SODIUM CARBONATE

(CAS #497-19-8)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: March 17, 2021

Expiration Date: March 17, 2026

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING
1367 Connecticut Ave., N.W., Suite 300
Washington, D.C. 20036

TABLE OF CONTENTS

TABLE OF FIGURES

TABLE OF TABLES

GreenScreen® Executive Summary for Sodium Carbonate (CAS #497-19-8)

Sodium carbonate is a non-flammable and non-reactive white solid. It is an inorganic compound that is soluble in water and non-volatile. Sodium carbonate is used as a chemical intermediate to synthesize other chemicals, an alkalizing agent in various applications, a builder in detergent formulations, a catalyst in coal liquification, a sealer of ponds to prevent leakage, and a stabilizer in food.

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

- Benchmark 2e
    - Very High Group II Human Hazard (acute toxicity – AT)

A data gap (DG) exists for chronic aquatic toxicity - CA. As outlined in GreenScreen® Guidance Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), sodium carbonate meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if sodium carbonate were assigned a Very High score for the data gap CA, it would be categorized as a Benchmark 1 Chemical.

GreenScreen® Hazard Summary Table for Sodium Carbonate

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

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.
* Sodium carbonate is an inorganic chemical; therefore, persistence is only considered in combination with chronic hazards when assigning the GreenScreen Benchmark™ Score.

GreenScreen® Chemical Assessment for Sodium Carbonate (CAS #497-19-8)

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

GreenScreen® Assessment (v.1.2) Prepared By:
Name: Zach Guerrette, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: June 18, 2015

Quality Control Performed By:
Name: Bingxuan Wang, Ph.D.,
Title: Toxicologist
Organization: ToxServices LLC
Date: June 20, 2015

GreenScreen® Assessment (v.1.4) Prepared By:
Name: Sara M. Ciotti, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: February 16, 2021; March 17, 2021

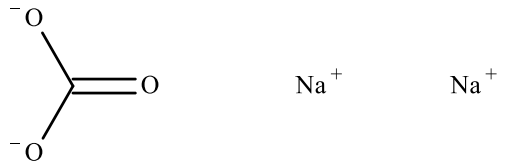
Quality Control Performed By:
Name: Bingxuan Wang, Ph.D., D.A.B.T.
Title: Senior Toxicologist
Organization: ToxServices LLC
Date: March 1, 2021; March 16, 2021

Expiration Date: March 17, 2026[2]

Chemical Name: Sodium Carbonate

CAS Number: 497-19-8

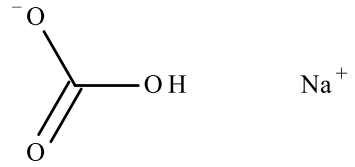
Chemical Structure(s):



Also called:
Carbonic acid, disodium salt; Soda Ash; Bisodium carbonate; Calcined soda; Carbonic acid sodium salt; Crystol carbonate; Disodium carbonate; EINECS 207-838-8; Soda, calcined; Sodium carbonate, anhydrous; Solvay soda; Washing soda; Carbonic acid disodium salt (ChemIDplus 2021)

Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
Limited data on sodium carbonate were identified for some endpoints. ToxServices identified sodium bicarbonate (CAS #144-55-8) as a suitable surrogate for sodium carbonate since the chemicals differ only by the additional sodium in sodium carbonate in place of a hydrogen in sodium bicarbonate. In addition, carbonate can be converted to bicarbonate as part of the buffering system found in the blood and interstitial fluid of vertebrates.

[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).



Surrogate: Sodium Bicarbonate (CAS #144-55-8)

Identify Applications/Functional Uses (HSDB 2018)**:**

1. Chemical intermediate
2. Alkalizing agent
3. Builder in detergent formulations
4. Catalyst in coal liquification
5. Sealer of ponds
6. Stabilizer in food

Known Impurities[3]:

Sodium carbonate may contain the following impurities at low levels: sodium chloride 0.035-0.15%), sodium sulfate (0.02-0.1%), calcium oxide (0.01%), magnesium oxide (0.003-0.02%), sodium bicarbonate, Fe_2O_3 (0.001-0.002%), and chlorine (<0.02%) (HSDB 2018). The screen is performed on the theoretical pure substance.

GreenScreen® Summary Rating for Sodium Carbonate[4,5 6,7]: Sodium carbonate was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes") (CPA 2018b). This score is based on the following hazard score:

- Benchmark 2e
  - Very High Group II Human Hazard (acute toxicity – AT)

A data gap (DG) exists for chronic aquatic toxicity - CA. As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), sodium carbonate meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if sodium carbonate were assigned a Very High score for the data gap CA, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Summary Table for Sodium Carbonate

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

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four

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

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.
* Sodium carbonate is an inorganic chemical; therefore, persistence is only considered in combination with chronic hazards when assigning the GreenScreen Benchmark™ Score (CPA 2018b).

Environmental Transformation Products

No transformation products were identified for sodium carbonate. Sodium carbonate is an inorganic chemical that does not undergo biodegradation and disassociates to sodium and carbonate ions upon dissolution in water. Based on the lack of transformation products identified for this chemical, the Benchmark Score for sodium carbonate was not modified by transformation products.

Introduction

Sodium carbonate is used in the decontamination of radioactive surfaces, glass production, detergent formulation, photography, adjustment of water pH, textile bleaching, and as a fungicide, cosmetic ingredient, food additive, and alkalizing agent in pharmaceuticals (HSDB 2018). It is also used as a builder in water softening formulations and is used as an additive in various cleaning products (HERA 2005). It is produced via processing of natural sodium carbonate bearing deposits, from lake brines or sea water via electrolysis, or by the ammonia soda (Solvay) process (HSDB 2018). Sodium carbonate is considered Generally Recognized As Safe (GRAS) by the United States Food and Drug Administration (U.S. FDA) (U.S. FDA 2021). In biology, carbonate is a component of the bicarbonate buffer system in blood and interstitial fluid of vertebrates (UNEP 2002).

ToxServices assessed sodium carbonate 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

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2020). 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 carbonate is listed on the U.S. EPA SCIL with a full green circle as a processing aid and additive.

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 output for sodium carbonate can be found in Appendix C.

- Sodium carbonate is an LT-UNK chemical 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 carbonate is not listed on the U.S. DOT list.
- Sodium carbonate is on the following lists for multiple endpoints. Specified lists for single endpoints are reported in individual hazard endpoints in the hazard assessment section below.
    - German FEA – Substances Hazardous to Waters – Class 1 Low Hazard to Waters
    - Quebec CSST – WHMIS 1988 – Class D2B – Toxic material causing other toxic effects
    - Quebec CSST – WHMIS 1988 – Class E – Corrosive materials

Hazard Statement and Occupational Control

Sodium carbonate is classified as a serious eye irritant in the European Union (EU) with the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) Hazard Statement of H319, as presented in Table 1, below. General personal protective equipment (PPE) recommendations are presented in Table 2, below. No occupational exposure limits (OEH) were identified.

Table 1: GHS H Statements for Sodium Carbonate (CAS #497-19-8) (Pharos 2021)

H Statement	H Statement Details
H319	Causes serious eye irritation

Table 2: Occupational Exposure Limits and Recommended Personal Protective Equipment for Sodium Carbonate (CAS #497-19-8)

Personal Protective Equipment (PPE)	Reference	Occupational Exposure Limits (OEL)	Reference
Use local exhaust or breathing protection; wear protective gloves; wear safety goggles	NIOSH 2004	None identified	

Physicochemical Properties of Sodium Carbonate

Sodium carbonate is a white inorganic powder under standard temperature and pressure. It has negligible vapor pressure and is very soluble in water (212,500 mg/L). It is not expected to be systemically available following oral, dermal, or inhalation exposures.

Table 3: Physical and Chemical Properties of Sodium Carbonate (CAS #497-19-8)

Property	Value	Reference
Molecular formula	C-H2-O3.2Na	ChemIDplus 2021
SMILES Notation	C(=O)([O-])[O-].[Na+].[Na+]	ChemIDplus 2021
Molecular weight	105.988	ChemIDplus 2021
Physical state	Solid	ECHA 2021
Appearance	White powder	ECHA 2021
Melting point	851°C	ECHA 2021
Boiling point	Decomposes before boiling	ECHA 2021
Vapor pressure	Negligible, ionizable inorganic chemical	UNEP 2002
Water solubility	212,500 mg/L at 20°C (OECD 105)	ECHA 2021
Dissociation constant	pKa1 = 10.25 pKa2 = 6.33	UNEP 2002
Density/specific gravity	Relative density = 2.52-2.53 at 20°C (OECD 109)	ECHA 2021
Partition coefficient	Not relevant, ionizable inorganic chemical	UNEP 2002

Toxicokinetics

Once sodium carbonate comes into contact with body fluids it dissociates into carbonate and sodium ions. If carbonate is absorbed it may increase the pH of the blood; however, its concentration is regulated by the bicarbonate buffering system which is described by the following equation:

$H_2O + CO_2 \longleftrightarrow H_2CO_3 \longleftrightarrow H^+ + HCO_3^-$

Therefore, carbonate is not expected to be systemically available. Following oral uptake, sodium carbonate is neutralized in the stomach by gastric acid. Sodium is an essential element in the body and it is primarily regulated in the kidney (HERA 2005). No other information regarding absorption by oral, dermal or inhalation routes, and excretion, is identified.

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *L*

Sodium carbonate was assigned a score of Low for carcinogenicity based on ToxServices not classifying it as a carcinogen under GHS. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as limited data are available.

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- UNEP 2002
  - Sodium carbonate is not likely to be systemically available following dissolution and neutralization in body fluids including blood and gastric acids. In addition, carbonate is a natural component of the bicarbonate buffering system in blood and interstitial fluids.
- HERA 2005
  - Sodium carbonate is not systemically available; therefore, it is not carcinogenic. Additionally, it contains no structural alerts for genotoxicity or DNA reactivity making a local carcinogenic effect also unlikely.
- UNEP 2003
  - *Oral: Surrogate: Sodium Bicarbonate (CAS #144-55-8)*: Male Fischer 344 rats (number not specified) were provided diets containing sodium bicarbonate (food additive grade) at 0.64% for 104 weeks. No increase in the incidence of urinary bladder tumors was observed with sodium bicarbonate treatment relative to controls.
- Based on the negative results for bladder carcinogenicity by the surrogate sodium bicarbonate, the lack of systemic availability for sodium carbonate, and carbonate's involvement in the natural buffering system of bodily fluids, ToxServices did not classify sodium carbonate as a carcinogen under GHS criteria (UN 2019).

