biodegradable (OECD 2009, ECHA 2021a), they are not expected to have relevant transformation products.

[4] 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.
[5] See Appendix A for a glossary of hazard endpoint acronyms.
[6] For inorganic chemicals only, see GreenScreen® Guidance v1.4 Section 12 (Inorganic Chemical Assessment Procedure).
[7] 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.

Introduction

Sodium lauryl sulfate, C10-C16 alkyl alcohol sulfuric acid, sodium salt, and related alkyl sulfates function primarily as ionic surfactants (OECD 2009). Sodium lauryl sulfate functions as a cleansing and foaming agent, denaturant, and surfactant (emulsifying and/or cleansing) in cosmetics and personal care products (EC 2021). Sodium lauryl sulfate is used in food manufacturing/processing as an emulsifier and surface-active agent (U.S. FDA 2021). The United States Food and Drug Administration (U.S. FDA) has permitted sodium lauryl sulfate as a direct food additive under 21 CFR §172.210 and §172.822; as an indirect food additive under 21 CFR §175.105, §175.300, §175.320, §176.170, §176.180, §176.210, §177.1200, §177.1210, §177.1630, §177.2600, §177.2800, and §178.1010; and as a packaging material for use during irradiation of prepackaged foods under 21 CFR §179.45. Sodium lauryl sulfate is produced via sulfation of lauryl alcohol followed by neutralization with sodium carbonate or sodium hydroxide (HSDB 2015).

C10-C16 alkyl alcohol sulfuric acid, sodium salt exists as four different mixtures, all of which mostly contain sodium lauryl sulfate (C12) (OECD 2009):

- Type A: 7-9% C10, 74-77% C12, 14-17% C14, 0.1-0.5% C16;
- Type B: 0-2% C10, 40-60% C12, - 20-30% C13, 5-15% C14;
- Type C: 1% C10, 65-71% C12, 22-28% C14, 4-8% C16; and
- Type D: 10.5-11.5% C10, 53-59% C12, 19-24% C14, 7-11% C16

ToxServices assessed sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt against GreenScreen® Version 1.4 (CPA 2018b) following procedures outlined in ToxServices' SOPs (GreenScreen® Hazard Assessment) (ToxServices 2020).

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

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2020a). 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 sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are both listed on the U.S. EPA SCIL as surfactants with full green circles.

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 2021) 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),[8] 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 outputs for sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt can be found in Appendix C.

- Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are LT-P1 chemicals when screened using Pharos, and therefore a full GreenScreen® is required.

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

- Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are not listed on the U.S. DOT list.
- Sodium lauryl sulfate is on the following lists for multiple endpoints:
  - Québec CSST - WHMIS 1988 - Class D2B - Toxic material causing other toxic effects.
  - EC - CEPA DSL - Inherently Toxic in the Environment (iTE).
  - EC - CEPA DSL - Inherently Toxic to Humans (iTH).
  - German FEA - Substances Hazardous to Waters - Class 2 - Hazard to Waters.
- C10-C16 Alkyl alcohol sulfuric acid, sodium salt is on the following list for multiple endpoints:
  - German FEA - Substances Hazardous to Waters - Class 2 - Hazard to Waters.
- Specified lists for single endpoints are reported in individual hazard endpoints in the hazard assessment section below.

Hazard Statement and Occupational Control

Globally Harmonized Systems of Classification and Labelling of Chemicals (GHS) classifications that are harmonized across European Union (EU) are not available for sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt as reported by the European Chemicals Agency (ECHA). The authors of the REACH dossier for sodium lauryl sulfate have classified it as a GHS Category 4 acute oral toxicant (H302), a GHS Category 2 skin irritant (H315), a GHS Category 1 eye irritant (H318), and GHS Category 3 chronic aquatic toxicant (H412) (ECHA 2021a). No REACH dossier is available for C10-C16 alkyl alcohol sulfuric acid, sodium salt. A majority of EU notifiers have self-classified it as a GHS Category 2 skin irritant (H315) and a GHS Category 1 eye irritant (H318) (ECHA 2021b). These hazard statements are presented in Table 1.

Table 1: GHS H Statements for Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #151-21-3, 68585-47-7) (ECHA 2021a,b)

H Statement	H Statement Details
Sodium Lauryl Sulfate (CAS #151-21-3)	
H302	Harmful if swallowed
H315	Causes skin irritation
H318	Causes serious eye damage
H412	Harmful to aquatic life with long lasting effects
C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #68585-47-7)	
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 Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #151-21-3, 68585-47-7)

Personal Protective Equipment (PPE)	Reference	Occupational Exposure Limits (OEL)	Reference
Gloves, goggles, protective clothing	ECHA 2021a	None identified	HSDB 2015, OSHA 2021

Physicochemical Properties of Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt

Limited data were identified for C10-C16 alkyl alcohol sulfuric acid, sodium salt. Therefore, sodium lauryl sulfate is discussed as a representative chemical below. Sodium lauryl sulfate is a white granular solid under standard temperature and pressure. It has a low vapor pressure (≤ 0.00135 mm Hg) indicating it exists mostly in the solid phase. It is highly soluble in water (> 130,000 mg/L) and is predicted to be more soluble in water than in octanol (log K_{ow} ≤ -2.03).

Table 3: Physical and Chemical Properties of Sodium Lauryl Sulfate (CAS #151-21-3)

Property	Value	Reference
Molecular formula	C12-H26-O4-S.Na	ChemIDplus 2021a
SMILES Notation	[Na+].CCCCCCCCCCCCOS(=O)(=O)[O-]	ChemIDplus 2021a
Molecular weight	288.3815 g/mol	ChemIDplus 2021a
Physical state	Solid	ECHA 2021a
Appearance	White granules	ECHA 2021a
Melting point	190-205°C	ECHA 2021a
Boiling point	Initially boils then decomposes at 216°C (OECD Guideline 103)	ECHA 2021a
Vapor pressure	≤ 0.18 Pa (≤ 0.00135 mm Hg) at 20°C (OECD Guideline 104)	ECHA 2021a
Water solubility	> 130 g/L (> 130,000 mg/L) at 20°C (OECD Guideline 105)	ECHA 2021a
Dissociation constant	pKa = 1.31 at 20°C (OECD Guideline 112)	ECHA 2021a
Density/specific gravity	Bulk density = 0.63 g/mL Specific gravity > 1.11 g/mL	ECHA 2021a
Partition coefficient	Log K_{ow} ≤ -2.03 at 20°C (estimated) (OECD Guideline 107)	ECHA 2021a

Toxicokinetics

Absorption:

Following oral dosing, alkyl sulfate salts are significantly absorbed from the gastrointestinal tract of rats, dogs, and humans, with up to 98% (≤ 98%) of administered sodium lauryl sulfate excreted in the urine (OECD 2009). In contrast, absorption across intact skin is limited since anionic surfactants have a binding affinity for skin surfaces. ToxServices identified no data for inhalation absorption.

Distribution:

Plasma concentrations of radiolabeled C16 alkyl alcohol sulfuric acid, erythromycin salt peaked 0.5-2 hours following oral dosing in dogs and humans and then declined rapidly, with 10% of the maximum concentration achieved after 6 hours (OECD 2009). Whole body autoradiography following intraperitoneal injection of rats with ^{35}S-radio labeled C10, C12, or C18 alkyl alcohol sulfuric acid, potassium salts indicated that only the liver and kidney exhibited measurable radioactivity. The radioactivity levels were highest one hour after dosing and cleared most rapidly for the C10 salt.

Metabolism:

Rats, dogs, and humans extensively metabolize alkyl sulfates via ω- and β-oxidation to yield metabolites containing C2 and C4 alkyl chains, including butyric acid 4-sulfate (CAS #16899-85-7) and 4-butyrolactone (CAS #96-48-0), for even-numbered alkyl chain sulfates (OECD 2009). Glycolic acid sulfate (CAS #N/A) has also been identified as a minor metabolite in the dog and human urine. For odd-numbered alkyl sulfates, specifically the C11 alkyl sulfate, propionic acid-3-sulfate (CAS #N/A), pentanoic acid-5-sulfate (CAS #N/A), and inorganic sulfate (CAS #14808-79-8) were identified as metabolites and were postulated to be produced via ω- and β-oxidation. The C2 alkyl chain metabolites are utilized by the body in energy production pathways, and ultimately eliminated from the body as carbon dioxide.

Excretion:

The major route of elimination for alkyl sulfates and their metabolites is via the urine (OECD 2009). Overall excretion rates do not differ between male and female rats, but alkyl sulfates of differing alkyl chain length exhibit different urinary excretion rates, with lauryl sulfates having faster elimination than C10, C11, or C18 chains following intraperitoneal or oral administration. This suggests that the lauryl sulfates are metabolized more rapidly than other alkyl sulfates. Fecal elimination occurs to a lesser extent and accounts for ≤ 19.9% of total excretion.

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): L
Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Low for carcinogenicity based on the lack of tumorigenicity identified for sodium lauryl sulfate and 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 high as it is based on reliable 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.
- ECHA 2021a
  - *Oral*: A pr-GLP chronic oral carcinogenicity test was performed with male Osborne-Mendel rats (number not specified) provided diets containing sodium lauryl sulfate (purity not specified) at 0, 0.25, 0.5 or 1% (providing doses of 0, 250, 500, and 1,000 mg/kg/day, respectively) for 104 weeks. Treatment did not increase the tumor rates (Klimisch Score 4, not assignable).
  - *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 surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts (purity not specified) 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 sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Low for mutagenicity/genotoxicity based on negative results for mutagenicity and clastogenicity in a battery of *in vitro* and *in vivo* studies of alkyl sulfates. 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 reliable 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.
- ECHA 2021a
  - *In vitro*: Sodium lauryl sulfate was negative for mutagenicity in a GLP-compliant bacterial reverse mutation assay conducted according to OECD Guideline 471 (only one strain evaluated, addendum to a previously-conducted assay (see below)). *Escherichia coli* strain WP_2 *uvr* A was exposed to sodium lauryl sulfate (97.8% purity) in water at ≤ 5,200 µg/plate with and without exogenous metabolic activation (S9 mix livers of rats induced with phenobarbital and β-naphthoflavone). Cytotoxicity was evident at ≥ 2,600 µg/plate, but sodium lauryl sulfate did not increase the mutation frequency in the presence or absence of metabolic activation. The vehicle and positive controls (2-aminoanthracene and 4-nitroquinoline-N-oxide) were valid (Klimisch Score 2, reliable with restrictions).
  - *In vitro*: Sodium lauryl sulfate was negative for mutagenicity in a GLP-compliant bacterial reverse mutation assay conducted according to OECD Guideline 471 (no *E. coli* strain tested, see above). *Salmonella typhimurium* tester strains TA1535, TA1537, TA98, TA100, and TA1538 were exposed to sodium lauryl sulfate (97% purity) in water at ≤ 5,000 µg/plate with and without exogenous metabolic activation (unspecified S9 mix). Cytotoxicity was evidence at ≥ 200 µg/plate, but sodium lauryl sulfate did not increase the mutation frequency in the presence or absence of metabolic activation. The vehicle and positive controls (sodium azide, 4-nitroquinoline-N-oxide, 9-aminoacridine, and 2-aminoanthracene) were valid (Klimisch Score 2, reliable with restrictions).
  - *In vitro*: Sodium lauryl sulfate was not mutagenic in a non-GLP-compliant mammalian cell gene mutation assay conducted in a manner similar to OECD Guideline 476 (lack of details on test substance). Mouse lymphoma L5178Y cells were exposed to sodium lauryl sulfate (purity not specified) in dimethyl sulfoxide (DMSO) at ≤ 100 µg/mL without and ≤ 95 µg/mL with exogenous metabolic activation (S9 mix from livers of male Fischer 344 rats induced with Aroclor 1254). Cytotoxicity was evident ≥ 70 µg/mL without and at 95 µg/mL with metabolic activation, but sodium lauryl sulfate did not increase the mutation frequency in the presence or absence of metabolic activation. The vehicle and positive (3-methylcholanthrene and methyl methane sulfonate) controls were valid (Klimisch Score 2, reliable with restrictions).
  - *In vitro*: Sodium lauryl sulfate was not genotoxic in a sister chromatid exchange (SCE) assay. Chinese hamster ovary (CHO) cells were exposed to sodium lauryl sulfate (purity not

specified) at ≤ 160 µg/mL with and without exogenous metabolic activation (metabolic system not specified). Cytotoxicity was evident at the highest concentration, but sodium lauryl sulfate did not increase the frequency of SCE. No details were provided for the performance of the controls (Klimisch Score 4, not assignable).

- *In vivo*: Sodium lauryl sulfate was negative for mutagenicity in a non-GLP-compliant dominant lethal assay conducted in a manner similar to OECD Guideline 478 (limited details on test substance and methodology available). Male CD-1 mice (30 in negative control group, 15 in treated and positive control groups) were administered single gavage doses of sodium lauryl sulfate (purity not specified) in water at 0, 120, 380, or 1,200 mg/kg or ethyl methane sulphonate (positive control). Each male was subsequently bred with two untreated, virgin females. The females were sacrificed during the gestation period and the uteri were isolated and examined for the number of live implantations, early deaths, and late deaths. Sodium lauryl sulfate did not affect these parameters or the pregnancy rate. No data were provided for the performance of the controls (Klimisch Score 2, reliable with restrictions).
- *In vivo*: *Surrogate: Sulfuric Acid, Mono-C16-18-Alkyl Esters, Sodium Salts (CAS #68955-20-4)*: The surrogate sulfuric acid, mono-C16-18-alkyl esters, sodium salts were not clastogenic in a GLP-compliant OECD Guideline 474 micronucleus test. CFW 1 mice (7/sex/group) were administered single gavage doses of the surrogate sulfuric acid, mono-C16-18-alkyl esters, sodium salts (purity not specified) in water at 400, 2,000, or 4,000 mg/kg. The animals were sacrificed after 24 hours (all three doses) or after 48 or 72 hours (4,000 mg/kg only), and bone marrow samples were isolated for the micronuclei assessment. The surrogate sulfuric acid, mono-C16-18-alkyl esters, sodium salts treatment did not produce signs of toxicity and did not increase the frequency of micronuclei. The vehicle and positive (chemical identity not specified) controls were valid (Klimisch Score 2, reliable with restrictions).
- *In vivo: Surrogate: Sulfuric Acid, Mono-C12-15-Alkyl Esters, Sodium Salts (CAS #68890-70-0)*: The surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts was not clastogenic in a non-GLP-compliant chromosome aberration assay conducted in a manner similar to OECD Guideline 475 (lacking details on test substance). Rats (6/sex/group, strain not specified) were provided diets containing sulfuric acid, mono-C12-15-alkyl esters, sodium salts (purity not specified) in water at 1.13% for 90 days. At the end of the exposure period, the animals were sacrificed and bone marrow cells were isolated for the chromosome aberration assessment. The surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts treatment did not produce signs of toxicity and did not increase the frequency of micronuclei. The vehicle and positive (chemical identity not specified) controls were valid (Klimisch Score 2, reliable with restrictions).

Reproductive Toxicity (R) Score (H, M, or L): DG

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Data Gap for reproductive toxicity based on insufficient data to fully characterize effects on male and female fertility and reproductive outcomes across generations.

- 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 2021a
  - A male fertility study was performed with male Swiss mice (10/group) provided diets containing sodium lauryl sulfate (purity not specified) at 1% for 2 weeks or 0.1% for 6

weeks. Treatment did not produce impairment of epididymal spermatozoa (specific endpoints were not identified) but the animals in the high dose group exhibited significant reductions in average body weight. The REACH dossier authors report a reproductive toxicity NOAEL of 1,000 mg/kg/day for this study (Klimisch Score 4, not assignable).

- OECD 2009
  - "No fertility studies were performed with alkyl sulfates."

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): L

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Low for developmental toxicity based on the lack of direct developmental toxicity identified in prenatal animals tests of sodium lauryl sulfate. The adverse effects identified in animal studies are considered secondary to maternal toxicity. 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 high as it is based on reliable 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.
- ECHA 2021a
  - A non-GLP-compliant prenatal developmental toxicity test was performed with pregnant female Wistar rats (15/group, 10 for dissection and 5 for natural parturition) administered gavage doses of sodium lauryl sulfate (purity not specified) at 0, 63, 125, 250, or 500 mg/kg/day on gestation days 6-15. The animals were sacrificed on gestation day 21 or allowed to give birth and wean the pups up to postnatal day 21. Maternal evaluations included body weight, food consumption, and uterine content (gravid uterus weight, uterine tissue weight, intrauterine mortality, and mean response per pregnancy). Fetal/pup examinations included fetal/pup body weights, crown to rump distance, placental weight, and incidence of external, visceral, and skeletal malformations. All dams in the high dose group exhibited diarrhea. As the course of treatment continued, gavage dosing became progressively more difficult, suggesting a dryness of the gastrointestinal tract, and the animals exhibited more aggressive behavior. In the high dose group, four dams died and one was killed in moribund condition between the 4th and 8th doses. All of the decedent animals exhibited irritation of the gastrointestinal tract and diffuse hemorrhaging of the stomach, and three animals exhibited lung congestion. A high dose dam exhibited a terminated pregnancy after the 9th dose. Treatment statistically significantly reduced maternal body weight gain and food consumption in the high dose group, but did not increase pre- or post-implantation loss. In the high dose group, treatment decreased the mean placental weight for male and female fetuses combined or considered separately ($p = 0.05$). Treatment did not affect the incidence of gross variants/anomalies or skeletal malformations. Three fetuses from separate litters in the high dose group exhibited malformations, which included protruding tongue, gross edema and shortening of the pubic bone; unossified metatarsus and claw in left hind foot; and agenesis of eyelids and cleft palate. Malformations were also identified in one live fetus in the 250 mg/kg/day group, characterized as reduced ossification of the 6th lumbar arch and scoliosis and hermi-centric lumbar centra with asymmetry, and one fetus in the 63 mg/kg/day group, characterized as unossified and dumbbell shaped thoracic centrae associated with branched ribs. Treatment did not affect postnatal mortality or the incidence of skeletal defects in pups on postnatal say 21. The REACH dossier authors identified a maternal toxicity NOAEL/LOAEL of 250/500 mg/kg/day based on changes to body weight gain and food consumption and a teratogenicity

NOAEL of 500 mg/kg/day, the highest dose tested (Klimisch Score 2, reliable with restrictions).

