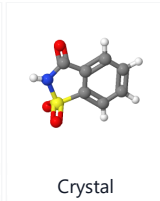
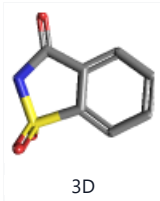
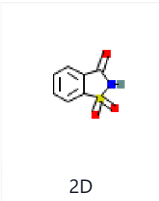


COMPOUND SUMMARY

Saccharin

PubChem CID	5143
Structure	 2D 3D Crystal
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	C ₇ H ₅ NO ₃ S
Synonyms	saccharin 81-07-2 o-Benzoic sulfimide o-Sulfobenzimide Saccharine View More...
Molecular Weight	183.19 g/mol <i>Computed by PubChem 2.2 (PubChem release 2021.10.14)</i>
Dates	Create: 2005-03-25 Modify: 2023-08-12
Description	Saccharin (manufacturing) appears as white crystals. Odorless or faintly aromatic odor. Sweet taste. (NTP, 1992) <i>National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.</i> ► CAMEO Chemicals Saccharin is a 1,2-benzisothiazole having a keto-group at the 3-position and two oxo substituents at the 1-position. It is used as an artificial sweetening agent. It has a role as a sweetening agent, a xenobiotic and an environmental contaminant. It is a 1,2-benzisothiazole and a N-sulfonylcarboxamide. ► ChEBI Saccharin has been investigated for the treatment of Hypertension and Hyperglycemia. ► DrugBank

[View More...](#)

Contents

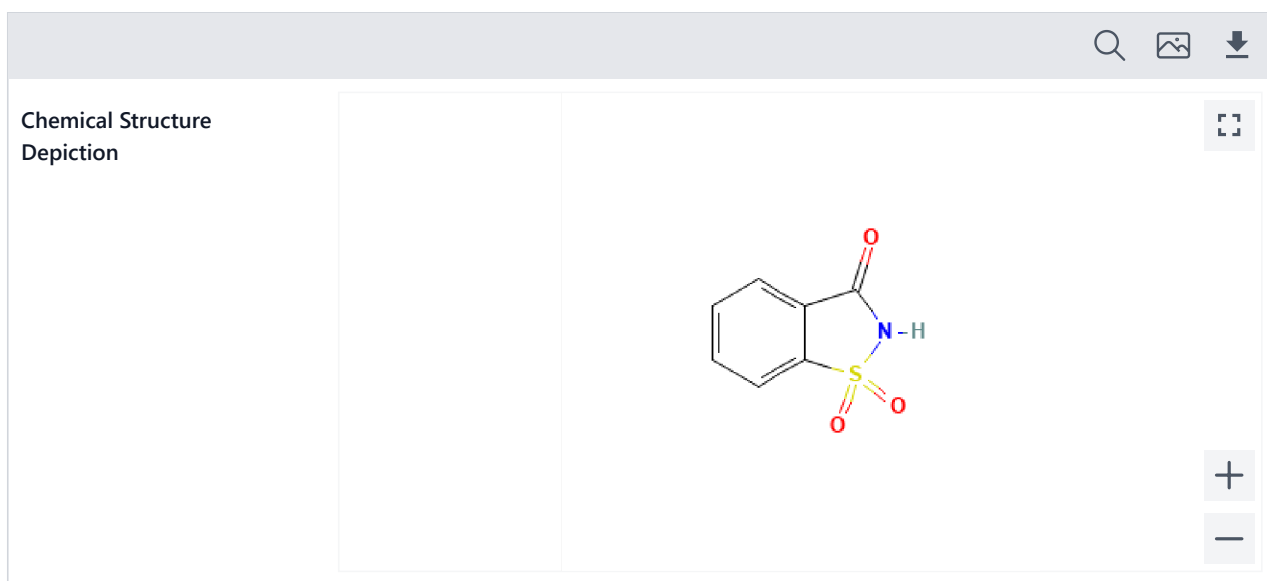
Title and Summary	
1 Structures	▼
2 Names and Identifiers	▼
3 Chemical and Physical Properties	▼
4 Spectral Information	▼
5 Related Records	▼
6 Chemical Vendors	
7 Drug and Medication Information	▼
8 Food Additives and Ingredients	▼
9 Agrochemical Information	▼
10 Pharmacology and Biochemistry	▼
11 Use and Manufacturing	▼
12 Identification	▼
13 Safety and Hazards	▼
14 Toxicity	▼
15 Associated Disorders and Diseases	
16 Literature	▼
17 Patents	▼
18 Interactions and Pathways	▼
19 Biological Test Results	▼
20 Taxonomy	
21 Classification	▼
22 Information Sources	

1 Structures



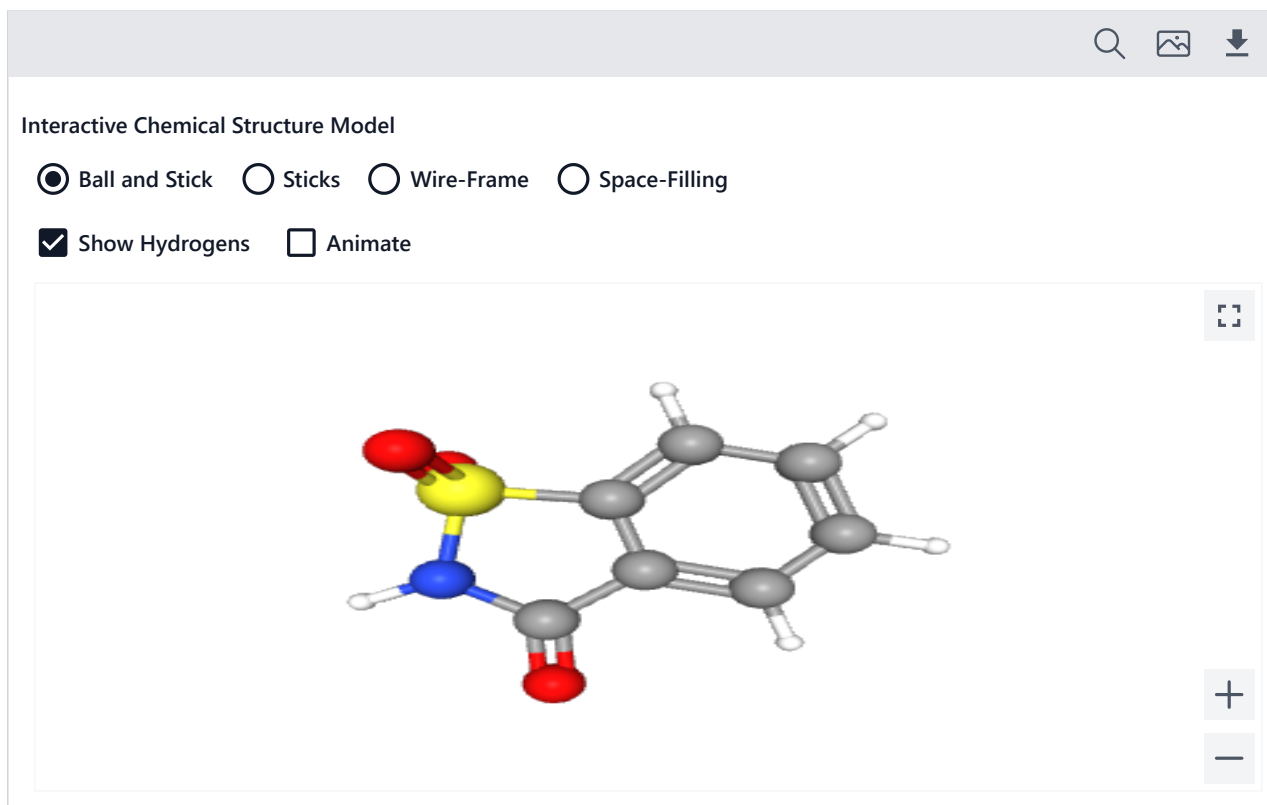
1.1 2D Structure





► PubChem

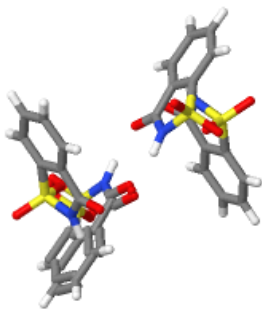
1.2 3D Conformer



► PubChem

1.3 Crystal Structures



1 of 9		View All 
CCDC Number	274592	
Associated Article	DOI:10.1107/S1600536805016600	
Crystal Structure Data	DOI:10.5517/cc96qt0	
Crystal Structure Depiction		

► [The Cambridge Structural Database](#)

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

1,1-dioxo-1,2-benzothiazol-3-one

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.2 InChI

InChI=1S/C₇H₅NO₃S/c9-7-5-3-1-2-4-6(5)12(10,11)8-7/h1-4H,(H,8,9)

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.3 InChIKey

CVHZOJJKTDOEJC-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

[► PubChem](#)

2.1.4 Canonical SMILES



C1=CC=C2C(=C1)C(=O)NS2(=O)=O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

[► PubChem](#)

2.2 Molecular Formula



C₇H₅NO₃S

Computed by PubChem 2.2 (PubChem release 2021.10.14)

[► CAMEO Chemicals; PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



81-07-2

[► CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals under the TSCA; EPA D...](#)

2.3.2 Deprecated CAS



126987-83-5, 474-91-9, 61255-27-4, 890126-34-8

[► ChemIDplus; EPA DSSTox](#)

2.3.3 European Community (EC) Number



201-321-0

[► European Chemicals Agency \(ECHA\)](#)

2.3.4 NSC Number



757878

[► DTP/NCI](#)

5349

[► DTP/NCI](#)

2.3.5 UN Number



3077

- ▶ NJDOH RTK Hazardous Substance List

2.3.6 UNII



FST467XS7D

- ▶ FDA Global Substance Registration System (GSRS)

2.3.7 DSSTox Substance ID



DTXSID5021251

- ▶ EPA DSSTox

2.3.8 Nikkaji Number



J747.663I

- ▶ Japan Chemical Substance Dictionary (Nikkaji)

J3.855E

- ▶ Japan Chemical Substance Dictionary (Nikkaji)

2.3.9 Wikipedia



Saccharin

- ▶ Wikipedia

2.3.10 Wikidata



Q191381

- ▶ Wikidata

2.3.11 NCI Thesaurus Code



C76515

- ▶ NCI Thesaurus (NCIt)

2.3.12 RXCUI



9509

► NLM RxNorm Terminology

2.3.13 Pharos Ligand ID



VR72KS9NK6KQ

► Pharos

2.3.14 Metabolomics Workbench ID



44013

► Metabolomics Workbench

2.3.15 ChEMBL ID



CHEMBL310671

► ChEMBL

2.4 Synonyms



2.4.1 MeSH Entry Terms



Calcium, Saccharin
Saccharin
Saccharin Calcium
Saccharin Sodium

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



saccharin	Benzosulphimide	Kandiset	Benzo-2-sulphimide
81-07-2	Saccharinol	Sacarina	Sweeta
o-Benzoic sulfimide	Saccharinose	Sucrette	Benzoylsulfonic Imide
o-Sulfobenzimide	Gluside	Zaharina	o-Benzosulphimide
Saccharine	Benzosulfinate	Saccharin insoluble	o-Sulfobenzoic acid imide
Saccharimide	Hermesetas	Sykose	Insoluble saccharin
Benzosulfimide	Saccharol	Saxin	1,2-Benzisothiazol-3(2H)-one 1,1-d

Benzoic sulfimide Glucid o-Benzoyl sulfimide Natreen
Garantose Saccharin acid Sucre edulcor Sacharin
o-Benzoylsulfimide Benzoic sulfimide 1,3-Benzisothiazol-2(1H)-one 1,1-dioxide o-Benzoylsulfimide

► PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	183.19 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3	0.9	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	182.99901420 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	182.99901420 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	71.6Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	12	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	303	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

► PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Saccharin (manufacturing) appears as white crystals. Odorless or faintly aromatic odor. Sweet taste. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

White solid; [CAMEO]

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

Solid

► [Human Metabolome Database \(HMDB\)](#)

3.2.2 Color / Form



Monoclinic crystals

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

Needles from [acetone](#); prisms from alcohol; leaflets from [water](#)

Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-458

► [Hazardous Substances Data Bank \(HSDB\)](#)

White, crystalline powder

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1102

► [Hazardous Substances Data Bank \(HSDB\)](#)

White crystals

FCC; Food Chemicals Codex. Committee on Food Chemicals Codex, Food and Nutrition Board, Institute of Medicine. 5th. Washington, DC: National Academy Press (2003)

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.3 Odor



ODORLESS OR HAS FAINT AROMATIC ODOR.

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 1236

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.4 Taste



In dilute aqueous solution it is 500 times as sweet as sugar; sweet taste detectable in 1:100,000 dilution.

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

Bitter, metallic aftertaste

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.5 Boiling Point



Sublimes (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. *National Toxicology Program Chemical Repository Database*. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

Sublimes

Lide, D.R. *CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008*. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-458

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.6 Melting Point



444 °F (decomposes) (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. *National Toxicology Program Chemical Repository Database*. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

228 °C decomposes

Lide, D.R. *CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008*. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-458

► [Hazardous Substances Data Bank \(HSDB\)](#)

224 °C

► [Human Metabolome Database \(HMDB\)](#)

3.2.7 Solubility



greater than or equal to 100 mg/mL at 75 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. *National Toxicology Program Chemical Repository Database*. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

1 G SOL IN 2.6 ML [WATER](#), 4.7 ML ALC /[CALCIUM SALT](#)/.

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 1236

► [Hazardous Substances Data Bank \(HSDB\)](#)

FREELY SOL IN [WATER](#). /AMMONIUM SALT/

Weed Science Society of America. Herbicide Handbook. 4th ed. Champaign, IL: Weed Science Society of America, 1979. of America, 1979., p. 371

► [Hazardous Substances Data Bank \(HSDB\)](#)

Slightly soluble in [benzene](#), [ethyl ether](#), [chloroform](#); soluble in [acetone](#), [ethanol](#)

Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-458

► [Hazardous Substances Data Bank \(HSDB\)](#)

Slightly soluble in deuterated dimethylsulfoxide

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V2: 1285

► [Hazardous Substances Data Bank \(HSDB\)](#)

1 g dissolves 31 mL alcohol, 12 mL [acetone](#), and in about 50 mL [glycerol](#); freely soluble in solution of alkali carbonates; slightly soluble in [chloroform](#), ether

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

Soluble in [amyl acetate](#), [ethyl acetate](#)

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1102

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Solubility (Complete) data for SACCHARIN (7 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

4 mg/mL at 25 °C

► [Human Metabolome Database \(HMDB\)](#)

3.2.8 Density



0.828 (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► CAMEO Chemicals

0.828 g/cu cm at 25 °C

Lide, D.R. *CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008*. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 3-458

► Hazardous Substances Data Bank (HSDB)

3.2.9 Vapor Pressure



0.00000064 [mmHg]

► Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

1.03X10⁻⁷ mm Hg at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Jan, 2010. Available from, as of May 27, 2011: <https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm>

► Hazardous Substances Data Bank (HSDB)

3.2.10 LogP



log Kow = 0.91

Hansch, C., Leo, A., D. Hoekman. *Exploring QSAR - Hydrophobic, Electronic, and Steric Constants*. Washington, DC: American Chemical Society, 1995., p. 27

► Hazardous Substances Data Bank (HSDB)

0.91

► Human Metabolome Database (HMDB)

3.2.11 Henry's Law Constant



Henry's Law constant = 1.23X10⁻⁹ atm-cu m/mol at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Jan, 2010. Available from, as of May 27, 2011: <https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm>

► Hazardous Substances Data Bank (HSDB)

3.2.12 Decomposition



When heated to decomposition it emits very toxic fumes of /nitrogen oxides/, /sulfur oxides/ and **sodium oxide**.

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3277

► Hazardous Substances Data Bank (HSDB)

3.2.13 Heat of Combustion



At constant volume: 4753.1 cal/g

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.14 pH



pH of 0.35% aqueous solution: 2.0

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.15 Ionization Efficiency



Ionization mode	Positive
logIE	0.22
pH	2.7
Instrument	Agilent XCT
Ion source	Electrospray ionization
Additive	formic acid (5.3nM)
Organic modifier	MeCN (80%)
Reference	DOI:

► [Kruve Lab, Ionization & Mass Spectrometry, Stockholm University](#)

3.2.16 Dissociation Constants



pKa = 1.31 at 25 °C for the conjugate acid

Serjeant, E.P., Dempsey B.; *Ionisation Constants of Organic Acids in Aqueous Solution*. International Union of Pure and Applied Chemistry (IUPAC). IUPAC Chemical Data Series No. 23, 1979. New York, New York: Pergamon Press, Inc.

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.17 Other Experimental Properties



Sugar equivalence value relative to **sucrose** = 300

Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Twinning on (001). Perfect 100 cleavage; acicular crystals by vacuum sublimation.

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

SOL: 30.5 G/100 G 92.5% [ETHANOL-WATER](#) MIXT @ 25 °C; 35.1 G/100 G [PROPYLENE](#) @ 25 °C; 36.3 G/100 ML GLYCOL @ 25 °C; 13.3 G/100 ML [GLYCERIN](#) @ 25 °C. /[CALCIUM](#) SALT/

Furia, T.E. (ed.). *CRC Handbook of Food Additives*. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 529

► [Hazardous Substances Data Bank \(HSDB\)](#)

SOL: 2.6 G/100 G 92.5% [ETHANOL-WATER](#) @ 25 °C; 44.7 G/100 G [PROPYLENE](#) @ 25 °C; 46.2 G/100 ML GLYCOL @ 25 °C; 55.8 G/100 G [GLYCERIN](#) @ 25 °C. /[SODIUM](#) SALT/

Furia, T.E. (ed.). *CRC Handbook of Food Additives*. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 529

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Other Experimental Properties (Complete) data for SACCHARIN (6 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.18 Chemical Classes



Other Uses -> Food Additives

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

3.3 SpringerMaterials Properties



[Crystal structure](#)
[Density](#)
[Formula unit](#)
[Formula weight](#)
[Fusion temperature](#)
[Melting temperature](#)
[Phase transition](#)
[Space group](#)
[Transition enthalpy](#)
[Unit cell](#)
[Unit cell parameter](#)

► [SpringerMaterials](#)

4 Spectral Information



4.1 1D NMR Spectra



1 of 2

1D NMR Spectra

1H NMR: 6667 (Sadtler Research Laboratories Spectral Collection)

[► Hazardous Substances Data Bank \(HSDB\)](#)

2 of 2

1D NMR Spectra

[NMRShiftDB Link](#)[► NMRShiftDB](#)

4.1.1 1H NMR Spectra



1 of 2

Instrument Name

BRUKER AC-300

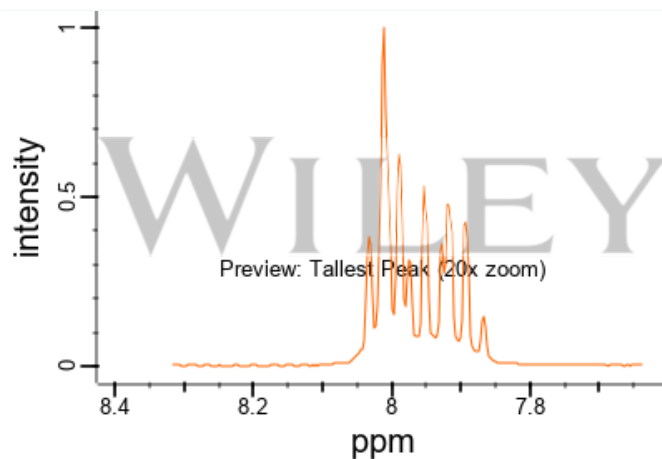
Source of Sample

Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan

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Thumbnail

[► SpectraBase](#)