Mutagenicity/Genotoxicity (M) Score (H, M, or L): *L*

Sodium carbonate was assigned a score of Low for mutagenicity/genotoxicity based on ToxServices not classifying it as a mutagen/genotoxicant under GHS criteria. 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 low as limited data are available.

- 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 2021
    - *In vitro*: Negative results for genotoxicity were obtained in a non-GLP-compliant *Escherichia coli* Chromotest. *E coli* tester strain PQ37 (uvrB-) was exposed to sodium carbonate (purity not specified) at 0.11-11,000 µg/mL without metabolic activation. Cytotoxicity was identified at 1,100 µg/mL. No increase in genotoxicity was observed with treatment in the absence of metabolic activation.
        - The Chromotest has not been validated for regulatory purposes and therefore has limited value for assessing genotoxicity.
- CCRIS 1997
    - *In vitro*: Sodium carbonate was negative in an Ames test. *Salmonella typhimurium* tester strains TA97 and TA102 were exposed to sodium carbonate (purity not specified) in distilled water at 0.1-10 mg/plate with and without metabolic activation. No increase in the mutation frequency was identified with treatment in the presence or absence of metabolic activation.
- Based on the limited negative results for mutagenicity and the fact that carbonate is a component of the natural buffering system of bodily fluids, ToxServices did not classify sodium carbonate as a mutagen under GHS criteria (UN 2019).

Reproductive Toxicity (R) Score (H, M, or L): *L*
Sodium carbonate was assigned a score of Low for reproductive toxicity based on ToxServices not classifying it as a reproductive toxicant under GHS criteria. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on expert judgment by United Nations Environment Programme (UNEP).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- UNEP 2002
    - No reproductive toxicity studies are available for sodium carbonate. However, it is not likely to reach the reproductive organs or the fetus following oral, dermal, or inhalation exposure as it is not systemically available.
- Based on the lack of availability for sodium carbonate to reach the reproductive organs or fetus and the fact that carbonate is a component of the natural buffering system of bodily fluids, ToxServices did not classify sodium carbonate as a reproductive toxicant under GHS criteria (UN 2019).

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): L
Sodium carbonate was assigned a score of Low for developmental toxicity based on ToxServices not classifying it as a developmental toxicant under GHS criteria. 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 experimental data.

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

- ECHA 2021
    - A non-GLP-compliant developmental toxicity test was performed with pregnant female Wistar rats (number not specified) administered oral doses of sodium carbonate (purity not specified) at 0, 2.45, 11.4, 52.9, or 245 mg/kg/day via gavage on gestational days (GD) 6-15. The dams were evaluated for body weight and ovarian and uterine content. The offspring were evaluated for litter size and weight, number of resorptions, and the incidence of skeletal and visceral malformations. No treatment-related effects were observed on these parameters and the study authors identified maternal toxicity and teratogenicity NOAELs of 245 mg/kg/day.
    - A non-GLP-compliant developmental toxicity study was performed with pregnant female CD-1 mice (number not specified) administered oral doses of sodium carbonate (purity not specified) at 3.4-340 mg/kg/day via gavage on GD 6-15. The dams were evaluated for body weight and ovarian and uterine content. The offspring were evaluated for litter size and weight, number of resorptions, and the incidence of skeletal and visceral malformations. No treatment-related effects were observed on these parameters and the study authors identified maternal toxicity and teratogenicity NOAELs of 340 mg/kg/day.
    - A non-GLP-compliant developmental toxicity study was performed with pregnant female Dutch rabbits (number not specified) administered oral doses of sodium carbonate (purity not specified) at 0, 1.79, 8.31, 38.6, or 179 mg/kg/day via gavage on GD 6-18. The dams were evaluated for body weight and ovarian and uterine content. The offspring were evaluated for litter size and weight, number of resorptions, and the incidence of skeletal and visceral malformations. No treatment-related effects were observed on these parameters and the study authors identified maternal toxicity and teratogenicity NOAELs of 179 mg/kg/day.
- UNEP 2002
    - There is a general consideration that sodium carbonate will not reach the fetus as it is not systemically available.
- Based on the negative results for developmental toxicity in studies performed with rats, mice, and rabbits, ToxServices did not classify sodium carbonate as a developmental toxicant under GHS criteria (UN 2019).

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

Sodium carbonate was assigned a score of Low for endocrine activity based on the lack of systemic availability for sodium carbonate and carbonate's role in the bicarbonate buffering system of bodily fluids. GreenScreen® criteria classify chemicals as a Low hazard for endocrine activity when adequate data are available and negative for estrogen agonism and antagonism, androgen agonism and antagonism, and thyroid hormone reactivity (CPA 2018b). The confidence in the score is low as limited data are available.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- No data were identified for this endpoint. However, sodium carbonate is not likely to be available to reach the endocrine organs as previously discussed (UNEP 2002, HERA 2005). Additionally, carbonate is a component of the natural buffering system of bodily fluids, and sodium is ubiquitous in mammalian cells. Therefore, ToxServices concludes that sodium carbonate is not likely to possess endocrine activity.

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 carbonate was assigned a score of Very High for acute toxicity based on inhalation LC_{50} values as low as 0.4 mg/L after adjustment for exposure duration. GreenScreen® criteria classify chemicals as a Very High hazard for acute toxicity when LC_{50} values are no greater than 0.5 mg/L for dusts, mists, and fumes (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data.

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* GHS - New Zealand - 6.1D (inhalation) – Acutely toxic
    - Based on an LC_{50} of 2.3 mg/L (2 hr) in rats
  - *Screening:* GHS – Japan – Acute toxicity (inhalation: dust, mist) – Category 4 [H332]
  - Screening: GHS – New Zealand – 6.1E (oral) – Acutely toxic
    - Based on an LD_{50} of 4,090 mg/kg in rats
- ChemIDplus 2021
  - *Oral*: LD_{50} (mouse) = 6,600 mg/kg
  - *Oral*: LD_{50} (rat) = 4,090 mg/kg
- ECHA 2021
  - *Oral*: LD_{50} (Wistar rat) = 2,800 mg/kg (non-GLP-compliant)
  - *Inhalation*: 2-hour whole body aerosol LC_{50} (male Wistar and Sprague-Dawley rat) = 2.3 mg/L (non-GLP-compliant)
    - Equivalent to a 4-hour LC_{50} of 2.3/2 = 1.15 mg/L
  - *Inhalation*: 2-hour whole body aerosol LC_{50} (male Hartley guinea pig) = 0.8 mg/L (non-GLP-compliant)
    - Equivalent to a 4-hour LC_{50} of 0.8/2 = 0.4 mg/L
  - *Inhalation*: 2-hour whole body aerosol LC_{50} (male Swiss Webster mouse) = 1.2 mg/L (non-GLP-compliant)
    - Equivalent to a 4-hour LC_{50} of 1.2/2 = 0.6 mg/L
  - *Dermal*: LD_{50} (New Zealand White rabbit) > 2,000 mg/kg (non-GLP-compliant, EPA 16 CFR 1500.40)
- Based on the weight of evidence, a score of Very High was assigned. Sodium carbonate was not toxic by the oral and dermal routes of exposure with LD_{50} values of > 2,000 mg/kg. Three inhalation toxicity studies were identified, but all of them used the exposure duration of two hours instead of 4 hours in standard toxicity guidelines. Both the GHS thresholds and GreenScreen® thresholds are based on 4-hour LC_{50} values. The GHS guidance indicates that a 1-hour LC_{50} can be converted to a 4-hour LC_{50} by dividing the value by 4 for dusts and mists (UN 2019). Following that approach, ToxServices divided the 2-hour LC_{50} values by 2 to compare to the guideline values. The lowest adjusted 4-hour LC_{50} of 0.4 mg/L warrants a Very High score.

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

Sodium carbonate was assigned a score of Moderate for systemic toxicity (single dose) based on ToxServices classifying it to GHS category 3 for respiratory irritation. GreenScreen® criteria classify chemicals as a Moderate hazard for systemic toxicity (single dose) when they are classified as GHS

Category 3 respiratory irritants (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data.

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* GHS – Australia – H335 – May cause respiratory irritation.
- ECHA 2021
    - *Oral*: In the acute oral toxicity test that identified an oral LD_{50} value of 2,800 mg/kg in Wistar rats, clinical signs of toxicity included muscle tremors, ataxia, red nasal discharge, urinary staining of the abdomen, soft stool, prostration, lethargy, piloerection, dyspnea, and fecal staining of the abdomen. The effects resolved by day 5 in the surviving animals. Animals that died prior to the scheduled sacrifice exhibited no body weight gain or reduced body weight. Necropsy findings included mottle liver at doses of 1,300 mg/kg and greater; red intestines, mottled or pale kidneys, and stomachs with red pyloric region or containing fluid at 2,600 mg/kg or greater; mottled or dark lungs at 3,600 mg/kg or greater and intestines filled with fluid at 5,000 mg/kg. The lowest dose tested was 1,300 mg/kg.
    - *Inhalation*: In the acute inhalation toxicity test that identified an inhalation LC_{50} value of 2.3 mg/L for male Wistar and Sprague-Dawley rats, clinical signs of toxicity included wheezing, dyspnea, excessive salivation, and distention of the abdomen immediately after exposure. Excessive salivation and repeated swallowing was observed in many animals during the first 2 hours after exposure. These signs subdued within 3-4 hours after the exposure but at 5 hours many animals exhibited inappetence and inspiratory and expiratory dyspnea. Animals that died prior to the scheduled sacrifice exhibited lesions of the posterior pharynx, anterior trachea, larynx, and, in approximately 3% of cases, the lungs. No concentrations were specified for these effects. The lowest concentration tested was 0.8 mg/L.
    - *Inhalation*: In the acute inhalation toxicity test that identified an inhalation LC_{50} value of 0.8 mg/L for male Hartley guinea pigs, clinical signs of toxicity included wheezing, excessive salivation, dyspnea, and distention of the stomach were observed immediately after the exposure. Excessive salivation and repeated swallowing was observed in many animals during the first 2 hours after exposure. These signs subdued within 3-4 hours after the exposure but at 5 hours many animals exhibited inappetence and inspiratory and expiratory dyspnea. Animals that died prior to the scheduled sacrifice exhibited lesions of the posterior pharynx, anterior trachea, larynx, and, in approximately 3% of cases, the lungs. No concentrations were specified for these effects. The lowest concentration tested was 0.5 mg/L.
    - *Inhalation*: In the acute inhalation toxicity test that identified an inhalation LC_{50} value of 1.2 mg/L in male Swiss Webster mice, clinical signs of toxicity included wheezing, excessive salivation, dyspnea, and distention of the stomach were observed immediately after the exposure. Excessive salivation and repeated swallowing was observed in many animals during the first 2 hours after exposure. These signs subdued within 3-4 hours after the exposure but at 5 hours many animals exhibited inappetence and inspiratory and expiratory dyspnea. Animals that died prior to the scheduled sacrifice exhibited lesions of the posterior pharynx, anterior trachea, larynx, and, in approximately 3% of cases, the lungs. No concentrations were specified for these effects. The lowest concentration tested was 0.6 mg/L.
    - *Dermal*: In the acute dermal toxicity test that identified a dermal LD_{50} value of greater than 2,000 mg/kg in New Zealand White rabbits, clinical signs of toxicity included well-defined to severe erythema and slight to severe edema 24 hours after application. Lethargy and