- ToxServices notes that the malformations observed in three fetuses at the high dose, one fetus at 250 mg/kg, and one fetus at 63 mg/kg are not likely to be treatment-related, due to lack of dose response and the low incidence of occurrence.

- A non-GLP-compliant prenatal developmental toxicity test conducted in a manner similar to OECD Guideline 414 (intervals in dose range and lack of details on test substance) was performed with pregnant female New Zealand White rabbits (13/group) administered gavage doses of sodium lauryl sulfate (purity not specified) in water at 0, 0.2, 2, 300, or 600 mg/kg/day on gestation days 6-18. The animals were sacrificed on gestation day 29. The maternal examinations included body weight, food consumption, ovaries, and uterine content. Fetal examinations included the incidence of visceral and skeletal malformations. Treatment produced unspecified maternal toxic effects in the high dose group, but no evidence of embryotoxicity or teratogenicity was detected at up to the highest dose tested. The REACH dossier authors identified a maternal toxicity NOAEL/LOAEL of 300/600 mg/kg/day and a developmental toxicity NOAEL of 600 mg/kg/day, the highest dose tested (Klimisch Score 2, reliable with restrictions).
- A non-GLP-compliant prenatal developmental toxicity test conducted in a manner similar to OECD Guideline 414 (intervals in dose range, lack of details on test substance) was performed with pregnant female CD rats (20/group) administered gavage doses of sodium lauryl sulfate (purity not specified) at 0, 0.2, 2, 300, or 600 mg/kg/day on gestation days 6-15. The animals were sacrificed on gestation day 20. The maternal examinations included body weight, food consumption, ovaries, and uterine content. Fetal examinations included the incidence of visceral and skeletal malformations. Treatment produced unspecified maternal toxic effects in the high dose group, but no evidence of embryotoxicity or teratogenicity was detected at up to the highest dose tested. No additional details were provided. The REACH dossier authors identified a maternal toxicity NOAEL/LOAEL of 300/600 mg/kg/day and a developmental toxicity NOAEL of 600 mg/kg/day, the highest dose tested (Klimisch Score 2, reliable with restrictions).
- *Surrogate: Sulfuric Acid, Mono-C12-14-Alkyl Esters, Sodium Salts (CAS #85586-07-8)*: A non-GLP-compliant prenatal developmental toxicity test conducted in a manner similar to OECD Guideline 414 (partially natural parturition) was performed with pregnant female Wistar rats (20/group, 15 for dissection, 5 for natural parturition) administered gavage doses of sulfuric acid, mono-C12-14-alkyl esters, sodium salts (as Alfol 12-14 sulphate, 100% purity) in water at 0, 63, 125, 250, or 500 mg/kg/day on gestation days 6-15. The animals were sacrificed on gestation day 21. Maternal examinations included clinical signs of toxicity, body weight, food consumption, ovaries, and uterine content. Fetal examinations included litter size, weight, survival, and incidence of external, visceral, and skeletal malformations. Maternal toxicity was evident in the high dose group as reduced food intake and body weight gain and an increased incidence of severe diarrhea. One high dose dam died and two were killed for humane reasons prior to the scheduled sacrifice. Surviving dams in the high dose group exhibited an increased number of intra-uterine fetal deaths and reduced live fetal body weights. These fetuses exhibited delayed ossification and an increased incidence of shortened thoracic ribs and supernumerary cervical ribs. Treatment at 500 mg/kg/day did not increase the incidence of external or visceral malformations. Treatment at lower doses did not negatively affect the number of live fetuses, fetal body weight or crown-rump distance, or the incidence of external, visceral, or skeletal malformations. Treatment did not produce adverse effects on pups born via natural parturition and reared through weaning at 21 days of age. The REACH dossier authors

concluded that the developmental deficits and decreased fetal survival at 500 mg/kg/day was secondary to maternal toxicity in this dose group; therefore, they identified maternal toxicity and developmental toxicity NOAELs of 250 mg/kg/day and LOAELs of 500 mg/kg/day (Klimisch Score 2, reliable with restrictions).

- *Surrogate: Sulfuric Acid, Mono-C16-18-Alkyl Esters, Sodium Salts (CAS #68955-20-4)*: A non-GLP-compliant prenatal developmental toxicity test was performed with pregnant female Wistar rats (15/group, 10 for dissection and 5 for natural parturition) administered gavage doses of sulfuric acid, mono-C16-18-alkyl esters, sodium salts (as Alfol 16-18 sulphate, purity not specified) at 0, 112, 225, 450, or 675 mg/kg/day on gestation days 6-15. The animals were sacrificed on gestation day 21 or allowed to give birth and wean the pups up to postnatal day 21. Maternal evaluations included clinical signs of toxicity, food consumption, body weight, ovaries, and uterine content. Treatment increased the incidence of diarrhea in the high dose group, and statistically significantly reduced mean maternal body weight gains on gestation days 6-10 for the 675 mg/kg/day group and on gestation days 10-15 for the 450 mg/kg/day group. No statistically significant differences in food consumption were identified between the control and treatment groups. Dams in the high dose group had a statistically significantly lower mean number of live fetuses per pregnancy than the concurrent control group. Treatment produced a statistically significantly decreased mean placental weight for male fetuses in the 450 mg/kg/day group. The incidence of macroscopically-observed hemorrhage under the capsule of the kidney was 4.95%, 3.73%, and 3.66% in the 112, 225, and 450 mg/kg groups, respectively (not clear if greater than the control incidence). Treatment increased the incidence of vertebral and head variations/anomalies in the 112 mg/kg/day group. Following natural parturition, 5/6 pups in a single litter born from a high dose dam were cannibalized during postnatal days 1-3. Additionally, two pups from a single litter born from a dam administered 450 mg/kg/day were cannibalized. No additional details were provided. The REACH dossier authors identified a maternal toxicity NOAEL/LOAEL of 225/450 mg/kg/day based on reduced body weight gains and a embryotoxicity NOAEL of 675 mg/kg/day, the highest dose tested (Klimisch Score 2, reliable with restrictions).
    - ToxServices notes that the decreased mean placental weight for male fetuses at 450 mg/kg, increased vertebral and head variations/anomalies at 112 mg/kg, and cannibalism of pups from a single litter each at 450 and 675 mg/kg are not likely treatment-related due to lack of dose response.

- In summary, while some studies identified increased incidences in skeletal and/or visceral variations or malformations following *in utero* exposure to sodium lauryl sulfate, these effects appear to be secondary to maternal toxicity, characterized as statistically significantly decreased body weight gains and/or food consumption and clinical signs of toxicity including diarrhea. The increase in fetal skeletal variations may reflect delayed development due to nutritional deficits following treatment (OECD 2009). Therefore, ToxServices assigned a Low score for this endpoint based on the lack of evidence for direct developmental toxicity by sodium lauryl sulfate.

Endocrine Activity (E) Score (H, M, or L): DG

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Data Gap for endocrine activity based on insufficient data identified for this endpoint.

- 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 2021
    - Sodium lauryl sulfate was active in 2/21 estrogen receptor (ER) assays, 2/15 androgen receptor (AR) assays, 0/2 steroidogenesis assays, and 9/17 thyroid receptor assays performed as part of the U.S. EPA's Endocrine Disruptor Screening Program (EDSP) in the 21st Century (Appendix D).
    - Sodium lauryl sulfate was predicted to be inactive for estrogen receptor agonism but to have very weak antagonism and binding using the CERAPP Potency Level (Consensus and From literature) models. It was predicted to be inactive for androgen receptor agonism, antagonism, and binding using the COMPARA (Consensus) model in ToxCast (Appendix E).
- VEGA 2020 (Note: ToxServices could not model the full structure of sodium lauryl sulfate in VEGA as it does not evaluate ionic substances. Therefore, ToxServices input the structure for lauryl sulfate (CAS #151-41-7) as the sodium moiety is not expected to contribute endocrine activity.)
    - Sodium lauryl sulfate was predicted to be active in the Estrogen Receptor Relative Binding Affinity model (IRFMN) with low reliability [Global applicability domain (AD) Index = 0] (Appendix F).
    - Sodium lauryl sulfate was predicted to be non-active in the Estrogen Receptor-mediated effect (IRFMN/CERAPP) 1.0.0 model with low reliability (Global AD Index = 0) (Appendix F).
    - Sodium lauryl sulfate was predicted to be non-active in the Androgen Receptor-mediated effect (IRFMN/COMPARA) 1.0.0 model with strong reliability (Global AD Index = 0.991, similarity index = 0.982, accuracy index = 1, concordance index = 1) (Appendix F).
    - Sodium lauryl sulfate was predicted to be inactive in the Thyroid Receptor Alpha effect (NRMEA) 1.0.0 model with strong reliability (Global AD Index = 0.982, similarity index = 0.965, accuracy index = 1, concordance index = 1) (Appendix F).
    - Sodium lauryl sulfate was predicted to be inactive in the Thyroid Receptor Beta effect (NRMEA) 1.0.0 model with strong reliability (Global AD Index = 0.982, similarity index = 0.965, accuracy index = 1, concordance index = 1) (Appendix F).
    - Sodium lauryl sulfate was predicted to be inactive in the Aromatase activity (IRFMN) 1.0.0 model with moderate reliability (Global AD Index = 0.775, similarity index = 0.831, accuracy index = 1, concordance index = 1) (Appendix F).
- DTU 2021
    - Sodium lauryl sulfate, its predicted metabolites from *in vivo* rat metabolism simulator, and predicted metabolites from the rat liver S9 metabolism simulator, contain no structural alerts for estrogen receptor binding (Appendix G).
    - Sodium lauryl sulfate was predicted to be negative and in domain by the Leadscope model for estrogen receptor activation, CERAPP data (*in vitro*) (Appendix G).
    - Sodium lauryl sulfate was predicted to be negative and in domain by the Leadscope model for androgen receptor binding, CoMPARA data (*in vitro*), androgen receptor inhibition, CoMPARA data (*in vitro*), and androgen receptor activation, CoMPARA data (*in vitro*) (Appendix G).
    - Sodium lauryl sulfate was predicted to be negative and in domain by thyroperoxidase (TPO) inhibition QSAR1 (Rat *in vitro*) and QSAR2 (Rat *in vitro*) models (Appendix G).
- Based on the weight of evidence, ToxServices assigned a Data Gap for endocrine activity. The available *in vitro* high through-put and modeling results indicate that sodium lauryl sulfate is not likely to interact with ER, AR, or thyroid receptors or affect steroidogenesis. However, no *in vivo* data are available to determine sodium lauryl sulfate's effects on circulating estrogen, androgen, and thyroid hormone levels. ToxServices identified no data for C10-C16 alkyl alcohol sulfuric acid,

sodium salt or other alkyl sulfates relevant to this endpoint. Therefore, ToxServices assigned a Data Gap for this endpoint.

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): *vH*

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Very High for acute toxicity based on a dermal LD_{50} of 200 mg/kg/day in male rabbits exposed to sodium lauryl sulfate. This dose equates to a GHS Category 2 acute dermal toxicity classification, which both Australia and Japan have applied to sodium lauryl sulfate. GreenScreen® criteria classify chemicals as a Very High hazard for acute toxicity when they are classified as GHS Category 2 acute toxicants for any route of exposure (CPA 2018b). The confidence in the score is low due to the limited details regarding the key study, as identified in the REACH dossier entry.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Australia - H302 - Harmful if swallowed.
      - Based on oral LD_{50} values of 977–1,427 mg/kg in rats (AICIS 2013).
    - GHS – Australia - H311 - Toxic in contact with skin.
      - Based on a dermal LD_{50} of ~200 mg/kg in rabbits (AICIS 2013).
    - GHS – Japan - Acute Toxicity (oral) - Category 4 [H302].
      - Based on an oral LD_{50} of 1,200 mg/kg in rats (NITE 2015).
    - GHS – Japan - Acute Toxicity (dermal) - Category 2 [H310].
      - Based on a dermal LD_{50} of ~200 mg/kg in rabbits (NITE 2015).
    - GHS - New Zealand - 6.1D (oral) - Acutely toxic (GHS Cat. 4).
      - Based on an oral LD_{50} of 977 mg/kg in rats (CCID 2021).
    - GHS - New Zealand - 6.1C (dermal) - Acutely toxic (GHS Cat. 3).
      - Based on a dermal LD_{50} of 580 mg/kg in rabbits (CCID 2021).
    - GHS - New Zealand - 6.1D (dermal) - Acutely toxic (GHS Cat. 4).
      - Applicable to solutions in a non-hazardous diluent containing >26 - 33% sodium lauryl sulfate (CCID 2021).
    - GHS - New Zealand - 6.1E (dermal) - Acutely toxic (GHS Cat. 5).
      - Applicable to solutions in a non-hazardous diluent containing >2 - 4% sodium lauryl sulfate (CCID 2021).
- ECHA 2021a
  - *Oral*: Sodium Lauryl Sulfate: LD_{50} (Wistar rats) = 977 mg/kg (female), 1,425 mg/kg (male) (non-GLP-compliant, OECD Guideline 401) (Klimisch Score 2, reliable with restrictions).
  - *Oral*: Sodium Lauryl Sulfate: LD_{50} (rat) > 1,500 mg active ingredient/kg (non-GLP-compliant, similar to OECD Guideline 401) (Klimisch Score 2, reliable with restrictions).
  - *Dermal*: Sodium Lauryl Sulfate: LD_{50} (male rabbits) = 200 mg active ingredient sodium lauryl sulfate/kg (non-GLP-compliant) (Klimisch Score 4, not assignable)
    - ToxServices notes that this study is described as "disregarded due to major methodological deficiencies" despite the Klimisch Score of 4 (not assignable), and as "not sufficient for risk assessment" due to limited data related to test conditions and/or experimental methods.

  - *Dermal*: *Surrogate: Sodium Octyl Sulphate (CAS #142-31-4)*: LD_{50} (Wistar rat) > 2,000 mg/kg (GLP-compliant, OECD Guideline 402) (Klimisch Score 2, reliable with restrictions).
  - *Dermal*: *Surrogate: Sulfuric acid, mono-C10-16-alkyl esters, ammonium salts (CAS #68081-96-9)*: LD_{50} (New Zealand White rabbits) > 500 mg active ingredient/kg (pre-GLP, similar to OECD Guideline 402) (Klimisch Score 2, reliable with restrictions).
  - *Dermal: Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Potassium Salts (CAS #91783-22-1)*: LD_{50} (New Zealand White rabbits) > 500 mg active ingredient/kg (pre-GLP, similar to OECD Guideline 402) (Klimisch Score 2, reliable with restrictions).
  - *Dermal: Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Magnesium Salts (CAS #68081-97-0)*: LD_{50} (New Zealand White rabbits) > 500 mg active ingredient/kg (pre-GLP, similar to OECD Guideline 402) (Klimisch Score 2, reliable with restrictions).
- OECD 2009
  - *Oral*: C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt: LD_{50} (Cox CD rats) = 1,830 mg/kg (similar to OECD Guideline 401)

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

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Moderate for systemic toxicity (single dose) based on ToxServices classifying them as Category 3 specific target organ toxicants following single exposures for respiratory irritation under GHS criteria. 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 irritation (CPA 2018b). The confidence in the score is high as it is based on measured animal data and effects in exposed human populations.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Australia - H335 - May cause respiratory irritation.
      - Sodium lauryl sulfate is reported as irritating to the respiratory tract in exposed human populations (AICIS 2013).
- ECHA 2021a
  - *Oral*: In the non-GLP-compliant, OECD Guideline 401 acute oral toxicity test that identified oral LD_{50}s of 977-1,425 mg/kg for sodium lauryl sulfate (>98% purity) in Wistar rats, clinical signs of toxicity included decreased activity, diarrhea, spastic gait, hunched posture, lateral position, labored respiration, and coma with dose-dependent frequencies. No body weight data were provided. At the end of the 14-day recovery period, none of the surviving animals exhibited treatment-related gross pathological changes. In contrast, the decedent animals exhibited vascular congestion in the liver and hemorrhaging in gastrointestinal tract (dose groups not specified) (Klimisch Score 2, reliable with restrictions).
  - *Oral*: No data on clinical signs of toxicity, body weight, or gross pathological changes were presented for the study that identified an oral LD_{50} > 1,500 mg active ingredient/kg for sodium lauryl sulfate in rats (Klimisch Score 2, reliable with restrictions).
  - *Dermal*: In the non-GLP-compliant acute dermal toxicity test that identified a dermal LD_{50} of 200 mg active ingredient/kg for sodium lauryl sulfate in male rabbits, clinical signs of toxicity included tonic-clonic convulsions, respiratory failure, tremors, and slight scaling to leathery appearance of skin at the application site. Treatment decreased body weight at doses of 300 and 600 mg/kg. No gross pathological data were provided (Klimisch Score 4,

not assignable).
    - ToxServices notes that this study is described as "disregarded due to major methodological deficiencies" despite the Klimisch Score of 4 (not assignable), and as "not sufficient for risk assessment" due to limited data related to test conditions and/or experimental methods.
  - *Dermal*: *Surrogate: Sodium Octyl Sulphate (CAS #142-31-4)*: In the GLP-compliant, OECD Guideline 402 acute dermal toxicity test that identified a dermal LD_{50} > 2,000 mg/kg for the surrogate sodium octyl sulfate in Wistar rats, treatment did not produce clinical signs of toxicity, changes to body weight, or gross pathological alterations (Klimisch Score 2, reliable with restrictions).
  - *Dermal*: *Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Ammonium Salts (CAS #68081-96-9)*: In the pre-GLP acute dermal toxicity test that identified a dermal LD_{50} > 500 mg active ingredient/kg (the only dose tested) for the surrogate sulfuric acid, mono-C10-16-alkyl esters, ammonium salts in New Zealand White rabbits, clinical signs of toxicity were limited to dermal irritation which was characterized as severe erythema and slight eschar formation at 24 hours, necrosis on days 2-14, sloughing of the skin on days 8-14, and hyper-pigmentation of new skin by day 14. Treatment decreased the body weight of one animal with intact skin during the observation period. No gross pathological data were provided (Klimisch Score 2, reliable with restrictions).
  - *Dermal: Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Potassium Salts (CAS #91783-22-1)*: In the pre-GLP acute dermal toxicity test that identified a dermal LD_{50} > 500 mg active ingredient/kg for the surrogate sulfuric acid, mono-C12-13-alkyl esters, potassium salts in New Zealand White rabbits, clinical signs of toxicity were limited to moderate to severe atonia (loss of muscle strength) and dermal irritation which was characterized as moderate to severe erythema and edema. Treatment produced desquamation and fissuring, slight to marked desquamation, eschar formation, and exfoliation at the application site by the end of the observation period. Treatment did not affect body weights during the observation period. No gross pathological data were provided (Klimisch Score 2, reliable with restrictions).
  - *Dermal: Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Magnesium Salts (CAS #68081-97-0)*: In the pre-GLP acute dermal toxicity test that identified a dermal LD_{50} > 500 mg active ingredient/kg for the surrogate sulfuric acid, mono-C10-16-alkyl esters, magnesium salts in New Zealand White rabbits, clinical signs of toxicity were limited to dermal irritation which was characterized as severe erythema and eschar formation at 24 hours, necrosis on days 5-21, and sloughing of necrotic tissues and hyper-pigmentation of skin on day 21. Two of the three animals exhibited decreased body weights during the observation period. No gross pathological data were provided (Klimisch Score 2, reliable with restrictions).
- Ciuchta and Dodd 1978, ECHA 2021a
  - The results of a mouse upper respiratory tract irritation study with sodium lauryl sulfate indicate an RD_{50} (the concentration producing a 50% reduction in respiration rate) of 88 µg/L.
- OECD 2009
  - *Oral*: In the acute oral toxicity test that identified an oral LD_{50} of 1,830 mg/kg in Cox CD rats for C10-C16 alkyl alcohol sulfuric acid, sodium salt, clinical signs of toxicity included abdominal griping and diarrhea, decreased motor activity and respiratory rate, blanching, and loss of corneal reflex and pupillary response. No body weight data were provided. Surviving animals exhibited no treatment-related gross pathological changes.