2 of 2

Instrument Name

Varian A-60

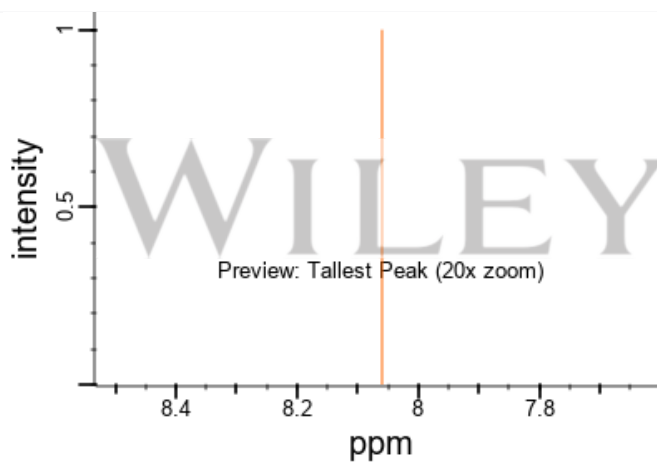
Source of Sample

H. Hettler, Max-Planck Society, Goettingen, Germany

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Thumbnail

[► SpectraBase](#)

4.1.2 13C NMR Spectra



1 of 2

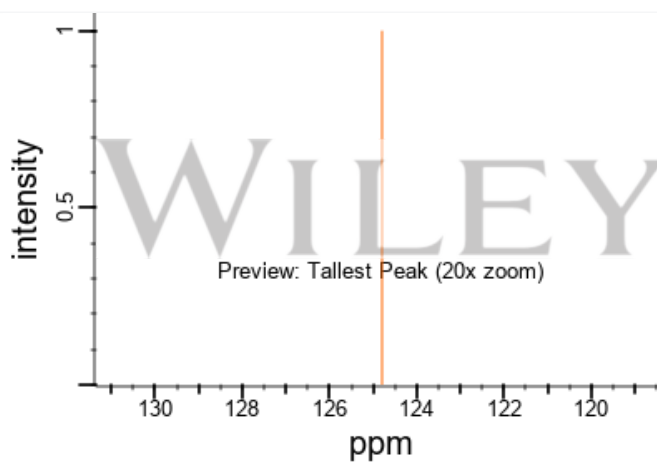
Source of Sample

Aldrich Chemical Company, Inc., Milwaukee, Wisconsin

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Thumbnail

[► SpectraBase](#)

2 of 2

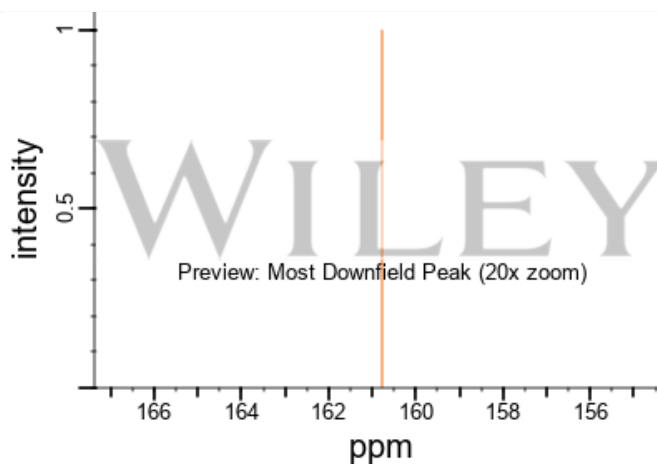
Instrument Name

Bruker AM-270

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Thumbnail

[► SpectraBase](#)

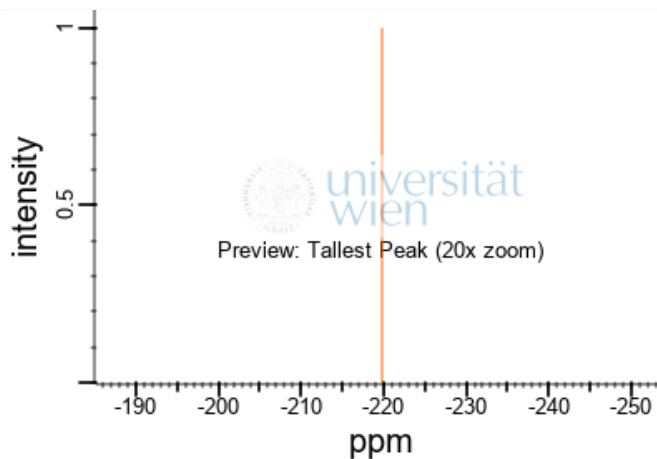
4.1.3 15N NMR Spectra



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Thumbnail

[► SpectraBase](#)

4.2 Mass Spectrometry



4.2.1 GC-MS

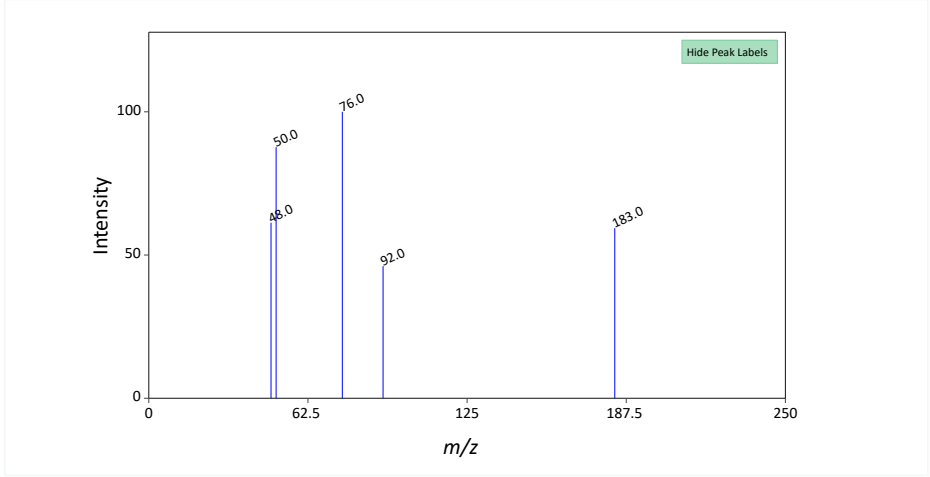


1 of 12

[View All](#)Spectra ID [27762](#)

Instrument Type EI-B

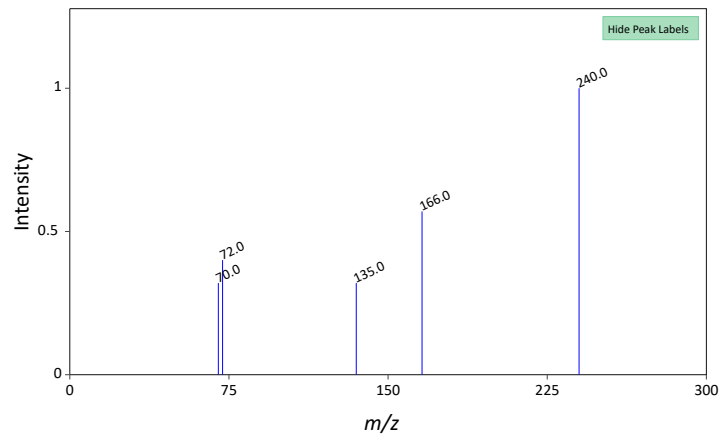
Ionization Mode positive

SPLASH	splash10-0fiv-9200000000-3cbd853d90d67ac630ab
Top 5 Peaks	76.0 99.99 50.0 87.65 48.0 61.29 183.0 59.39 92.0 46.12
Thumbnail	
Notes	instrument=JEOL JMS-HX-100

► [Human Metabolome Database \(HMDB\)](#)

2 of 12	View All
Spectra ID	31602
Instrument Type	GC-MS
SPLASH	splash10-006x-5940000000-c3d4fc7537245087aa01
Top 5 Peaks	240.0 1 166.0 0.57 72.0 0.40 135.0 0.32 70.0 0.32

Thumbnail



► [Human Metabolome Database \(HMDB\)](#)

4.2.2 MS-MS



1 of 6

[View All](#)

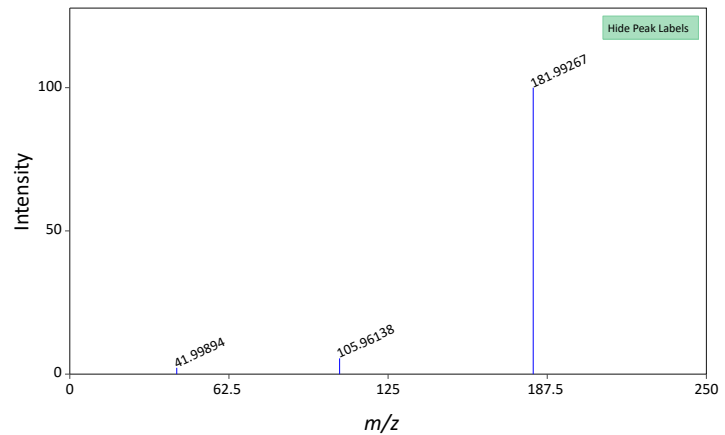
Spectra ID [2233520](#)

Ionization Mode Negative

SPLASH [splash10-001i-0900000000-8541df3050a01079f8cb](#)

Top 5 Peaks
181.99267 100
105.96138 5.50
41.99894 2.20

Thumbnail

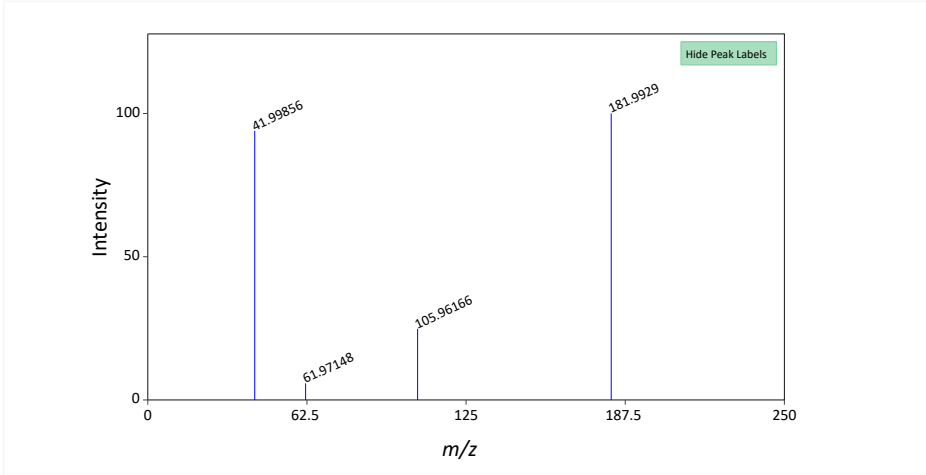


► [Human Metabolome Database \(HMDB\)](#)

2 of 6

[View All](#)

Spectra ID [2235403](#)

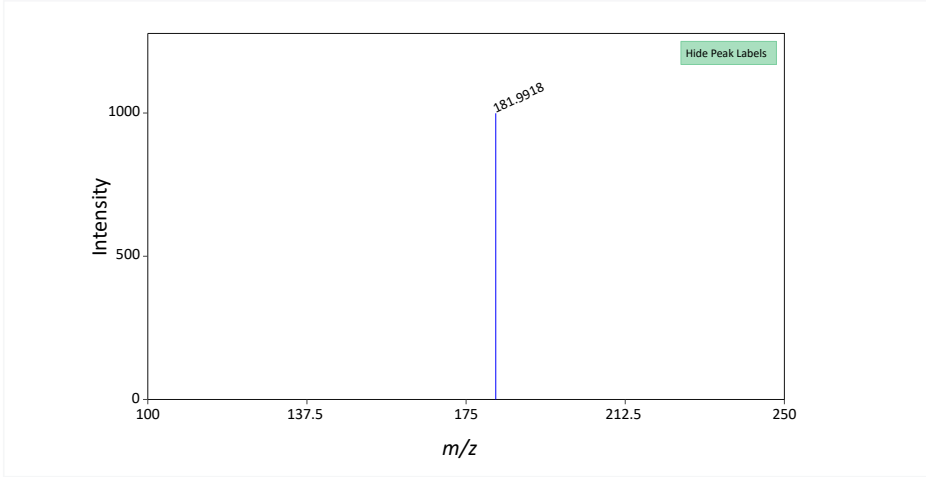
Ionization Mode	Negative
SPLASH	splash10-001l-7900000000-b92b2b5563f0682cf4c5
Top 5 Peaks	181.9929 100 41.99856 94 105.96166 24.80 61.97148 5.80
Thumbnail	

► [Human Metabolome Database \(HMDB\)](#)

4.2.3 LC-MS

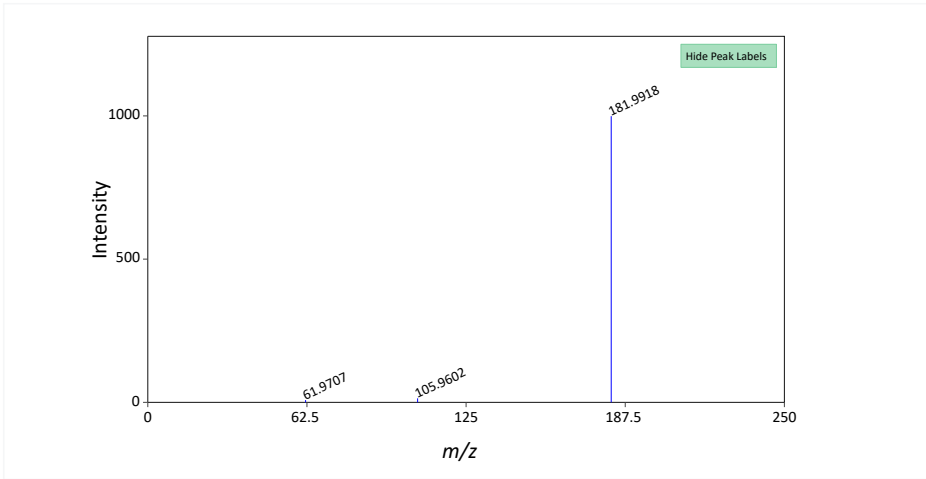


1 of 19	View All
Accession ID	MSBNK-CASMI_2016-SM867051
Authors	Krauss M, Schymanski EL, Weidauer C, Schupke H, UFZ and Eawag
Instrument	Q Exactive Plus Orbitrap Thermo Scientific
Instrument Type	LC-ESI-QFT
MS Level	MS2
Ionization Mode	NEGATIVE
Ionization	ESI
Collision Energy	35 (nominal)
Fragmentation Mode	HCD
Column Name	Kinetex C18 EVO 2.6 um, 2.1x50 mm, precolumn 2.1x5 mm, Phenomenex
Retention Time	2.874 min
Precursor m/z	181.9917
Precursor Adduct	[M-H]-

Top 5 Peaks	181.9918 999
SPLASH	splash10-001i-0900000000-1548a4ac4e5c19442679
Thumbnail	
License	CC BY
Reference	Schymanski, E. L.; Ruttkies, C.; Krauss, M.; Brouard, C.; Kind, T.; Dührkop, K.; Allen, F.; Vaniya, A.; Verdegem, D.; Böcker, S.; et al. Critical Assessment of Small Molecule Identification 2016: Automated Methods. Journal of Cheminformatics 2017, 9 (1). DOI:10.1186/s13321-017-0207-1

► [MassBank Europe](#)

2 of 19		View All 
Accession ID	MSBNK-Eawag-EA281651	
Authors	Stravs M, Schymanski E, Singer H, Department of Environmental Chemistry, Eawag	
Instrument	LTQ Orbitrap XL Thermo Scientific	
Instrument Type	LC-ESI-ITFT	
MS Level	MS2	
Ionization Mode	NEGATIVE	
Ionization	ESI	
Collision Energy	35 % (nominal)	
Fragmentation Mode	CID	
Column Name	XBridge C18 3.5um, 2.1x50mm, Waters	
Retention Time	2.5 min	
Precursor m/z	181.9917	
Precursor Adduct	[M-H] ⁻	
Top 5 Peaks	181.9918 999	

	105.9602 14 61.9707 8
SPLASH	splash10-001i-0900000000-4b6ed2bc790c007ba1d2
Thumbnail	
License	CC BY

► [MassBank Europe](#)

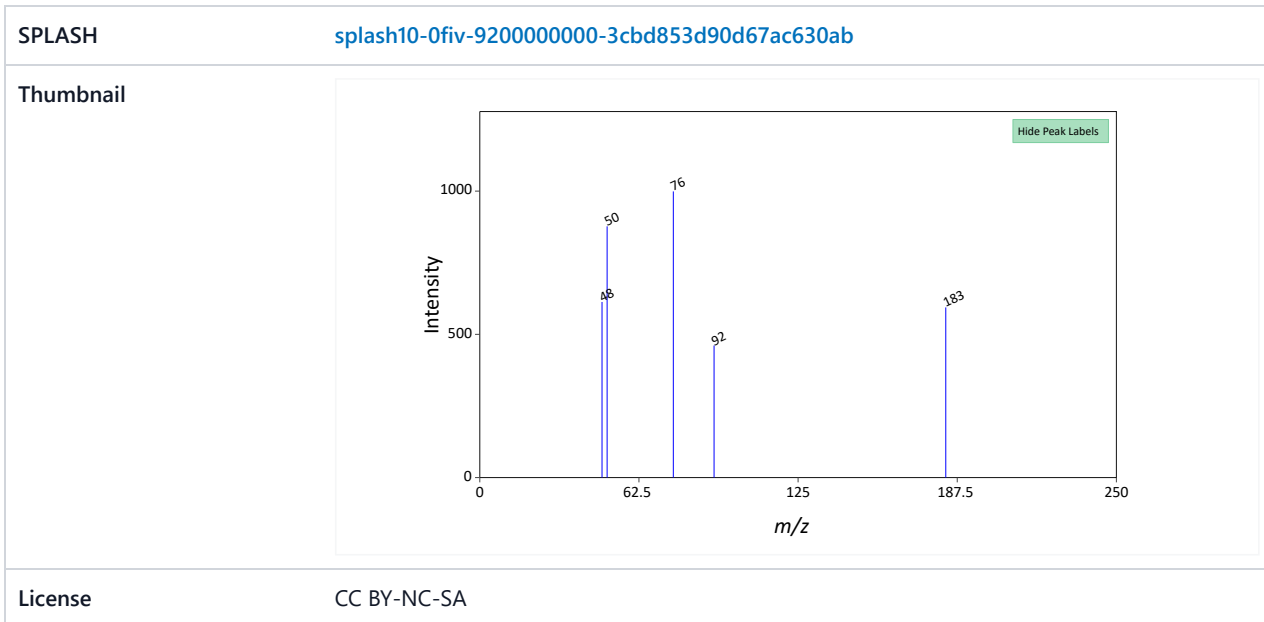
4.2.4 Other MS



1 of 5	View All
Other MS	MASS: 7732 (NIST/EPA/ MSDC Mass Spectral Database, 1990 Version)

► [Hazardous Substances Data Bank \(HSDB\)](#)

2 of 5	View All
Accession ID	MSBNK-Fac_Eng_Univ_Tokyo-JP004570
Authors	HAYASHI A, DEPT. OF CHEMISTRY, FAC. OF SCI. AND TECHNOLOGY, KINKI UNIV.
Instrument	JEOL JMS-HX-100
Instrument Type	EI-B
MS Level	MS
Ionization Mode	POSITIVE
Ionization	ENERGY 70 eV
Top 5 Peaks	76 999 50 877 48 613 183 594 92 461



► [MassBank Europe](#)

4.3 UV Spectra



UV max absorption (0.1 N NaOH): 267.3 nm (epsilon = 1570)

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

UV: 15734 (Sadtler Research Laboratories Spectral Collection)

Lide, D.R., G.W.A. Milne (eds.). *Handbook of Data on Organic Compounds. Volume I. 3rd ed.* CRC Press, Inc. Boca Raton ,FL. 1994., p. V2: 1285

► [Hazardous Substances Data Bank \(HSDB\)](#)

4.4 IR Spectra



IR Spectra	IR: 5038 (Coblentz Society Spectral Collection)
-------------------	---

► [Hazardous Substances Data Bank \(HSDB\)](#)