hypernea were also observed 24 hours after dosing. Half of the animals gained weight during the observation period while the other half lost weight or did not gain weight. No gross pathological findings were reported.

- UNEP 2002
    - Due to its alkaline properties, sodium carbonate may cause respiratory tract irritation.
- Although local effects in the lungs were observed following inhalation exposures in rats, guinea pigs and mice, no systemic toxicity is expected from sodium carbonate as it is not anticipated to be systemically available. Furthermore, carbonate is involved in the bicarbonate buffering system in blood and interstitial fluids of vertebrates. However, signs of respiratory irritation were observed in multiple inhalation toxicity studies across species. Therefore, ToxServices classified sodium carbonate to GHS Category 3 (respiratory irritation).

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

Sodium carbonate was assigned a score of Low for systemic toxicity (repeated dose) based on ToxServices not classifying it as a systemic toxicant following repeated dose under GHS criteria. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when adequate data are available and they are not classified under GHS (CPA 2018b). The confidence in the score is low because limited experimental data are available.

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* Not listed on any screening lists for this endpoint.
- UNEP 2002
    - *Inhalation*: A repeated inhalation exposure study was performed with male rats (strain and number not specified) exposed to a 2% aqueous sodium carbonate aerosol for 4 hours/day, 5 days/week for 3.5 months. The final concentration was 0.07 mg/L and the particle size was reported as not exceeding 5 µm. The animals were evaluated for body weight, blood parameters, and histopathology. No treatment-related effects were observed on body weight gain, organ weights, or several blood parameters (no further details provided). Pulmonary ascorbic acid levels decreased with treatment. Treated animals exhibited hyperplasia and desquamation of the bronchiolar epithelium and perivascular edema. These effects were expected due to the alkaline nature of the sodium carbonate solution (pH = 11.6).
    - Carbonate is not expected to be systemically available in the body due to neutralization by gastric acid or by blood. The hazard of sodium dietary intake is well characterized and has been focused on the prevention and control of hypertension. The recommended daily dietary sodium intake is 3,100-6,000 mg/day for normal intake and 2,000-3,000 mg for moderately restricted intake. UNEP conclude that additional testing for the repeated dose endpoint is not necessary and highlight the fact that sodium carbonate is considered GRAS.
- Although local effects in the lungs were observed following inhalation exposures in rats, no systemic toxicity is expected from sodium carbonate as it is not anticipated to be systemically available. Furthermore, carbonate is involved in the bicarbonate buffering system in blood and interstitial fluids of vertebrates. Therefore, ToxServices did not classify sodium carbonate as a systemic toxicant following repeated exposures under GHS criteria (UN 2019).

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

Sodium carbonate was assigned a score of Low for neurotoxicity (single dose) based on the lack of systemic availability for sodium carbonate and carbonate's role in the bicarbonate buffering system of bodily fluids. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (single dose)

when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is low as no experimental data were identified.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- No data were identified for this endpoint. However, sodium carbonate is not likely to be available to reach the nervous tissues (UNEP 2002, HERA 2005). Additionally, carbonate is a component of the natural buffering system of bodily fluids. Therefore, ToxServices concludes that sodium carbonate is not likely to exhibit neurotoxicity.

Neurotoxicity (repeated dose, N-repeated) (Group II*) Score (H, M, or L): *L*
Sodium carbonate was assigned a score of Low for neurotoxicity (repeated dose) based on the lack of systemic availability for sodium carbonate and carbonate's role in the bicarbonate buffering system of bodily fluids. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (repeated dose) when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is low as no experimental data were identified.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- No data were identified for this endpoint. However, sodium carbonate is not likely to be available to reach the nervous tissues (UNEP 2002, HERA 2005). Additionally, carbonate is a component of the natural buffering system of bodily fluids. Therefore, ToxServices concludes that sodium carbonate is not likely to exhibit neurotoxicity.

Skin Sensitization (SnS) (Group II*) Score (H, M, or L): *L*
Sodium carbonate was assigned a score of Low for skin sensitization based on the results of modeled data. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on modeling results.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECB 2000
  - Sodium carbonate is not known to be a skin sensitizer.
- Payne and Walsh 1994
  - Sodium carbonate is not predicted to be a skin sensitizer based on the absence of structural alerts identified by Payne and Walsh (1994). See Appendix D for complete list of structural alerts.
- OECD 2020
  - Calcium carbonate is predicted to not be a skin sensitizer using the OECD Toolbox model using the read-across methodology (OECD 2012). See Appendix E for justification.
- Toxtree 2018
  - Calcium carbonate is predicted to not be a skin sensitizer using the Toxtree model using decision tree methodology. This chemical has not been identified as a substrate for any of the 5 electrophilic mechanisms known to produce a skin sensitization reaction. See Appendix F for justification.

- VEGA 2019
    - Calcium carbonate is predicted to not be a skin sensitizer using the CEASAR and IRFMN/JRC VEGA models. However, the reliability of these predictions is low as calcium carbonate is out of the applicability domains for the models with global acceptability domain indices (ADI) of 0. Therefore, ToxServices discounted the results of this model. See Appendix G for justification.
- In summary, all four prediction tools indicated that calcium carbonate is not a skin sensitizer. Although the VEGA result was discounted, the remaining three results still indicate that calcium carbonate is not predicted to be a skin sensitizer. Therefore, ToxServices did not classify calcium carbonate as a skin sensitizer under GHS criteria.

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

Sodium carbonate was assigned a score of Low for respiratory sensitization based on ECHA guidance regarding the assessment of respiratory sensitization. GreenScreen® criteria classify chemicals as a Low hazard for respiratory sensitization when adequate data are available and negative and 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 carbonate 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 was 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 carbonate was predicted to not be sensitizing to the skin (see skin sensitization section above), and a literature search did not find any human evidence of respiratory sensitization by sodium carbonate, and as sodium carbonate does not contain any structural alerts for respiratory sensitization (OECD 2020), sodium carbonate is not expected to be a respiratory sensitizer.

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

Sodium carbonate was assigned a score of Low for skin irritation/corrosivity based on negative results in studies in rabbits and a patch test in humans. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* GHS – New Zealand – 6.3A – Irritating to the skin (Cat. 2).
        - Based on moderate skin irritation in rabbit studies.

- ECHA 2021
    - A GLP-compliant dermal irritation test conducted in a manner similar to OECD Guideline 404 was performed with New Zealand White rabbits (6 total, sex not specified) administered topical applications of 500 mg sodium carbonate (purity not specified) under occlusive dressing for 4 hours. The mean erythema and edema scores at 24, 48, and 72 hours were both 0/4. The study authors concluded that sodium carbonate was not irritating to the skin in this study.
    - A non-GLP-compliant dermal irritation test conducted according to EPA 16 CFR 1500.3 was performed with New Zealand White rabbits (6 total, sex not specified) administered topical applications of 500 mg sodium carbonate (purity not specified) under occlusive dressing for 24 hours. The mean erythema and edema score were 0/4 at an unspecified time(s). The study authors concluded that sodium carbonate was not irritating to the skin in this study.
    - A GLP-compliant human patch test was performed with human volunteers (26 total) administered topical applications of 200 mg sodium carbonate (98% purity) in water for 4 hours. No evidence of dermal irritation was observed with treatment and the study authors concluded that sodium carbonate was not irritating to the skin in this study.
- UNEP 2002
    - The authors of the SIDS profile concluded that sodium carbonate has no or low skin irritation potential.
- Based on the weight of evidence, a score of Low was assigned. Undiluted sodium carbonate was not irritating to the skin of rabbits in studies conducted according to study guidelines. Additionally, it was not irritating in a patch test in humans. Therefore, a score of Low was assigned.

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

Sodium carbonate was assigned a score of High for eye irritation/corrosivity based on authoritative lists and results of studies in rabbits. GreenScreen® criteria classify chemicals as a High hazard for eye irritation/corrosivity when they are associated with the GHS Hazard Statement H319 (CPA 2018b). The confidence in the score is high as it is based on an authoritative list and well-conducted animal studies.