- In summary, treatment-related effects identified in the single exposure studies include clinical signs of toxicity and dermal irritation at the site of application (dermal toxicity studies only). The neurological signs of toxicity are discussed under the neurotoxicity section below. Clinical signs of toxicity included labored respiration or decreased respiratory rate in acute oral toxicity tests of sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt in rats, possibly indicating respiratory irritation. Ciuchta and Dodd (1978) identified an RD_{50} for sodium lauryl sulfate and Australia classified this chemical as a respiratory irritant under GHS criteria (UN 2019) based on effects in exposed human populations. Therefore, ToxServices classified sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt as a Category 3 specific target organ toxicant following single exposures for respiratory irritation under GHS criteria (UN 2019).

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

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Low for systemic toxicity (repeated dose) based on ToxServices not classifying them as specific target organ toxicants following repeated exposures under GHS criteria. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when they are not classified as GHS specific target organ toxicants following repeated exposures (CPA 2018b). The confidence in the score is high as it is based on reliable measured data from subchronic and chronic duration studies.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Japan - Specific target organs/systemic toxicity following repeated exposure - Category 2 [H373].
      - Based on adverse effects to the liver, including increased liver weights, increased serum ALT and AP activities, and hepatocytic hypertrophy in a 28-day rat study of sodium lauryl sulfate (NITE 2015). The key dose is described as 0.5%, equivalent to a converted guidance value of 76.2 mg/kg/day.
- ECHA 2021a
  - *Oral:* A subchronic repeated dose toxicity study (GLP status not specified) conducted in a manner similar to OECD Guideline 408 was performed with male and female rats (strain and number not specified) provided diets containing sodium lauryl sulfate (86% purity) at 0, 40, 200, 1,000, or 5,000 ppm (contributing doses equivalent to 0, 3, 17, 86, and 430 mg/kg/day, respectively) for 90 days. The animals were evaluated for clinical signs of toxicity, body weight, food consumption, urinalysis, clinical signs of toxicity, hematology, gross pathology, and histopathology. The only treatment-related effect identified was increased liver weights in high dose female rats, which the authors considered to be an adaptive effect. The authors identified a NOAEL of 430 mg/kg/day, the highest dose tested (Klimisch Score 2, reliable with restrictions).
  - *Oral:* A pre-GLP subchronic repeated dose toxicity test conducted in a manner similar to OECD Guideline 408 was performed with Sprague-Dawley (Charles River CD) rats (20/sex/group) provided diets containing C10-C16 alkyl alcohol sulfuric acid, sodium salt (purity not specified) at 0, 0.25, 0.5, or 1% (contributing doses equivalent to 0, 55.5, 112.48, and 201.28 mg/kg/day for males and 0, 59.94, 122.84, and 254.56 mg/kg/day for females, respectively) for 90 days. The animals were evaluated for clinical signs of toxicity, body weight, food consumption and efficiency, ophthalmology, hematology, clinical chemistry, urinalysis, gross pathology, and histopathology. Treatment did not adversely affect these

parameters and the REACH dossier authors identified a NOAEL of 1% (equivalent to 201.28-254.56 mg/kg/day), the highest dose tested (Klimisch Score 1, reliable without restriction).

- *Oral*: A GLP-compliant repeated dose toxicity test conducted in a manner similar to OECD Guideline 40/EU Method B.7 (no neurobehavioral assessment, some hematology and organ weight values are missing) was performed with CD rats (10/sex/group) administered gavage doses of sodium lauryl sulfate (> 90% purity) in water at 0, 30, 100, or 300 mg test substance/kg/day (equivalent to 27, 90, and 270 mg sodium lauryl sulfate/kg/day, respectively) five days/week for 28 days. The high dose group was increased to 600 mg/kg/day (equivalent to 540 mg sodium lauryl sulfate/kg/day) after 10 doses. Additional control and high dose groups of 5 animals/sex/group were dosed as above and then maintained for 29 days without treatment (recovery groups). The animals were evaluated for clinical signs of toxicity, body weight, food and water consumption, ophthalmology, hematology, clinical chemistry, gross pathology, and histopathology. Two high dose animals, one male and one female, died prior to the scheduled sacrifice. Clinical signs of toxicity were limited to excess salivation in the high dose group. Treatment produced decreased body weight gain and food consumption in high dose males (described as non-adverse by the REACH dossier authors), and increased water consumption in the high dose group during the fourth week of exposure. High dose males exhibited increased leukocyte counts and decreased lymphocyte counts, hematocrit, and mean corpuscular volume MCV, and high dose females exhibited increased leukocyte counts and hematocrit and decreased lymphocyte counts. High dose males and females exhibited decreased serum cholesterol and bilirubin levels and increased GPT activity. Treatment-related changes to organ weights were limited to the high dose group and included increased absolute and relative adrenal weights in males and females; increased relative liver weight in females; and increased relative brain, gonads, and kidney weights and decreased absolute and relative thymus weights in males. Treatment produced gross pathological changes to the stomach, characterized as bleeding and ulcerations, in high dose animals. Treatment-related histopathological changes included alterations to the myocard (muscular heart tissue) and tongue, both of which were reversible, and to the forestomach cutaneous mucous membrane which was only partially reversible. The study authors identified a NOAEL of 100 mg/kg/day (equivalent to 90 mg sodium lauryl sulfate/kg/day) and a LOAEL of 300-600 mg/kg/day (equivalent to 270-540 mg sodium lauryl sulfate/kg/day) based on local effects to the forestomach mucous membrane, reduced body weight gains, and decreased food and water intake (Klimisch Score 4, not assignable).
    - Note: the REACH dossier authors states that this study is "disregarded due major methodological deficiencies." This may be due to the use of gavage dosing rather than dietary dosing for an irritating substance.
- *Oral*: *Surrogate: Sulfuric Acid, Mono-C12-15-Alkyl Esters, Sodium Salts (CAS #68890-70-0)*: A non-GLP-compliant subchronic repeated dose toxicity study conducted in a manner similar to OECD Guideline 408 was performed with Colworth Wistar-derived rats (20/sex in control group, 10/sex in treatment groups) provided diets containing the surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts (purity not specified) at 0.07, 0.14, 0.28, 0.56, 1.13, or 2.25% (resulting in equivalent doses of 58, 113, 228, 470, 961, and 1,944 mg/kg/day for males and 66, 131, 261, 506, 1,070 and 2,218 mg/kg/day for females, respectively) for 13 weeks. The animals were evaluated for clinical signs of toxicity, body weight, food and water intake, hematology, clinical chemistry, organ weights, gross pathology, and histopathology. One male in each of the 0.14% and 1.13% groups were sacrificed during the course of the study due to morbidity the authors reported as arising from lesions

occasionally observed in this strain of rat. The authors did not consider these effects to be treatment-related. Treatment significantly reduced body weight gain in high dose females (16% decrease) and in males in the 1.13% group (10% decrease) and high dose group (20% decrease). The effects on body weight correlated with significantly decreased food consumption values in high dose males (9% decrease) and females (6% decrease), and significantly decreased food utilization in high dose males (13% decrease) and females (10% decrease) and in males in the 1.13% group (5% decrease). High dose females also exhibited a 15% decrease in water intake. Treatment did not adversely affect hematology parameters, but treatment-related effects on clinical chemistry parameters included significantly decreased protein, magnesium, and cholesterin levels and increased aspartate aminotransferase (AST, GOP), alanine aminotransferase (ALT, GPT), and alkaline phosphatase (AP) in high dose males; increased AP in high dose females; increased AP in 1.13% treatment group males; increased GPT in 1.13% treatment group females; and increased AP in 0.28% and 0.56% males. Treatment altered organ weights as indicated in the following table.

Organ	**Weight**	**Dietary Concentration (%)**					
		0.07	0.14	0.38	0.56	1.13	2.25
Liver	Relative				↑ m/f	↑ m/f	↑ m/f
	Absolute					↑ f	↑ f
Spleen	Relative						
	Absolute					↓ m	↓ m/f
Kidney	Relative					↑ f	↑ f
	Absolute						↓ m
Brain	Relative					↑ m	↑ m/f
	Absolute						
Testes	Relative					↑ m	↑ m
	Absolute						
Heart	Relative						↑ m
	Absolute					↓ m	↓ m/f

Treatment-related gross pathological changes included changes and color of the intestinal contents in high dose males and females and in males in the 1.13% treatment group, and no abdominal fat in high dose males. Treatment produced histopathological changes in the liver, kidney, alimentary tract, and connective tissue. In the liver, increased incidences of diffuse and periportal hypertrophy, reduced cytoplasmic (glycogenic) vacuolation, reduced hepatic parenchyma cytoplasmic and Kupffer cell hemosiderin content, and decreased hepatic parenchyma cytoplasmic neutral fat in the high dose group. Additionally, the incidence of diffuse hypertrophy increased in females in the 1.13% group and the incidence of periportal hypertrophy increased in males and females in this dose group. Females in the 0.28% group also exhibited an increased incidence of periportal hypertrophy. Decreased cytoplasmic neutral fat, hemosiderin content, and cytoplasmic (glycogenic) vacuolation were also detected in males and/or females in the 0.56-2.25% groups. The authors considered the histopathological changes in the liver to be adaptive responses to the treatment, rather than adverse. In the kidney, high dose females exhibited decreased incidences and/or severity of nephrocalcinosis, cortical interstitial fibrosis, small foci of cortical tubular atrophy, and focal lymphocytic infiltration, which are commonly identified in females of this rat strain. High dose animals exhibited lymphatic dilation of the small intestine, attributable to an increased

extent of dilation of individual vessels and an increase in the number of visible lymphatic channels, and an increased incidence of protozoan parasite colonization. Treatment also decreased the quantity of stromal lipid in the pancreas and parotid salivary glands. The authors identified a NOAEL of 0.56% (equivalent to 470-506 mg/kg/day) based on increased testicular weights in males at 1.13% (961 mg/kg/day) (Klimisch Score 2, reliable with restrictions).

- *Oral: Surrogate: Sulfuric Acid, Mono-C13-15-Alkyl Esters, Sodium Salts (CAS #86014-79-1):* A non-GLP-compliant subchronic repeated dose toxicity test conducted in a manner similar to OECD Guideline 408 was performed with Wistar rats (20/sex in control group, 10/sex in treatment groups) provided diets containing the surrogate sulfuric acid, mono-C13-15-alkyl esters, sodium salts (purity not specified) at 0, 0.07, 0.14, 0.28, 0.56, 1.13, or 2.25% (resulting in equivalent doses of 0, 64, 134, 253, 512, 1,007, and 2,096 mg/kg/day, respectively) for 13 weeks. Treatment only produced adaptive changes in the liver, characterized as increased liver weights and hepatic hypertrophy, and the REACH dossier authors identified a NOAEL/LOAEL of 512/1,007 mg/kg/day. No additional details were provided (Klimisch Score 2, reliable with restrictions).
- *Oral*: *Surrogate: Sulfuric Acid, Mono-C12-15-Alkyl Esters, Sodium Salts (CAS #68890-70-0)*: A non-GLP-compliant combined chronic toxicity/carcinogenicity test conducted in a manner similar to OECD Guideline 453 was performed with Colworth Wistar rats (45/sex/group) provided diets containing the surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts (purity not specified) at 0.015, 0.15, or 1.5% (contributing doses equivalent to 11, 113, and 1,125 mg/kg/day, respectively) for two years. The animals were evaluated for clinical signs of toxicity, body weight, food and water consumption, hematology, clinical chemistry, gross pathology, and histopathology. Treatment did not adversely affect survival, but high dose animals exhibited decreased body weight gain, food consumption, and water consumption relative to the control group. High dose females also exhibited a decreased total white blood cell count. High dose males exhibited increased serum ALT and AP activities and increased urea levels, while high dose females exhibited decreased lactate dehydrogenase and hydroxybutyrate dehydrogenase activities. The authors attributed the increased AP activity to hepatic parenchymal hypertrophy and the increased ALT activity to multifocal sub-lobular hepatic necrosis. High dose males exhibited reduced relative weights for the heart, kidneys, spleen, and adrenal glands and increased absolute and relative testes weights, while high dose males and females exhibited increased absolute and relative liver weights. Treatment produced an increased incidence of diffuse hepatic enlargement in the high dose group. This gross pathological finding correlated with increased incidences and severity of hepatic parenchymal hypertrophy, focal coagulative and/or hemorrhagic necrosis and pigmented lipid granuloma in the liver of high dose animals. The authors considered the pathological changes to the liver to be representative of adaptive changes and/or changes typically identified in aging rats of this strain. In high dose females, treatment reduced the severity of splenic extramedullary erythropoiesis and the incidence of splenic myelopoiesis and stem cell hyperplasia but increased the severity of red pulp hemosiderin deposition. High dose rats exhibited decreased incidences and/or severity of chronic nephropathy and pelvic nephrocalcinosis in the kidney and/or arterial medial hypertrophy in the heart. The authors identified a NOAEL/LOAEL of 113/1,125 mg/kg/day based on the adaptive changes to the liver and increased severity of red pulp hemosiderin deposition in the spleen (Klimisch Score 2, reliable with restrictions).
- *Oral: Surrogate: Sulfuric Acid, Mono-C16-18-Alkyl Esters, Sodium Salts (CAS #68955-20-4)*: A non-GLP-compliant subchronic repeated dose toxicity study conducted in a manner similar to OECD Guideline 408 was performed with Wistar rats (20/sex in the control group,

10/sex in the treatment groups) provided diets containing the surrogate sulfuric acid, mono-C16-18-alkyl esters, sodium salts (purity not specified) at 0, 0.07, 0.14, 0.28, 0.56, 1.13, or 2.25% (resulting in equivalent doses of 0, 61, 123, 230, 482, 970, and 2,067 mg/kg/day, respectively) for 13 weeks. Treatment only produced adaptive changes in the liver, characterized as increased liver weights and hepatic hypertrophy, and the REACH dossier authors identified a NOAEL/LOAEL of 482/970 mg/kg/day. No additional details were provided (Klimisch Score 2, reliable with restrictions).

- *Oral: Surrogate: Sulfuric Acid, Mono-C16-18-Alkyl Esters, Sodium Salts (CAS #68955-20-4)*: A GLP-compliant subchronic repeated dose toxicity test conducted in a manner similar to OECD Guideline 408 was performed with rats (10/sex/group, strain not specified) administered gavage doses of the surrogate sulfuric acid, mono-C16-18-alkyl esters, sodium salts (55% purity) in water at 0, 100, 300, or 900 mg test substance/kg/day (equivalent to 0, 55, 165, and 495 mg/kg/day active substance, respectively) for 90 days. The animals were evaluated for body weight, food consumption, and organ weights. Treatment reduced body weight gain and food consumption and increased relative liver weights in the high dose group. The authors concluded that other changes were non-specific and/or likely due to the irritative properties of the test substance on the stomach mucosa. The authors identified a NOAEL of 300 mg test substance/kg/day (equivalent to 165 mg sulfuric acid, mono-C16-18-alkyl esters, sodium salts/kg/day) based on the changes to body and liver weights detected in the high dose group (Klimisch Score 4, not assignable).
  - Note: the REACH dossier authors states that this study is "disregarded due major methodological deficiencies" and that "application via gavage is not appropriate to derive a NOAEL for risk assessment."
- *Dermal*: *Surrogate: Sulfuric Acid, Mono-C12-15-Alkyl Esters, Sodium Salts (CAS #68890-70-0)*: A non-GLP-compliant subchronic dermal repeated dose toxicity test conducted prior to implementation of but in a manner similar to OECD Guideline 411 (applications only twice per week, deficiencies in hematology and clinical chemistry data) was performed with C57BL mice (10/sex/group) administered topical applications of 0.2 mL of the surrogate sulfuric acid, mono-C12-15-alkyl esters, sodium salts (30.1% purity) in water at nominal concentrations of 0, 5, 10, 12.5, or 15% (calculated by the REACH dossier authors as equivalent to doses of 0, 200, 400, 500, and 600 mg/kg/day, respectively, assuming 20 g/mouse and 5 days/week exposure frequency) twice weekly for 13 weeks. The type of coverage was not specified. The animals were evaluated for body weight, water intake, hematology (white cell count, packed cell volume, hemoglobin level, and mean corpuscular hemoglobin concentration), and organ weights and histopathology (liver, spleen, kidney, brain, heart, and testes). One animal in the 12.5% group died after one week of treatment due to anorexia and dehydration. Water intake increased for all animals provided ≥ 10% test substance. High dose males exhibited decreased hemoglobin levels and increased white blood cell counts. High dose females exhibited increased absolute and relative heart weights, while females in the 12.5% group and males and females in the 15% group exhibited increased relative liver weights. High dose males and females also exhibited increased absolute an relative kidney weights, respectively. Gross pathological and histopathological changes were limited to the skin of the application site and included cytotoxic effects in the epidermis at 12.5% and 15%, exudate adherent to skin (4/20 animals) in the high dose group, loss of hair color lateral and ventral to application site in all dose groups, and dose-related ulceration of the epidermis (4/20 animals) with inflammatory exudate (11/20 animals) in the two highest dose groups. The decedent animal exhibited extensive ulceration and necrosis of the epidermis. The REACH dossier authors identified a NOAEL/LOAEL of 400/500 mg/kg/day based on effects on organ weights, hematology

parameters, and gross pathological changes to the skin in the two highest dose groups (Klimisch Score 2, reliable with restrictions).