4.4.1 FTIR Spectra

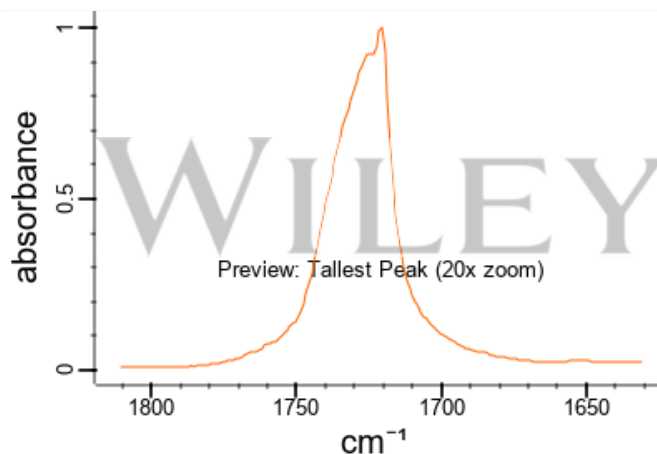


1 of 2	
Technique	KBr WAFER
Source of Sample	The Matheson Company, Inc., East Rutherford, New Jersey

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Thumbnail

[► SpectraBase](#)

2 of 2

Instrument Name

Bruker IFS 85

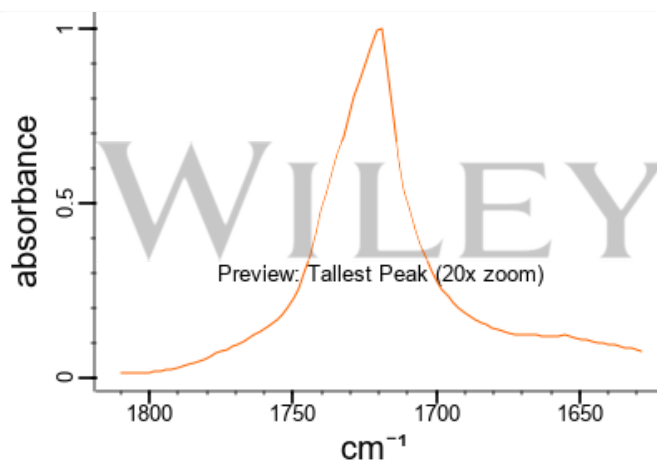
Technique

KBr-Pellet

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Thumbnail

[► SpectraBase](#)

4.4.2 ATR-IR Spectra



1 of 2

Instrument Name

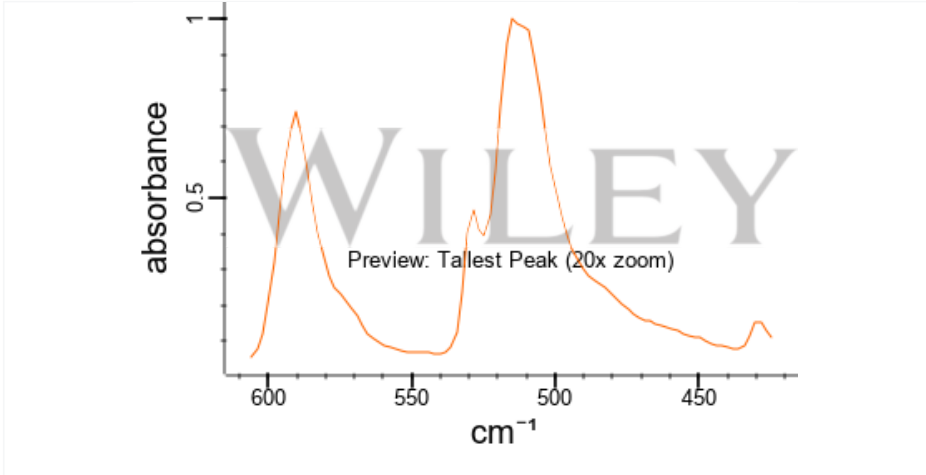
Bio-Rad FTS

Technique

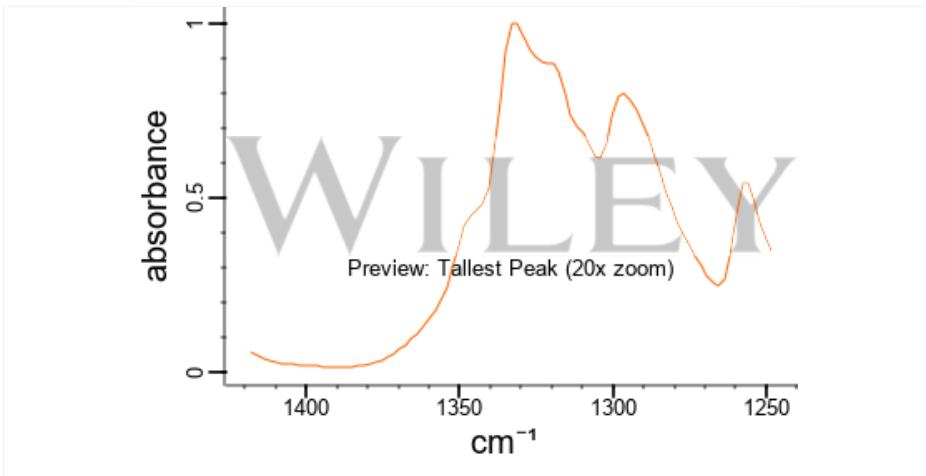
ATR-Neat (DuraSamplIR II) ground

Source of Spectrum

Forensic Spectral Research

Source of Sample	Sigma-Aldrich Chemie GmbH
Catalog Number	24093-1
Lot Number	S23444-458
Copyright	Copyright © 2009-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

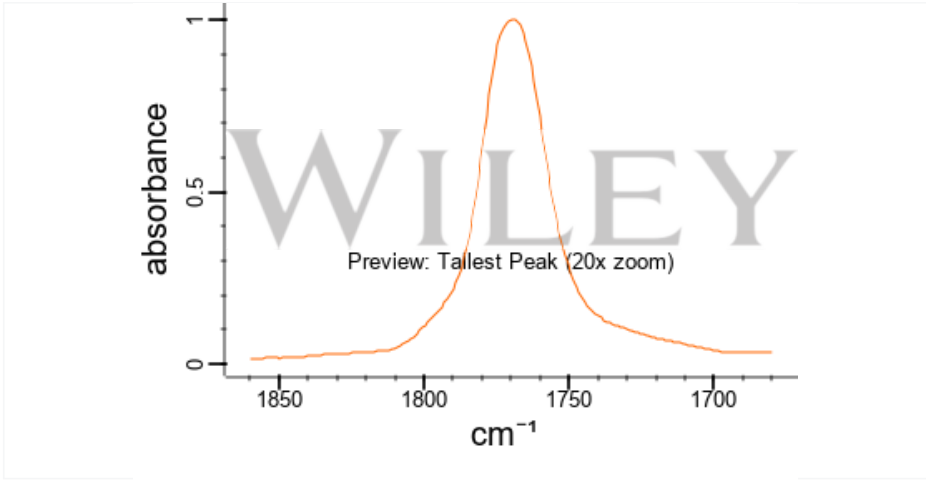
[► SpectraBase](#)

2 of 2	
Source of Sample	Aldrich
Catalog Number	109185
Copyright	Copyright © 2018-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

[► SpectraBase](#)

4.4.3 Vapor Phase IR Spectra



Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

4.5 Raman Spectra

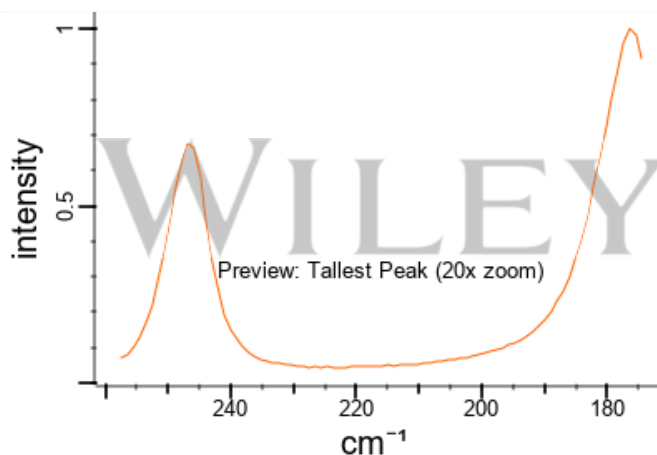


1 of 3	View All
Raman Spectra	Raman: 126 (Sadtler Research Laboratories Spectral Collection)

► Hazardous Substances Data Bank (HSDB)

2 of 3	View All
Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Sigma-Aldrich Company LLC
Catalog Number	240931
Lot Number	S23444-458
Copyright	Copyright © 2015-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

[► SpectraBase](#)

4.6 Other Spectra



SADTLER REF NUMBER: 322 (IR, PRISM); 110 (IR, GRATING)

Weast, R.C. (ed.) Handbook of Chemistry and Physics. 69th ed. Boca Raton, FL: CRC Press Inc., 1988-1989., p. C-485[► Hazardous Substances Data Bank \(HSDB\)](#)

5 Related Records



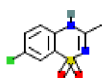
5.1 Related Compounds with Annotation



3,007 items



SORT BY Neighbor Type - A to Z



diazoxide, 364-98-7, Proglycem, Hyperstat, Hypertonalum, ...

Compound CID: [3019](#)

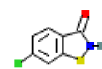
Neighbor Type: 2D+3D Annotation Types Count: 13



saccharin, 81-07-2, o-Benzoic sulfimide, o-Sulfobenzimide, Saccharine, ...

Compound CID: [5143](#)

Neighbor Type: 2D+3D Annotation Types Count: 17



TICLATONE, 70-10-0, 6-Chlorobenzo[d]isothiazol-3(2H)-one, Landromil, FER-1443, ...

Compound CID: [6258](#)

Neighbor Type: 2D+3D Annotation Types Count: 6



85-40-5, Tetrahydrophthalimide, 1,2,3,6-Tetrahydrophthalimide, 3a,4,7,7a-Tetrahydro-1H-isoindole-1,3(2H)-dione, 4-Cyclohexene-1,2-dicarboximide, ...

Compound CID: [6808](#)

Neighbor Type: 2D+3D Annotation Types Count: 12



PHTHALIMIDE, 85-41-6, Isoindole-1,3-dione, 1H-Isoindole-1,3(2H)-dione, isoindoline-1,3-dione, ...

Compound CID: [6809](#)

Neighbor Type: 2D+3D Annotation Types Count: 12

<< First < Previous Page 1 of 602 Next > Last >>

► [PubChem](#)

5.2 Related Compounds



Same Connectivity Count	11
Same Parent, Connectivity Count	197
Same Parent, Exact Count	187
Mixtures, Components, and Neutralized Forms Count	758
Similar Compounds Count	301
Similar Conformers Count	2751

► [PubChem](#)

5.3 Substances



5.3.1 Related Substances



All Count	1996
Same Count	309
Mixture Count	1687

► [PubChem](#)

5.3.2 Substances by Category



8 categories	↓
Chemical Vendors (90)	+

Curation Efforts (20)	+
Governmental Organizations (36)	+
Journal Publishers (6)	+
NIH Initiatives (12)	+
Research and Development (47)	+
Subscription Services (3)	+
Legacy Depositors (129)	+

► PubChem

5.4 Entrez Crosslinks



PubMed Count	7287
Protein Structures Count	7
Taxonomy Count	4
OMIM Count	5
Gene Count	45

► PubChem

5.5 Associated Chemicals



Sodium saccharin;128-44-9

► Hazardous Substances Data Bank (HSDB)

Calcium saccharin;6485-34-3

► Hazardous Substances Data Bank (HSDB)

5.6 NCBI LinkOut



Provider	Information
Ingenuity Pathways Analysis	Chemical Information: molecular interactions

► NCBI

6 Chemical Vendors



61 vendors



Sigma-Aldrich

PubChem SID: [24846892](#)Purchasable Chemical: [109185_ALDRICH](#)PubChem SID: [329751066](#)Purchasable Chemical: [1607007_USP](#)PubChem SID: [24854444](#)Purchasable Chemical: [240931_ALDRICH](#)

CSNpharm

PubChem SID: [384653337](#)Purchasable Chemical: [CSN22579](#)

MolCore BioPharmatech

PubChem SID: [446276532](#)Purchasable Chemical: [DY572779](#)PubChem SID: [405503908](#)Purchasable Chemical: [MC572779](#)

THE BioTek

PubChem SID: [446310500](#)Purchasable Chemical: [bt-1169157](#)

AKos Consulting & Solutions

PubChem SID: [104668904](#)Purchasable Chemical: [AKOS000120481](#)PubChem SID: [212309691](#)Purchasable Chemical: [AKOS017272711](#)

Biosynth

PubChem SID: [255371525](#)Purchasable Chemical: [W-200289](#)

AbaChemScene

PubChem SID: [354273823](#)Purchasable Chemical: [CS-0013120](#)

BLD Pharm

PubChem SID: [375288679](#)Purchasable Chemical: [BD105965](#)

Thermo Fisher Scientific

PubChem SID: [459197096](#)Purchasable Chemical: [GID_900000000171288](#)PubChem SID: [459197097](#)Purchasable Chemical: [GID_900000000171289](#)PubChem SID: [459218185](#)Purchasable Chemical: [GID_900000004982671](#)

Yuhao Chemical

PubChem SID: [463754297](#)Purchasable Chemical: [LL0154](#)PubChem SID: [318239939](#)Purchasable Chemical: [RT10372](#)

Alichem

PubChem SID: [377962752](#)Purchasable Chemical: [059006195](#)

Alfa Chemistry

PubChem SID: [347752035](#)Purchasable Chemical: [1189466-17-8](#)PubChem SID: [347759876](#)Purchasable Chemical: [81-07-2](#)PubChem SID: [445523521](#)Purchasable Chemical: [ACM81072](#)

LEAPCHEM

PubChem SID: [439959799](#)Purchasable Chemical: [LP070591](#)

Hunan Huateng Pharmaceutical Co., Ltd.

PubChem SID: [405072869](#)Purchasable Chemical: [F92844](#)

Aaron Chemicals LLC

PubChem SID: [406537257](#)Purchasable Chemical: [AR003UVG](#)

ClinivexPubChem SID: [463927353](#)Purchasable Chemical: [RCLTRS080800](#)**3WAY PHARM INC**PubChem SID: [438526457](#)Purchasable Chemical: [SWOT-0103585](#)**A2B Chem**PubChem SID: [444068545](#)Purchasable Chemical: [AB78880](#)PubChem SID: [480591746](#)Purchasable Chemical: [AE16112](#)PubChem SID: [480596060](#)Purchasable Chemical: [AW55433](#)**eNovation Chemicals**PubChem SID: [376013564](#)Purchasable Chemical: [D154409](#)**Chem-Space.com Database**PubChem SID: [434437304](#)Purchasable Chemical: [CSSB00000195689](#)**VladaChem**PubChem SID: [381002094](#)Purchasable Chemical: [VL164726](#)PubChem SID: [381019459](#)Purchasable Chemical: [VL274753-100G](#)**Enamine**PubChem SID: [473974284](#)Purchasable Chemical: [EN300-18624](#)PubChem SID: [335421898](#)Purchasable Chemical: [Z256708526](#)**MuseChem**PubChem SID: [355201312](#)Purchasable Chemical: [R011114](#)**BOC Sciences**PubChem SID: [441147813](#)Purchasable Chemical: [1981/7/2](#)PubChem SID: [254785320](#)Purchasable Chemical: [81-07-2](#)**Clearsynth**PubChem SID: [387197816](#)Purchasable Chemical: [CS-T-85174](#)**BenchChem**PubChem SID: [446466155](#)Purchasable Chemical: [B028170](#)**Key Organics/BIONET**PubChem SID: [404335484](#)Purchasable Chemical: [STR03759](#)**Norris Pharm**PubChem SID: [383460164](#)Purchasable Chemical: [NSZB-A270530](#)**Chemenu Inc.**PubChem SID: [443412127](#)Purchasable Chemical: [CM157269](#)**MedChemexpress MCE**PubChem SID: [406168261](#)Purchasable Chemical: [HY-Y0272](#)**Vitas-M Laboratory**PubChem SID: [131289932](#)Purchasable Chemical: [BBL015343](#)PubChem SID: [85280705](#)Purchasable Chemical: [STK803263](#)**Ambinter**PubChem SID: [369741376](#)Purchasable Chemical: [Amb22058725](#)**Selleck Chemicals**

PubChem SID: 404639137	Purchasable Chemical: S4819
MolPort	
PubChem SID: 88529690	Purchasable Chemical: MolPort-000-881-701
Achemo Scientific Limited	
PubChem SID: 316959406	Purchasable Chemical: AC-77203
Finetech Industry Limited	
PubChem SID: 164764925	Purchasable Chemical: FT-0674493
PubChem SID: 164764926	Purchasable Chemical: FT-0674494
AstaTech, Inc.	
PubChem SID: 458763989	Purchasable Chemical: D70140
LGC Standards	
PubChem SID: 340510549	Purchasable Chemical: DRE-C16901000
Yick-Vic Chemicals & Pharmaceuticals (HK) Ltd.	
PubChem SID: 441073256	Purchasable Chemical: PH-1258A
Starshine Chemical	
PubChem SID: 480457690	Purchasable Chemical: 2023-05-1B031883
Acadechem	
PubChem SID: 321910474	Purchasable Chemical: ACDS-025323
Sinfoo Biotech	
PubChem SID: 404788197	Purchasable Chemical: S009666
Oakwood Products	
PubChem SID: 117674072	Purchasable Chemical: 055150
RR Scientific	
PubChem SID: 472452871	Purchasable Chemical: R911859
Combi-Blocks	
PubChem SID: 374062485	Purchasable Chemical: QE-7604
abcr GmbH	
PubChem SID: 316403546	Purchasable Chemical: AB131633
OtavaChemicals	
PubChem SID: 441630911	Purchasable Chemical: 2925293
Santa Cruz Biotechnology, Inc.	
PubChem SID: 472963248	Purchasable Chemical: sc-212902
CymitQuimica	
PubChem SID: 470725745	Purchasable Chemical: CQ_81-07-2
Smolecule	
PubChem SID: 442866893	Purchasable Chemical: S1485461
Ambeed	
PubChem SID: 376124133	Purchasable Chemical: A239294
BioChemPartner	
PubChem SID: 375561470	Purchasable Chemical: BCP29068

001Chemical

PubChem SID: [440050564](#)Purchasable Chemical: [DY572779](#)

AA BLOCKS

PubChem SID: [374183193](#)Purchasable Chemical: [AA003U3O](#)

PubChem SID: [479827768](#)

Purchasable Chemical: [AA008X5G](#)

PubChem SID: 479871508

Purchasable Chemical: [AA01CCDP](#)

Matrix Scientific

PubChem SID: [406613498](#)

Purchasable Chemical: 032615

Achemtek

PubChem SID: [381354704](#)

Purchasable Chemical: 0102-026778

TargetMol

PubChem SID: 312995332

Purchasable Chemical: [T0889](#)

TCI (Tokyo Chemical Industry)

PubChem SID: 87563220

Purchasable Chemical: B0004

3B Scientific (Wuhan) Corp

PubChem SID: 375088568

Purchasable Chemical: [3B8-00183](#)

Life Chemicals

PubChem SID: [347811681](#)

Purchasable Chemical: [F0001-2092](#)

J&H Chemical Co.,Ltd

PubChem SID: [477504644](#)Purchasable Chemical: [JH488744](#)

► PubChem

7 Drug and Medication Information



7.1 FDA National Drug Code Directory



13 items



Q Search

SORT BY **Start Marketing Date - Most Recent** 

[illegible]

[illegible]

<< First < Previous Page 1 of 3 Next > Last >>

► National Drug Code (NDC) Directory

7.2 Drug Labels



Drug and label

1 item



SACCHARINUM (SACCHARIN) LIQUID

Drug: SACCHARIN Download: [PDF label](#) Data File: [XML](#)

Ingredient (UNII): SACCHARIN (UNII:FST467XS7D)