- Authoritative and Screening Lists
    - *Authoritative:* EU – GHS – H319 – Causes serious eye irritation
    - *Screening:* GHS – Australia – H318 – Causes serious eye damage
    - *Screening:* GHS – Japan – Serious eye damage / eye irritation – Category 1 [H318]
        - Based on rabbit studies reporting irreversible effects described in UNEP (2002), and on its pH of 11.58 as a 5% aqueous solution at 25°C as reported in HSDB (2003) (NITE 2008). *ToxServices notes that this pH is no longer reported in the most recent version of HSDB (2018).*
    - *Screening:* GHS - New Zealand - 6.4A – Irritating to the eye (Cat. 2A)
        - Based on sodium carbonate being highly irritating to the eyes of rabbits.
- ECHA 2021
    - A non-GLP-compliant ocular irritation test conducted according to EPA 16 CFR 1500.42 was performed with New Zealand White rabbits (9 total, sex not specified) administered ocular instillations of 0.1 mL undiluted sodium carbonate monohydrate (CAS #5968-11-6; purity not specified). Three animals had their eyes rinsed 4 seconds after instillation while the remaining six animals did not have their eyes rinsed. An observation period of 14 days followed the instillation. A mean overall irritation score based on the maximal scores from observations at 1, 2, 3, 4, 7, 10, and 14 days was 105/110 for the animals that did not have their eyes rinsed and 13/110 in the animals that had their eyes rinsed. The irritation effects

were not fully reversible within 14 days and included positive results for corneal, iris, conjunctival and chemosis effects for all six animals without rinsing and 1/3 animals that had their eyes rinsed. Five of the unwashed eyes had evidence of ulceration. Two of the animals with unwashed eyes suffered ruptured eyes at the end of the observation period. The study authors concluded that sodium carbonate was irritating to the eyes in this study.
    - A non-GLP-complaint ocular irritation test was performed with rabbits (18 total, strain and sex not specified) in a manner similar to OECD Guideline 405. Rabbits were administered ocular instillations of 0.1 mL undiluted sodium carbonate (purity not specified) for 24 hours. Six animals had their eyes rinsed for 2 minutes 30 seconds after the instillation and 12 animals did not have their eyes rinsed. For un-rinsed eyes, the mean corneal score at 72 hours was 3.8/4 and the mean iris score at 24, 48, 72, and 168 hours was 2/2. For rinsed eyes, the mean corneal score at 48 hours was 0.8/4 and the mean iris score at 1 hour was 1/2. The effects to rinsed eyes were fully reversible within 3 (iris effects) or 7 (corneal effects) days. The effects to un-rinsed eyes were not fully reversible within 7 days. The study authors concluded that sodium carbonate was highly irritating to the eyes in this study.
    - A GLP-compliant ocular irritation test conducted according to OECD Guideline 405 (minor deviations) was performed with New Zealand White rabbits (6 total, sex not specified) administered ocular instillations of 100 mg undiluted sodium carbonate (purity not specified) for 72 hours. Ocular reactions were evaluated at 1, 24, 48, and 72 hours after instillation. For the 1, 24, 48, and 72 hour readings, the mean iris score was 0.25/2, the mean corneal score was 0/4, the mean conjunctival score was 1.67/3, and the mean chemosis score was 1.38/4. In general, the ocular irritation effects were fully reversible within 72 hours, but the conjunctival and chemosis effects were not fully reversible within 72 hours in one animal. The study authors concluded that sodium carbonate was not irritating to the eyes in this study.
- UNEP 2002
    - Following their review of the above studies, the authors of the SIDS profile concluded that sodium carbonate is irritating to the eyes.

Ecotoxicity (Ecotox)

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

Sodium carbonate was assigned a score of Low for acute aquatic toxicity based on based on acute aquatic toxicity values as low as 200 mg/L. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when acute aquatic toxicity values are greater than 100 mg/L (CPA 2018b). The confidence in the score is high as it is based on measured data on all three trophic levels.

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* Not listed on any screening lists for this endpoint.
- ECHA 2021
    - 96-hour LC_{50} (*Lepomis macrochirus*, bluegill) = 300 mg/L (non-GLP-compliant)
    - 96-hour LC_{50} (*Gambusia affinis*, mosquitofish) = 740 mg/L (non-GLP-compliant)
    - 48-hour mobility EC_{50} (Ceriodaphnia sp.) = 200-227 mg/L (non-GLP-compliant)
- UNEP 2002
    - No acute aquatic toxicity studies have been identified for algae. However, the results can be predicted by the rise in the pH of the growth medium following the addition of sodium carbonate. At pH values greater than 9, algal growth will be reduced, with the theoretical

NOEC at 1-10 mg/L and an EC_{50} in the range of 10-100 mg/L. The actual value will depend on the algal species, the growth medium, and the growth conditions.
    - ToxServices did not use the predicted EC_{50} of 10 – 100 mg/L for this endpoint, as this was based on a pH of greater than 9, which is not likely to occur in natural waters with adequate buffering capacities.
- ECB 2000
    - 5-day EC_{50} (Nitzschia sp., diatoms) = 242 mg/L

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): DG
Sodium carbonate was assigned a score of DG for chronic aquatic toxicity based on insufficient 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.
- UNEP 2002
    - No aquatic toxicity studies have been identified for algae. However, the results can be predicted by the rise in the pH of the growth medium following the addition of sodium carbonate. At pH values greater than 9, algal growth will be reduced, with the theoretical NOEC at 1-10 mg/L. The actual value will depend on the algal species, growth medium, and growth conditions.
        - ToxServices did not use the predicted NOEC of 1-10 mg/L for this endpoint, as this is based on a pH of greater than 9, which is not likely to occur in natural waters with adequate buffering capacities.

<u>Environmental Fate (Fate)</u>

Persistence (P) Score (vH, H, M, L, or vL): *vH*
Sodium carbonate was assigned a score of Very High for persistence based on it being an inorganic salt and being on a screening list. GreenScreen® criteria classify chemicals as a Very High hazard for persistence when they are recalcitrant (CPA 2018b). The confidence in the score is low as no measured data were identified.
- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* EC – CEPA DSL - Persistent
- UNEP 2002
    - Sodium carbonate is an inorganic salt. It will not undergo biodegradation.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vL*
Sodium carbonate was assigned a score of Very Low for bioaccumulation based on it being an inorganic chemical that will not undergo bioaccumulation. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when chemicals are not expected to undergo bioaccumulation (CPA 2018b). The confidence in the score is low as no measured data were available.
- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* Not listed on any screening lists for this endpoint.
- UNEP 2002
    - Sodium carbonate is an inorganic salt. It will not undergo bioaccumulation.
- ECHA 2021
    - Sodium carbonate does not bioaccumulate.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Sodium carbonate was assigned a score of Low for reactivity based on ToxServices not classifying it as a reactive chemical under GHS criteria. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when they are not explosive and not oxidizing (CPA 2018b). The confidence in the score was low as no measured data were available.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- No measured data were identified. Therefore, screening procedures for explosivity were used here to estimate the reactivity property of sodium carbonate. These procedures are listed in the GHS (UN 2019).
  - Based on the structure of its components or moieties, sodium carbonate is 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 carbonate is not considered to have oxidizing properties as it does not contain any structural groups known to be correlated with a tendency to react exothermally with combustible materials.
- UNEP 2002
  - Sodium carbonate does not possess oxidizing properties.
- ECB 2000
  - Sodium carbonate does not exhibit explosive or oxidizing properties.
- Based on the lack of oxidizing and explosive properties, ToxServices did not classify sodium carbonate as a reactive chemical under GHS criteria (UN 2019).

Flammability (F) Score (vH, H, M, or L): L
Sodium carbonate was assigned a score of Low for flammability based on ToxServices not classifying it as a flammable solid under GHS criteria. GreenScreen® criteria classify chemicals as a Low hazard for flammability when they are non-flammable (CPA 2018b). The confidence in the score was high as it is based on the results of a well-conducted study.

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- ECHA 2021
  - No propagation of combustion was observed with sodium carbonate in a GLP-compliant EU Method A.10 (Flammability (Solids)) test.
- Based on the negative results for flammability in an EU Method A.10 test, ToxServices did not classify sodium carbonate as a flammable solid under GHS criteria (UN 2019).

Use of New Approach Methodologies (NAMs)[9] in the Assessment

Table 4: Summary of NAMs Used in the GreenScreen® Assessment		
Endpoint	**NAMs Data Available and Evaluated? (Y/N)**	**Types of NAMs Data (*in silico* modeling/*in vitro* biological profiling/frameworks)**
Carcinogenicity	N	
Mutagenicity	N	
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	N	
Acute mammalian toxicity	N	
Single exposure systemic toxicity	N	
Repeated exposure systemic toxicity	N	
Single exposure neurotoxicity	N	
Repeated exposure neurotoxicity	N	
Skin sensitization	Y	*In silico* modeling: VEGA/Payne and Walsh (1994) structural alerts/Danish QSAR/Toxtree/ OECD Toolbox
Respiratory sensitization	Y	*In silico* modeling: OECD Toolbox structural alerts
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	
Chronic aquatic toxicity	N	
Persistence	N	
Bioaccumulation	N	

[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).

References

Chemical Carcinogenesis Research Information System (CCRIS). 1997. Entry for Sodium Carbonate (CAS #497-19-8). CCRIS Record Number 7319. Last revision date February 4, 1997. United States National Library of Medicine. Available at: https://toxplanet.com/

ChemIDplus. 2021. Sodium Carbonate (CAS #497-19-8). United States National Library of Medicine. Available: http://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp.

Clean Production Action (CPA). 2018a. GreenScreen® Assessment Expiration Policy. October 2, 2018.