- In summary, the liver is the target organ following repeated oral dosing of sodium lauryl sulfate, C10-C16 alkyl alcohol sulfuric acid, sodium salt, or related alkyl sulfates based on altered serum enzymes, increased liver weights, and histopathological changes. The NOAELs for the subchronic repeated dose toxicity studies were greater than the GHS oral threshold of 100 mg/kg/day (UN 2019). The 28-day study of sodium lauryl sulfate in CD rats identified a NOAEL of 90 mg/kg/day based on effects at 270-540 mg/kg/day. The LOAEL of 270 mg/kg/day is less than the GHS guidance value of 300 mg/kg/day adjusted for study length (28 days is approximately one-third of 90 days). Although this study and the basis of the Japanese GHS classification suggest effects following sub-acute exposures, the NOAELs of subchronic and chronic studies do not support classification under GHS criteria. In addition, the 28-day study used the gavage dosing method, which aggravates the local irritation effects of the test article, which is a highly irritating substance. Therefore, ToxServices assigned a Low score for this endpoint.

Neurotoxicity (single dose, N-single) (Group II) Score (vH, H, M, or L): DG
Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Data Gap for neurotoxicity (single dose) due to lack of sufficient study details for GHS classification.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Japan - Specific target organs/systemic toxicity following single exposure - Category 1 [H370].
      - Based on effects to the central nervous system in single dose animal studies including decreased locomotor activity, decreased respiratory rate, and coma after single oral doses and tremors and tonic-clonic convulsions following single dermal doses of 200 mg/kg (NITE 2015).
- ECHA 2021a
  - *Oral*: In the non-GLP-compliant, OECD Guideline 401 acute oral toxicity test that identified oral LD_{50}s of 977-1,425 mg/kg for sodium lauryl sulfate (>98% purity) in Wistar rats, clinical signs of toxicity included decreased activity, diarrhea, spastic gait, hunched posture, lateral position, labored respiration, and coma with dose-dependent frequencies. No body weight data were provided. At the end of the 14-day recovery period, none of the surviving animals exhibited treatment-related gross pathological changes. In contrast, the decedent animals exhibited vascular congestion in the liver and hemorrhaging in gastrointestinal tract (dose groups not specified) (Klimisch Score 2, reliable with restrictions).
  - *Oral*: No data on clinical signs of toxicity, body weight, or gross pathological changes were presented for the study that identified an oral LD_{50} > 1,500 mg active ingredient/kg for sodium lauryl sulfate in rats (Klimisch Score 2, reliable with restrictions).
  - *Dermal*: In the non-GLP-compliant acute dermal toxicity test that identified a dermal LD_{50} of 200 mg active ingredient/kg for sodium lauryl sulfate in male rabbits, clinical signs of toxicity included tonic-clonic convulsions, respiratory failure, tremors, and slight scaling to leathery appearance of skin at the application site. Treatment decreased body weight at doses of 300 and 600 mg/kg. No gross pathological data were provided (Klimisch Score 4, not assignable).
    - ToxServices notes that this study is described as "disregarded due to major methodological deficiencies" despite the Klimisch Score of 4 (not assignable), and

as "not sufficient for risk assessment" due to limited data related to test conditions and/or experimental methods.

- *Dermal*: *Surrogate: Sodium Octyl Sulphate (CAS #142-31-4)*: In the GLP-compliant, OECD Guideline 402 acute dermal toxicity test that identified a dermal LD_{50} > 2,000 mg/kg for the surrogate sodium octyl sulfate in Wistar rats, treatment did not produce clinical signs of toxicity, changes to body weight, or gross pathological alterations (Klimisch Score 2, reliable with restrictions).
- *Dermal*: *Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Ammonium Salts (CAS #68081-96-9)*: In the pre-GLP acute dermal toxicity test that identified a dermal LD_{50} > 500 mg active ingredient/kg (the only dose tested) for the surrogate sulfuric acid, mono-C10-16-alkyl esters, ammonium salts in New Zealand White rabbits, clinical signs of toxicity were limited to dermal irritation which was characterized as severe erythema and slight eschar formation at 24 hours, necrosis on days 2-14, sloughing of the skin on days 8-14, and hyper-pigmentation of new skin by day 14. Treatment decreased the body weight of one animal with intact skin during the observation period. No gross pathological data were provided (Klimisch Score 2, reliable with restrictions).
- *Dermal: Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Potassium Salts (CAS #91783-22-1)*: In the pre-GLP acute dermal toxicity test that identified a dermal LD_{50} > 500 mg active ingredient/kg for the surrogate sulfuric acid, mono-C12-13-alkyl esters, potassium salts in New Zealand White rabbits, clinical signs of toxicity were limited to moderate to severe atonia (loss of muscle strength) and dermal irritation which was characterized as moderate to severe erythema and edema. Treatment produced desquamation and fissuring, slight to marked desquamation, eschar formation, and exfoliation at the application site by the end of the observation period. Treatment did not affect body weights during the observation period. No gross pathological data were provided (Klimisch Score 2, reliable with restrictions).
- *Dermal: Surrogate: Sulfuric Acid, Mono-C10-16-Alkyl Esters, Magnesium Salts (CAS #68081-97-0)*: In the pre-GLP acute dermal toxicity test that identified a dermal LD_{50} > 500 mg active ingredient/kg for the surrogate sulfuric acid, mono-C10-16-alkyl esters, magnesium salts in New Zealand White rabbits, clinical signs of toxicity were limited to dermal irritation which was characterized as severe erythema and eschar formation at 24 hours, necrosis on days 5-21, and sloughing of necrotic tissues and hyper-pigmentation of skin on day 21. Two of the three animals exhibited decreased body weights during the observation period. No gross pathological data were provided (Klimisch Score 2, reliable with restrictions).

- OECD 2009
  - *Oral*: In the acute oral toxicity test that identified an oral LD_{50} of 1,830 mg/kg in Cox CD rats on C10-C16 alkyl alcohol sulfuric acid, sodium salt, clinical signs of toxicity included abdominal griping and diarrhea, decreased motor activity and respiratory rate, blanching, and loss of corneal reflex and pupillary response. No body weight data were provided. Surviving animals exhibited no treatment-related gross pathological changes.
- In summary, several single dose study identified neurological clinical signs of toxicity, including effects on motor activity, changes to gait, reflexes, and/or responses to stimuli, coma, and/or convulsions. These effects may be related to discomfort following exposure to an irritating substance, or specifically neurologic in nature. No data regarding the reversibility of these effects were provided. Most of the studies did not list the doses at which these effects were observed. In addition, effects occurring at or above lethal doses should not be used as the basis to classify chemicals for this endpoint. Therefore, ToxServices did not consider neurological effects at a

dermal dose of 200 mg/kg/day in rats that were the basis of Japanese GHS classification for sodium lauryl sulfate to be appropriate for classification, as this study established an LD_{50} of 200 mg/kg. Due to lack of sufficient data, a Data Gap was assigned.

Neurotoxicity (repeated dose, N-repeated) (Group II*) Score (H, M, or L): DG
Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Data Gap for neurotoxicity (repeated dose) based on the lack of data identified for this endpoint.

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

Skin Sensitization (SnS) (Group II*) Score (H, M, or L): L
Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Low for skin sensitization based on negative results in a guinea pig maximization test and in one local lymph node assay. The positive results obtained in other local lymph node assays were attributed to its irritancy. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate and negative data and no GHS classification are available (CPA 2018b). The confidence in the score is high as it is based on reliable 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.
- ECHA 2021a
  - 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 lauryl sulfate (purity not specified) in DMSO on three consecutive days, or intradermal injections of 0.05%, 0.5%, or 5% sodium lauryl sulfate in saline followed five day later with topical applications of 5% sodium lauryl 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 lauryl sulfate was not sensitizing to the skin under the tested conditions (Klimisch Score 2, reliable with restrictions).
  - *Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Sodium Salts (CAS #91783-23-2):* A GLP-compliant guinea pig maximization test conducted in a manner similar to OECD Guideline 406 (no concentration provided for epicutaneous induction dose, lack test substance details) was performed with male and female Hartley guinea pigs (10 in control group, 20 treatment animals) administered dermal doses of sulfuric acid, mono-C12-13-alkyl esters, sodium salts (purity not specified). The induction doses were administered as intradermal injections of 25% sulfuric acid, mono-C12-13-alkyl esters, sodium salts in water and Freund's Complete Adjuvant (FCA) and a topical application of 12.5% sulfuric acid, mono-C12-13-alkyl esters, sodium salts in water under semi-occlusive dressing. The challenge dose was administered as a topical application of 12.5% sulfuric acid, mono-C12-13-alkyl esters, sodium salts (described as 3.35% active substance) in water. The dermal reactions were evaluated 48 and 72 hours after the challenge dose. The test substance

produced positive reactions in 2/20 and 0/20 animals 48 and 72 hours after the challenge dose, respectively. The negative controls treatment produced positive reactions in 2/20 and 0/20 animals 48 and 72 hours after the challenge dose, respectively. Since the treatment and negative control treatment produced the same degree of positive dermal reactions, the REACH dossier authors concluded that sulfuric acid, mono-C12-13-alkyl esters, sodium salts were not sensitizing to the skin under the tested conditions (Klimisch Score 2, reliable with restrictions).

- Montelius et al. 1994, ECHA 2021a
  - Two LLNAs were performed with female CBA/Ca mice (4/dose) administered dermal doses of sodium lauryl sulfate (purity not specified) at 4%, 10%, or 25% in dimethylformamide (DMF) or 5%, 10%, or 25% in DMF. The SIs were 4.1, 5.1, and 6.7 for the 4%, 10%, and 25% solutions, respectively, and 4.0, 5.1, and 7.6 for the 5%, 10%, and 25% solutions, respectively. While sodium lauryl sulfate produced SIs > 3.0, typically indicative of positive sensitization results, the authors concluded that sodium lauryl sulfate did not have a positive skin sensitization potential and that the induced lymphocyte proliferation was due to its skin irritation potential.
    - The REACH dossier authors indicated that this study was "disregarded due to major methodological deficiencies" although they assigned a Klimisch Score of 4 (not assignable) and indicated that the "[s]tudy [was] well documented, meets generally accepted scientific principles, acceptable for assessment."
- Basketter et al. 1994, ECHA 2021a
  - An LLNA was performed with mice (4/group, strain and sex not specified) administered topical doses of sodium lauryl sulfate (purity not specified) at 5%, 10%, or 25% in DMSO. The SIs were 3.2, 4, and 4.2 for the 5%, 10%, and 25% solutions, respectively. The authors concluded that sodium lauryl sulfate was sensitizing to the skin under the tested conditions.
    - The REACH dossier indicated that this study was "disregarded due to major methodological deficiencies" although they assigned a Klimisch Score of 4 (not assignable) and indicated that the "[s]tudy [was] well documented, meets generally accepted scientific principles, acceptable for assessment."
- In summary, sodium lauryl sulfate was negative for skin sensitization in a guinea pig maximization test. The inconsistent results in local lymph node assays were attributed to differences in irritating potential of the test substance, and additional research indicate that sodium lauryl sulfate produces "lymph node cell changes […] characteristic of irritancy and not of allergy" (OECD 2009). Therefore, ToxServices assigned a Low score for this endpoint.

Respiratory Sensitization (SnR) (Group II*) Score (H, M, or L): *L*

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were 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 2020
  - Sodium lauryl sulfate does not contain any structural alerts for respiratory sensitization (Appendix H).

- 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 sulfate 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 sulfate, and as sodium lauryl sulfate does not contain any structural alerts for respiratory sensitization (OECD 2020), sodium lauryl sulfate is not expected to be a respiratory sensitizer.

Skin Irritation/Corrosivity (IrS) (Group II) Score (vH, H, M, or L): H

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of High for skin irritation/corrosivity based on ToxServices classifying them as GHS Category 2 skin irritants (H315). GreenScreen® criteria classify chemicals as a High hazard for skin irritation/corrosivity when they are classified as GHS Category 2 skin irritants (CPA 2018b). The confidence in the score is high as it is based on reliable measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Australia - H315 - Causes skin irritation.
      - Based on 5–25 % solutions of sodium lauryl sulfate producing erythema and edema on unabraded rabbit skin after a four-hour application (AICIS 2013).
    - GHS – Japan - Skin corrosion / irritation - Category 2 [H315].
      - Based on moderate to severe irritation in animal studies (NITE 2015).
    - GHS - New Zealand - 6.3B - Mildly irritating to the skin.
      - Based on mild irritation reported in numerous human studies (CCID 2021).
- ECHA 2021a
  - A non-GLP-compliant dermal irritation test conducted in a manner similar to OECD Guideline 404 (24-hour occluded exposure, observation period of only 72 hours, and 48-hour scoring missing) was performed with New Zealand White rabbits (6 total) administered topical applications of 0.5 mL undiluted sodium lauryl sulfate (100% active ingredient) to shaved skin under occlusive dressing for 24 hours. An observation period of 72 hours followed the exposure period. At 24 and 72 hours, the mean erythema score was 2.2/4 and the mean edema score was 1.7/4. The erythema and edema were not fully reversible within 72 hours. The REACH dossier authors concluded that sodium lauryl sulfate was irritating under the tested conditions (Klimisch Score 2, reliable with restrictions).
  - An acute irritation patch test was performed with 22 human volunteers administered topical applications of 20% sodium lauryl sulfate (purity not specified) in water under occlusive dressing for 2 hours. Two subjects had a weak (+) reaction after the two-hour patch. One subject dropped out of the study after the first week. During the second week, 8 subjects exhibited no reactions, 10 subjects exhibited weak (+) reactions, and three subjects exhibited moderate (++) reactions. During the third week, 7 subjects exhibited weak (+) reactions and one subject exhibited a moderate (++) reaction. The REACH dossier authors concluded that sodium lauryl sulfate was irritating under the tested conditions (Klimisch Score 2, reliable with restrictions).

  - A human patch test was performed with an unspecified number of volunteers administered topical applications of 20% sodium lauryl sulfate (purity not specified) under occlusive dressing for 4 hours. The REACH dossier authors concluded that the test substance was irritating to the skin under the tested conditions. No further details were provided (Klimisch Score 2, reliable with restrictions).
  - A Draize test was performed with rabbits (strain and number not specified) administered topical applications of 2%, 10%, or 20% sodium lauryl sulfate (purity not specified) in water under occlusive dressing for 24 hours. The primary irritancy indices (PIIs) were 5-5.5, 6, and 6 for the 2%, 10%, and 20% solutions, respectively. The REACH dossier authors concluded that sodium lauryl sulfate was irritating to the skin under the tested conditions (Klimisch Score 2, reliable with restrictions).
  - A Burckhardt test was performed with human volunteers (number not specified) administered topical applications of 1% sodium lauryl sulfate (> 98% C12) for 30 minutes without coverage (open). The test substance was reported as not irritating under the tested conditions (Klimisch Score 4, not assignable).
  - A dermal irritation test was performed with New Zealand White rabbits (8 total) administered topical applications of 5% sodium lauryl sulfate (purity not specified) in water under semi-occlusive dressing for 4 hours. An observation period of 72 hours followed the exposures. Two assessors evaluated the dermal reactions, and the scores ranged from 4 (moderate) to 6 (severe) for all 8 animals at an unspecified time period (Klimisch Score 4, not assignable).
  - A non-GLP-compliant dermal irritation test conducted according to OECD Guideline 404 (occlusive coverage used rather than semi-occlusive) was performed with Kleinrusse rabbits (5 total) administered topical applications of 0.5 mL sodium lauryl sulfate (purity not specified) to shaved skin under occlusive dressing for 4 hours. An observation period of 21 days followed the exposure period. At 24, 48, and 72 hours, the mean erythema score was 4/4 and the mean edema score was 3.7/4. The erythema and edema were not fully reversible within 21 days, and the REACH dossier authors concluded that sodium lauryl sulfate was irritating to the skin under the tested conditions (Klimisch Score 2, reliable with restrictions).
  - In a series of human patch tests performed across three laboratories, sodium lauryl sulfate (purity not specified) was positive in 21/100, 15/100, and 16/31 (52%) subjects when administered as a 1% solution, and was positive in 79/100, 53/100, and 29/31 (94%) subjects when administered as a 10% solution. All exposures were for 4 hours under occlusive coverage. The REACH dossier authors concluded that sodium lauryl sulfate was irritating under the tested conditions (Klimisch Score 2, reliable with restrictions).
  - In a human patch test, 20% sodium lauryl sulfate (purity not specified) was irritating to 54/65 (83%) subjects following a 4-hour exposure under occlusive dressing. The REACH dossier authors concluded that sodium lauryl sulfate was irritating under the tested conditions (Klimisch Score 2, reliable with restrictions).
- Based on the weight of evidence, sodium lauryl sulfate is irritating to the skin. Although some of the dermal irritation effects were not fully reversible by the end of the observation periods in one study, this study used a more conservative occlusive exposure condition, rather than the semiocclusive condition recommended by current OECD Guideline. Further, corrosive effects, as evidenced by necrosis or other forms of tissue death, were not observed in any study. Therefore, ToxServices classified sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt as GHS Category 2 skin irritants (H315).