Indication: Indications: SACCHARINUM Indifference

Category: Homeopathic Company: Washington Homeopathic Products Date: 2010-09-30

► DailyMed

Active ingredient and drug

17 items ↓				
Search		SORT BY Ingredient - A to Z ▼		
Ingredient	Drug	Label	Data File	Data SetID
ACONITUM NAPELLUS (UNII:U0NQ8555JD); PROPYL PARABEN (UNII:Z8IX2SC1OH); LEDUM PALUSTRE TWIG (UNII:877L01IZ0P); LYCOPERDON UTRIFORME FRUITING BODY (UNII:K2A74U428F); CINNAMON (UNII:5S29HWU6QB); HERRING, UNSPECIFIED (UNII:34EX28T4C1); GELSEMIUM SEMPERVIRENS ROOT (UNII:639KR60Q1Q); AMARANTH (UNII:37RBV3X49K); GINGER (UNII:C5529G5JPQ); QUAAHOG, UNSPECIFIED (UNII:226LY0AFR9); SHRIMP, UNSPECIFIED (UNII:1891LE191T); TOXICODENDRON PUBESCENS LEAF (UNII:6IO182RP7A); SULFUR (UNII:70FD1KFU70); HAZELNUT, UNSPECIFIED (UNII:IW0OM96F6O); LAMB (UNII:FOF26T73HA); COD, UNSPECIFIED (UNII:8D6Q5LNG3D); TUNA, UNSPECIFIED (UNII:V2T3IHT3E2); SCALLOP, UNSPECIFIED (UNII:D380C73WOU); SODIUM COPPER CHLOROPHYLLIN (UNII:1D276TYV9O); ASPARTAME (UNII:Z0H242BBR1); FD&C RED NO. 3 (UNII:PN2ZH5LOQY); SACCHAROMYCES CEREVISIAE (UNII:978D8U419H); FD&C YELLOW NO. 5 (UNII:I753WB2F1M); USTILAGO MAYDIS (UNII:4K7Z7K7SWG); LACTOSE (UNII:J2B2A4N98G); PORK (UNII:O138UB266J); ACID GREEN 50 (UNII:9B7E8Y9D0X); SODIUM TRIPOLYPHOSPHATE (UNII:5HK03SA80J); ABRUS PRECATORIUS SEED (UNII:3OM8I6L7CD); POTASSIUM BENZOATE (UNII:763YQN2K7K); CRAB LEG, UNSPECIFIED (UNII:S1VF61QLO9); LACHESIS MUTA VENOM (UNII:VSW71SS07I); TURKEY (UNII:8E9NT44R8I); SACCHARIN (UNII:FST467XS7D); BLACK MUSTARD SEED (UNII:8LTY55LQ8D); TROUT, UNSPECIFIED (UNII:7TI7U5PF2U); GARLIC (UNII:V1V998DC17); PODOPHYLLUM (UNII:2S713A4VP3); IPECAC (UNII:62I3C8233L); PEANUT (UNII:QE1QX6B99R); SOLANUM NIGRUM WHOLE (UNII:0FMD6WV47M); ASCORBIC ACID (UNII:PQ6CK8PD0R); SODIUM NITRITE (UNII:M0KG633D4F); SODIUM CHLORIDE (UNII:451W47IQ8X); ARSENIC TRIOXIDE (UNII:S7V92P67HO); SODIUM DITHIONATE (UNII:RPF7Z41GAW); IRIS VERSICOLOR ROOT (UNII:X43D4L3DQC); CHICKEN (UNII:0X8Q245Y7B); ALLYLTHIOUREA (UNII:706IDJ14B7); CYNARA SCOLYMUS LEAF (UNII:B71UA545DE); FD&C BLUE NO. 2 (UNII:L06K8R7DQK); SODIUM BENZOATE (UNII:OJ245FE5EU); OYSTER, UNSPECIFIED (UNII:S614XWR17V); AMANITA MUSCARIA FRUITING BODY (UNII:DIF093I037); MONOSODIUM GLUTAMATE (UNII:W81N5U6R6U); FD&C YELLOW NO. 6 (UNII:H77VEI93A8); ANACARDIUM OCCIDENTALE FRUIT (UNII:4A10JR4E7E); CARMOISINE (UNII:DR4641L47F); 2-PHENYLPHENOL (UNII:D343Z75HT8);	E102 Tartrazine, E104 Quinoline yellow, E110 Sunset/Orange yellow, E122 Carmoisine, E123 Armamaranth, E124 Cochineal red A, E127 Erythrosine, D128 Red 2G, E 132 Indigotine, E141 Copper/Chlorophyll Complex, E142 Green S, E211 Sodium benzoate, E212 Potassium benzoate, E216 Propyl P-hydroxybenzoate, E223 Sodium metabisulphate, E231 Orthophenylphenol, E250 Sodium nitrate, E300 Ascorbic acid, E399 Sodium mono/bi/triphosphate, E951 Aspartame, Monosodium glutamate, Beef, Pork, Lamb, Chicken, Turkey, Clam	Drug PDF label	XML	ed359bb8-4e91-1486-1dc0-6d39e6ed1f54

URTICA URENS (UNII:IHN2NQ5OF9); ONION (UNII:492225Q21H); MENTHA PIPERITA (UNII:79M2M2UDA9); ANTIMONY TRISULFIDE (UNII:F79059A38U); SALMON, UNSPECIFIED (UNII:6122W2M0GB); NUTMEG (UNII:AE24M3MQ9); ALPINE STRAWBERRY (UNII:CG6IX3GCMU); HISTAMINE DIHYDROCHLORIDE (UNII:3POA0Q644U); D&A;C YELLOW NO. 10 (UNII:35SW5USQ3G); SOLANUM TUBEROSUM (UNII:2A8I57T4MX); PULSATILLA VULGARIS (UNII:I76KB35JEV); PHOSPHORUS (UNII:27YLU75U4W); GLYCYRRHIZA GLABRA (UNII:2788Z9758H); EGG (UNII:291P45F896); BEEF (UNII:4PIB2155QP); SEPIA OFFICINALIS JUICE (UNII:QDL83WN8C2); BRAZIL NUT (UNII:XKR79OET1K); ACID RED 1 (UNII:3365R6427R); SOLANUM LYCOPERSICUM (UNII:0243Q4990L); SOLIDAGO VIRGAUREA FLOWERING TOP (UNII:5405K23S50); CAPSICUM (UNII:00UK7646FG); PONCEAU 4R (UNII:Z525CBK9PG); CAFFEINE (UNII:3G6A5W338E); BAPTISIA TINCTORIA ROOT (UNII:5EF0HWI5WU); CINCHONA OFFICINALIS BARK (UNII:S003A158SB); LYCOPodium CLAVATUM SPORE (UNII:C88X29Y479)

LYCOPUS VIRGINICUS (UNII:TWH5125Q6F); ACONITUM NAPELLUS (UNII:U0NQ8555JD); EUPHRASIA STRICTA (UNII:C9642I91WL); SANGUINARIA CANADENSIS ROOT (UNII:N9288CD508); TRILLIUM ERECTUM ROOT (UNII:AHW6F0T2X0); PROPYLPARABEN (UNII:Z8IX2SC1OH); PHYTOLACCA AMERICANA ROOT (UNII:11E6VI8VEG); MELEAGRIS GALLOPAVO FEATHER (UNII:CAC78E2Q9S); LYCOPERDON UTRIFORME FRUITING BODY (UNII:K2A74U428F); LEDUM PALUSTRE TWIG (UNII:877L01I20P); FELIS CATUS HAIR (UNII:1564HD0N96); ROSA CANINA FLOWER (UNII:81MCR2UQ6Q); CINNAMON (UNII:5S29HWU6QB); HERRING, UNSPECIFIED (UNII:34EX28T4C1); HELIANTHEMUM CANADENSE (UNII:46G3W789Q3); ANTHOXANTHUM ODORATUM POLLEN (UNII:2KIK19R45Y); POA PRATENSIS POLLEN (UNII:SCB8J7LS3T); GELSEMIUM SEMPERVIRENS ROOT (UNII:639KR60Q1Q); AMARANTH (UNII:37RBV3X49K); PHLEUM PRATENSE POLLEN (UNII:65M88RW2EG); GINGER (UNII:C5529G5JPQ); ANSER ANSER FEATHER (UNII:15XI414745); QUAHOG, UNSPECIFIED (UNII:226LY0AFR9); FESTUCA PRATENSIS POLLEN (UNII:A0WFQ8P6N1); GOLDENSEAL (UNII:ZW3Z11D0JV); HADDOCK (UNII:0WLY635722); EQUUS CABALLUS SKIN (UNII:88VZV9HGT4); CHELIDONIUM MAJUS (UNII:7E889U5RNN); SERINUS CANARIA FEATHER (UNII:9EL3384IQY); SHRIMP, UNSPECIFIED (UNII:1891LE191T); HOUSE DUST (UNII:EYO007VX98); CASEIN, LACTOCOCCUS LACTIS CULTURED, PENICILLIUM ROQUEFORTI CULTURED, AGED (UNII:IYI0G2057S); YUCCA FILAMENTOSA (UNII:T6VR38UJ9I); WHEAT GLUTEN (UNII:1534K8653J); TOXICODENDRON PUBESCENS LEAF (UNII:6IO182RP7A); SAMBUCUS NIGRA FLOWERING TOP (UNII:CT03BSA18U); CAPRA HIRCUS HAIR (UNII:16M9MK8C4W); OYSTER SHELL CALCIUM CARBONATE, CRUDE (UNII:2E32821G6I); AMBROSIA ARTEMISIIFOLIA (UNII:9W34L2CQ9A); DATURA STRAMONIUM (UNII:G6W4F0V8Z3); ULEX EUROPAEUS FLOWER

Cow milk, Skim milk, Cow milk fat, Casein Lactococcus Lactis cultured, Casein lactococcus lactis penicilium roqueforti cultured, Casein lactococcus lactis cultured penicillium camemberti cultured, Egg, Felis catus skin, Canis lupus familiaris skin, Oryctolagus cuniculus skin, Equus caballus skin, Serinus canaria feather, gallus gallus feather, Anas platyrhynchos feather, Anser anser feather, melopsittacus undulatus feather, Phasianus colchicus feather, Meleagris gallopavo feather, Felis catus hair

Drug XML 4adb1459-a7c4-4912-f235-8838c2dfcca8
PDF
label

(UNII:398DBS1PXN); BELLIS PERENNIS (UNII:2HU33I03UY); TOBACCO LEAF (UNII:6YR2608RSU); GALLUS GALLUS FEATHER (UNII:1FCM16V0FV); SULFUR (UNII:70FD1KFU70); HAZELNUT, UNSPECIFIED (UNII:IW0OM96F6O); RYE (UNII:0R4AQI398X); LAMB (UNII:FOF26T73HA); COD, UNSPECIFIED (UNII:8D6Q5LNG3D); PTELEA TRIFOLIATA BARK (UNII:5KQR6FTT0D); ULMUS GLABRA POLLEN (UNII:T2K08L297Q); CANIS LUPUS FAMILIARIS HAIR (UNII:05S7L91ZTR); TUNA, UNSPECIFIED (UNII:V2T3IHT3E2); SCALLOP, UNSPECIFIED (UNII:D380C73WOU); CLADOSPORIUM HERBARUM (UNII:O64JF1198); SODIUM COPPER CHLOROPHYLLIN (UNII:1D276TYV9O); ASPARTAME (UNII:Z0H242BBR1); POPULUS NIGRA POLLEN (UNII:0MGE63QPFJ); HUMAN SKIN (UNII:0EE2343509); ELYMUS REPENS ROOT (UNII:3IXW0F6P8W); FD&C RED NO. 3 (UNII:PN2ZH5LOQY); ASPERGILLUS NIGER VAR. NIGER (UNII:9IOA40ANG6); FELIS CATUS SKIN (UNII:5308ED00EL); SACCHAROMYCES CEREVISIAE (UNII:978D8U419H); FD&C YELLOW NO. 5 (UNII:I753WB2F1M); ARTEMISIA VULGARIS ROOT (UNII:32MP823R8S); MESOCRICETUS AURATUS HAIR (UNII:EFG2YD102P); USTILAGO MAYDIS (UNII:4K7Z7K7SWG); LACTOSE (UNII:J2B2A4N98G); CORN (UNII:0N8672707O); OAT (UNII:Z6J799EAJK); CALLUNA VULGARIS POLLEN (UNII:5Q1IE9V5YZ); PORK (UNII:O138UB266J); POPULUS TREMULOIDES BARK (UNII:5543O0CEID); ACID GREEN 50 (UNII:9B7E8Y9D0X); SODIUM TRIPOLYPHOSPHATE (UNII:5HK03SA80J); MATRICARIA RECUTITA (UNII:G0R4UBI2ZZ); ORYCTOLAGUS CUNICULUS HAIR (UNII:09N62XQ70Y); HUMAN HAIR (UNII:1AWP0DKL4I); POTASSIUM IODIDE (UNII:1C4QK22F9J); BROMINE (UNII:SBV4XY874G); PHASIANUS COLCHICUS FEATHER (UNII:95ZNE214EZ); ABRUS PRECATORIUS SEED (UNII:3OM8I6L7CD); TARAXACUM OFFICINALE (UNII:39981FM375); LOLIUM PERENNE POLLEN (UNII:4T81LB52R0); POTASSIUM BENZOATE (UNII:763YQN2K7K); FAGUS SYLVATICA POLLEN (UNII:63218N1ZBI); BROMUS SECALINUS POLLEN (UNII:Q4T1SJ3046); CAVIA PORCELLUS HAIR (UNII:KBA5Y6X57N); CRAB LEG, UNSPECIFIED (UNII:S1VF61QLO9); XEROPHYLLUM ASPHODELOIDES (UNII:9I4XB1GP2B); WHITE RICE (UNII:A195V20H7A); BARLEY (UNII:5PWM7YLI7R); SHEEP WOOL (UNII:503LYG631H); CYTISUS SCOPARIUS POLLEN (UNII:I0NS0040GH); ALFALFA (UNII:DJO934BRBD); TURKEY (UNII:8E9NT44R8I); SACCHARIN (UNII:FST467XS7D); BLACK MUSTARD SEED (UNII:8LTY55LQ8D); TROUT, UNSPECIFIED (UNII:7TI7U5PF2U); GARLIC (UNII:V1V998DC17); CORYLUS AMERICANA POLLEN (UNII:ZGS382Y3AV); APIS MELLIFERA (UNII:7S82P3R43Z); PEANUT (UNII:QE1QX6B99R); COW MILK FAT (UNII:463JZS0XJ3); SOLANUM NIGRUM WHOLE (UNII:0FMD6WV47M); HOLCUS LANATUS POLLEN (UNII:70O1TP6H01); ATROPA BELLADONNA (UNII:WQZ3G9PF0H); SKIM MILK (UNII:6A001Y4M5A); ASCORBIC ACID (UNII:PQ6CK8PD0R); SODIUM NITRITE (UNII:M0KG633D4F); HUMAN DANDER (UNII:30X630U81C); DIANTHUS CARYOPHYLLUS FLOWER (UNII:B0D836E90S); BOS TAURUS HAIR (UNII:TOQ97Z8644); NARCISSUS

PSEUDONARCISSUS (UNII:Q2D0SKW2P4); BETULA PENDULA POLLEN (UNII:ZL5TV40C5Y); SODIUM CHLORIDE (UNII:451W471Q8X); ARSENIC TRIOXIDE (UNII:S7V92P67HO); SODIUM DITHIONATE (UNII:RPF7Z41GAW); ALOPECURUS PRATENSIS POLLEN (UNII:DG1ZL6W96V); EQUUS CABALLUS HAIR (UNII:4F35XG0149); CHICKEN (UNII:0X8Q245Y7B); ALETRIS FARINOSA ROOT (UNII:O021JGR97X); CYNARA SCOLYMUS LEAF (UNII:B71UA545DE); ALLYLTHIOUREA (UNII:706IDJ14B7); FD&C BLUE NO. 2 (UNII:L06K8R7DQK); SODIUM BENZOATE (UNII:OJ245FE5EU); POPULUS TREMULOIDES LEAF (UNII:7IIH57D9E0); AVENA SATIVA POLLEN (UNII:A7IKY24TR7); ORYCTOLAGUS CUNICULUS SKIN (UNII:Z91WAU43WC); OYSTER, UNSPECIFIED (UNII:S614XWR17V); CASEIN, LACTOCOCCUS LACTIS CULTURED, AGED (UNII:CJP9NL7JSJ); FD&C YELLOW NO. 6 (UNII:H77VEI93A8); MONOSODIUM GLUTAMATE (UNII:W81N5U6R6U); AMANITA MUSCARIA FRUITING BODY (UNII:DIF093I037); FRAXINUS EXCELSIOR POLLEN (UNII:1824QUA0U3); ANACARDIUM OCCIDENTALE FRUIT (UNII:4A10JR4E7E); ENGLISH WALNUT (UNII:1V3SHR7QB7); QUERCUS ALBA POLLEN (UNII:Z4Y9ZSV4KK); PRIMULA VULGARIS (UNII:KZ3PRK2V0J); CRATAEGUS MONOGYNA POLLEN (UNII:X6049S3TX1); CARMOISINE (UNII:DR4641L47F); AETHUSA CYNAPIUM (UNII:M6936L953C); 2-PHENYLPHENOL (UNII:D343Z75HT8); ECHINACEA, UNSPECIFIED (UNII:4N9P6CC1DX); URTICA URENS (UNII:IHN2NQ5OF9); ONION (UNII:492225Q21H); MENTHA PIPERITA (UNII:79M2M2UDA9); CYNOSURUS CRISTATUS POLLEN (UNII:SES68PF95U); BRYONIA ALBA ROOT (UNII:T7J046YI2B); LILIUM CANDIDUM FLOWER (UNII:COV655U2CJ); SALMON, UNSPECIFIED (UNII:6122W2M0GB); DYSPHANIA AMBROSIOIDES (UNII:4H5RSU087I); WYETHIA HELENIOIDES ROOT (UNII:J10PD1AQ0N); HYOSCYAMUS NIGER (UNII:4WRK2153H3); ARUNDO PLINIANA ROOT (UNII:ZXE7LB03WC); ALPINE STRAWBERRY (UNII:CG6IX3GCMU); NUTMEG (UNII:AE24M3MQ9); HISTAMINE DIHYDROCHLORIDE (UNII:3POA0Q644U); D&C YELLOW NO. 10 (UNII:35SW5USQ3G); SOLANUM TUBEROSUM (UNII:2A8I57T4MX); PULSATILLA VULGARIS (UNII:I76KB35JEV); GLYCYRRHIZA GLABRA (UNII:2788Z9758H); SCHOENOCALON OFFICINALE SEED (UNII:6NAF1689IO); EGG (UNII:291P45F896); DROSEROTA ROTUNDIFOLIA (UNII:QR44N9XPJQ); BEEF (UNII:4PIB2155QP); ANAS PLATYRHYNCHOS FEATHER (UNII:83B65P4796); SALIX ALBA POLLEN (UNII:WQ580684IZ); COW MILK (UNII:917J3173FT); JUNIPERUS VIRGINIANA TWIG (UNII:532BCG080L); SUCROSE (UNII:C151H8M554); ACID RED 1 (UNII:3365R6427R); BRAZIL NUT (UNII:XKR79OET1K); SOLANUM LYCOPERSICUM (UNII:0243Q4990L); MELOPSITTACUS UNDULATUS FEATHER (UNII:1XY644QKWG); ECHINOCHLOA CRUS-GALLI POLLEN (UNII:6941ZR795V); SOLANUM DULCAMARA TOP (UNII:KPS1B1162N); PONCEAU 4R (UNII:Z525CBK9PG); CAPSICUM (UNII:00UK7646FG); CAFFEINE (UNII:3G6A5W338E); CASEIN, LACTOCOCCUS LACTIS CULTURED, PENICILLIUM CAMEMBERTI CULTURED, AGED (UNII:G44KT17KIS); LYCOPODIUM CLAVATUM SPORE (UNII:C88X29Y479); AGROSTIS GIGANTEA POLLEN (UNII:HU8V6E7HOA); WHEAT