Clean Production Action (CPA). 2018b. The GreenScreen® for Safer Chemicals Guidance. Version 1.4 Guidance. Dated January, 2018. Available: https://www.greenscreenchemicals.org/static/ee_images/uploads/resources/GreenScreen_Guidance_v1_4_2018_01_Final.pdf

European Chemical Bureau (ECB). 2000. IUCLID Dataset for Sodium Carbonate (CAS #497-19-8). European Chemicals Bureau. Available at: https://toxplanet.com/

European Chemicals Agency (ECHA). 2017. Guidance on information requirements and Chemical Safety Assessment. Chapter R.7a: Endpoint specific guidance. Version 6.0. Dated: July 2017. Available: https://echa.europa.eu/documents/10162/13632/information_requirements_r7a_en.pdf

European Chemicals Agency (ECHA). 2021. REACH dossier for sodium carbonate. Available : https://echa.europa.eu/registration-dossier/-/registered-dossier/15432

Hazardous Substances Data Bank (HSDB). 2018. Entry for sodium carbonate (CAS #497-19-8). Last revision date December 18, 2018. United States National Library of Medicine. Available at: https://pubchem.ncbi.nlm.nih.gov/source/hsdb/5018#section=Administrative-Information

Human and Environmental Risk Assessment on Ingredients of Household Cleaning Products (HERA). 2005. Sodium carbonate (CAS #497-19-8). Edition 2.0. Available : https://www.heraproject.com/files/10-F-05_HERA_sodium_carbonate_revised_version2%20.pdf

National Institute for Occupational Safety and Health (NIOSH). 2004. Sodium carbonate (anhydrous) (CAS #497-19-8). October 2004. Available: https://www.ilo.org/dyn/icsc/showcard.display?p_lang=en&p_card_id=1135&p_version=2

National Institute of Technology and Evaluation (NTE). 2008. GHS classification result for sodium carbonate (CAS #497-19-8). Available: https://www.nite.go.jp/chem/english/ghs/08-mhlw-0051e.html

Organisation for Economic Co-operation and Development (OECD). 2020. OECD QSAR Toolbox for Grouping Chemicals into Categories Version 4.4.1. Available: http://toolbox.oasis-lmc.org/?section=download&version=latest.

Payne, M.P., and P.T. Walsh. 1994. Structure-activity relationships for skin sensitization potential: development of structural alerts for use in knowledge-based toxicity prediction systems. *J Chem Inf Comput Sci*. 34:154-161.

Pharos. 2021. Pharos Chemical and Material Library Entry for Sodium Carbonate (CAS #497-19-8). Available: http://www.pharosproject.net/material/.

ToxServices. 2020. SOP 1.37: GreenScreen® Hazard Assessments. Dated: February 3, 2020.

Toxtree. 2018. Estimation of Toxic Hazard- A Decision Tree Approach v3.1.0. Available: http://toxtree.sourceforge.net.

United Nations (UN). 2019. Globally Harmonized System of Classification and Labelling of Chemicals (GHS). Eighth revised edition.

United Nations Environment Programme (UNEP). 2002. Screening Information Data Sheet (SIDS) Initial Assessment Report for Sodium Carbonate (CAS #497-19-8). Organization for Economic Cooperation and Development (OECD) SIDS. Available at: https://hpvchemicals.oecd.org/ui/SIDS_Details.aspx?id=7bcd380e-ada2-4baf-b2f7-ded360d32d7d

United Nations Environment Programme (UNEP). 2003. Screening Information Data Sheet (SIDS) Initial Assessment Report for Sodium Bicarbonate (CAS #144-55-8). Organization for Economic Cooperation and Development (OECD) SIDS. Available at: https://hpvchemicals.oecd.org/UI/SIDS_Details.aspx?key=aa25b3d9-90a4-461d-b279-2332758304fa&idx=0

United States Department of Transportation (U.S. DOT). 2008a. Chemicals Listed with Classification. 49 CFR § 172.101. Available: http://www.gpo.gov/fdsys/pkg/CFR-2008-title49-vol2/pdf/CFR-2008-title49-vol2-sec172-101.pdf.

United States Department of Transportation (U.S. DOT). 2008b. Classification Criteria. 49 CFR § 173. Available: http://www.ecfr.gov/cgi-bin/text-idx?c=ecfr&tpl=/ecfrbrowse/Title49/49cfr173_main_02.tpl

United States Environmental Protection Agency (U.S. EPA). 2015. Safer Choice Standard. Available: https://www.epa.gov/saferchoice/standard

United States Environmental Protection Agency (U.S. EPA). 2020. Safer Chemical Ingredients List (SCIL). Available: https://www.epa.gov/saferchoice/safer-ingredients

United States Food and Drug Administration (U.S. FDA). 2021. Substances added to food inventory. Available: https://www.fda.gov/food/food-additives-petitions/substances-added-food-formerly-eafus

Virtual Models for Evaluating the Properties of Chemicals within a Global Architecture (VEGA). 2019. Predictive Model Platform version 1.1.5. Available: http://www.vega-qsar.eu/index.php.

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 Carbonate (CAS #497-19-8)

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
Yes	**Sodium Carbonate**	**497-19-8**	*L*	*L*	*L*	**L**	*L*	**vH**	**M**	*L*	*L*	*L*	*L*	*L*	**L**	**H**	**L**	DG	*vH*	*vL*	*L*	**L**

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Sodium Carbonate	2

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

Table 6

Chemical Name	Final GreenScreen® Benchmark Score
Sodium Carbonate	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												

* Sodium carbonate is an inorganic chemical; therefore, persistence is only considered in combination with chronic hazards when assigning the GreenScreen Benchmark™ Score (CPA 2018b).

APPENDIX C: Pharos Output for Sodium Carbonate (CAS #497-19-8)

497-19-8
Sodium carbonate
ALSO CALLED 1314087-39-2, 1332-57-6, 1977561-09-3, Bisodium carbonate, Calcined soda, carbonate sodium, Carbonat...
View all synonyms (64)

Share Profile

Hazards | Properties | Functional Uses | Process Chemistry | Resources

GreenScreen Only View

Show PubMed Results | Request Assessment | Add to Comparison

		Group I Human					Group II and II* Human								Ecotox			Fate		Physical		Mult
	GS Score	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult
GreenScreen List Hazards	LT-UNK	-	-	-	-	-	M	M	-	-	-	-	-	H	H	-	-	-	vH-H	-	-	-	M

Hazard Lists

Download Lists

ENDPOINT	HAZARD LEVEL	GS SCORE	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Acute Mammalian Toxicity	M	LT-UNK	GHS - Japan	Acute toxicity (inhalation: dust, mist) - Category 4 [H332]	+3
	M	LT-UNK	GHS - New Zealand	6.1D (inhalation) - Acutely toxic	
	L	LT-UNK	GHS - New Zealand	6.1E (oral) - Acutely toxic	
	pC	NoGS	US EPA - OPP - Registered Pesticides	FIFRA Registered Pesticide	
Systemic Toxicity/Organ Effects-Single Exposure	M	LT-UNK	GHS - Australia	H335 - May cause respiratory irritation	
Skin Irritation/Corrosivity	H	LT-UNK	GHS - New Zealand	6.3A - Irritating to the skin (Cat. 2)	+1
	M	LT-UNK	GHS - New Zealand	6.3B - Mildly irritating to the skin	
Eye Irritation/Corrosivity	H	LT-UNK	EU - GHS (H-Statements)	H319 - Causes serious eye irritation	+4
	vH	LT-UNK	GHS - Australia	H318 - Causes serious eye damage	
	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	H319 - Causes serious eye irritation (unverified)
Persistence	vH-H	LT-UNK	EC - CEPA DSL	Persistent
Human and/or Aquatic toxicity and/or Persistence and/or Bioaccumulation	U	LT-UNK	German FEA - Substances Hazardous to Waters	Class 1 - Low Hazard to Waters
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
Reactivity and/or Eye Irritation/Corrosivity and/or Skin Irritation/Corrosivity	U	LT-UNK	Québec CSST - WHMIS 1988	Class E - Corrosive materials
Systemic Toxicity/Organ Effects [Single Exposure] and/or Neurotoxicity [Single Exposure]	M	LT-UNK	GHS - Japan	Specific target organs/systemic toxicity following single exposure - Category 3 [H335 or H336]

Restricted Substance Lists (1)

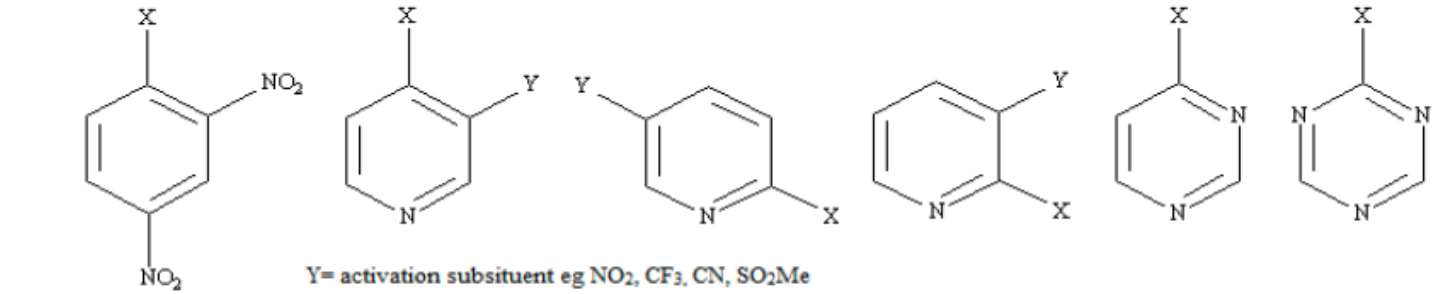
- EU - PACT-RMOA Substances: Substances selected for RMOA or hazard assessment

Positive Lists (3)

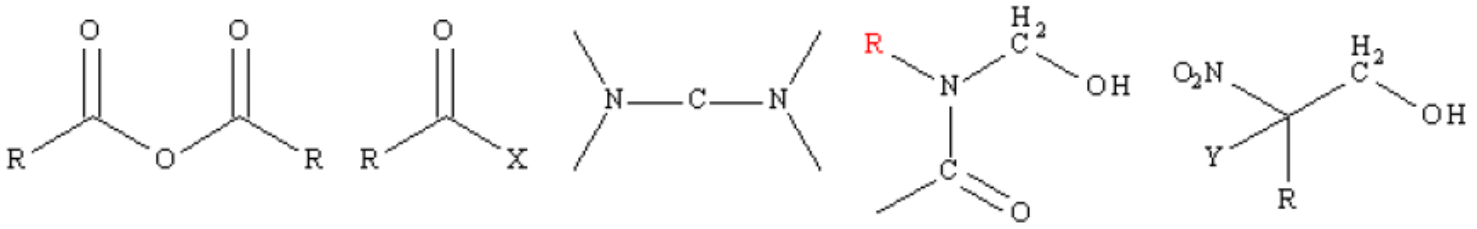
- Cosmetic Ingredient Review (CIR): Safe as Used
- Inventory of Existing Cosmetic Ingredients in China (IECIC 2015): Cosmetic Ingredients
- US EPA - DfE SCIL: Green Circle - Verified Low Concern

APPENDIX D: Known Structural Alerts for Skin Sensitization

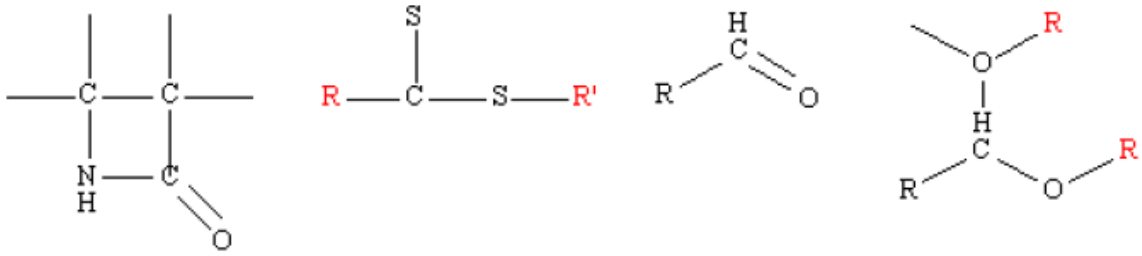
Below are known structural alerts for skin sensitizers (Payne and Walsh 1994). Sodium carbonate possesses no known structural alerts.