Eye Irritation/Corrosivity (IrE) (Group II) Score (vH, H, M, or L): vH

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Very High for eye irritation/corrosivity based on ToxServices classifying them as GHS Category 1 ocular irritants (H318). GreenScreen® criteria classify chemicals as a Very High hazard for eye irritation/corrosivity when they are classified as GHS Category 1 ocular irritants (CPA 2018b). The confidence in the score is high as it is based on reliable measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Australia - H318 - Causes serious eye damage.
      - Based on irreversible effects to rabbit eyes produced by a 25% sodium lauryl sulfate solution (AICIS 2013).
    - GHS – Japan - Serious eye damage / eye irritation - Category 1 [H318].
      - Based on irreversible effects produced following ocular instillation of a 25% aqueous solution in rabbits (NITE 2015).
    - GHS - New Zealand - 6.4A - Irritating to the eye (Cat. 2A).
      - Based on severe conjunctivitis produced by a 25% solution instilled to rabbit eyes (CCID 2021).
- ECHA 2021a
  - A non-GLP-compliant ocular irritation test conducted according to OECD Guideline 405 was performed with Kleinrusse rabbits (4 total) administered ocular instillations of 0.1 mL sodium lauryl sulfate (purity and concentration not specified). An observation period of 21 days followed the instillations. At 24, 48, and 72 hours, the mean corneal opacity score was 1/4, the mean iris score was 0/2, the mean conjunctival redness score was 2.6/3, and the mean chemosis score was 1.1/4. The corneal opacity and conjunctival redness were not fully reversible within 21 days, while the chemosis was fully reversible within 14 days. The authors concluded that sodium lauryl sulfate was irritating under the conditions of this test (Klimisch Score 2, reliable with restrictions).
  - A non-GLP-compliant ocular irritation test conducted in a manner similar to OECD Guideline 405 (observation period was only 7 days rather than 21 days) was performed with New Zealand White rabbits (3 total) administered ocular instillations of 0.1 mL undiluted C10-C16 alkyl alcohol sulfuric acid, sodium salt (sodium tetradecyl sulfate, purity not specified). The animals were observed for 7 days following the instillations. At 24, 48, and 72 hours, the mean corneal opacity score was 1.4/4 (grade 1 in 1 animal), the mean iris score was 0.7/2, the mean conjunctival redness score was 2/3 (grade 1 in 2 animals), and the mean chemosis score was 1.6/4. The chemosis and iris effects were fully reversible by the end of the observation period, while the corneal opacity and conjunctival redness were not fully reversible (Klimisch Score 2, reliable with restrictions).
  - A non-GLP-compliant ocular irritation study conducted in a manner similar to OECD Guideline 405 (recovery period of 14 days rather than 21 days) was performed with New Zealand White rabbits (3 total) administered ocular instillations of 0.1 mL undiluted C10-C16 alkyl alcohol sulfuric acid, sodium salt (sodium tetradecyl sulfate, purity not specified). An observation period of 14 days followed the instillations. At 24, 48, and 72 hours, the mean corneal opacity was 0.9/4, the mean iris score was 0.7/2, the mean conjunctival redness score was 1.9/3, and the mean chemosis score was 1.6/4. All of the ocular irritation effects were fully reversible by the end of the observation period (Klimisch Score 2, reliable with restrictions).

- *Surrogate: Sulfuric Acid, Mono-C12-13-Alkyl Esters, Potassium Salts (CAS #91783-22-1)*: A pre-GLP ocular irritation test conducted according to OECD Guideline 405 was performed with New Zealand White rabbits (6 total) administered ocular instillations of 0.1 mL 50% w/w sulfuric acid, mono-C12-13-alkyl esters, potassium salts (22% active ingredient) in water. Three animals had their eye rinsed 4 seconds after instillation with 20 mL lukewarm tap water; the remaining three animals did not have their eyes rinsed. An observation period of up to 28 days followed the instillations. At 24, 48, and 72 hours, the mean overall irritation scores were 6.56 (daily scores of 7.67, 6.67, and 5.33) for unrinsed eyes and 5.33 (daily scores of 6.34, 5.44, and 4.33) for rinsed eyes. At 24, 48, and 72 hours, the mean corneal opacity score was 2/4, the mean iris score was 0.8/2, the mean conjunctival redness score was 2.1/3, and the mean chemosis score was 1.7/4 (the REACH dossier authors did not specify whether these values were for rinsed or non-rinsed eyes). The corneal opacity, conjunctival redness, and chemosis were not fully reversible within 21 days, while the iris effects were fully reversible (Klimisch Score 2, reliable with restrictions).

- Based on the weight of evidence, sodium lauryl sulfate, C10-C16 alkyl alcohol sulfuric acid, sodium salt, and related alkyl sulfates are irritating to the eyes. As some of the ocular irritation effects were not fully reversible by the end of 21-day observation periods (UN 2019), ToxServices classified sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt as GHS Category 1 ocular irritants (H318).

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): vH

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Very High for acute aquatic toxicity based on measured acute aquatic toxicity values as low as 0.12 mg/L across all three trophic levels. GreenScreen® criteria classify chemicals as a Very High hazard for acute aquatic toxicity when acute aquatic toxicity values are ≤ 1 mg/L (CPA 2018b). The confidence in the score is high as it is based on reliable measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:*
    - GHS – Japan - Hazardous to the aquatic environment (acute) - Category 1 [H400].
      - Based on a 96-hor E/LC_{50} of 0.12 mg/L for crustacea (*Acartia tonsa*) (NITE 2015).
    - GHS - New Zealand 9.1D (fish, crustacean, algae) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action.
      - Based on a 96-hour LC_{50} of 1.25 mg/L in fish (*Fundulus heteroclitus*), a 48-hour EC_{50} of 1.5 mg/L for crustacea (*Artemia salina*), and a 72-hour EC_{50} of 53 mg/L in algae (*Scenedesmus subspicatus*) (CCID 2021).
    - EC - CEPA DSL - Inherently Toxic in the Environment (iTE).
      - Based on a 96-hour LC_{50} of 0.55 mg/L for crustacea (*Acartia tonsa*) (OECD 2021).
- ECHA 2021a
  - The following studies on sodium lauryl sulfate were assigned Klimisch Scores of 1 (reliable without restriction).
    - 96-hour LC_{50} (*Pimephales promelas*, fathead minnow) = 29 mg/L (measured) (non-GLP-compliant, similar to OECD Guideline 203)

- 48-hour LC_{50} (*Pseudosida ramose*, cladoceran) = 11.1 mg/L (nominal) (OECD Guideline 202)
- 48-hour LC_{50} (*Daphnia pulex*) = 5.34 mg/L (nominal) (OECD Guideline 202)
- 48-hour LC_{50} (*Simocephalus mixtus*) = 4.5 mg/L (nominal) (OECD Guideline 202)
- 48-hour LC_{50} (*Ceriodaphnia dubia*) = 8.59 mg/L (nominal) (OECD Guideline 202)
- 72-hour EC_{50} (*Desmodesmus subspicatus*, algae) = 53 mg/L (biomass), > 12 mg/L (growth rate) (both nominal) (GLP-compliant, DIN 38412, part 9)

o The following studies on sodium lauryl sulfate were assigned Klimisch Scores of 2 (reliable with restrictions).

- 96-hour LC_{50} (*Channa punctatus*, potted snakehead) = 19.5 mg/L (nominal)
- 96-hour LC_{50} (*Saccobranchus (Heteropneustes) fossilis*, Asian stinging catfish)
- 96-hour LC_{50} (*Oncorhynchus mykiss*, rainbow trout) = 4.62 mg/L (nominal) (non-GLP-compliant)
- 96-hour LC_{50} (*Danio rerio*, zebrafish) = 7.97 mg/L (nominal) (non-GLP-compliant)
- 96-hour LC_{50} (*Jordanella floridae*, flagfish) = 8.1 mg/L (nominal) (non-GLP-compliant)
- 96-hour LC_{50} (*Piaractus brachypomus*, pirapitinga (fish)) (nominal) (EPA-821-R-02-012)
- 96-hour LC_{50} (*Sparus auratus*, gilt-head bream (fish)) = 6.1 mg/L (nominal) (similar to OECD Guideline 203)
- 96-hour LC_{50} (*Dicentrarchus labrax*, European bass) = 7.34 mg/L (nominal) (similar to OECD Guideline 203)
- 96-hour LC_{50} (*Oreochromis mossambicus*, Mozambique tilapia) = 19.7 mg/L (nominal) (NIEA B902.10T, Taiwan EPA)
- 96-hour LC_{50} (*Oryzias latipes*, Japanese rice fish) = 12.5 mg/L (nominal) (NIEA B902.10T, Taiwan EPA)
- 96-hour LC_{50} (Gambusia holbrooki, Eastern mosquitofish) = 15.1 mg/L (nominal) (similar to OECD Guideline 203)
- 96-hour LC_{50} (*Lepomis macrochirus*, bluegill) = 4.5 mg/L (non-GLP-compliant, EPA 660/3-75-009)
- 96-hour LC_{50} (*Cyprinodon variegatus*, sheepshead minnow) = 4.1 mg/L (measured) (ASTM E-35)
- 96-hour LC_{50} (*Menidia*, Atlantic silverside) = 2.8 mg/L (measured) (ASTM E-35)
- 96-hour LC_{50} (*Thalassoma pavo*, ornate wrasse (fish)) = 5.23 mg/L (nominal) (EPA-821-R-02-012)
- 96-hour LC_{50} (*Rasbora daniconius*, slender rasbora (fish)) = 6.3 mg/L (nominal) (non-GLP-compliant, APHA guideline)
- 96-hour LC_{50} (*Scophthalmus maximus*, turbot) = 7.5 mg/L (nominal) (non-GLP-compliant, similar to OECD Guideline 203)
- 96-hour LC_{50} (*Ctenopharyngodon idella*, grass carp) = 7.7 mg/L (nominal) (APHA guideline)
- 96-hour LC_{50} (*P. promelas*, fathead minnow) = 10.2 mg/L (nominal)
- 96-hour LC_{50} (*Cichlasoma nigrofasciatum*, convict cichlid) = 16.1 g/L (nominal)
- 96-hour LC_{50} (*Carassius auratus*, goldfish) = 28.4 mg/L (nominal)
- 96-hour LC_{50} (*Poecilia reticulata*, guppy) = 13.5 mg/L (nominal)
- 96-hour LC_{50} (*Menidia beryllina*, inland silverside) = 9.5 mg/L (nominal) (EPA 821-R-02-012)
- 48-hour LC_{50} (*P. promelas*, fathead minnow) = 31.9 mg/L (nominal) (non-GLP-compliant, similar to OECD Guideline 203)

- 96-hour LC_{50} (*Cynopoecilus melanotaenia*, killfish) = 14.9 mg/L (nominal) (EPA 600/4-90/027F)
- 48-hour LC_{50} (*Artemia salina*, brine shrimp) = 3.15 mg/L (nominal) (non-GLP-compliant)
- 48-hour LC_{50} (*C. dubia*) = 5.55 mg/L (nominal or measured not specified) (non-GLP-compliant, similar to OECD Guideline 202)
- 48-hour mobility EC_{50} (*Artemia parthenogenetica*, brine shrimp) =12.2 mg/L (nominal) (OECD Guideline 202)
- 96-hour LC_{50} (*Allorchestes compressa*, amphipod) = 3.6 mg/L (nominal)
- 48-hour LC_{50} (*Paracentrotus lividus*, sea urchin) = 2.65-4.05 mg/L (nominal)
- 48-hour mobility EC_{50} (*Cypris subglobosa*) = 2.05 mg/L (nominal)
- 72-hour LC_{50} (*Moina mongolica*) = 3.5 mg/L (nominal)
- 96-hour LC_{50} (*Artemia parthenogenetica*, brine shrimp) = 13.9 mg/L (nominal)
- 48-hour LC_{50} (*Brachionus calyciflorus*, rotifer) = 1.2 mg/L (nominal) (non-GLP-compliant)
- 48-hour LC_{50} (*Arenicola marina*, aquatic worm) = 15.2 mg/L (nominal)
- 96-hour LC_{50} (*Nitocra spinipes*, copepod) = 14.4 mg/L (nominal)
- 24-hour LC_{50} (*Crassostrea rhizophorae*, mollusc) = 1.36 mg/L (nominal)
- 96-hour LC_{50} (*Mysidopsis juniae*, mysid shrimp) = 2.2-2.3 mg/L (nominal)
- 1-hour fertilization rate EC_{50} (*P. lividus*, sea urchin) = 3.2 mg/L (nominal)
- 48-hour LC_{50} (*Tiburonella viscana*, amphipod) = 3.41 mg/L (nominal) (ASTM E 1367-99)
- 48-hour LC_{50} (*Perna*, mollusc) = 0.85 mg/L (ASTM E 724/89)
- 96-hour LC_{50} (*Neomysis americana*, opossum shrimp) = 7.24 mg/L (nominal) (ASTM E-35)
- 96-hour LC_{50} (*Americamysis bahia)*, shrimp) = 6.62 mg/L (nominal) (ASTM E-35)
- 48-hour mobility EC_{50} (*Daphnia obtuse*) = 9.8 mg/L (nominal)
- 96-hour LC_{50} (*Gammarus pulex*, amphipod) = 4.1 mg/L (nominal)
- 96-hour LC_{50} (*Lymnea palustris*, snail) = 7 mg/L (nominal)
- 48-hour larval development EC_{50} (*Mytilus galloprovincialis*, mollusk) = 2.35 mg/L (nominal)
- 96-hour LC_{50} (*Siriella armata*) = 8.47 mg/L (nominal)
- 48-hour LC_{50} (*Daphnia magna*) = 1.8 mg/L (non-GLP-compliant, EPA 660/3-75-009)
- 48-hour larval development EC_{50} (*Chlamys asperrima*) = 1 mg/L (nominal)
- 48-hour LC_{50} (*Temora stylifera*, copepod) = 2.6 mg/L (nominal)
- 48-hour LC_{50} (*Acartia lilljeborgi*, copepod) = 1.9 mg/L (nominal)
- 1-hour fertilization rate EC_{50} (*P. lividus*, sea urchin) = 3.2 mg/L (nominal) (EPA: ERL-N-SOP)
- 96-hour mobility EC_{50} (*Tigriopus fulvus*, copepod) = 7.4 mg/L (ISO/FDSI 14669)
- 28-hour LC_{50} (*Paracentrotus lividus*) = 1.48 mg/L (nominal) (EPA 600/R-95-136\EPA 600/-94/025)
- 38-hour LC_{50} (*Arbacia lixula*) = 1.55 mg/L (nominal) (EPA 600/R-95-136\EPA 600/-94/025)
- 38-hour LC_{50} (*Sphaerechinus granularis*) = 1.59 mg/L (nominal) (EPA 600/R-95-136\EPA 600/-94/025)
- 72-hour LC_{50} (*A. bahia*) = 3.8 mg/L (nominal) (APHA guideline)
- 48-hour mobility EC_{50} (*Daphnia ambigua*) = 2.44 mg/L (ASTM E-729- 88a)
- 48-hour mobility EC_{50} (*C. dubia*) = 1.26 mg/L (ASTM E-729- 88a)

        - 96-hour LC_{50} (*Corophium orientale*, amphipod) = 8.7 mg/L (nominal)
        - 96-hour growth rate EC_{50} (*Tetraselmis chuii*) = 30.2 mg/L (nominal) (OECD Guideline 201)
        - 72-hour biomass EC_{50} (*Chlamydomonas reinhardtii*) = 18.8 mg/L (nominal)
        - 7-day root length EC_{50} (*Lemna minor*) = 18 mg/L (nominal)
        - 96-hour growth rate EC_{50} (*Pseudokirchneriella subcapitata*) = (nominal)
- OECD 2009
    - Sodium lauryl sulfate: 96-hour EC_{50} (*Acartia tonsa*) = 0.12 mg/L (nominal) (EPA-600/9-76-010) (Klimisch Score 2, reliable with restrictions)
    - C10-C16 alkyl alcohol sulfuric acid, sodium salt: 48-hour EC_{50} (*Ceriodaphnia dubia*) = 1.37 mg/L (nominal) (Klimisch Score 2, reliable with restrictions)
    - C10-C16 alkyl alcohol sulfuric acid, sodium salt: 72-hour cell number EC_{50} (*Pseudokirchneriella subcapitata*) = 60 mg/L (nominal) (Klimisch Score 2, reliable with restrictions)
    - C10-C16 alkyl alcohol sulfuric acid, sodium salt: 72-hour growth rate EC_{50} (*D. subspicatus*, algae) = 3.5-6.2 mg/L (nominal) (OECD Guideline 201) (Klimisch Score 4, not assignable)

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): H

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of High for chronic aquatic toxicity based on chronic aquatic toxicity values as low as 0.88 mg/L across all three trophic levels. GreenScreen® criteria classify chemicals as a High hazard for chronic aquatic toxicity when chronic aquatic toxicity values are > 0.1 to 1.0 mg/L (CPA 2018b). The confidence in the score is high as it is based on reliable measured data.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:*
        - EC - CEPA DSL - Inherently Toxic in the Environment (iTE).
            - Based on a 96-hour LC_{50} of 0.55 mg/L for crustacea (*Acartia tonsa*) (OECD 2021). It is not classified as persistent or bioaccumulative.
    - *Other:*
        - GHS – Japan - Hazardous to the aquatic environment (chronic) - Category 3 [H412].
            - Based on a 7-day reproductive NOEC of 0.88 mg/L for crustacea (*Ceriodaphnia dubia*) and its rapid biodegradability (NITE 2015).
- ECHA 2021a (the studies below are conducted on sodium lauryl sulfate)
    - 42-day weight and mortality NOEC (*P. promelas*, fathead minnow) ≥ 1.357 mg/L (measured, no effects detected at up to the highest concentration tested) (Klimisch Score 2, reliable with restrictions).
    - 28-day LC_{10} (*P. promelas*, fathead minnow) = 3.6 mg/L (measured) (non-GLP-compliant, similar to OECD Guideline 210) (Klimisch Score 2, reliable with restrictions).
    - 7-day reproduction NOEC (*C. dubia*) = 0.88 mg/L (measured) (non-GLP-compliant, EPA-600/489/001) (Klimisch Score 1, reliable without restriction).
    - 21-day reproduction NOEC (*Daphnia magna*) = 3.2 mg/L (measured) (OECD Guideline 202) (Klimisch Score 2, reliable with restrictions).
    - 7-day growth NOEC (*Mysidopsis intii*) = 1.41 mg/L (nominal) (non-GLP-compliant, EPA/600/4-87/028) (Klimisch Score 2, reliable with restrictions).
    - 7-day mortality NOEC (*Holmesimysis costata*) = 1.41 mg/L (nominal) (non-GLP-compliant, EPA/600/4-87/028) (Klimisch Score 2, reliable with restrictions).