(UNII:4J2I0SN84Y); ONOSMODIUM VIRGINIANUM WHOLE
(UNII:604NK4250S); PLATANUS ORIENTALIS POLLEN
(UNII:Y1A4835L6K)

LYCOPUS VIRGINICUS (UNII:TW5125Q6F); ACONITUM
NAPELLUS (UNII:U0NQ8555JD); EUPHRASIA STRICTA
(UNII:C9642I91WL); SANGUINARIA CANADENSIS ROOT
(UNII:N9288CD508); TRILLIUM ERECTUM ROOT
(UNII:AHW6F0T2X0); PROPYL PARABEN (UNII:Z8IX2SC1OH);
PHYTOLACCA AMERICANA ROOT (UNII:11E6VI8VEG);
MELEAGRIS GALLOPAVO FEATHER (UNII:CAC78E2Q9S);
LYCOPERDON UTRIFORME FRUITING BODY
(UNII:K2A74U428F); LEDUM PALUSTRE TWIG
(UNII:877L01IZ0P); FELIS CATUS HAIR (UNII:1564HD0N96);
ROSA CANINA FLOWER (UNII:81MCR2UQ6Q); CINNAMON
(UNII:5S29HWU6QB); HERRING, UNSPECIFIED
(UNII:34EX28T4C1); HELIANTHEMUM CANADENSE
(UNII:46G3W789Q3); ANTHOXANTHUM ODORATUM POLLEN
(UNII:2KIK19R45Y); POA PRATENSIS POLLEN
(UNII:SCB8J7LS3T); GELSEMIUM SEMPERVIRENS ROOT
(UNII:639KR60Q1Q); AMARANTH (UNII:37RBV3X49K); PHLEUM
PRATENSE POLLEN (UNII:65M88RW2EG); GINGER
(UNII:C5529G5JPQ); ANSER ANSER FEATHER
(UNII:15XI414745); QUAHOG, UNSPECIFIED (UNII:226LY0AFR9);
FESTUCA PRATENSIS POLLEN (UNII:A0WFQ8P6N1);
GOLDENSEAL (UNII:ZW3Z11D0JV); HADDOCK
(UNII:0WLY635722); EQUUS CABALLUS SKIN
(UNII:88VZV9HGT4); CHELIDONIUM MAJUS
(UNII:7E889U5RNN); SERINUS CANARIA FEATHER
(UNII:9EL3384IQY); SHRIMP, UNSPECIFIED (UNII:1891LE191T);
HOUSE DUST (UNII:EYO007VX98); CASEIN, LACTOCOCCUS
LACTIS CULTURED, PENICILLIUM ROQUEFORTI CULTURED,
AGED (UNII:IYI0G2057S); YUCCA FILAMENTOSA
(UNII:T6VR38UJ9I); WHEAT GLUTEN (UNII:1534K8653J);
TOXICODENDRON PUBESCENS LEAF (UNII:6IO182RP7A);
SAMBUCUS NIGRA FLOWERING TOP (UNII:CT03BSA18U);
CAPRA HIRCUS HAIR (UNII:16M9MK8C4W); OYSTER SHELL
CALCIUM CARBONATE, CRUDE (UNII:2E32821G6I); AMBROSIA
ARTEMISIIFOLIA (UNII:9W34L2CQ9A); DATURA STRAMONIUM
(UNII:G6W4F0V8Z3); ULEX EUROPAEUS FLOWER
(UNII:398DBS1PXN); BELLIS PERENNIS (UNII:2HU33I03UY);
TOBACCO LEAF (UNII:6YR2608RSU); GALLUS GALLUS FEATHER
(UNII:1FCM16V0FV); SULFUR (UNII:70FD1KFU70); HAZELNUT,
UNSPECIFIED (UNII:IW0OM96F6O); RYE (UNII:0R4AQI398X);
LAMB (UNII:FOF26T73HA); COD, UNSPECIFIED
(UNII:8D6Q5LNG3D); PTELEA TRIFOLIATA BARK
(UNII:5KQR6FTT0D); ULMUS GLABRA POLLEN
(UNII:T2K08L297Q); CANIS LUPUS FAMILIARIS HAIR
(UNII:05S7L91ZTR); TUNA, UNSPECIFIED (UNII:V2T3IHT3E2);
SCALLOP, UNSPECIFIED (UNII:D380C73WOU); CLADOSPORIUM
HERBARUM (UNII:O64JF1198); SODIUM COPPER
CHLOROPHYLLIN (UNII:1D276TYV9O); ASPARTAME
(UNII:Z0H242BBR1); POPULUS NIGRA POLLEN
(UNII:0MGE63QPFJ); HUMAN SKIN (UNII:0EE2343509);
ELYMUS REPENS ROOT (UNII:3IXW0F6P8W); FD&C RED
NO. 3 (UNII:PN2ZH5LOQY); ASPERGILLUS NIGER VAR. NIGER
(UNII:9IOA40ANG6); FELIS CATUS SKIN (UNII:5308ED00EL);

Cow milk, Skim milk,
Cow milk fat, Casein
Lactococcus Lactis
cultured, Casein
lactococcus lactis
penicillium roqueforti
cultured, Casein
lactococcus lactis
cultured penicillium
camemberti cultured,
Egg, Felis catus skin,
Canis lupus familiaris
skin, Oryzctolagus
cuniculus skin, Equus
caballus skin, Serinus
canaria feather, gallus
gallus feather, Anas
platyrhynchos feather,
Anser anser feather,
melopsittacus undulatus
feather, Phasianus
colchicus feather,
Meleagris gallopavo
feather, Felis catus hair

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label aa4f-
12dd73dffe77

SACCHAROMYCES CEREVISIAE (UNII:978D8U419H); FD&C YELLOW NO. 5 (UNII:I753WB2F1M); ARTEMISIA VULGARIS ROOT (UNII:32MP823R8S); MESOCRICETUS AURATUS HAIR (UNII:EFG2YD102P); USTILAGO MAYDIS (UNII:4K7Z7K7SWG); LACTOSE (UNII:J2B2A4N98G); CORN (UNII:0N8672707O); OAT (UNII:Z6J799EAJK); CALLUNA VULGARIS POLLEN (UNII:5Q1IE9V5YZ); PORK (UNII:O138UB266J); POPULUS TREMULOIDES BARK (UNII:5543O0CEID); ACID GREEN 50 (UNII:9B7E8Y9D0X); SODIUM TRIPOLYPHOSPHATE (UNII:5HK03SA80J); MATRICARIA RECUTITA (UNII:G0R4UBI2ZZ); ORYCTOLAGUS CUNICULUS HAIR (UNII:09N62XQ70Y); HUMAN HAIR (UNII:1AWP0DKL4I); POTASSIUM IODIDE (UNII:1C4QK22F9J); BROMINE (UNII:SBV4XY874G); PHASIANUS COLCHICUS FEATHER (UNII:95ZNE214EZ); ABRUS PRECATORIUS SEED (UNII:3OM8I6L7CD); TARAXACUM OFFICINALE (UNII:39981FM375); LOLIUM PERENNE POLLEN (UNII:4T81LB52R0); POTASSIUM BENZOATE (UNII:763YQN2K7K); FAGUS SYLVATICA POLLEN (UNII:63218N1ZBI); BROMUS SECALINUS POLLEN (UNII:Q4T1SJ3046); CAVIA PORCELLUS HAIR (UNII:KBA5Y6X57N); CRAB LEG, UNSPECIFIED (UNII:S1VF61QLO9); XEROPHYLLUM ASPHODELOIDES (UNII:9I4XB1GP2B); WHITE RICE (UNII:A195V20H7A); BARLEY (UNII:5PWM7YLI7R); SHEEP WOOL (UNII:503LYG631H); CYTISUS SCOPARIUS POLLEN (UNII:I0NS0040GH); ALFALFA (UNII:DJO934BRBD); TURKEY (UNII:8E9NT44R8I); SACCHARIN (UNII:FST467XS7D); BLACK MUSTARD SEED (UNII:8LTY55LQ8D); TROUT, UNSPECIFIED (UNII:7T17U5PF2U); GARLIC (UNII:V1V998DC17); CORYLUS AMERICANA POLLEN (UNII:ZGS382Y3AV); APIS MELLIFERA (UNII:7S82P3R43Z); PEANUT (UNII:QE1QX6B99R); SOLANUM NIGRUM WHOLE (UNII:0FMD6WV47M); COW MILK FAT (UNII:463JZS0XJ3); HOLCUS LANATUS POLLEN (UNII:70O1TP6H01); ATROPA BELLADONNA (UNII:WQZ3G9PF0H); ASCORBIC ACID (UNII:PQCK8PD0R); SKIM MILK (UNII:6A001Y4M5A); SODIUM NITRITE (UNII:M0KG633D4F); HUMAN DANDER (UNII:30X630U81C); DIANTHUS CARYOPHYLLUS FLOWER (UNII:B0D836E90S); BOS TAURUS HAIR (UNII:TOQ97Z8644); NARCISSUS PSEUDONARCISSUS (UNII:Q2D0SKW2P4); BETULA PENDULA POLLEN (UNII:ZL5TV40C5Y); SODIUM CHLORIDE (UNII:451W47IQ8X); ARSENIC TRIOXIDE (UNII:S7V92P67HO); SODIUM DITHIONATE (UNII:RPF7Z41GAW); ALOPECURUS PRATENSIS POLLEN (UNII:DG1ZL6W96V); EQUUS CABALLUS HAIR (UNII:4F35XG0149); CHICKEN (UNII:0X8Q245Y7B); ALETRIS FARINOSA ROOT (UNII:O021JGR97X); ALLYLTHIOUREA (UNII:706IDJ14B7); CYNARA SCOLYMUS LEAF (UNII:B71UA545DE); FD&C BLUE NO. 2 (UNII:L06K8R7DQK); SODIUM BENZOATE (UNII:OJ245FE5EU); POPULUS TREMULOIDES LEAF (UNII:7IIH57D9E0); AVENA SATIVA POLLEN (UNII:A7IKY24TR7); OYSTER, UNSPECIFIED (UNII:S614XWR17V); ORYCTOLAGUS CUNICULUS SKIN (UNII:Z91WAU43WC); CASEIN, LACTOCOCCUS LACTIS CULTURED, AGED (UNII:CJP9NL7JSJ); AMANITA MUSCARIA FRUITING BODY (UNII:DIF093I037); MONOSODIUM GLUTAMATE (UNII:W81N5U6R6U); FD&C YELLOW NO. 6 (UNII:H77VEI93A8); FRAXINUS EXCELSIOR POLLEN

(UNII:1824QUA0U3); ANACARDIUM OCCIDENTALE FRUIT (UNII:4A10JR4E7E); ENGLISH WALNUT (UNII:1V3SHR7QB7); QUERCUS ALBA POLLEN (UNII:Z4Y9ZSV4KK); PRIMULA VULGARIS (UNII:KZ3PRK2V0J); CRATAEGUS MONOGYNA POLLEN (UNII:X6049S3TX1); CARMOISINE (UNII:DR4641L47F); AETHUSA CYNAPIUM (UNII:M6936L953C); 2-PHENYLPHENOL (UNII:D343Z75HT8); ECHINACEA, UNSPECIFIED (UNII:4N9P6CC1DX); URTICA URENS (UNII:IHN2NQ5OF9); ONION (UNII:492225Q21H); MENTHA PIPERITA (UNII:79M2M2UDA9); CYNOSURUS CRISTATUS POLLEN (UNII:SES68PF95U); BRYONIA ALBA ROOT (UNII:T7J046YI2B); LILIUM CANDIDUM FLOWER (UNII:COV655U2CJ); SALMON, UNSPECIFIED (UNII:6122W2M0GB); DYSPHANIA AMBROSIOIDES (UNII:4H5RSU087I); HYOSCYAMUS NIGER (UNII:4WRK2153H3); WYETHIA HELENIOIDES ROOT (UNII:J10PD1AQ0N); NUTMEG (UNII:AE24M3MQ9); ALPINE STRAWBERRY (UNII:CG6IX3GCMU); ARUNDO PLINIANA ROOT (UNII:ZXE7LB03WC); HISTAMINE DIHYDROCHLORIDE (UNII:3POA0Q644U); D&A;C YELLOW NO. 10 (UNII:35SW5USQ3G); SOLANUM TUBEROSUM (UNII:2A8I57T4MX); PULSATILLA VULGARIS (UNII:I76KB35JEV); GLYCYRRHIZA GLABRA (UNII:2788Z9758H); SCHOENOCALON OFFICINALE SEED (UNII:6NAF1689IO); DROSER A ROTUNDIFOLIA (UNII:QR44N9XPJQ); EGG (UNII:291P45F896); BEEF (UNII:4PIB2155QP); ANAS PLATYRHYNCHOS FEATHER (UNII:83B65P4796); SALIX ALBA POLLEN (UNII:WQ580684IZ); COW MILK (UNII:917J3173FT); JUNIPERUS VIRGINIANA TWIG (UNII:532BCG080L); BRAZIL NUT (UNII:XKR79OET1K); ACID RED 1 (UNII:3365R6427R); SOLANUM LYCOPERSICUM (UNII:0243Q4990L); MELOPSITTACUS UNDULATUS FEATHER (UNII:1XY644QKWG); ECHINOCHLOA CRUS-GALLI POLLEN (UNII:6941ZR795V); SOLANUM DULCAMARA TOP (UNII:KPS1B1162N); CAPSICUM (UNII:00UK7646FG); PONCEAU 4R (UNII:Z525CBK9PG); CAFFEINE (UNII:3G6A5W338E); CASEIN, LACTOCOCCUS LACTIS CULTURED, PENICILLIUM CAMEMBERTI CULTURED, AGED (UNII:G44KT17KIS); LYCOPODIUM CLAVATUM SPORE (UNII:C88X29Y479); AGROSTIS GIGANTEA POLLEN (UNII:HU8V6E7HOA); ONOSMODIUM VIRGINIANUM WHOLE (UNII:604NK4250S); WHEAT (UNII:4J2I0SN84Y); PLATANUS ORIENTALIS POLLEN (UNII:Y1A4835L6K)

PEANUT (UNII:QE1QX6B99R); PROPYL PARABEN (UNII:Z8IX2SC1OH); SODIUM NITRITE (UNII:M0KG633D4F); MODIFIED CORN STARCH (1-OCTENYL SUCCINIC ANHYDRIDE) (UNII:461P5CJN6T); AMARANTH (UNII:37RBV3X49K); CITRULLUS COLOCYNTHIS FRUIT PULP (UNII:23H32AOH17); SODIUM CHLORIDE (UNII:451W471Q8X); ARSENIC ACID (UNII:N7CIZ75ZPN); WHEAT GLUTEN (UNII:1534K8653J); CASEIN (UNII:48268V50D5); SODIUM BENZOATE (UNII:OJ245FE5EU); SOYBEAN (UNII:L7HT8F1ZOD); MONOSODIUM GLUTAMATE (UNII:W81N5U6R6U); FD&A;C YELLOW NO. 6 (UNII:H77VEI93A8); ENGLISH WALNUT (UNII:1V3SHR7QB7); URTICA URENS (UNII:IHN2NQ5OF9); HYOSCYAMUS NIGER (UNII:4WRK2153H3); FD&A;C YELLOW NO. 5 (UNII:I753WB2F1M); HISTAMINE DIHYDROCHLORIDE (UNII:3POA0Q644U); D&A;C YELLOW NO. 11

Apis 30c, Arsenicum 30c, Baptisia 30c, Caseinum 30c, Colocynthis 30c, Corn 30c, Food Dye Additives 30c, Food Preservatives 30c, Histaminum 30c, Hyoscyamus 30c, Mixed Nuts 30c, Modified Corn Starch 30c, MSG 30c, Natrum Mur 30c, Phosphorous 30c, Sacharrin 30c, Soy 30c, Strawberry 30c, Uritca

Drug XML 05fc002c-
PDF b306-4e10-
label 9b68-
32c3c8a8bf0c

(UNII:44F3HYL954); APIS MELLIFERA VENOM
(UNII:76013O881M); PHOSPHORUS (UNII:27YLU75U4W); EGG
(UNII:291P45F896); CORN (UNII:0N8672707O); STRAWBERRY
(UNII:4J2TY8Y81V); METHYLPARABEN (UNII:A2I8C7HI9T);
BAPTISIA TINCTORIA (UNII:5K1UO2888Y); ALMOND
(UNII:3Z252A2K9G); SACCHARIN (UNII:FST467XS7D)

Urens 30c, Wheat Gluten
30c, Whole Egg 30c

PHYTOLACCA AMERICANA ROOT (UNII:11E6VI8VEG); SODIUM
NITRITE (UNII:M0KG633D4F); FORMIC ACID
(UNII:0YIW783RG1); STRYCHNOS NUX-VOMICA SEED
(UNII:269XH13919); PHOSPHORIC ACID (UNII:E4GA8884NN);
SODIUM SULFITE (UNII:VTK01UQK3G); GAMBOGE
(UNII:7556HJ7587); SODIUM BICARBONATE
(UNII:8MDF5V39QO); SODIUM NITRATE (UNII:8M4L3H2ZVZ);
SACCHARIN (UNII:FST467XS7D)

Natural Medicine

Drug
PDF
label

XML

cc46b3e6-
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► [DailyMed](#)

7.3 Clinical Trials



7.3.1 ClinicalTrials.gov



4 items



Pretympanoplasty Assessment of Patency and Mucociliary Function of Eustachian Tube

CTID: [NCT05229380](#)

Status: Not yet recruiting

Date: 2022-02-08

Microbiome and Non-caloric Sweeteners in Humans

CTID: [NCT03708939](#)

Phase: N/A Status: Completed

Date: 2021-08-04

Effect of Stevioside in Postprandial Glucose in Healthy Adults

CTID: [NCT01488383](#)

Phase: N/A Status: Withdrawn

Date: 2015-09-09

Efficacy Study of Folic Acid Supplementation in Adolescent Epileptics

CTID: [NCT02318446](#)

Phase: Phase 3 Status: Unknown status

Date: 2014-12-17

► [ClinicalTrials.gov](#)

7.4 Drug Idiosyncrasies



Idiosyncratic effects of saccharin on the liver were reported in a 70-year-old woman. Increased activities of [alanine](#) aminotransferase, [aspartate](#) aminotransferase, gamma-glutamyl transferase and alkaline phosphatase were found after oral administration of three pharmaceutical drugs of which saccharin was the only common constituent. The drugs were [lorazepam](#), [dihydroergocristine](#) and [chlordemethyldiazepam](#). Exposure to saccharin alone reproduced the effects.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 574 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

8 Food Additives and Ingredients



8.1 Food Additive Classes



JECFA Functional Classes

Food Additives -> SWEETENER;

► [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

8.2 FDA Substances Added to Food



Substance	SACCHARIN
Used for (Technical Effect)	NON-NUTRITIVE SWEETENER
Document Number (21 CFR)	172.812 180.37

► [FDA Center for Food Safety and Applied Nutrition \(CFSAN\)](#)

8.3 Evaluations of the Joint FAO / WHO Expert Committee on Food Additives - JECFA



Chemical Name	SACCHARIN
Evaluation Year	1993

ADI	0-5 mg/kg bw
Comments	GROUP ADI FOR SACCHARIN AND ITS CALCIUM , POTASSIUM AND SODIUM SALTS
Report	TRS 837-JECFA 41/17
Tox Monograph	FAS 32-JECFA 41/105

► [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

9 Agrochemical Information



9.1 Agrochemical Transformations



[1,2-benzisothiazol-3\(2H\)-one](#),1,1-dioxide is a known environmental transformation product of [oxasulfuron](#), [metsulfuron](#), [metsulfuron-methyl](#), [propoxycarbazone](#), and [tribenuron-methyl](#).

S78 | [SLUPESTTPS](#) | *Pesticides and TPs from SLU, Sweden* | [DOI:10.5281/zenodo.4687924](#)

► [NORMAN Suspect List Exchange](#)

[1,2-benzisothiazol-3\(2H\)-one](#),1,1-dioxide is a known environmental transformation product of [Oxasulfuron](#).