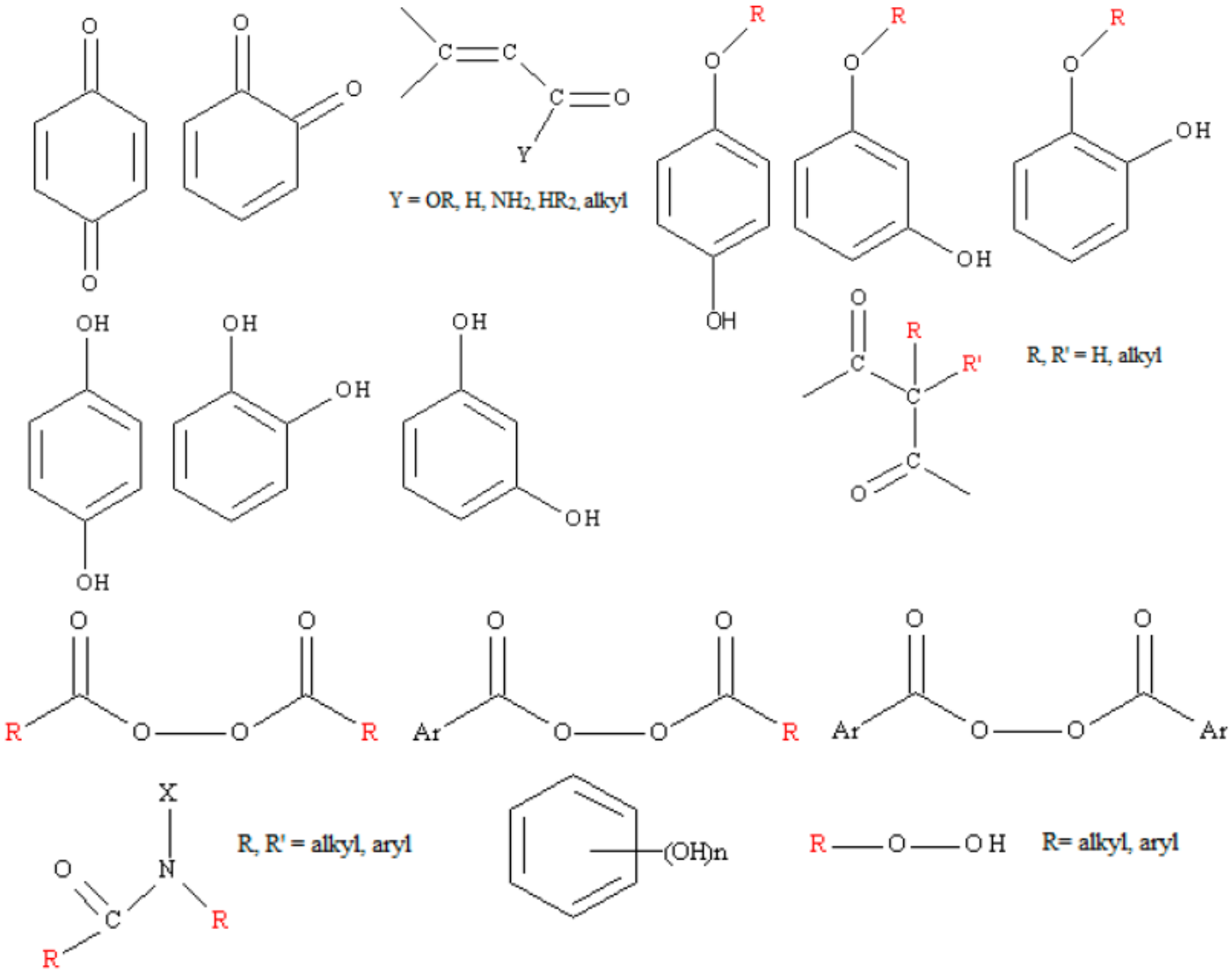


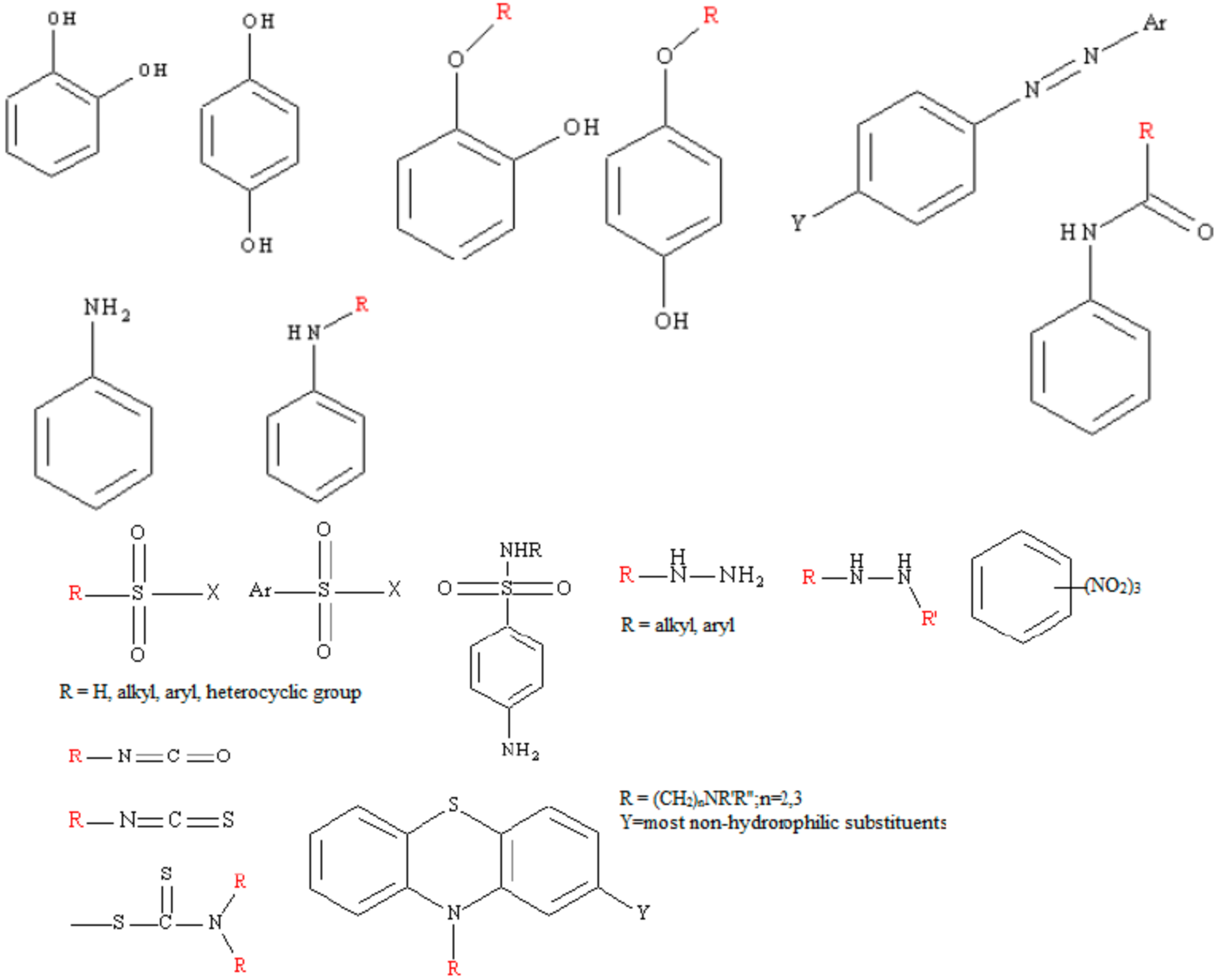
Y= activation subsituent eg NO_2, CF_3, CN, SO_2Me