  - 21-day reproduction NOEC (*Pseudosida ramosa*) = 1 mg/L (nominal) (non-GLP-compliant, OECD Guideline 211) (Klimisch Score 2, reliable with restrictions).
  - 21-day budding rate NOEC (*Hydra attenuata*) = 5.76 mg/L (nominal) (non-GLP-compliant)
  - 40-day mortality NOEC (*D. magna*) = 2-4 mg/L (nominal) (Klimisch Score 2, reliable with restrictions).
  - 72-hour biomass NOEC (*D. subspicatus*, algae) = 30 mg/L (nominal) (GLP-compliant, DIN 38412, part 9) (Klimisch Score 1, reliable without restriction).
- OECD 2009
  - C10-C16 alkyl alcohol sulfuric acid, sodium salt: 72-hour growth rate NOEC (*D. subspicatus*, algae) = 1.0 mg/L (nominal) (OECD Guideline 201) (Klimisch Score 4, not assignable)

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): vL

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Very Low for persistence based on sodium lauryl sulfate meeting the 10-day window in an OECD Guideline 301 B ready biodegradation test and water expected to be the dominant environmental compartment. GreenScreen® criteria classify chemicals as a Very Low hazard for persistence when water is the dominant environmental compartment and the 10-day biodegradation window is met (CPA 2018b). The confidence in the score is high as it is based on 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.
- ECHA 2021a
  - A GLP-compliant ready biodegradability test conducted according to OECD Guideline 301 B (CO_2 evolution test) was performed with non-adapted, activated domestic sludge exposed to sodium lauryl sulfate (purity not specified) at 20 mg/L (DOC) for 28 days. The test substance degraded 81.5% and 95% after 10 and 28 days. The positive control (sodium benzoate) performed as expected. As sodium lauryl sulfate met the 10-day window, ToxServices concluded that it was readily biodegradable under the tested conditions (Klimisch Score 1, reliable without restriction).
  - A GLP-compliant ready biodegradability test conducted according to OECD Guideline 301 D (closed bottle test) was performed with domestic sewage treatment plant effluent exposed to sodium lauryl sulfate (purity not specified) at 2 or 5 mg/L for 28 days. At the end of the treatment period, the level of degradation was 97% and 94% for the 2 and 5 mg/L solutions, respectively. The positive control (sodium benzoate) performed as expected. No details regarding the 10-day window were provided. ToxServices concludes that sodium lauryl sulfate was at least rapidly degradable under the tested conditions.
- OECD 2009
  - Based on their physicochemical properties, alkyl sulfates are expected to partition mostly in water (i.e., the hydrosphere). No partitioning to the atmosphere is expected due to their ionic structure. Alkyl sulfates are not expected to undergo hydrolysis in water due to the lack of hydrolysable functional groups.
  - Alkyl sulfates are readily biodegradable.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vL
Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Very Low for bioaccumulation based on measured BCFs ≤ 82 for alkyl sulfates with ≤ C16 alkyl chains. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when BCF/BAF values are ≤ 100 (CPA 2018b). The confidence in the score is high as it is based on reliable 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.
- ECHA 2021a
  - A non-GLP-compliant bioaccumulation test was performed with carp (*Cyprinus carpio*) exposed to sodium lauryl 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).
  - A non-GLP-compliant bioaccumulation test was performed with carp (*C. carpio*) exposed to radiolabeled sodium lauryl 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).
  - A non-GLP-compliant bioaccumulation test was performed with goldfish (*C. auratus*) exposed to ^{14}C or ^{35}S-radiolabeled sodium lauryl 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).
  - A non-GLP-compliant bioaccumulation test was performed with carp (*C. carpio*) exposed to sodium lauryl 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).
  - A bioaccumulation test (GLP status not specified) was performed with goby (*Proterorhinus marmoratus*) exposed to sodium lauryl sulfate (purity not specified) at 4 mg/L for 240 days. The whole-body BCF was calculated as 7.15 (Klimisch Score 4, not assignable).
  - A non-GLP-compliant bioaccumulation test was performed with carp (*C. carpio*) exposed to ^{35}S-radiolabeled sodium lauryl 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 2009
  - Alkyl sulfates with ≤ C16 alkyl chains have BCFs ≤ 73.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Low for reactivity based on ToxServices not classifying them as reactive under GHS criteria. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when no GHS classifications are available (CPA 2018b). The confidence in the score was low as it is not based on measured data or authoritative listings.

- 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 2021a
    - Sodium lauryl sulfate lacks structural alerts for explosive and oxidizing properties.
- No measured data were identified. Therefore, screening procedures for explosivity were used here to estimate the reactivity properties of sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt. These procedures are listed in the GHS (UN 2019).
    - Based on the structure of its components or moieties, sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are not considered explosive or self-reactive due to lack of functional groups associated with explosive or self-reactive properties (See Appendix I).
    - Based on the structure of its components or moieties, sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt are 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.
- Based on the above information, ToxServices did not classify sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt for reactivity under GHS criteria (UN 2019).

Flammability (F) Score (vH, H, M, or L): M

Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt were assigned a score of Moderate for flammability based on ToxServices classifying it as a Category 2 flammable solid under GHS criteria. GreenScreen® criteria classify chemicals as a Moderate hazard for flammability when they are classified as GHS Category 2 flammable solids (CPA 2018b). The confidence in the score was high as it is based on 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.
- ECHA 2021a
    - Sodium lauryl sulfate (purity not specified) has a flash point of 170-180°C as identified in three EU Method A.9 tests (GLP status not specified) (Klimisch Score 2, reliable with restrictions).
    - Sodium lauryl sulfate (purity not specified) did not ignite on contact with air (i.e., is not pyrophoric) and had a burning time of 27 seconds and a combustion velocity (burning rate) of 3.7 mm/second in an EU Method A.10 (Flammability (Solids)) test (GLP status not specified) (Klimisch Score 2, reliable with restrictions).
    - Sodium lauryl sulfate (purity not specified) has a self-ignition temperature of 310.5°C as identified in a VDI 2263 test (GLP status not specified) (Klimisch Score 2, reliable with restrictions). It had no self-heating properties up to 186°C.
- As sodium lauryl sulfate is not flammable in contact with water and has a burning rate of 3.7 mm/second, ToxServices classified it as a Category 2 flammable solid under GHS criteria (UN 2019). GHS Category 2 flammable solids have burning times < 45 seconds or burning rates > 2.2 mm/second and are not flammable in contact with water.

Use of New Approach Methodologies (NAMs)[9] in the Assessment, Including Uncertainty Analyses of Input and Output

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* genotoxicity assays, *in vitro* and *in silico* endocrine activity assessments, and use of structural alerts to evaluate respiratory sensitization. NAMs are non-animal alternative 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 2020b, OECD 2020b). 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 2020b):

- 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 sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt's NAMs dataset include no *in vivo* and/or *in vitro* experimental data for endocrine activity and respiratory sensitization. Sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt's Type II (extrapolation output) uncertainties include limitations in the applicability domains of the (Quantitative) Structure Activity Relationship ((Q)SAR) models applied in this assessment and exogenous metabolic systems used in *in vitro* genotoxicity tests that do not entirely mirror *in vivo* metabolism. Some of sodium lauryl sulfate and C10-C16 alkyl alcohol sulfuric acid, sodium salt's type II uncertainties were alleviated by the use of *in vitro* test batteries in combination of *in vivo* data.

Table 4: Summary of NAMs Used in the GreenScreen® Assessment, Including Uncertainty Analyses	
Uncertainty Analyses (OECD 2020b)	
Type I Uncertainty: Data/Model Input	**Endocrine activity**: No *in vivo* experimental data are available. **Respiratory sensitization**: No experimental data are available.
Type II Uncertainty: Extrapolation Output	**Genotoxicity:** The bacterial reverse mutation assay (OECD 471) only tests point-mutation inducing activity in non-mammalian cells, and the exogenous metabolic activation system does not entirely mimic *in vivo* conditions[10]. The mammalian cell gene mutation assay (OECD 476) only detects gene mutations, and the exogenous metabolic activation system does not entirely mirror *in vivo* metabolism[11]. The exogenous metabolic activation system used in these studies does not entirely mirror *in vivo* metabolism[12].

[9] 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).

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

[11] https://www.oecd-ilibrary.org/docserver/9789264264809-en.pdf?expires=1614097800&id=id&accname=guest&checksum=C0DE371FB9C5A878E66C9AB7F84E6BBE

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

	Endocrine activity: VEGA tool does not evaluate ionic substances (VEGA 2020). Sodium lauryl sulfate is outside of the applicability domain for several endocrine-related model batteries (DTU 2021). **Respiratory sensitization**: The OECD Toolbox (OECD 2020) only identifies structural alerts and does not define applicability domains.	
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* gene mutation assay
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	Y	*In vitro* high throughput data: EDSP Tox 21 screening assays *In silico* modeling: VEGA/Danish QSAR/ToxCast
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/Danish QSAR
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	
Chronic aquatic toxicity	N	
Persistence	N	
Bioaccumulation	N	

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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 Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #151-21-3, 68585-47-7)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

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
							S	R *	S	R *	*	*								
Table 2: Chemical Details																				
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 Sulfate and C10-C16 Alkyl	151-21-3, 68585-47-7	L	L	DG	L	DG	*vH*	M	L	DG	DG	L	*L*	H	vH	vH	H	vL	vL	*L*	M

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 Sulfate and C10-C16 Alkyl Alcohol	2

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

Table 6

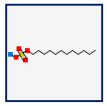
Chemical Name	Final GreenScreen® Benchmark Score
Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol	2

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 Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt (CAS #151-21-3, 68585-47-7)



151-21-3

Sodium lauryl sulfate

ALSO CALLED [12738-53-3] SODIUM LAURYL SULFATE (primary CASRN is 151-21-3), [1335-72-4] Sodium lauryl sulfate (p...

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		Group I Human					Group II and II* Human								Ecotox			Fate		Physical		Mult	Non-GSLT				
	GS Score	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
All Hazards	LT-P1	-	-	pC	-	-	vH	M	-	-	-	-	-	H	vH	vH	-	M	-	-	-	pC	vH	-	-	-	R

Hazard Lists

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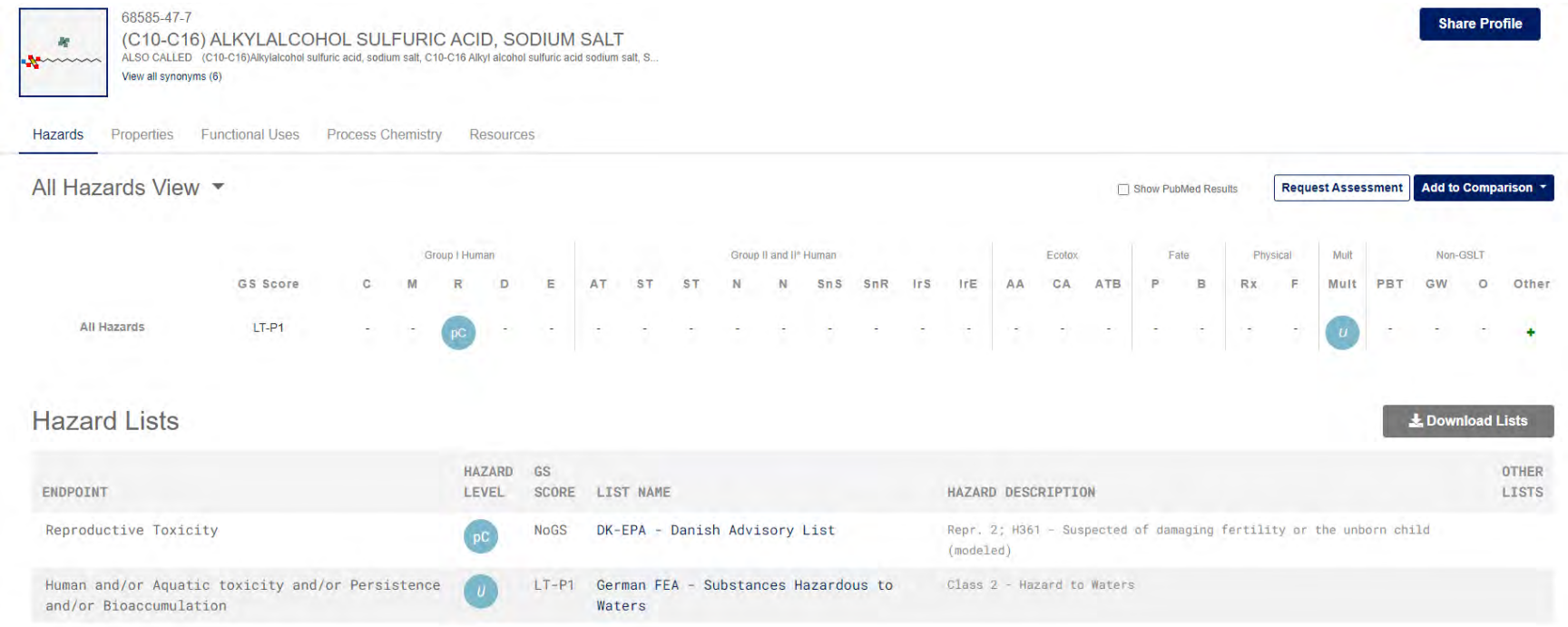
ENDPOINT	HAZARD LEVEL	GS SCORE	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Reproductive Toxicity	pC	NoGS	DK-EPA - Danish Advisory List	Repr. 2; H361 - Suspected of damaging fertility or the unborn child (modeled)	

Acute Mammalian Toxicity	vH	LT-UNK	GHS - Japan	Acute Toxicity (dermal) - Category 2 [H310]	+13
	vH-H	LT-UNK	GHS - Australia	H311 - Toxic in contact with skin	
	H	LT-UNK	GHS - New Zealand	6.1C (dermal) - Acutely toxic	
	H-M	LT-UNK	GHS - Australia	H302 - Harmful if swallowed	
	M	LT-UNK	GHS - Japan	Acute Toxicity (oral) - Category 4 [H302]	
	M	LT-UNK	GHS - New Zealand	6.1D (dermal) - Acutely toxic	
	M	LT-UNK	GHS - New Zealand	6.1D (oral) - Acutely toxic	
	L	LT-UNK	GHS - New Zealand	6.1E (dermal) - Acutely toxic	
	pC	NoGS	US EPA - OPP - Registered Pesticides	FIFRA Registered Pesticide	
	pC	NoGS	DK-EPA - Danish Advisory List	Acute Tox. 4 - Harmful if swallowed (modeled)	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H302 - Harmful if swallowed (unverified)	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H311 - Toxic in contact with skin (unverified)	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H312 - Harmful in contact with skin (unverified)	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H332 - Harmful if inhaled (unverified)	

Systemic Toxicity/Organ Effects-Single Exposure	M	LT-UNK	GHS - Australia	H335 - May cause respiratory irritation	+1
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H335 - May cause respiratory irritation (unverified)	
Skin Irritation/Corrosivity	H	LT-UNK	GHS - Japan	Skin corrosion / irritation - Category 2 [H315]	+3
	H	LT-UNK	GHS - Australia	H315 - Causes skin irritation	
	M	LT-UNK	GHS - New Zealand	6.3B - Mildly irritating to the skin	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H315 - Causes skin irritation (unverified)	
Eye Irritation/Corrosivity	vH	LT-UNK	GHS - Australia	H318 - Causes serious eye damage	+4
	vH	LT-UNK	GHS - Japan	Serious eye damage / eye irritation - Category 1 [H318]	
	H	LT-UNK	GHS - New Zealand	6.4A - Irritating to the eye (Cat. 2A)	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H318 - Causes serious eye damage (unverified)	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H319 - Causes serious eye irritation (unverified)	
Acute Aquatic Toxicity	vH	LT-UNK	GHS - Japan	Hazardous to the aquatic environment (acute) - Category 1 [H400]	+1
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H400 - Very toxic to aquatic life (unverified)	

Terrestrial Ecotoxicity	M	NoGS	GHS - New Zealand	9.3C - Harmful to terrestrial vertebrates	+1
	pC	NoGS	GHS - New Zealand	9.2D - Slightly harmful in the soil environment	
Flammability	pC	NoGS	EU - Manufacturer REACH hazard submissions	H228 - Flammable solid (unverified)	
Human and/or Aquatic toxicity and/or Persistence and/or Bioaccumulation	U	LT-P1	German FEA - Substances Hazardous to Waters	Class 2 - Hazard to Waters	
Carcinogenicity,Mutagenicity/Genotoxicity Reproductive Toxicity, Developmental Toxicity, Acute Mammalian Toxicity, or System Toxicity/Organ Effects.	U	LT-UNK	Québec CSST - WHMIS 1988	Class D2B - Toxic material causing other toxic effects	+1
	U	LT-UNK	EC - CEPA DSL	Inherently Toxic to Humans (iTH)	
T & P and/or B [(Chronic Aquatic Toxicity and Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	U	LT-UNK	GHS - Japan	Hazardous to the aquatic environment (chronic) - Category 3 [H412]	+4
	U	LT-UNK	GHS - New Zealand	9.1D (algal) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action	
	U	LT-UNK	GHS - New Zealand	9.1D (crustacean) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action	
	U	LT-UNK	GHS - New Zealand	9.1D (fish) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action	
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H412 - Harmful to aquatic life with long lasting effects (unverified)	
Systemic Toxicity/Organ Effects [Repeated Exposure] and/or Neurotoxicity [Repeated Exposure]	M	LT-UNK	GHS - Japan	Specific target organs/systemic toxicity following repeated exposure - Category 2 [H373]	
Systemic Toxicity/Organ Effects [Single Exposure] and/or Neurotoxicity [Single Exposure]	vH	LT-UNK	GHS - Japan	Specific target organs/systemic toxicity following single exposure - Category 1 [H370]	
Acute aquatic toxicity; Chronic aquatic toxicity	U	LT-UNK	EC - CEPA DSL	Inherently Toxic in the Environment (iTE)	



68585-47-7

(C10-C16) ALKYLALCOHOL SULFURIC ACID, SODIUM SALT

ALSO CALLED (C10-C16)Alkylalcohol sulfuric acid, sodium salt, C10-C16 Alkyl alcohol sulfuric acid sodium salt, S...