M07 (saccharin) is a known environmental transformation product of [Propoxycarbazone](#).

Saccharin (IN-00581) is a known environmental transformation product of [Tribenuron-methyl](#) and [Metsulfuron-methyl](#).

S60 | [SWISSEST19](#) | *Swiss Pesticides and Metabolites from Kiefer et al 2019* | [DOI:10.5281/zenodo.3544759](#)

► [NORMAN Suspect List Exchange](#)

10 Pharmacology and Biochemistry



10.1 MeSH Pharmacological Classification



Sweetening Agents

Substances that sweeten food, beverages, medications, etc., such as sugar, saccharine or other low-calorie synthetic products. (From Random House Unabridged Dictionary, 2d ed) (See [all compounds classified as Sweetening Agents](#).)

► [Medical Subject Headings \(MeSH\)](#)

10.2 Absorption, Distribution and Excretion



TRANSPLACENTAL TRANSFER OF ... (14)C-SACCHARIN ADMIN BY IV INFUSION TO RHESUS MONKEYS IN LATE PREGNANCY, WAS RAPID, BUT SLIGHT. (14)C WAS CLEARED MORE SLOWLY FROM FETAL THAN FROM MATERNAL BLOOD, & WAS DISTRIBUTED IN ALL FETAL TISSUES EXAMINED ... WAS ONLY BIOTRANSFORMED TO LIMITED EXTENT & WAS RAPIDLY EXCRETED

The Chemical Society. Foreign Compound Metabolism in Mammals. Volume 2: A Review of the Literature Published Between 1970 and 1971. London: The Chemical Society, 1972., p. 150

► [Hazardous Substances Data Bank \(HSDB\)](#)

Three groups of five men were given [sodium saccharin](#) in single oral doses of 50, 150 or 333 mg/60 kg bw. Peak plasma concentrations occurred between 30 and 60 min after dosing, and 60 and 76% was excreted unchanged in urine at 6 and 24 h, respectively. /[Sodium saccharin](#)/

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 570 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

IN 3 VOLUNTEERS, 85-92% OF DOSES OF 1 G 3-(14)C-SACCHARIN ADMIN ORALLY FOR 21 DAYS WAS EXCRETED UNCHANGED IN THE URINE WITHIN 24 HR; NO METABOLITES WERE FOUND. WITHIN 48 HR, 92.3% OF A DOSE OF 500 MG (14)C-SACCHARIN WAS EXCRETED IN THE URINE & 5.8% IN THE FECES.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 151 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

After administration of 1-g doses of soluble ([sodium](#)) saccharin [form not specified] to three men, saccharin was excreted in the urine quantitatively unchanged by two of the subjects within 48 hr. In a subsequent experiment involving six subjects, none excreted the dose quantitatively within 72 hr, but no metabolism of saccharin was detected. /[Sodium saccharin](#)/

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 570 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Absorption, Distribution and Excretion (Complete) data for SACCHARIN (13 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

10.3 Metabolism / Metabolites



... 3-(14)C-SACCHARIN WAS EXCRETED UNCHANGED, MAINLY IN THE URINE (85-92% IN 24 HR) BY ADULT HUMAN SUBJECTS, BOTH BEFORE & AFTER TAKING 1 G OF SACCHARIN DAILY FOR 21 DAYS; NO METABOLITE OF SACCHARIN WAS FOUND. THESE RESULTS WERE AMPLY CONFIRMED IN ANIMAL EXPERIMENTS, IN WHICH ORALLY ADMIN (14)C-SACCHARIN WAS EXCRETED ENTIRELY UNCHANGED BY RATS ON A NORMAL DIET & BY RATS ON A DIET CONTAINING 1% & 5% OF SACCHARIN FOR UP TO 12 MO. 80-90% OF THE DOSE WAS EXCRETED IN THE URINE, 10-20% IN THE FECES; NO (14)CO₂ WAS FOUND IN THE EXHALED AIR, & NO (14)CO₃(2-) OR [2-SULFAMOYL BENZOIC ACID](#) IN THE URINE.

The Chemical Society. Foreign Compound Metabolism in Mammals. Volume 5: A Review of the Literature Published during 1976 and 1977. London: The Chemical Society, 1979., p. 419

► [Hazardous Substances Data Bank \(HSDB\)](#)

YIELDS IN MONKEYS [SULFAMOYLBENZOIC ACID](#) & [O-SULFOBENZOIC ACID](#). /FROM TABLE/

Goodwin, B.L. Handbook of Intermediary Metabolism of Aromatic Compounds. New York: Wiley, 1976., p. S-1

► [Hazardous Substances Data Bank \(HSDB\)](#)

EXPOSURE OF MALE CHARLES RIVER [CDI](#) RATS TO 5% SACCHARIN DIET IN UTERO & THROUGHOUT WEANING, DID NOT INDUCE DETECTABLE METABOLISM. NO METABOLITES WERE DETECTED IN URINE OF NORMAL RATS GIVEN TRACER DOSE. PRETREATMENT WITH [3-METHYLCHOLANTHRENE](#) DID NOT INDUCE SACCHARIN METABOLISM.

PMID:472722

SWEATMAN TW, RENWICK AG; SCIENCE 205 (4410): 1019 (1979)

► [Hazardous Substances Data Bank \(HSDB\)](#)

One female and two male volunteers excreted 85-92% of a dose of 1g (3-14)C- saccharin unchanged in the urine within 24 hr, before or after taking 1 g saccharin daily for 21 days; no metabolites were found.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 570 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Within 48 h, 92% of a dose of 500 mg [¹⁴C]saccharin taken by six male volunteers was excreted in the urine and 5.8% in the faeces. Analysis of urine and feces by highperformance liquid chromatography and thin-layer chromatography revealed only unmetabolized saccharin.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 570 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

10.4 Biological Half-Life



In three adult men given an intravenous bolus of 10 mg/kg bw [sodium saccharin](#), the plasma concentration-time curve fitted a two-compartment open model with a terminal half-life of 70 min. /[Sodium saccharin](#)/

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 570 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Six women with an average oral daily intake of 100-300 mg saccharin (form not specified) had maximum plasma concentrations after 0.5-1 hr and an elimination half-life of 7.5 hr.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 569 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

10.5 Mechanism of Action



...it has been shown that the activation of particular T2R bitter taste receptors is partially involved with the bitter aftertaste sensation of saccharin and [acesulfame-K](#). ... /This study/ addressed the question of whether /they/ could stimulate transient receptor potential vanilloid-1 (TRPV1) receptors, as these receptors are activated by a large range of structurally different chemicals. Moreover, TRPV1 receptors and/or their variants are found in taste receptor cells and in nerve terminals throughout the oral cavity. Hence, TRPV1 activation could be involved in the ... aftertaste or even contribute to the poorly understood metallic taste sensation. Using Ca(2+) imaging on TRPV1 receptors heterologously expressed in the human embryonic kidney (HEK) 293 cells and on dissociated primary sensory neurons,... /it was found/ that in both systems, .../sweeteners/ activate TRPV1 receptors, and, moreover, they sensitize these channels to acid and heat. ... /it was/also found that TRPV1 receptors were activated by CuSO(4), ZnSO(4), and FeSO(4), three salts known to produce a metallic taste sensation. In summary, .../the/ results identify a novel group of compounds that activate TRPV1 and, consequently, provide a molecular mechanism that may account for off tastes of sweeteners and metallic tasting salts.

Riera CE, et al; *Am J Physiol Regul Integr Comp Physiol* 293 (2): R626-34 (2007)

► [Hazardous Substances Data Bank \(HSDB\)](#)

10.6 Human Metabolite Information



10.6.1 Cellular Locations

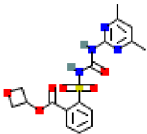


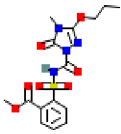
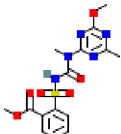
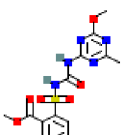
Cytoplasm
Extracellular

► [Human Metabolome Database \(HMDB\)](#)

10.7 Transformations



9 items					
Search			SORT BY Predecessor Name - A to Z		
Predecessor	Predecessor Name	Successor	Successor Name	Transformation	Evidence DOI
	oxasulfuron		1,2-benzisothiazol-3(2H)-one,1,1-dioxide	Environmental	10.1021/acs.est.1c0046

	propoxycarbazone		1,2-benzisothiazol-3(2H)-one,1,1-dioxide	Environmental	10.1021/acs.est.1c0046
	tribenuron-methyl		1,2-benzisothiazol-3(2H)-one,1,1-dioxide	Environmental	10.1021/acs.est.1c0046
	metsulfuron-methyl		1,2-benzisothiazol-3(2H)-one,1,1-dioxide	Environmental	10.1021/acs.est.1c0046
	metsulfuron		1,2-benzisothiazol-3(2H)-one,1,1-dioxide	Environmental	10.1021/acs.est.1c0046

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► NORMAN Suspect List Exchange

11 Use and Manufacturing



11.1 Uses



EPA CPDat Chemical and Product Categories

19 items	↓
Search	SORT BY Category - A to Z ▼
artificial sweetener Categorization Type: Reported Functional Use	
artificial sweeteners Categorization Type: Reported Functional Use	
cosmetics Categorization Type: Reported Functional Use	
flavoring agent Categorization Type: Reported Functional Use	
flavoring and nutrient Categorization Type: OECD Functional Use	

<< First < Previous Page 1 of 4 Next > Last >>

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

► [EPA Chemical and Products Database \(CPDat\)](#)

Sources/Uses

Used as a non-nutritive sweetener, pharmaceutical aid (flavor), and in electroplating-bath brighteners; [Merck Index] Used as a cattle feed additive and in tobacco processing; [HSDB] Permitted for use as an inert ingredient in non-food pesticide products; [EPA]

Merck Index - O'Neil MJ, Heckelman PE, Dobbelaar PH, Roman KJ (eds). The Merck Index, An Encyclopedia of Chemicals, Drugs, and Biologicals, 15th Ed. Cambridge, UK: The Royal Society of Chemistry, 2013.

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

Industrial Processes with risk of exposure

[Electroplating](#) [Category: Plate]

[Farming \(Feed Additives\)](#) [Category: Industry]

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

Non-nutritive sweetener; pharmaceutical aid (flavor). In formulations for electroplating-bath brighteners

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1435

► [Hazardous Substances Data Bank \(HSDB\)](#)

A sweetening agent in Aromatic Cascara Sagrada Fluid extract and highly alcoholic preparations. ... It is used as a sweetening agent in vehicles, canned foods, and beverages and in diets for diabetics to replace [sucrose](#).

Troy, D.B. (Ed); Remington The Science and Practice of Pharmacy. 21 st Edition. Lippincott Williams & Williams, Philadelphia, PA 2005, p. 1067

► [Hazardous Substances Data Bank \(HSDB\)](#)

Add sweetness with or without the extra calories ... /in/ beverages, baked goods, confections, table-top sugar, substitutes, many processed foods

FDA; Food Ingredients and Colors. Revised April 2010. Available from, as of Jun 7, 2011:

<https://www.fda.gov/Food/FoodIngredientsPackaging/ucm094211.htm>

► [Hazardous Substances Data Bank \(HSDB\)](#)

NON-CALORIC SYNTHETIC SWEETENER IN TABLETS, LIQ PRODUCTS, SOFT DRINKS, DIETETIC FOODS, MISC PHARMACEUTICALS, CHEWING GUM, TOOTH PASTE, SMOKELESS TOBACCO PRODUCTS; ELECTROPLATING BATH ADDITIVE; CATTLE FEED ADDITIVE; ANTISEPTIC (FORMER USE); PRESERVATIVE TO RETARD FERMENTATION OF FOOD (FORMER USE).

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

Saccharin has been used in the sweetening of pharmaceutical tablets and in processing of tobacco.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at:

<https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 125 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.1.1 Use Classification



Food Additives -> SWEETENER; -> JECFA Functional Classes

► [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

Cosmetics -> Masking; Oral care

S13 | *EUCOSMETICS* | *Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)* | [DOI:10.5281/zenodo.2624118](https://doi.org/10.5281/zenodo.2624118)

► [NORMAN Suspect List Exchange](#)

Environmental transformation -> Pesticide transformation products (metabolite, successor)

S60 | *SWISSPEST19* | *Swiss Pesticides and Metabolites from Kiefer et al 2019* | [DOI:10.5281/zenodo.3544759](https://doi.org/10.5281/zenodo.3544759)

► [NORMAN Suspect List Exchange](#)

11.1.2 Industry Uses



Adhesives and sealant chemicals

Other (specify)

<https://www.epa.gov/chemical-data-reporting>

► [EPA Chemicals under the TSCA](#)

11.1.3 Household Products



Household & Commercial/Institutional Products

Information on 1 consumer products that contain Saccharin in the following categories is provided:

- Home Maintenance

► [Consumer Product Information Database \(CPID\)](#)

11.2 Methods of Manufacturing



In most countries, commercial saccharin is produced by the Remsen-Fahlberg process ... **Toluene** is used as the starting material and reacted with **chlorosulfonic acid** to a mixture of isomeric **toluene** sulfochlorides. In the presence of **ammonia**, 2-toluene **sulfochloride** forms 2-toluene sulfonic acid amide which is oxidized under appropriate conditions to saccharin. Potential oxidizing agents are **potassium permanganate** or **chromic acid**.

von Rymon Lipinski GW; *Ullmann's Encyclopedia of Industrial Chemistry* 7th ed. (2010). NY, NY: John Wiley & Sons; Sweeteners.
Online Posting Date: June 15, 2000

► [Hazardous Substances Data Bank \(HSDB\)](#)

In the United States, the Maumee process is used. This starts from either [anthranilic acid](#) or its methyl ester, which can be obtained from [phthalic acid anhydride](#). With [sodium nitrite](#), [anthranilic acid](#) forms a diazonium compound, which is reacted with [sulfur dioxide](#) or sulfites, and chlorinated to [2-chlorosulfonylbenzoic acid methyl ester](#). In the presence of [ammonia](#), this ester yields the respective amide, from which, after de-esterification, saccharin is obtained. Reaction with [sodium hydroxide](#) or [calcium hydroxide](#) forms the respective saccharin salts.

von Rymon Lipinski GW; Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (2010). NY, NY: John Wiley & Sons; Sweeteners. Online Posting Date: June 15, 2000

► [Hazardous Substances Data Bank \(HSDB\)](#)

Saccharin is dissolved in an equimolar quantity of aqueous [sodium hydroxide](#), and the solution is concentrated to crystallization. /[Saccharin sodium](#)/

Troy, D.B. (Ed); Remington The Science and Practice of Pharmacy. 21 st Edition. Lippincott Williams & Williams, Philadelphia, PA 2005, p. 1067

► [Hazardous Substances Data Bank \(HSDB\)](#)

Saccharin is reacted with a semimolar quantity of [calcium hydroxide](#) in aqueous medium, and the resulting solution is concentrated to crystallization. /[Saccharin calcium](#)/

Troy, D.B. (Ed); Remington The Science and Practice of Pharmacy. 21 st Edition. Lippincott Williams & Williams, Philadelphia, PA 2005, p. 1067

► [Hazardous Substances Data Bank \(HSDB\)](#)

A mixture of toluenesulfonic acids is converted into the [sodium](#) salt then distilled with [phosphorus trichloride](#) and [chlorine](#) to obtain the [o-toluene sulfonyl chloride](#) which, by means of [ammonia](#), is converted into o-toluenesulfamide. This is oxidized with [permanganate](#), treated with acid, and saccharin crystallized out.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1102

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.3 Impurities



o- & [p-Toluenesulfonamide](#); 1,2-benzisothiazol-1,1-dioxide; [1,2-benzisothiazoline-1,1-dioxide](#); 3-aminobenzisothiazol-1,1-dioxide; 5- & [6-chlorosaccharin](#); [ammonium saccharin](#); methyl saccharin; [diphenyl sulfone](#); ditolylsulphone isomers; o- & [p-sulfamoylbenzoic acid](#); [o-chlorobenzoic acid](#); [o-sulfobenzoic acid](#) (& ammonium salt); [n-tetracosane](#); bis(4-carboxyphenyl)sulfone; [toluene-2,4-disulfonamide](#); saccharin-o-[toluenesulfonamide](#); saccharin-6-sulfonamide; N-methyl-o-toluene-sulfonamide; [methyl-o-chlorobenzoate](#); 4,4'-dibenzoylsulfone; 2- or 3-carboxy thioxanthone-5-dioxide; o-sulfobenzamide; methyl-o-sulfamoylbenzoate; methyl-N-methylsulfamoylbenzoate; saccharin-o-toluenesulfoxylimide; & other /Reported impurities in saccharin & [sodium saccharin](#)/

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 113 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.4 Formulations / Preparations



Grades: Commercial; CP /Chemically pure: A grade designation signifying a minimum of impurities, but not 100% pure;/ USP /United States Pharmacopeia;/ FCC /Food Chemicals Codex/.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1102

► [Hazardous Substances Data Bank \(HSDB\)](#)

Sodium saccharin FCC (Food Chemicals Codex) is available in the USA in four grades: spray-dried, containing 3.0% moisture; powder, containing 5.0-5.8% moisture; pelletized, containing 10.5-11.5% moisture; and granular, containing 14.0-15.0% moisture. Each of these grades meets or exceeds the following Food Chemicals Codex specifications: 98-101% active ingredient on an anhydrous basis, 3-15% [water](#), 100 mg/kg toluenesulphonamides, 30 mg/kg [selenium](#), 10 mg/kg heavy metals (as lead) and 3 mg/kg [arsenic](#). /**Sodium saccharin**/

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 119 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Trade Names: **Assugrin** vollsuss (also contains [sodium cyclamate](#)); Garantose; Glucid; Gluside; Hermesetas; Kandiset; Natreen (also contains [sodium cyclamate](#)); Sacarina; 550 Saccharin; Saccharina; Saccharinol; Saccharinose; Saccharol; Saxin; Sucre Edulcor; Sucrette; Sykose; Zaharina.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 111 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Available in the USA as saccharin insoluble powder FCC (Food Chemicals Codex): 98-101% active ingredient on an anhydrous basis, a maximum of 100 mg/kg toluenesulphonamides, 30 mg/kg [selenium](#), 10 mg/kg heavy metals (as lead) & 3 mg/kg [arsenic](#) ... Available in the USA as a USP grade containing 98-101% active ingredient on an anhydrous basis.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 112 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.5 Consumption Patterns



Global consumption (1000 tons): 37

Buerge IJ et al; Environ Sci Technol 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

The USA consumption pattern for saccharin (all forms) in 1976 has been estimated as follows: 77% in food uses: 45% in soft drinks, 18% in 'tabletop' sweetener, and 14% in other foods such as fruits, premixes, juices, sweets, chewing gum and jellies; and 23% in nonfood items: 10% in cosmetics such as toothpaste, mouthwash and lipstick, 7% in pharmaceuticals such as coatings on pills, 2% in smokeless tobacco products such as chewing tobacco and snuff, 2% in electroplating, 1% in cattle feed and 1% in miscellaneous uses. /Saccharin (all forms)/

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at:

<https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 125 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.6 U.S. Production



Aggregated Product Volume

2019: <1,000,000 lb

2018: <1,000,000 lb

2017: <1,000,000 lb

2016: <1,000,000 lb

<https://www.epa.gov/chemical-data-reporting>

► [EPA Chemicals under the TSCA](#)

(1977) AT LEAST 2.18X10+9 G (EST-INCL SALT)

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

(1982) AT LEAST 2.00X10+9 G (EST)

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

(1985) Not reported

USITC. SYN ORG CHEM-U.S. PROD/SALES 1985 p.125

► [Hazardous Substances Data Bank \(HSDB\)](#)

1,2-Benzisothiazol-3(2H)-one, 1,1-dioxide is listed as a High Production Volume (HPV) chemical (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. 1,2-Benzisothiazol-3(2H)-one, 1,1-dioxide (81-07-2). Available from, as of July 5, 2011: <https://www.epa.gov/hpv/pubs/general/opptsrch.htm>

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more U.S. Production (Complete) data for SACCHARIN (6 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.7 U.S. Imports



(1977) 1.35X10+9 G

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

(1982) 1.34X10+9 G

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

(1985) 8.07X10+8 g.