Y= electronegative subsituent eg halogen, nitro group

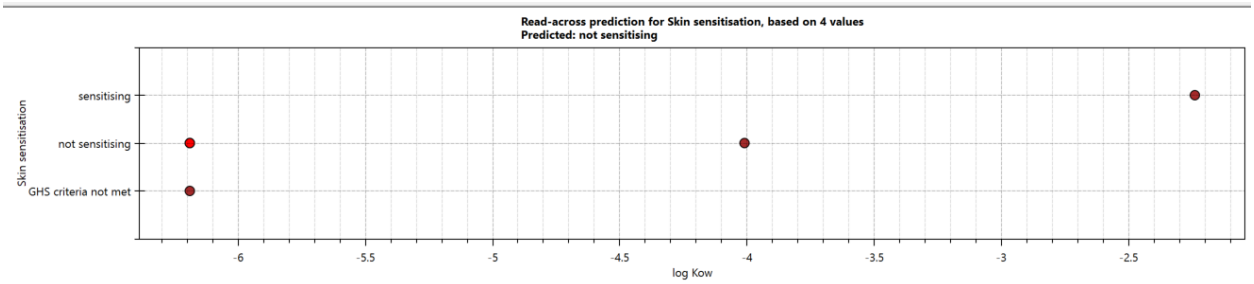




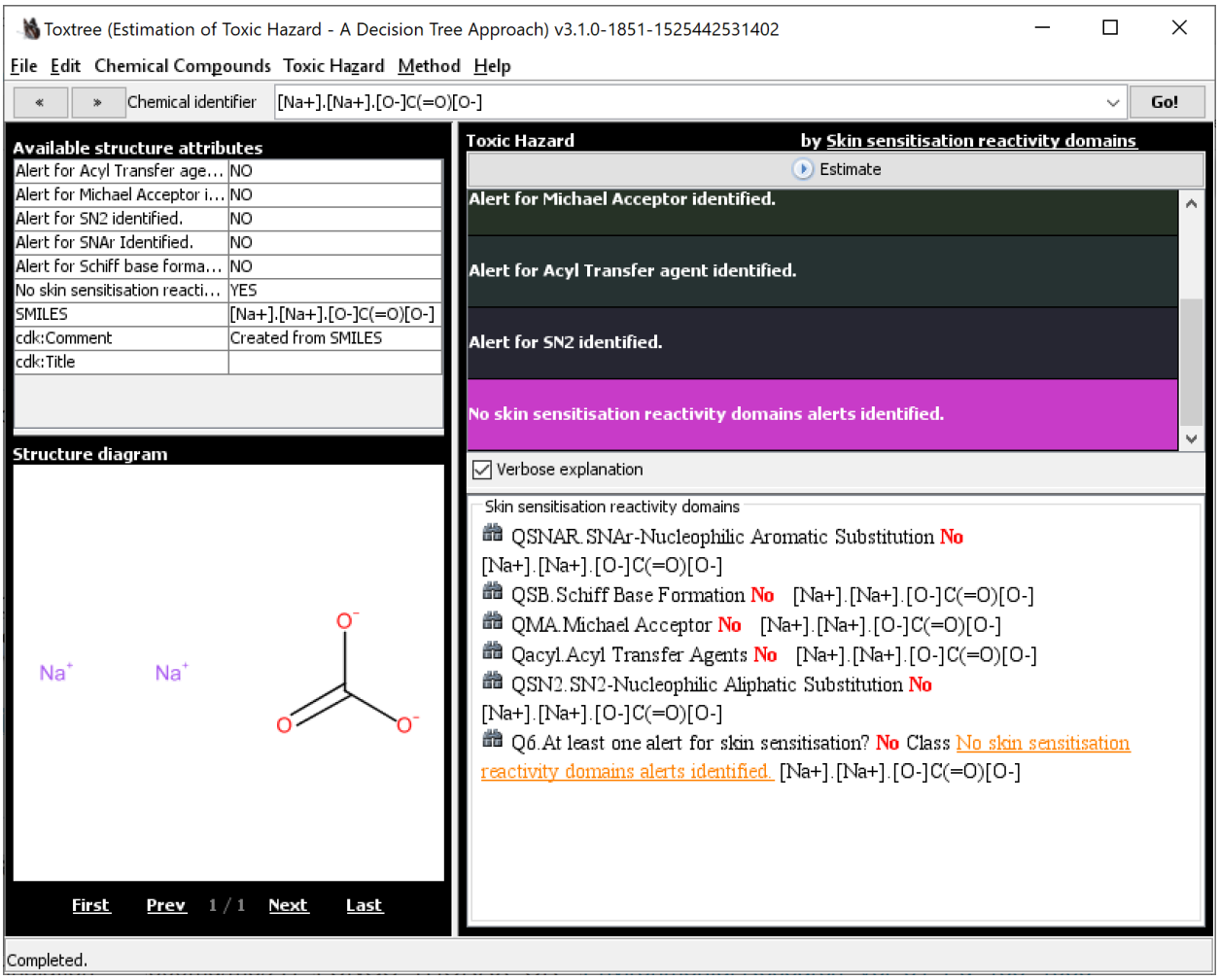


APPENDIX E: OECD Toolbox Skin Sensitization Results for Sodium Carbonate (CAS #497-19-8)

Sodium carbonate was profiled as a carbonate/hydrocarbonate under OECD HPV Chemical Categories. No subcategorization was necessary.



APPENDIX F: Toxtree Skin Sensitization Results for Sodium Carbonate (CAS #497-19-8)

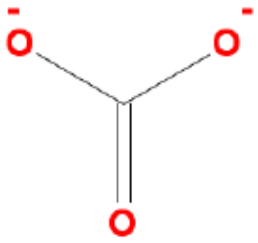


APPENDIX G: VEGA Skin Sensitization Results for Sodium Carbonate (CAS #497-19-8)

VEGA Skin Sensitization model (CAESAR) 2.1.6 page 1

1. Prediction Summary

Prediction for compound Molecule 0

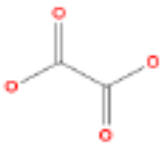
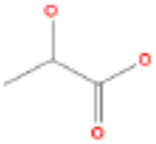
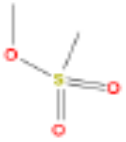
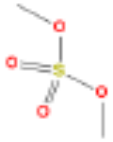


Prediction: Reliability:

Prediction is NON-Sensitizer, 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
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=C([O-])[O-]
Experimental value: -
Predicted skin sensitization activity: NON-Sensitizer
O(Active): 0.32
O(Inactive): 0.68
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: 144-62-7 Dataset Id: 169 (Training set) SMILES: O=C(O)C(=O)O Similarity: 0.704 Experimental value: Sensitizer Predicted value: Sensitizer
	Compound #2 CAS: 107-22-2 Dataset Id: 103 (Training set) SMILES: O=CC=O Similarity: 0.669 Experimental value: Sensitizer Predicted value: Sensitizer
	Compound #3 CAS: 50-00-0 Dataset Id: 96 (Test set) SMILES: O=C Similarity: 0.646 Experimental value: Sensitizer Predicted value: NON-Sensitizer
	Compound #4 CAS: 50-21-5 Dataset Id: 127 (Training set) SMILES: O=C(O)C(O)C Similarity: 0.644 Experimental value: NON-Sensitizer Predicted value: NON-Sensitizer
	Compound #5 CAS: 66-27-3 Dataset Id: 153 (Training set) SMILES: O=S(=O)(OC)C Similarity: 0.627 Experimental value: Sensitizer Predicted value: Sensitizer
	Compound #6 CAS: 77-78-1 Dataset Id: 83 (Training set) SMILES: O=S(=O)(OC)OC Similarity: 0.615 Experimental value: Sensitizer Predicted value: Sensitizer

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 = 0.686
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.

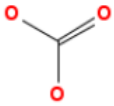
Atom Centered Fragments similarity check
ACF index = 0.6
Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found).

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

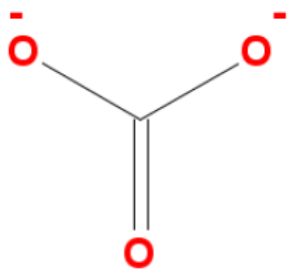
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: O=C(O)O
The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0

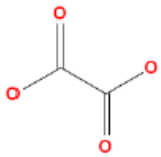


Prediction: Reliability:

Prediction is NON-Sensitizer, 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
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=C([O-])[O-]
Experimental value: -
Predicted skin sensitization activity: NON-Sensitizer
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

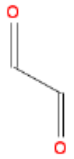
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 144-62-7
Dataset id: 67 (Training set)
SMILES: O=C(O)C(=O)O
Similarity: 0.704

Experimental value: Sensitizer
Predicted value: Sensitizer



Compound #2

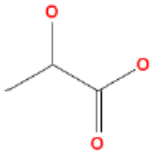
CAS: 107-22-2
Dataset id: 40 (Training set)
SMILES: O=CC=O
Similarity: 0.669

Experimental value: Sensitizer
Predicted value: Sensitizer

Compound #3

CAS: 50-00-0
Dataset id: 38 (Training set)
SMILES: O=C
Similarity: 0.646

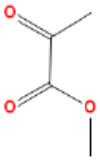
Experimental value: Sensitizer
Predicted value: NON-Sensitizer



Compound #4

CAS: 50-21-5
Dataset id: 197 (Training set)
SMILES: O=C(O)C(O)C
Similarity: 0.644

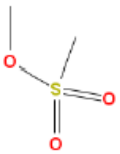
Experimental value: NON-Sensitizer
Predicted value: Sensitizer



Compound #5

CAS: 600-22-6
Dataset id: 165 (Training set)
SMILES: O=C(OC)C(=O)C
Similarity: 0.635

Experimental value: Sensitizer
Predicted value: Sensitizer



Compound #6

CAS: 66-27-3
Dataset id: 60 (Training set)
SMILES: O=S(=O)(OC)C
Similarity: 0.627

Experimental value: Sensitizer
Predicted value: Sensitizer

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 = 0.686 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 = 0.6 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found).

Symbols explanation:

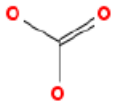
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ 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.