View all synonyms (6)

Share Profile

Hazards | Properties | Functional Uses | Process Chemistry | Resources

All Hazards View

Show PubMed Results | Request Assessment | Add to Comparison

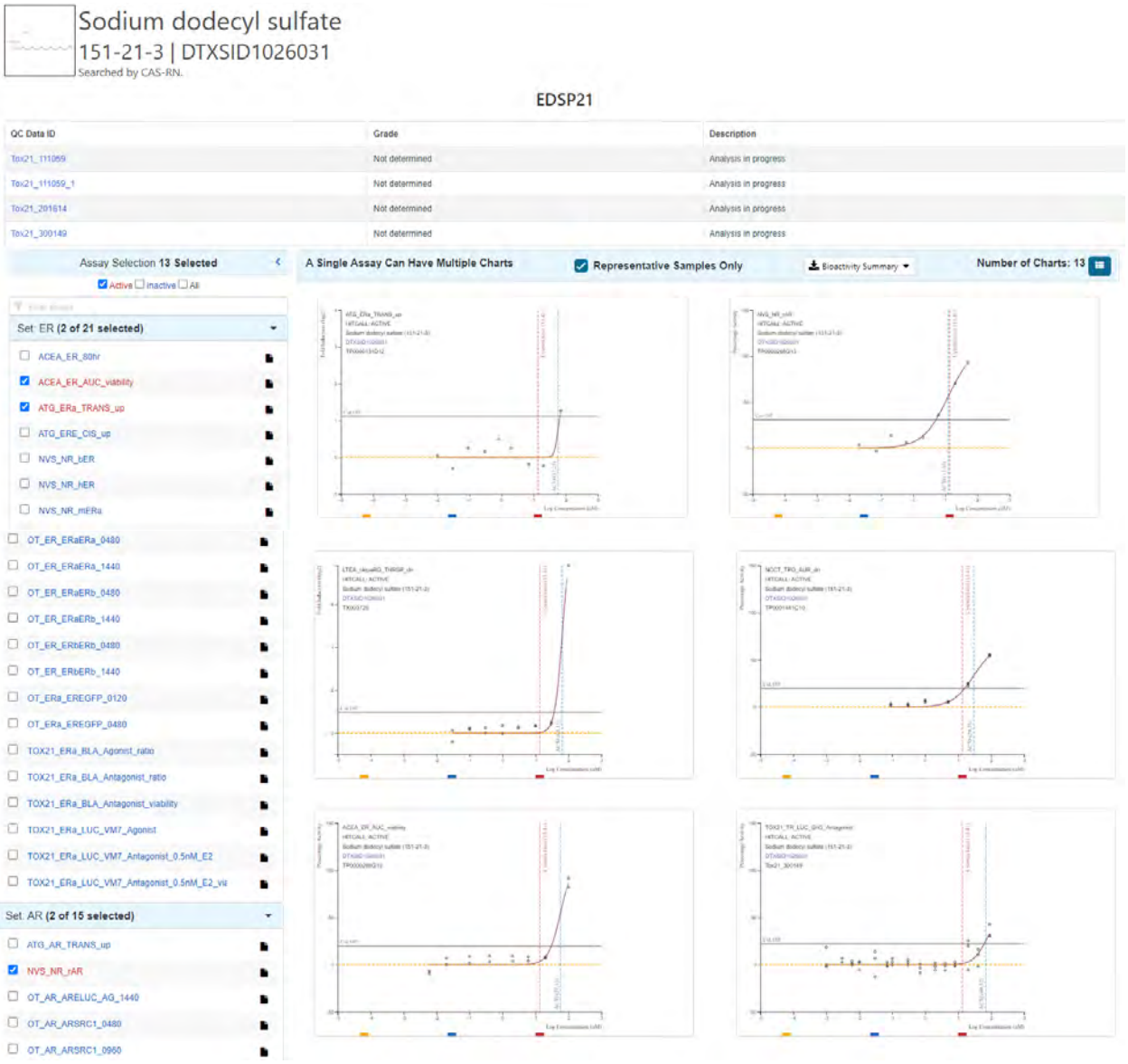
		Group I Human					Group II and II* Human									Ecotox			Fate		Physical		Mult	Non-GSLT			
	GS Score	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
All Hazards	LT-P1	-	-	pC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	U	-	-	-	+

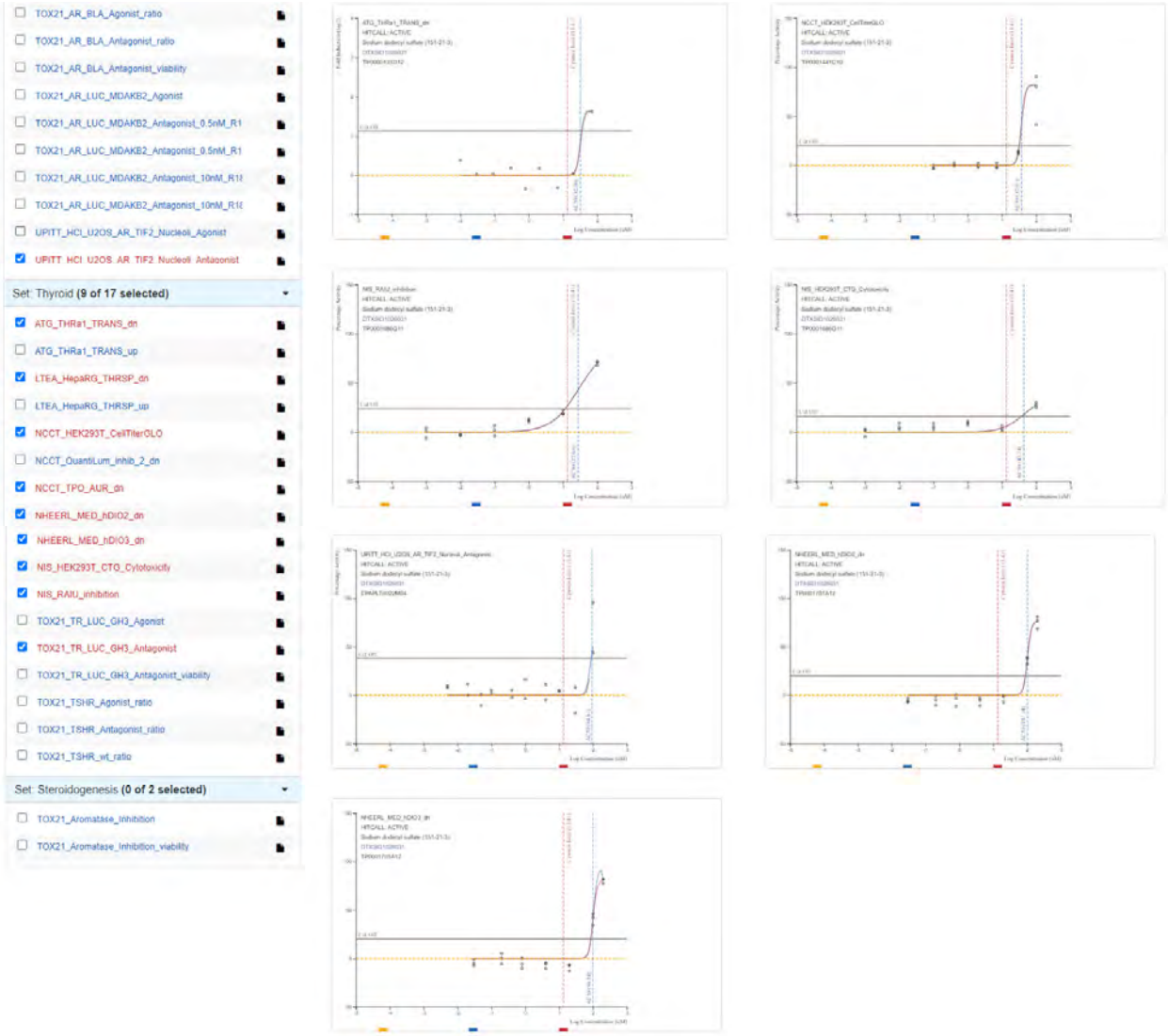
Hazard Lists

Download Lists

ENDPOINT	HAZARD LEVEL	GS SCORE	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)	
Human and/or Aquatic toxicity and/or Persistence and/or Bioaccumulation	U	LT-P1	German FEA - Substances Hazardous to Waters	Class 2 - Hazard to Waters	

APPENDIX D: CompTox EDSP21 Results for Sodium Lauryl Sulfate (CAS #151-21-3)





APPENDIX E: ToxCast Model Predictions for Sodium Lauryl Sulfate (CAS #151-21-3)

Sodium dodecyl sulfate
151-21-3 | DTXSID1026031
Searched by CAS-RN.

ToxCast: Models
ToxCast Model Predictions

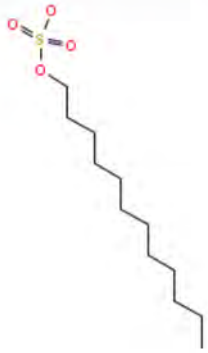
Download ToxCast Model Predictions

Model	Receptor	Agonist	Antagonist	Binding
ToxCast Pathway Model (AUC)	Androgen	0.00	5.49e-5	-
ToxCast Pathway Model (AUC)	Estrogen	0.00	0.00	-
COMPARA (Consensus)	Androgen	Inactive	Inactive	Inactive
CERAPP Potency Level (From Literature)	Estrogen	Inactive (Inactive)	-	Active (Very weak)
CERAPP Potency Level (Consensus)	Estrogen	Inactive (Inactive)	Active (VeryWeak)	Active (VeryWeak)

APPENDIX F: VEGA Endocrine Endpoint for Sodium Lauryl Sulfate (CAS #151-21-3)

1. Prediction Summary

Prediction for compound Molecule 0



Prediction: Reliability:

Prediction is Active, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 infrequent fragments found)

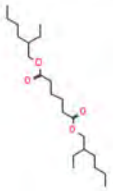
Compound: Molecule 0
Compound SMILES: O=S(=O)([O-])OCCCCCCCCCCCC
Experimental value: -
Predicted activity: Active
Classification tree final node: 18
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 126-73-8
Dataset id: 18 (Training set)
SMILES: O=P(OCCCC)(OCCCC)OCCCC
Similarity: 0.777

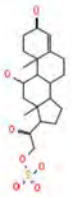
Experimental value: Inactive
Predicted value: Inactive



Compound #2

CAS: 103-23-1
Dataset id: 9 (Training set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.749

Experimental value: Inactive
Predicted value: Inactive



Compound #3

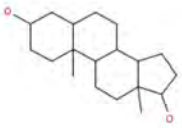
CAS: 100775-23-3
Dataset id: 139 (Training set)
SMILES: O=C3C=C2CCC1C4CCC(C(=O)COS(=O)(=O)O)C4(C)(CC(O)C1C2(C)CC3)
Similarity: 0.728

Experimental value: Inactive
Predicted value: Inactive

Compound #4

CAS: 2664-60-0
Dataset id: 220 (Training set)
SMILES: O=C(OCCCCCCCCCCCC)c1ccc(O)cc1
Similarity: 0.716

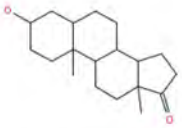
Experimental value: Active
Predicted value: Active



Compound #5

CAS: 571-20-0
Dataset id: 83 (Test set)
SMILES: OC4CCC2(C)(C(CCC1C3CCC(O)C3(C)(CCC12))C4)
Similarity: 0.714

Experimental value: Active
Predicted value: Active



Compound #6

CAS: 53-41-8
Dataset id: 78 (Training set)
SMILES: O=C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.711

Experimental value: Inactive
Predicted value: Active

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.762
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 0.85
Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 infrequent fragments found).

Symbols explanation:

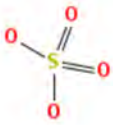
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

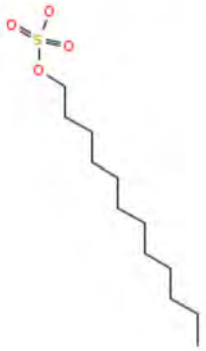


Fragment defined by the SMILES: O=S(=O)(O)O
The fragment has less than 3 occurrences in the model's training set

Fragment defined by the SMILES: OS
The fragment has less than 3 occurrences in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0



Prediction: Reliability:

Prediction is Not predicted, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: O=S(=O)([O-])OCCCCCCCCCCCC
Experimental value: -
Predicted ER-mediated effect: Not predicted
No. alerts for activity: 0
No. alerts for possible activity: 0
No. alerts for non-activity: 0
No. alerts for possible non-activity: 0
Structural alerts: -
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: N.A.
Dataset id: 1014 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCCC
Similarity: 0.976

Experimental value: NON-active
Predicted value: Not predicted

Compound #2

CAS: N.A.
Dataset id: 682 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCC
Similarity: 0.964

Experimental value: NON-active
Predicted value: Not predicted

Compound #3

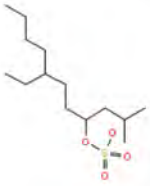
CAS: N.A.
Dataset id: 889 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCCCC
Similarity: 0.963

Experimental value: NON-active
Predicted value: Not predicted

Compound #4

CAS: N.A.
Dataset id: 874 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCC
Similarity: 0.947

Experimental value: Active
Predicted value: Not predicted



Compound #5

CAS: N.A.
Dataset id: 661 (Training set)
SMILES: O=S(=O)(O)OC(CCC(CC)CCCC)CC(C)C
Similarity: 0.942

Experimental value: NON-active
Predicted value: Not predicted

Compound #6

CAS: N.A.
Dataset id: 683 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCCCCC
Similarity: 0.94

Experimental value: NON-active
Predicted value: Not predicted

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	**Global AD Index** AD index = 0 Explanation: the predicted compound is outside the Applicability Domain of the model.
✔	**Similar molecules with known experimental value** Similarity index = 0.968 Explanation: strongly similar compounds with known experimental value in the training set have been found.
✖	**Accuracy of prediction for similar molecules** Accuracy index = 0 Explanation: accuracy of prediction for similar molecules found in the training set is not adequate.
✖	**Concordance for similar molecules** Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.
✔	**Atom Centered Fragments similarity check** ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

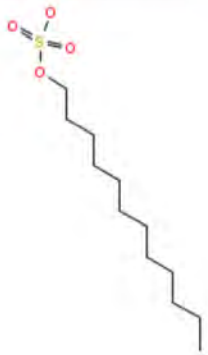
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0



Prediction: Reliability:

Prediction is NON-active, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.
The following relevant fragments have been found: ER alert no. 27, inactive

Compound: Molecule 0
Compound SMILES: O=S(=O)([O-])OCCCCCCCCCCCC
Experimental value: -
Predicted AR binding activity: NON-active
No. alerts for binding activity: 0
No. alerts for non-binding activity: 1
Structural alerts: ER alert no. 27, inactive
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: N.A.
Dataset id: 849 (Training set)
SMILES: CCCCCCCCCCCCOS(O)(=O)=O
Similarity: 0.988

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

Compound #2

CAS: 3026-63-9
Dataset id: 1034 (Training set)
SMILES: CCCCCCCCCCCCCCOS(O)(=O)=O
Similarity: 0.976

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

Compound #3

CAS: 142-87-0
Dataset id: 1179 (Training set)
SMILES: CCCCCCCCCCOS(O)(=O)=O
Similarity: 0.964

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

Compound #4

CAS: 1191-50-0
Dataset id: 999 (Training set)
SMILES: CCCCCCCCCCCCCCOS(O)(=O)=O
Similarity: 0.963

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

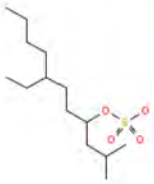
Compound #5

CAS: 1072-15-7
Dataset id: 1459 (Training set)
SMILES: CCCCCCCCCOS(O)(=O)=O
Similarity: 0.947

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 139-88-8
Dataset id: 1268 (Training set)
SMILES: CC(C)CC(CCC(CCCC)CC)OS(O)(=O)=O
Similarity: 0.942

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.991
Explanation: the predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.982
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts:

Fragment found: ER alert no. 27, inactive

Fragment related to ER inactivity (high reliability), defined by the SMARTS: CCOS(=O)

Following, the most similar compounds from the model's dataset having the same fragment.