BUREAU OF THE CENSUS. U.S. IMPORTS FOR CONSUMPTION AND GENERAL IMPORTS 1985 p.1-564

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.8 General Manufacturing Information



Industry Processing Sectors

Adhesive Manufacturing

Computer and Electronic Product Manufacturing

► [EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

1,2-Benzisothiazol-3(2H)-one, 1,1-dioxide: ACTIVE

<https://www.epa.gov/tsc-inventory>

► [EPA Chemicals under the TSCA](#)

In 1977, the FDA proposed a ban on saccharin because of the discovery of bladder tumors in some male rats fed with high doses of saccharin. Because no other nonnutritive sweetener was available at that time, the proposed ban faced strong opposition. Legislation to stay the ban has been passed in the U.S. Congress periodically. In December, 1991, the FDA withdrew its proposed ban. All saccharin-containing packaged products were required to carry a warning label indicating that saccharin has been determined to cause cancer in laboratory animals. In 2001, the warning label requirement was lifted by the Congress. In 2003, saccharin was delisted from California Proposition 65 (the so-called carcinogen list).

Lee TD; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). New York, NY: John Wiley & Sons; Sweeteners. Online Posting Date: 24 March 2006

► [Hazardous Substances Data Bank \(HSDB\)](#)

Industrial grade **sodium saccharin** is reportedly used as a brightener in **nickel**-plating baths, as an antistatic agent in plastics and textiles, as a polymer modifier and accelerator in photosensitive dispersions, and as a light fastness aid in nylon dyes. /[Sodium saccharin](#)/

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 125 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Compared with dilute [sucrose](#) solutions, the sweetness intensity of saccharin is about 550, whereas the values for its salts are about 450. At medium or elevated use levels, saccharin sweetness is accompanied by a metallic or bitter aftertaste. Several masking agents for this side-taste have been suggested, and sweetener blends, especially a blend of 1 part [sodium saccharin](#) to 9 - 10 parts [sodium cyclamate](#), are often used.

von Rymon Lipinski GW; *Ullmann's Encyclopedia of Industrial Chemistry* 7th ed. (2010). NY, NY: John Wiley & Sons; *Sweeteners*. Online Posting Date: June 15, 2000

► [Hazardous Substances Data Bank \(HSDB\)](#)

12 Identification



12.1 Analytic Laboratory Methods



Method: AOAC 969.27; Procedure: qualitative thin-layer chromatography; Analyte: saccharin; Matrix: nonalcoholic beverages; Detection Limit: not provided.

Official Methods of Analysis of AOAC International, 18th Edition Online. Saccharin (81-07-2). Available from, as of July 12, 2011: <https://www.aoac.org>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Method: AOAC 941.10; Procedure: qualitative test (organoleptic test, [phenol-sulfuric acid](#) test); Analyte: saccharin; Matrix: foods; Detection Limit: not provided.

Official Methods of Analysis of AOAC International, 18th Edition Online. Saccharin (81-07-2). Available from, as of July 12, 2011: <https://www.aoac.org>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Method: AOAC 973.29; Procedure: gravimetric method; Analyte: saccharin; Matrix: food; Detection Limit: not provided.

Official Methods of Analysis of AOAC International, 18th Edition Online. Saccharin (81-07-2). Available from, as of July 12, 2011: <https://www.aoac.org>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Method: AOAC 980.18; Procedure: differential pulse polarographic method; Analyte: saccharin; Matrix: food; Detection Limit: not provided.

Official Methods of Analysis of AOAC International, 18th Edition Online. Saccharin (81-07-2). Available from, as of July 12, 2011: <https://www.aoac.org>

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Analytic Laboratory Methods (Complete) data for SACCHARIN (10 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

12.2 Clinical Laboratory Methods



Gas chromatography/Electron Capture detection (GC/ECD) is used for determination of saccharin in blood. Limit of detection is 10 ug/l.

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 123 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

13 Safety and Hazards



13.1 Hazards Identification



13.1.1 GHS Classification



GHS Hazard Statements	Not Classified Reported as not meeting GHS hazard criteria by 510 of 525 companies (only ~ 2.9% companies provided GHS information). For more detailed information, please visit ECHA C&L website .
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► [European Chemicals Agency \(ECHA\)](#)

13.1.2 Health Hazards



SYMPTOMS: Symptoms of exposure to this compound include anorexia, nausea, vomiting, diarrhea and gastric hyperacidity. Other symptoms include coughing, chest pain and irritation of the eyes, nose and throat.

ACUTE/CHRONIC HAZARDS: When heated to decomposition this chemical emits very toxic fumes of NO_x, SO_x, **carbon monoxide** and **carbon dioxide**. This compound may cause skin, nose and throat irritation. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

13.1.3 Fire Hazards



Flash point data for this chemical are not available; however, it is probably combustible. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

13.1.4 Hazards Summary



May cause irritation; [Sigma-Aldrich MSDS]

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

13.2 First Aid Measures



13.2.1 First Aid



EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with [water](#) or [normal saline](#) solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician.

IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

SKIN: IMMEDIATELY flood affected skin with [water](#) while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and [water](#). If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of [water](#) to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital.

OTHER: Since this chemical is a known or suspected carcinogen you should contact a physician for advice regarding the possible long term health effects and potential recommendation for medical monitoring.

Recommendations from the physician will depend upon the specific compound, its chemical, physical and toxicity properties, the exposure level, length of exposure, and the route of exposure. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

13.3 Fire Fighting



Fires involving this material can be controlled with a dry chemical, [carbon dioxide](#) or [Halon](#) extinguisher. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

13.4 Accidental Release Measures



13.4.1 Disposal Methods



SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or [water](#); effects on animal and plant life; and conformance with environmental and public health regulations.

► [Hazardous Substances Data Bank \(HSDB\)](#)

Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U202, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

40 CFR 240-280, 300-306, 702-799 (7/1/89)

► [Hazardous Substances Data Bank \(HSDB\)](#)

A potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids. A potential candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids.

USEPA; Engineering Handbook for Hazardous Waste Incineration p.3-15 (1981) EPA 68-03-3025

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.4.2 Preventive Measures



SRP: In bulk storage or manufacturing situations where combustible dusts can collect in sufficient concentrations to give rise to an explosion/deflagration, reasonable precautions shall be taken to reduce or eliminate the hazard. Efforts shall be made to control or eliminate the five elements necessary to initiate a dust explosion. These include combustible dust (fuel), ignition source (heat), [oxygen](#) in air (oxidizer), and dispersion of dust particles in sufficient quantity and concentration as well as confinement of the dust cloud. General guidance in these efforts can be found in OSHA's "Combustible Dust in Industry; Preventing and Mitigating the Effects of Fire and Explosions", which list measures to control dusts, eliminate ignition sources, and limit the effects of explosions.

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.5 Handling and Storage



13.5.1 Nonfire Spill Response



SMALL SPILLS AND LEAKAGE: If you spill this chemical, you should dampen the solid spill material with [water](#), then transfer the dampened material to a suitable container. Use absorbent paper dampened with [water](#) to pick

up any remaining material. Seal your contaminated clothing and the absorbent paper in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with a soap and [water](#) solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should store this chemical under ambient temperatures, and keep it away from oxidizing materials. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

13.6 Exposure Control and Personal Protection



13.6.1 Other Standards Regulations and Guidelines



In 1977, the FDA proposed a ban on saccharin because of the discovery of bladder tumors in some male rats fed with high doses of saccharin. Because no other nonnutritive sweetener was available at that time, the proposed ban faced strong opposition. Legislation to stay the ban has been passed in the U.S. Congress periodically. In December, 1991, the FDA withdrew its proposed ban. All saccharin-containing packaged products were required to carry a warning label indicating that saccharin has been determined to cause cancer in laboratory animals. In 2001, the warning label requirement was lifted by the Congress. In 2003, saccharin was delisted from California Proposition 65 (the so-called carcinogen list).

Lee TD; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). New York, NY: John Wiley & Sons; Sweeteners. Online Posting Date: 24 March 2006

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.6.2 Personal Protective Equipment (PPE)



RECOMMENDED RESPIRATOR: Where the neat test chemical is weighed and diluted, wear a NIOSH-approved half face respirator equipped with a combination filter cartridge, i.e. organic vapor/acid gas/HEPA (specific for organic vapors, HCl, acid gas, SO₂ and a high efficiency particulate filter). (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

► [CAMEO Chemicals](#)

13.7 Stability and Reactivity



13.7.1 Air and Water Reactions



Slightly soluble in [water](#).

► [CAMEO Chemicals](#)

13.7.2 Reactive Group



Amides and Imides

Sulfonates, Phosphonates, and Thiophosphonates, Organic

► [CAMEO Chemicals](#)

13.7.3 Reactivity Profile



An amide. Acid to litmus. pH of 0.35% aqueous solution: 2.0. Organic amides/imides react with azo and diazo compounds to generate toxic gases. Flammable gases are formed by the reaction of organic amides/imides with strong reducing agents. Amides are very weak bases (weaker than [water](#)). Imides are less basic yet and in fact react with strong bases to form salts. That is, they can react as acids. Mixing amides with dehydrating agents such as P2O5 or SOCl2 generates the corresponding nitrile. The combustion of these compounds generates mixed oxides of nitrogen (NOx).

► [CAMEO Chemicals](#)

13.8 Regulatory Information



13.8.1 TSCA Requirements



Section 8(a) of [TSCA](#) requires manufacturers of this chemical substance to report preliminary assessment information concerned with production, exposure, and use to EPA as cited in the preamble in 51 FR 41329. Effective date 9/29/2006; Reporting date: 11/28/2006.

40 CFR 712.30 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 5, 2011: <https://www.ecfr.gov>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Pursuant to section 8(d) of [TSCA](#), EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. [1,2-Benzisothiazol-3\(2H\)-one](#), 1,1-dioxide is included on this list. Effective date: 9/29/2006; Sunset date: 11/28/2006.

40 CFR 716.120 (USPEA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 5, 2011: <https://www.ecfr.gov>

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.8.2 FDA Requirements



The food additives saccharin, [ammonium saccharin](#), [calcium saccharin](#), and [sodium saccharin](#) may be safely used as sweetening agents in food in accordance with the following conditions /in part 180, section 37/, if the substitution for nutritive sweeteners is for a valid special dietary purpose and is in accord with current special dietary food regulations and policies or if the use or intended use is for an authorized technological purpose other than calorie reduction.

21 CFR 180.37 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 12, 2011: <https://www.ecfr.gov>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Drug products containing certain active ingredients offered over-the-counter (OTC) for certain uses. A number of active ingredients have been present in OTC drug products for various uses, as described below. However, based on evidence currently available, there are inadequate data to establish general recognition of the safety and effectiveness of these ingredients for the specified uses: Saccharin is included in weight control drugs.

21 CFR 310.545(a)(20) (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 5, 2011: <https://www.ecfr.gov>

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.9 Other Safety Information



13.9.1 Special Reports



Toxicity of Food Additives (Excluding Antioxidants), January 1978-July 1989. Govt Reports Announcements & Index (GRA&I) Issue 6 (1990). This bibliography contains citations concerning the toxicity of food additives, incl saccharin, and their effects on the liver, kidneys, bladder, and other organs.

► [Hazardous Substances Data Bank \(HSDB\)](#)

Arnold DL, Boyes BG; The Toxicological Effects Of Saccharin in Short-Term Genotoxicity Assays. Mutat Res 221 (2): 69-132 (1989).

► [Hazardous Substances Data Bank \(HSDB\)](#)

National Toxicology Program. Eleventh Report on Carcinogens (2005). The Report on Carcinogens is an informational scientific and public health document that identifies and discusses substances (including agents, mixtures, or exposure circumstances) that may pose a carcinogenic hazard to human health. Saccharin (81-07-2) is delisted as reasonably anticipated to be a human carcinogen.[Available from, as of July 31, 2009: <http://ntp.niehs.nih.gov/ntp/roc/eleventh/profiles/append/appb.pdf>]

► [Hazardous Substances Data Bank \(HSDB\)](#)

14 Toxicity



14.1 Toxicological Information



14.1.1 Evidence for Carcinogenicity



Evaluation: There is inadequate evidence in humans for the carcinogenicity of saccharin salts used as sweeteners. There is sufficient evidence in experimental animals for the carcinogenicity of **sodium saccharin**. There is inadequate evidence in experimental animals for the carcinogenicity of saccharin (acid form) and **calcium saccharin**. Overall evaluation: In making the evaluation, the Working Group concluded that **sodium saccharin** produced urothelial bladder tumors in rats by a non-DNA reactive mechanism that involves the formation of a

urinary **calcium phosphate** containing precipitate, cytotoxicity and enhanced cell proliferation. The mechanism is not relative to humans because of critical interspecies differences in urine composition. Saccharin and its salts are not classifiable as to the carcinogenicity to humans (Group 3).

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. 73 607 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Saccharin: delisted as reasonably anticipated to be a human carcinogen.

DHHS/National Toxicology Program; *Eleventh Report on Carcinogens Saccharin (81-07-2) (January 2005)*. Available from, as of July 31, 2009: <https://ntp.niehs.nih.gov/ntp/roc/eleventh/profiles/append/appb.pdf>

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.2 Carcinogen Classification



IARC Carcinogenic Agent	Saccharin and its salts
IARC Carcinogenic Classes	Group 3: Not classifiable as to its carcinogenicity to humans
IARC Monographs	Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print) Volume 73: (1999) Some Chemicals that Cause Tumours of the Kidney or Urinary Bladder in Rodents and Some Other Substances

► [International Agency for Research on Cancer \(IARC\)](#)

14.1.3 Effects During Pregnancy and Lactation



● Summary of Use during Lactation

Because of the low levels of saccharin in breastmilk, amounts ingested by the infant after typical maternal intake are small and would not be expected to cause any adverse effects in breastfed infants and not likely to reach an intake greater than the acceptable daily intake. Ingestion of diet drinks containing low-calorie sweeteners might increase the risk of vomiting in breastfed infants. However, some authors suggest that women may wish to limit the consumption of nonnutritive sweeteners while breastfeeding because their effect on the nursing infants are unknown.

● Effects in Breastfed Infants

A cross-sectional survey assessed the dietary history of US mothers nursing infants between 11 and 15 weeks of age. The survey was used to estimate the amount of diet soda and fruit drinks consumed by the women. There were no statistically significant differences in infants' weight or z-scores based on low calorie sweetener exposure. However, infants exposed to low calorie sweetener in milk once or less per week had a statistically significantly higher risk of vomiting than those who were not exposed. Greater exposure was not associated with vomiting. It was not possible to assess the effects of specific sweeteners.

● Effects on Lactation and Breastmilk

Relevant published information was not found as of the revision date.

► [Drugs and Lactation Database \(LactMed\)](#)

14.1.4 Acute Effects



1 item 					
Compound CID	Organism	Test Type	Route	Dose	Reference
5143	mouse	LD50	oral	17 gm/kg	Experientia., 35(1364), 1979 [PMID:499424]

► [ChemiDplus](#)

14.1.5 Interactions



IT IS NOW WELL ESTABLISHED THAT THE INTERACTION OF MULTIPLE ENVIRONMENTAL FACTORS MAY INCR THE INCIDENCE OF SOME HUMAN CANCERS MORE THAN EXPOSURE TO A SINGLE CARCINOGEN. WITH AN IN VIVO EXPERIMENTAL RAT MODEL, SYNERGISTIC EFFECT IN BLADDER CARCINOGENESIS BETWEEN A SUBCARCINOGENIC DOSE OF THE STRONG BLADDER CARCINOGEN, [N-METHYL-N-NITROSOUREA](#) & SACCHARIN WAS DEMONSTRATED.

[PMID:872124](#)

HICKS RM, CHOWANIEC J; *CANCER RES* 37 (8 PT 2): 2943 (1977)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Since both [sodium L-ascorbate](#) and [sodium saccharin](#) promote two-stage bladder carcinogenesis in rats, synergism of the two chemicals was investigated with special reference to the role of urinary pH and [sodium](#)+ concentration. Male F344 rats were given 0.05% [N-butyl-N-\(4-hydroxybutyl\)nitrosamine](#) in the drinking water for 4 wk and then treated with basal diet containing 5% [sodium saccharin](#), 5% [sodium L-ascorbate](#), 5% [sodium saccharin](#) plus 5% [sodium L-ascorbate](#), 5% [L-ascorbic acid](#), 5% [sodium saccharin](#) plus 5% [L-ascorbic acid](#), or no added chemical for 32 wk. Treatment with [sodium saccharin](#) or [sodium L-ascorbate](#) alone significantly increased the induction of neoplastic and preneoplastic lesions of the bladder. [Sodium saccharin](#) plus [sodium L-ascorbate](#) also induced these bladder lesions significantly when compared with the controls, and the number of lesions was greater than the sum of the lesions in the group treated with [sodium saccharin](#) alone or [sodium L-ascorbate](#) alone. In contrast, the induction of carcinomas and papillomas in rats treated with [sodium saccharin](#) plus [sodium L-ascorbate](#) produced an elevation of urinary pH and [sodium](#)+ concentrations, although the increases were not different from those in rats fed [sodium saccharin](#) or [sodium L-ascorbate](#) alone. [Sodium saccharin](#) plus [L-ascorbic acid](#), however, did not cause elevation of urinary pH, although it increased urinary [sodium](#)+ concentration. Thus, the bladder carcinogenesis promotion by [sodium saccharin](#) was synergized by [sodium L-ascorbate](#) and inhibited by [L-ascorbic acid](#). This modulation was associated with changes of urinary pH and Na+ concentration. /[Sodium saccharin](#)/

[PMID:2364375](#)

Fukushima S et al; *Cancer Res* 50 (14): 4195-8 (1990)

► [Hazardous Substances Data Bank \(HSDB\)](#)

CHRONIC RAT FEEDING STUDIES WERE CONDUCTED ON A 10:1 [CYCLAMATE](#)/SACCHARIN MIXT. THE TEST MIXT WAS FED AT DIETARY LEVELS DESIGNED TO FURNISH 500, 1120, & 2500 MG/KG TO GROUPS OF 35 MALE & 45 FEMALE RATS. THE ONLY POS FINDING WHICH PROVED TO HAVE CRUCIAL SIGNIFICANCE WAS THE OCCURRENCE OF PAPILLARY CARCINOMAS IN THE BLADDERS OF 12 OF THE 70 RATS FED THE MAX DIETARY LEVEL OF THE MIXT (EQUIV TO ABOUT 2500 MG/KG) FOR PERIODS RANGING FROM 78 TO 105 WK.

[PMID:1154429](#)

OSER BL ET AL; TOXICOLOGY 4 (3): 315 (1975)

► [Hazardous Substances Data Bank \(HSDB\)](#)

[N-METHYL-N-NITROSOUREA](#) WAS USED AS INITIATING CARCINOGEN AND GREATLY INCR YIELD OF BLADDER CANCERS IN SACCHARIN TREATED RATS. SACCHARIN IS A WEAK INITIATOR BUT A POWERFUL PROMOTER OF CARCINOGENESIS IN THE RAT BLADDER.