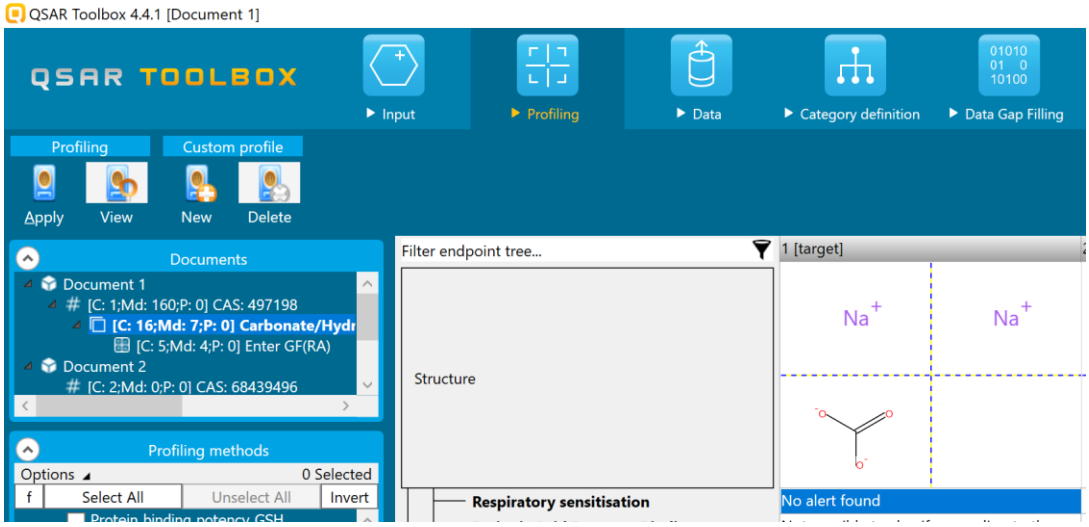
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(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:



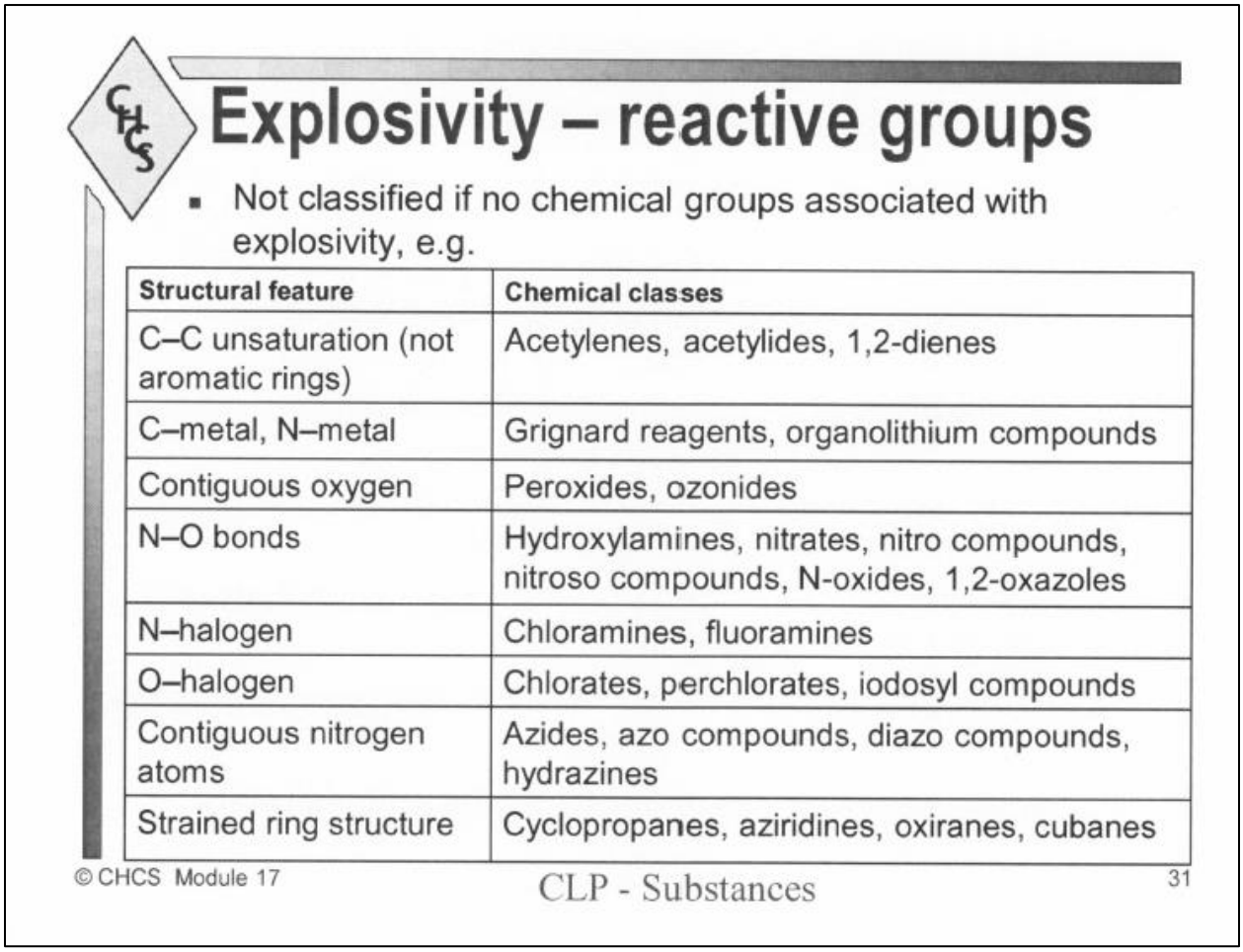
Fragment defined by the SMILES: O=C(O)O
The fragment has never been found in the model's training set

APPENDIX H: OECD Toolbox Respiratory Sensitization Results



APPENDIX I: Known Structural Alerts for Reactivity

Explosivity – Abbreviated List



Explosivity – reactive groups

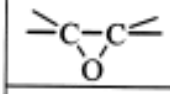
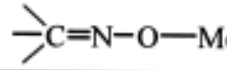
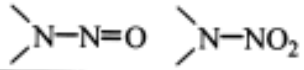
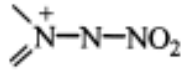
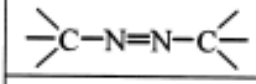
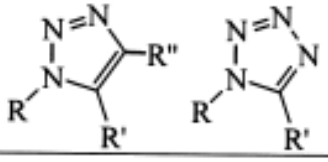
- Not classified if no chemical groups associated with explosivity, e.g.

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

© CHCS Module 17 CLP - Substances 31

Explosivity – Full List

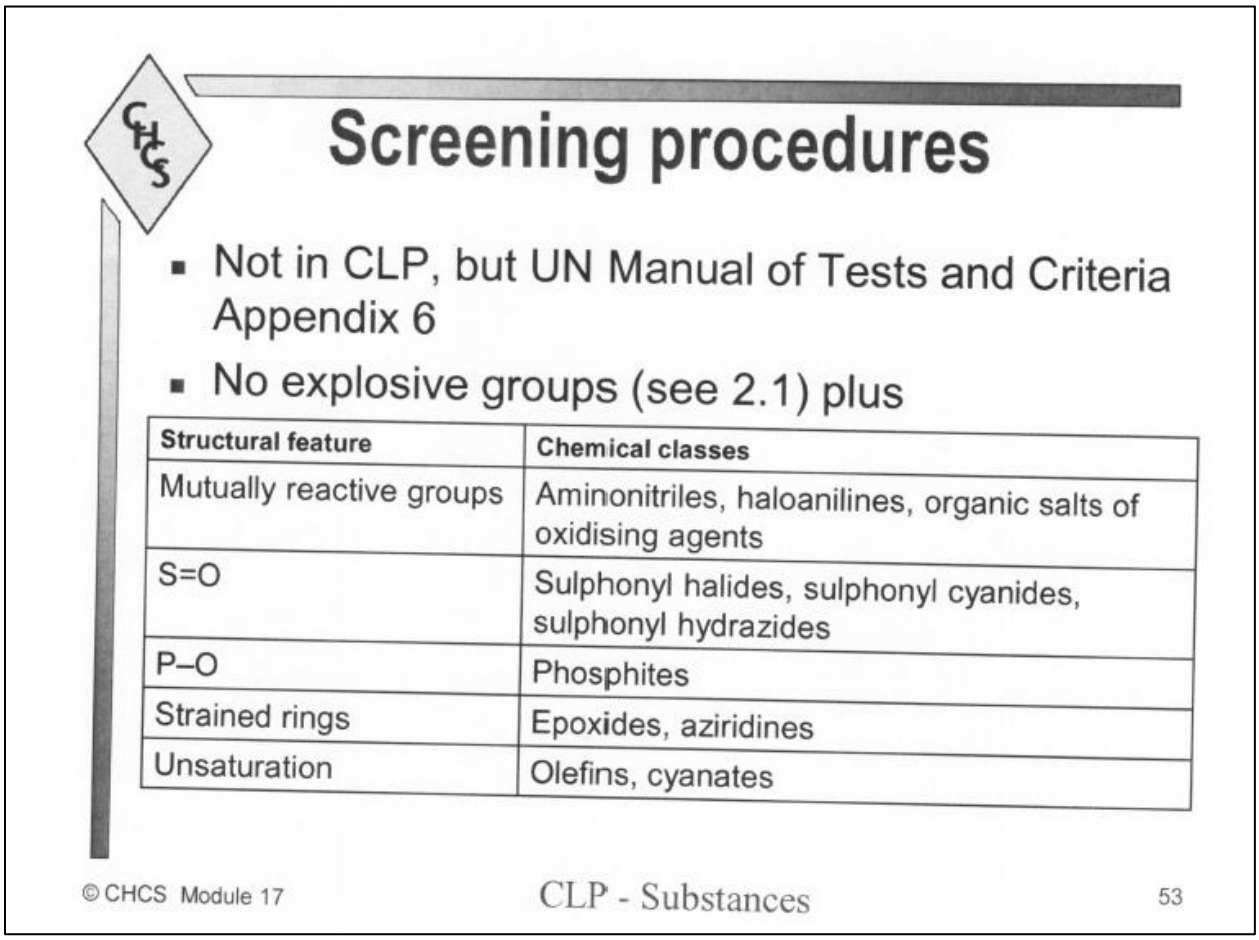
Table R.7.1-28 Chemical groups associated with explosive properties

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] —C(=O)OOR'	Peroxy Compounds: [1] Alkyl hydroperoxides (R'=H), Peroxides (R'=organic); [2] Peroxo acids (R'=H), Peroxyesters (R'=organic)
[1] ROOMetal, [2] —C(=O)OO⁻ Metal⁺	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 Carbonate GreenScreen® v1.2 Evaluation Prepared by:

SIGNATURE BLOCK

Zach Guerrette, Ph.D.
Toxicologist
ToxServices LLC

Sodium Carbonate GreenScreen® v1.4 Evaluation Prepared by:

SIGNATURE BLOCK

Sara Ciotti, Ph.D.
Toxicologist
ToxServices LLC

Sodium Carbonate GreenScreen® v1.2 Evaluation QC'd by:

SIGNATURE BLOCK

Bingxuan Wang, Ph.D.
Toxicologist
ToxServices LLC

Sodium Carbonate GreenScreen® v1.4 Evaluation QC'd by:

SIGNATURE BLOCK

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