CAS: N.A.
Dataset id: 849 (Training set)
SMILES: CCCCCCCCCCCCOS(O)(=O)=O
Similarity: 0.988

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

CAS: 3026-63-9
Dataset id: 1034 (Training set)
SMILES: CCCCCCCCCCCCCOS(O)(=O)=O
Similarity: 0.976

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

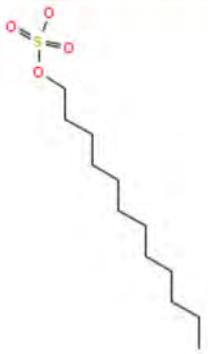
CAS: 142-87-0
Dataset id: 1179 (Training set)
SMILES: CCCCCCCCCCOS(O)(=O)=O
Similarity: 0.964

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER alert no. 27, inactive

1. Prediction Summary

Prediction for compound Molecule 0



Prediction: Reliability:

Prediction is Inactive, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: O=S(=O)([O-])OCCCCCCCCCCCC
Experimental value: -
Predicted TR alpha class: Inactive
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 151-21-3
Dataset id: 4205 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCC
Similarity: 0.988

Experimental value: Inactive
Predicted value: Inactive

Compound #2

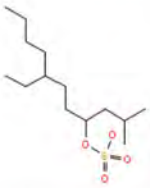
CAS: 142-87-0
Dataset id: 4204 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCC
Similarity: 0.964

Experimental value: Inactive
Predicted value: Inactive

Compound #3

CAS: 1072-15-7
Dataset id: 4203 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCC
Similarity: 0.947

Experimental value: Inactive
Predicted value: Inactive



Compound #4

CAS: 139-88-8
Dataset id: 4200 (Training set)
SMILES: O=S(=O)(O)OC(CCC(CC)CCCC)CC(C)C
Similarity: 0.942

Experimental value: Inactive
Predicted value: Inactive

Compound #5

CAS: 1120-01-0
Dataset id: 4206 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCCCCCC
Similarity: 0.94

Experimental value: Inactive
Predicted value: Inactive

Compound #6

CAS: 142-31-4
Dataset id: 4202 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCC
Similarity: 0.927

Experimental value: Inactive
Predicted value: Inactive

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.982
Explanation: the predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.965
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

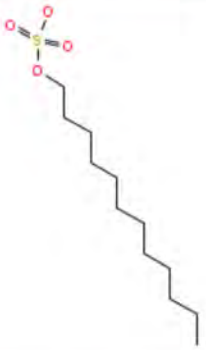
Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0



Prediction: Reliability:

Prediction is Inactive, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: O=S(=O)([O-])OCCCCCCCCCCCC
Experimental value: -
Predicted TR beta class: Inactive
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 151-21-3
Dataset id: 4223 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCC
Similarity: 0.988

Experimental value: Inactive
Predicted value: Inactive

Compound #2

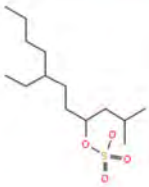
CAS: 142-87-0
Dataset id: 4222 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCC
Similarity: 0.964

Experimental value: Inactive
Predicted value: Inactive

Compound #3

CAS: 1072-15-7
Dataset id: 4221 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCC
Similarity: 0.947

Experimental value: Inactive
Predicted value: Inactive



Compound #4

CAS: 139-88-8
Dataset id: 4218 (Training set)
SMILES: O=S(=O)(O)OC(CCC(CC)CCCC)CC(C)C
Similarity: 0.942

Experimental value: Inactive
Predicted value: Inactive

Compound #5

CAS: 1120-01-0
Dataset id: 4224 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCCCCCCCCCC
Similarity: 0.94

Experimental value: Inactive
Predicted value: Inactive

Compound #6

CAS: 142-31-4
Dataset id: 4220 (Training set)
SMILES: O=S(=O)(O)OCCCCCCCC
Similarity: 0.927

Experimental value: Inactive
Predicted value: Inactive

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.982
Explanation: the predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.965
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

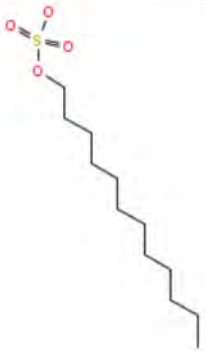
Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0



Prediction: Reliability:

Prediction is Inactive, but the result shows some critical aspects, which require to be checked:
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found)

Compound: Molecule 0
Compound SMILES: O=S(=O)([O-])OCCCCCCCCCCCC
Experimental value: -
Aromatase activity: Inactive
Probability(Active Agonist): 0.014
Probability(Active Antagonist): 0.038
Probability(Inactive): 0.948
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

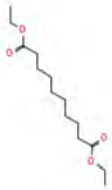
CAS: N.A.
Dataset id: 1553 (Test set)
SMILES: O=C(O)CCCCCCCCCCC(=O)O
Similarity: 0.837

Experimental value: Inactive
Predicted value: Inactive

Compound #2

CAS: N.A.
Dataset id: 1510 (Training set)
SMILES: O=C(OC)CCCCCCCCC(=O)OC
Similarity: 0.825

Experimental value: Inactive
Predicted value: Inactive



Compound #3

CAS: N.A.
Dataset id: 1461 (Test set)
SMILES: O=C(OCC)CCCCCCCCC(=O)OCC
Similarity: 0.824

Experimental value: Inactive
Predicted value: Inactive

Compound #4

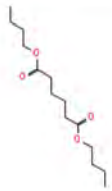
CAS: N.A.
Dataset id: 3102 (Test set)
SMILES: O=C(O)CCCCCCCCCC(=O)O
Similarity: 0.822

Experimental value: Inactive
Predicted value: Inactive

Compound #5

CAS: N.A.
Dataset id: 1372 (Test set)
SMILES: O=C(O)CCCCCCCCC(=O)O
Similarity: 0.806

Experimental value: Inactive
Predicted value: Inactive



Compound #6

CAS: N.A.
Dataset id: 1435 (Test set)
SMILES: O=C(OCCCC)CCCCC(=O)OCCCC
Similarity: 0.804

Experimental value: Inactive
Predicted value: Inactive

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.775
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.831
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

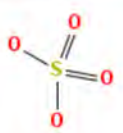
Atom Centered Fragments similarity check
ACF index = 0.85
Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found).

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: O=S(=O)(O)O
The fragment has less than 3 occurrences in the model's training set

APPENDIX G: Danish (Q)SAR Endocrine and Molecular Endpoints for Sodium Lauryl Sulfate (CAS #151-21-3)

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Estrogen Receptor α Binding, Full training set (Human *in vitro*)		INC_OUT	NEG_OUT	NEG_OUT	NEG_OUT
Estrogen Receptor α Binding, Balanced Training Set (Human *in vitro*)		INC_OUT	INC_OUT	NEG_OUT	NEG_OUT
Estrogen Receptor α Activation (Human *in vitro*)		INC_OUT	INC_OUT	NEG_OUT	POS_OUT
Estrogen Receptor Activation, CERAPP data (*in vitro*)		N/A	N/A	NEG_IN	N/A
Androgen Receptor Inhibition (Human *in vitro*)		INC_OUT	NEG_OUT	NEG_OUT	NEG_OUT
Androgen Receptor Binding, CoMPARA data (*in vitro*)	NEG	N/A	N/A	NEG_IN	N/A
Androgen Receptor Inhibition, CoMPARA data (*in vitro*)	NEG	N/A	N/A	NEG_IN	N/A
Androgen Receptor Activation, CoMPARA data (*in vitro*)		N/A	N/A	NEG_IN	N/A
Thyroperoxidase (TPO) inhibition QSAR1 (Rat *in vitro*)		N/A	N/A	NEG_IN	N/A
Thyroperoxidase (TPO) inhibition QSAR2 (Rat *in vitro*)		N/A	N/A	NEG_IN	N/A
Thyroid Receptor α Binding (Human *in vitro*)					
- mg/L				4420.632	
- µM				16593.96	
- Positive for IC_{50} ≤ 10 µM					
- Positive for IC_{50} ≤ 100 µM					
- Domain				OUT	OUT
Thyroid Receptor β Binding (Human *in vitro*)					
- mg/L				135.5015	
- µM				508.6393	
- Positive for IC_{50} ≤ 10 µM					
- Positive for IC_{50} ≤ 100 µM					
- Domain				OUT	OUT
Arylhydrocarbon (AhR) Activation – Rational final model (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Arylhydrocarbon (AhR) Activation – Random final model (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Pregnane X Receptor (PXR) Binding (Human *in vitro*)	N/A	INC_OUT	INC_OUT	INC_OUT	NEG_OUT
Pregnane X Receptor (PXR) Binding (Human *in vitro*) NEW		N/A	N/A	INC_OUT	N/A
Pregnane X Receptor (PXR) Activation (Human *in vitro*)	NEG	N/A	N/A	NEG_IN	N/A

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Pregnane X Receptor (PXR) Activation (Rat *in vitro*)	NEG	N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Activation at max. 20 µM (*in vitro*)		N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Activation at max. 50 µM (*in vitro*)	NEG	N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Inhibition at max. 20 µM (*in vitro*)		N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Inhibition at max. 50 µM (*in vitro*)		N/A	N/A	NEG_IN	N/A

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
CYP3A4 Induction (Human *in vitro*)	NEG	N/A	N/A	NEG_IN	N/A

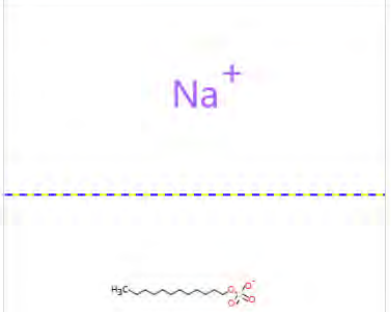
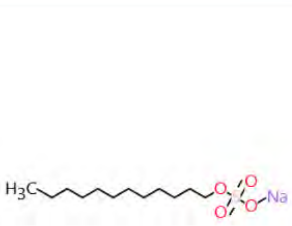
DTU-developed models

Estrogen Receptor Binding, alerts in:	
- parent only	Non binder, non cyclic structure
- metabolites from *in vivo* Rat metabolism simulator only	
- metabolites from Rat liver S9 metabolism simulator only	Non binder, non cyclic structure
rtER Expert System - USEPA, alerts in:	
- parent only	No alert found
- metabolites from *in vivo* Rat metabolism simulator only	
- metabolites from Rat liver S9 metabolism simulator only	No alert found

OECD QSAR Toolbox v.4.2 profilers

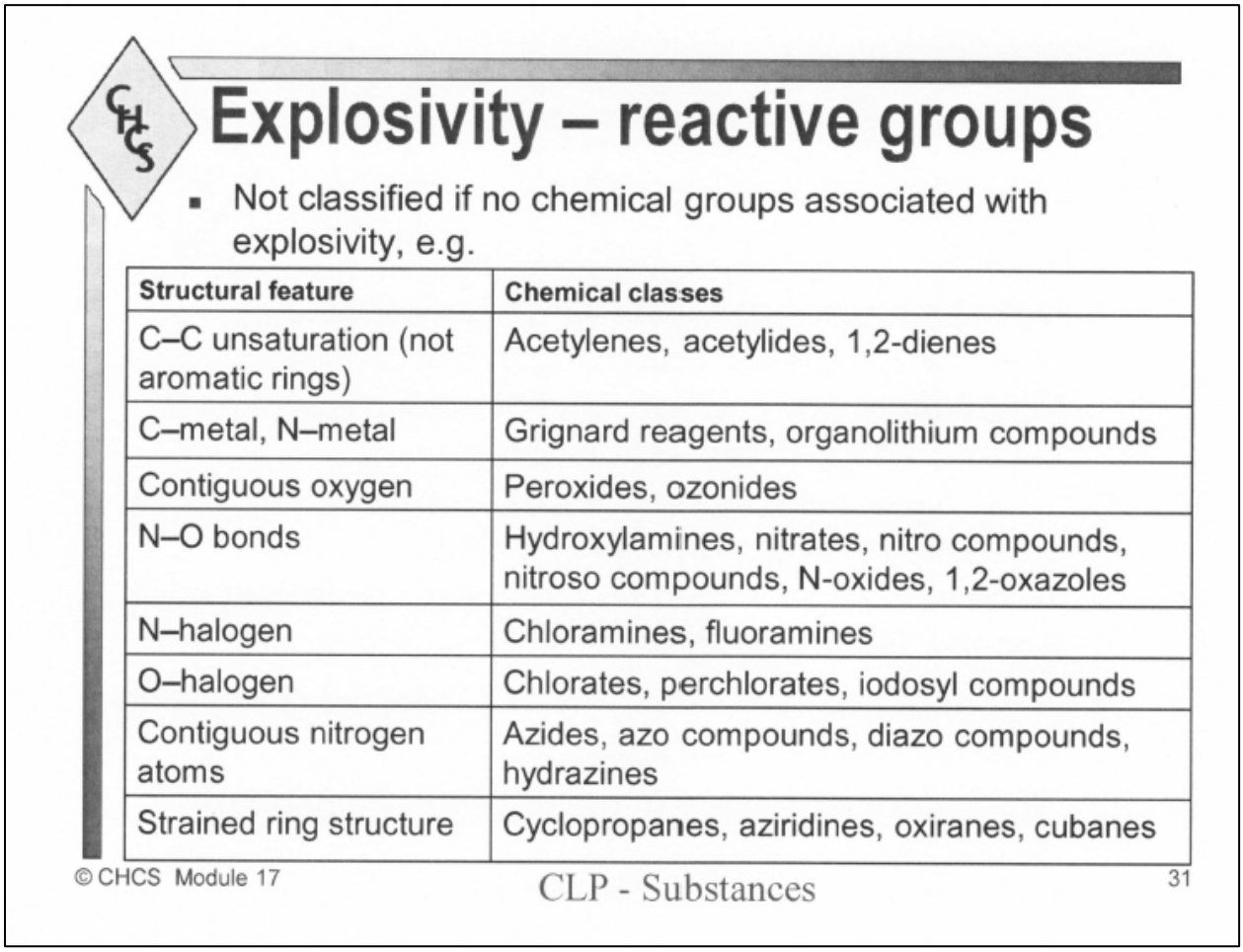
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

APPENDIX H: OECD Toolbox Respiratory Sensitization Results for Sodium Lauryl Sulfate (CAS #151-21-3)

Filter endpoint tree...	1	2	3
Structure			
⊞ Structure info			
⊞ Parameters			
⊞ Physical Chemical Properties			
⊞ Environmental Fate and Transport			
⊞ Ecotoxicological Information			
⊞ Human Health Hazards			
⊟ Profiling			
⊟ Endpoint Specific			
Respiratory sensitisation	No alert found	No alert found	No alert found

APPENDIX I: 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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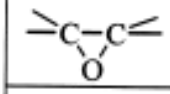
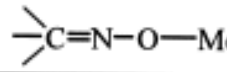
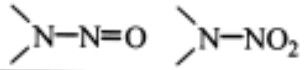
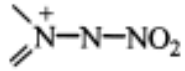
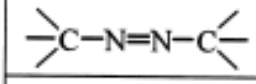
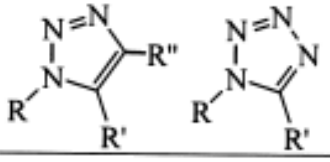
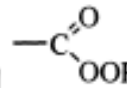
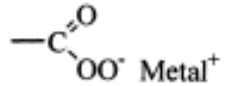
Explosivity – Full List

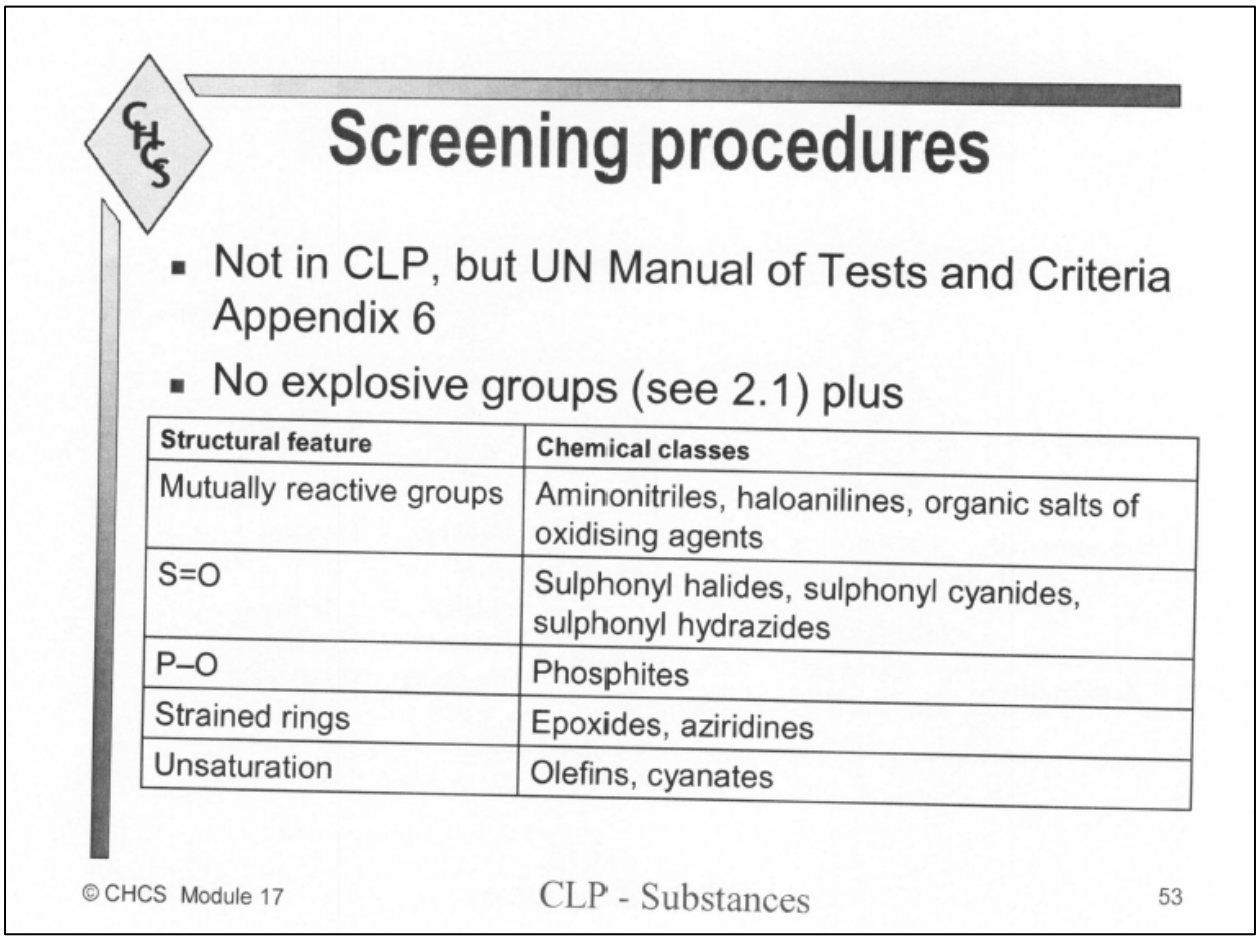
Table R.7.1-28 Chemical groups associated with explosive properties

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



Licensed GreenScreen® Profilers

Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt GreenScreen® Evaluation Prepared by:

SIGNATURE BLOCK

Zach Guerrette, Ph.D., D.A.B.T.
Senior Toxicologist
ToxServices LLC

Sodium Lauryl Sulfate and C10-C16 Alkyl Alcohol Sulfuric Acid, Sodium Salt GreenScreen® Evaluation QC'd by:

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Bingxuan Wang, Ph.D., D.A.B.T.
Senior Toxicologist
ToxServices LLC