HICKS RM ET AL; TOXICOLOGY RESEARCH PROJECTS DIRECTORY 04: 10 (1979)

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Interactions (Complete) data for SACCHARIN (15 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.6 Antidote and Emergency Treatment



Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing [water](#). Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; *Emergency Care For Hazardous Materials Exposure*. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160

► [Hazardous Substances Data Bank \(HSDB\)](#)

Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer [oxygen](#) by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary Monitor for shock and treat if necessary Anticipate seizures and treat if necessary For eye contamination, flush eyes immediately with [water](#). Irrigate each eye continuously with 0.9% saline (NS) during transport Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of [water](#) for dilution if the patient can swallow, has a strong gag reflex, and does not drool Cover skin burns with dry sterile dressings after decontamination /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; *Emergency Care For Hazardous Materials Exposure*. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160

► [Hazardous Substances Data Bank \(HSDB\)](#)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation

techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema Consider administering a beta agonist such as [albuterol](#) for severe bronchospasm Monitor cardiac rhythm and treat arrhythmias as necessary Start IV administration of D5W /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload Treat seizures with [diazepam](#) or [lorazepam](#) Use [proparacaine hydrochloride](#) to assist eye irrigation /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160-1

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.7 Human Toxicity Excerpts



/HUMAN EXPOSURE STUDIES/ Randomised, double-blind, placebo-controlled N-of-1 trial with a cross-over design /was conducted in order/ to determine whether there was a connection between the complaint of restless legs and the ingestion of artificial sweeteners in a patient with these symptoms after drinking certain 'light' beverages. During a period of 48 days, the patient took 4 capsules per day containing either 150 mg of [cyclamate](#), 22.5 mg of saccharine, both sweeteners, or placebo on two successive days. Between each of these 2-day periods there was a 2-day rest period during which no capsules were taken. The hospital pharmacist had prepared the capsules and determined the sequence of the 2-day periods on a random basis. The patient did not know which capsules he was taking. Every day on arising, starting 3 weeks before the trial period, the patient noted the intensity and duration of the symptoms in the late evening and previous night. For this notation he used an 11-point scale, from 0 (= no restless legs) to 10 (= almost total inability to sleep because of restless legs). A score of 1-3 corresponded to mild symptoms that had no effect on the patient's sleep; at a score of 4-6 his sleep was disturbed and at a score of 7-10 the patient hardly slept at all. The patient had symptoms more often while using saccharine or the combination of saccharine and [cyclamate](#) than when taking the placebo (4 and 4 versus 2 of the 6 nights); moreover, the average score was then statistically significantly higher (5.2 and 5.8 versus 3.3). There was a connection between the patient's complaints of restless legs and the use of saccharine, but not the use of [cyclamate](#).

[PMID:17216727](#)

de Groot S, Ned Tijdschr Geneesk 150 (51): 2796-2799 (2006)

► [Hazardous Substances Data Bank \(HSDB\)](#)

/CASE REPORTS/ Idiosyncratic effects of saccharin on the liver were reported in a 70-year-old woman. Increased activities of [alanine](#) aminotransferase, [aspartate](#) aminotransferase, gamma-glutamyl transferase and alkaline phosphatase were found after oral administration of three pharmaceutical drugs of which saccharin was the only common constituent. The drugs were [lorazepam](#), [dihydroergocristine](#) and [chlordemethyldiazepam](#). Exposure to saccharin alone reproduced the effects.

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 574 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

/CASE REPORTS/ ...reported 5 patients in whom oral administration of 0.1 g saccharin caused pruritis and edematous papules on the trunk and limbs.

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22 151 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

/EPIDEMIOLOGY STUDIES/ A SURVEY OF BLADDER CANCER PATIENTS & CONTROLS WITHOUT BLADDER CANCER SHOWED THAT IN GENERAL BLADDER CANCER RISK WAS NOT INCREASED BY NONNUTRITIVE SWEETENER SACCHARIN & [CYCLAMATE](#) USE. ADJUSTING FOR SMOKING HABITS, OCCUPATION, AGE, RACE, SEX, DIABETES MELLITUS, ETC DID NOT LEAD TO SIGNIFICANT CORRELATIONS BETWEEN THE SWEETENER USE & BLADDER CANCER.

KESSLER II; HEALTH SUGAR SUBSTITUTES PROC ERGOB CONF SUGAR SUBSTITUTES: 85 (1979)

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Human Toxicity Excerpts (Complete) data for SACCHARIN (11 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.8 Non-Human Toxicity Excerpts



/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ A total dose of 0.24 g saccharin (form not specified), made by the Remson-Fahlberg method, was applied as an 8% solution in [acetone](#) thrice weekly to the skin of 'S' strain mice. Twenty-five days after the start of the treatment, the animals were given 18 weekly applications of 0.17% croton oil in [acetone](#). At the end of the croton oil treatment, 15 skin papillomas were observed in seven of the 20 saccharin-treated animals, by comparison with four papillomas in four of 19 controls treated with croton oil only. The increase was not statistically significant.

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V73 550 (1999)

► [Hazardous Substances Data Bank \(HSDB\)](#)

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ The subacute toxicity of [sodium saccharin](#) and 2 hydrolytic derivatives, [o-sulfamoylbenzoic acid](#) (Compound I) and [ammonium o-carboxybenzene sulfonate](#) (Compound II) was evaluated by feeding each of the compounds alone at a dietary level of 20 000 ppm to both beagle dogs and albino rats. Additionally, groups of dogs and rats were fed combinations of the 3 materials at levels up to 20 000 ppm (2000 ppm [sodium saccharin](#), 9000 ppm of both Compound I and II). Dogs were maintained on the test diets for 16 weeks, rats for 13 weeks. No signs of a pharmacotoxic response to the test materials were observed. Parameters determined for treated animals, including growth, food consumption, hematologic profiles, clinical blood chemistry studies, urinalyses, organ weight and ratio data, and both gross and microscopic pathologic evaluation, were not significantly different from control values. From these findings, it is suggested that there is little toxicologic hazard associated with ingestion of the 2 hydrolytic derivatives of [sodium saccharin](#).

PMID:968910

Kennedy GL Jr et al; *Toxicology* 6 (2): 133-8 (1976)

► [Hazardous Substances Data Bank \(HSDB\)](#)

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Saccharin, administered to male albino rats at a dose of 65 mg/kg body weight/day (... /low/ dose) for a total period of 39 weeks resulted in a distinct decrease in the hepatic alkaline phosphatase (AkP, 86%), [lactate](#) dehydrogenase (LDH, 28%) and [glutamate pyruvate](#) transaminase (GPT, 67%) activities. The [glutamate oxaloacetate](#) transaminase (GOT) activity, however, increased 3.05 fold after 26 weeks of saccharin administration. The [urea](#) content showed 3.26% fold increase during the first 13 weeks of saccharin administration, which normalized subsequently. The [cholesterol](#) content and DNA content increased 7.7 fold and 2.6 fold after 26 weeks of saccharin administration. The soluble protein and RNA content, on the other hand, decreased 63% and 35% during the first 26 weeks of saccharin administration. After strong dose (260 mg/kg body wt/day) administration, various biochemical parameters followed the same pattern as for the weak dose, except for the extent of damage and for the DNA content, which decreased significantly when compared to weak dose experiment. Both concentrations of saccharin caused hypertrophy of hepatic cell, its nucleus and nucleoli in addition to excessive vacuolation. The number of nuclei/cell remained unaltered, whereas number of nucleoli/nucleus increased significantly after saccharin intoxication.

Shakoori AR et al; Pakistan Journal of Zoology 27 (1): 1-13 (1995)

► [Hazardous Substances Data Bank \(HSDB\)](#)

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ In studies primarily designed to evaluate the effects of saccharin and silicate on the urinary bladders of rodents, hemorrhage of the glandular stomach was observed in high incidence. It occurred in young rats with high doses of saccharin (7.5% [sodium saccharin](#); 6.3% acid saccharin), with no difference between male and female F344 rats fed during ages 5 to 15 weeks, no difference between [sodium saccharin](#) and acid saccharin, and was reversible, even with continued saccharin administration. [Sodium silicate](#) (0.38, 1.13, 2.26% of the diet) had no influence on gastric hemorrhage. [Iron](#) deficiency anemia has been observed in young rats fed high dietary levels of saccharin, and the present results suggest that gastric hemorrhage contributes to its etiology.

PMID:7940594

Okamura T et al; Toxicology Letters 74 (2): 129-40 (1994)

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Non-Human Toxicity Excerpts (Complete) data for SACCHARIN (65 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.9 Non-Human Toxicity Values



LD50 Rat ip 7100 mg/kg /[Sodium saccharin](#)/

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004, p. 3277

► [Hazardous Substances Data Bank \(HSDB\)](#)

LD50 Rat oral 14,200 mg/kg /[Sodium saccharin](#)/

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004, p. 3277

► [Hazardous Substances Data Bank \(HSDB\)](#)

LD50 Mouse oral 17,500 mg/kg /[Sodium saccharin](#)/

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3277

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.10 Ecotoxicity Values



LC50; Species: *Pimephales promelas* (fathead minnow, 30 day old); Concentration: 18.3 g/L for 96 hr (confidence limit 16.4 - 20.4 g/L). Dilution factor: 0%, 20%, 40%, 60%, 80% and 100% of the stock solution. Behavioral observations were not recorded. Increased alkalinity values were due to a reaction between the titrant and toxicant. /[Saccharin, sodium salt hydrate](#)/

Geiger D.L., Call D.J., Brooke L.T. (eds). *Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas)*. Vol. IV. Superior Wisconsin: University of Wisconsin-Superior, 1988., p. 141

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.1.11 National Toxicology Program Studies



[Sodium saccharin](#) (NaSac) ... was tested for potential effects on reproduction & fertility in Swiss CD-1 mice using the RACB protocol. Data on food & [water](#) consumptions, body weights, & clinical signs from the dose-range-finding study (Task 1) were used to set exposure concns for the continuous cohabitation phase (Task 2) at 1.25, 2.5, & 5% weight/volume in the drinking [water](#). While [water](#) consumption was decreased at the high dose by nearly equal to 10-20%, it was increased at the low & middle dose levels by nearly =40% & 20%, respectively. Consequently, the high dose animals gained slightly less weight during Task 2. Measures of body weights & [water](#) consumption allowed the calculation of daily exposure estimates: 3.5, 5.9, & 8.1 g/kg/day. In Task 2, 3, 0, 1, & 8 mice died in the control, low, middle, & high dose groups, respectively. The increased mortality at 5% NaSac was attributed to complications of dehydration. For the surviving pairs, there was no reduction in the mean number of litters/pair, although at the high dose, the number of live pups/litter decreased by 16% & the pup weight adjusted for litter size was decreased by 6%. There was no decr in the viability of the offspring. These effects were considered secondary to the decreased [water](#) intake seen at the high dose, & since the middle dose level had a relative incr in intake & showed no reproductive toxicity, Task 2 was judged to be essentially negative for reproductive toxicity, & the evaluation of the second generation was performed with only the controls & the middle dose level. Thus, the last litter from the control & middle dose groups was nursed, weaned, & reared to mating at nearly equal to 70-80 days of age. There was no effect of exposure to NaSac on viability or growth to weaning, or on body weights at the start of the cohabitation wk. [Water](#) consumption was increased by nearly =30 in the 2.5% NaSac group, although this did not translate to a change in body weight. In the mating trial, there were no differences due to NaSac consumption in the percent of F1 pairs mating or delivering a litter, or in the number, weight, or viability of pups in that litter. After the F2 pups were evaluated & discarded, the F1 controls & 2.5% NaSac-exposed mice were killed & necropsied. There were no differences between the groups in terminal body weights or organ weights. The concn, % motile, or % morphologically abnormal sperm in the epididymis were unchanged by NaSac exposure, as was the length or characteristics of the estrous cycle. In summary, NaSac reduced fertility only at a concn that also significantly reduced [water](#) consumption & increased mortality. At concns that increased [water](#) consumption, there were no measurable effects on reproductive performance or necropsy endpoints. /[Sodium saccharin](#)/

Department of Health & Human Services/National Institute of Environmental Health Sciences, National Toxicology Program; Sodium Saccharin (CAS #128-44-9): Reproduction and Fertility Assessment in CD-1 Mice When Administered in Drinking Water,

NTP Study No. RACB83072 (April 1985) Available from, as of August 14, 2002: <https://ntp.niehs.nih.gov/index.cfm?objectid=0847F35A-0850-D1E7-B02ED4DDD150F990>

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2 Ecological Information



14.2.1 Environmental Fate / Exposure Summary



Saccharin's production and use as an artificial, non-nutritive sweetener, pharmaceutical aid (flavor), and in formulations for electroplating-bath brighteners may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 1.0×10^{-7} mm Hg at 25 °C indicates saccharin will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase saccharin will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 22 hours. Particulate-phase saccharin will be removed from the atmosphere by wet or dry deposition. Saccharin contains chromophores that absorb at wavelengths >290 nm, and therefore may be susceptible to direct photolysis by sunlight. If released to soil, saccharin is expected to have very high mobility based upon an estimated Koc of 23. The pKa of saccharin is 1.31, indicating that this compound will partially exist in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.2×10^{-9} atm-cu m/mole. Saccharin may not volatilize from dry soil surfaces based upon its vapor pressure. Incubation experiments with activated sludge resulted in a first order half-life of 90 minutes with 78% removal efficiency after 3 hours suggesting that biodegradation may be an important environmental fate process. If released into water, saccharin is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of three suggests the potential for bioconcentration in aquatic organisms is low. Saccharin is stable in aqueous solution for most normal food applications, especially beverages. Therefore, saccharin is not expected to hydrolyze rapidly in environmental media. Occupational exposure to saccharin may occur through inhalation and dermal contact with this compound at workplaces where saccharin is produced or used. Monitoring and use data indicate that the general population may be exposed to saccharin via ingestion and contaminated drinking water, and consumer products containing saccharin. (SRC)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.2 Natural Pollution Sources



Saccharin, sodium and calcium saccharin and o-toluenesulphonamide do not occur as natural products.

IARC. *Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans*. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <https://monographs.iarc.fr/ENG/Classification/index.php>, p. V22: 128 (1980)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.3 Artificial Pollution Sources



Saccharin's production and use as an artificial, non-nutritive sweetener, pharmaceutical aid (flavor), and in formulations for electroplating-bath brighteners(1) may result in its release to the environment through various waste streams(SRC).

(1) O'Neil MJ; *Merck Index*, 14th ed, Whitehouse Station, NJ Merck & Co. p 1435 (2007)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.4 Environmental Fate



TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 23(SRC), determined from a log Kow of 0.91(2) and a regression-derived equation(3), indicates that saccharin is expected to have very mobility in soil(SRC). Volatilization of saccharin from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 1.2×10^{-9} atm-cu m/mole(SRC), using a fragment constant estimation method(4). The pKa of saccharin is 1.31(5), indicating that this compound will partially exist in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(6). Saccharin is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 1.0×10^{-7} mm Hg at 25 °C(SRC), determined from a fragment constant method(7). Incubation experiments with activated sludge resulted in a first order half-life of 90 minutes with 78% removal efficiency after 3 hours(8) suggesting that biodegradation may be an important environmental fate process in soil(SRC).

(1) Swann RL et al; *Res Rev* 85: 17-28 (1983) (2) measured log Kow ref e.g. Hansch C et al; *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants*. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. nn (1995) OR logS ref (3) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.1. Jan, 2010. Available from, as of June 1, 2011: <https://www.epa.gov/oppt/exposure/pubs/episuite.html> (4) Meylan WM, Howard PH; *Environ Toxicol Chem* 10: 1283-93 (1991) (5) Serjeant EP, Dempsey B; *Ionisation Constants of Organic Acids in Aqueous Solution*. International Union of Pure and Applied Chemistry (IUPAC). IUPAC Chemical Data Series No. 23. New York, NY: Pergamon Press, Inc. (1979) (6) Doucette WJ; pp. 141-188 in *Handbook of Property Estimation Methods for Chemicals*. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (7) Lyman WJ; p. 31 in *Environmental Exposure From Chemicals Vol I*, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985) (8) Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 23(SRC), determined from a log Kow of 0.91(2) and a regression-derived equation(3), indicates that saccharin is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is not expected(4) based upon an estimated Henry's Law constant of 1.2×10^{-9} atm-cu m/mole(SRC), developed using a fragment constant estimation method(5). According to a classification scheme(6), an estimated BCF of three(SRC), from its log Kow(2) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Incubation experiments with activated sludge resulted in a first order half-life of 90 minutes with 78% removal efficiency after 3 hours(7) suggesting that biodegradation may be an important environmental fate process in water(SRC).

(1) Swann RL et al; *Res Rev* 85: 17-28 (1983) (2) Hansch C et al; *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants*. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 27 (1995) (3) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.1. Jan, 2010. Available from, as of Jun 1, 2011: <https://www.epa.gov/oppt/exposure/pubs/episuite.html> (4) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (5) Meylan WM, Howard PH; *Environ Toxicol Chem* 10: 1283-93 (1991) (6) Franke C et al; *Chemosphere* 29: 1501-14 (1994) (7) Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), saccharin, which has an estimated vapor pressure of 1.0×10^{-7} mm Hg at 25 °C(SRC), determined from a fragment constant method(2), will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase saccharin is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 22 hours(SRC), calculated from its rate constant of 5.9×10^{-12} cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(3). Particulate-phase saccharin may be removed from the air by wet or dry deposition(SRC). Saccharin contains chromophores that absorb at wavelengths >290 nm(4), and therefore may be susceptible to direct photolysis by sunlight(SRC).

(1) Bidleman TF; *Environ Sci Technol* 22: 361-367 (1988) (2) Lyman WJ; p. 31 in *Environmental Exposure From Chemicals Vol I*, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985) (3) Meylan WM, Howard PH; *Chemosphere* 26: 2293-99 (1993) (4) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.5 Environmental Biodegradation



AEROBIC: The importance of biodegradation of saccharin in soil and [water](#) is unknown, but amides are usually susceptible to microbial metabolism(1). Saccharin was eliminated in wastewater treatment plants with activated sludge processes sampled in Zurich Switzerland; a mean removal efficiency of 90% was observed. Incubation experiments with activated sludge resulted in a first order half-life of 90 minutes with 78% removal efficiency after 3 hours. No loss was observed using sterile controls(2).

(1) Boethling RS et al; *Environ Sci Technol* 28: 459-65 (1994) (2) Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.6 Environmental Abiotic Degradation



The rate constant for the vapor-phase reaction of saccharin with photochemically-produced hydroxyl radicals has been estimated as 5.9×10^{-12} cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 22 hours at an atmospheric concentration of 5×10^5 hydroxyl radicals per cu cm(1). The respective acid and alkaline hydrolysis products of saccharin are [o-sulfamoylbenzoic acid](#) and [ammonium o-sulfobenzoic acid](#)(2). Rate data for the hydrolysis of saccharin in aqueous solutions were not located in the available literature(SRC). However, saccharin is stable in aqueous solution for most normal food applications, especially beverages. Therefore, saccharin is not expected to hydrolyze rapidly in environmental media(SRC). Saccharin contains chromophores that absorb at wavelengths >290 nm(3), and therefore may be susceptible to direct photolysis by sunlight(SRC).

(1) Meylan WM, Howard PH; *Chemosphere* 26: 2293-99 (1993) (2) O'Neil MJ; *Merck Index*, 14th ed, Whitehouse Station, NJ Merck & Co. p. 1435 (2007) (3) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.7 Environmental Bioconcentration



An estimated BCF of three was calculated in fish for saccharin(SRC), using a log Kow of 0.91(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration

in aquatic organisms is low(SRC). Bioconcentration of the substance was tested as a breakdown product of 3-(allyloxy)-1,1-dioxo-1 λ (6),2-benzothiazole; results indicated low bioconcentration potential(4).

(1) Hansch C et al; *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants*. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 27 (1995) (2) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.1. Jan, 2010. Available from, as of June 1, 2011: <https://www.epa.gov/oppt/exposure/pubs/episuite.html> (3) Franke C et al; *Chemosphere* 29: 1501-14 (1994) (4) NITE; *Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration*. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 1, 2011: <https://www.safe.nite.go.jp/english/db.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.8 Soil Adsorption / Mobility



The Koc of saccharin is estimated as 20(SRC), using a log Kow of 0.91(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that saccharin is expected to have very high mobility in soil. The pKa of saccharin is 1.31(4), indicating that this compound will partially exist in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

(1) Hansch C et al; *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants*. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 27 (1995) (2) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.1. Jan, 2010. Available from, as of June 1, 2011: <https://www.epa.gov/oppt/exposure/pubs/episuite.html> (3) Swann RL et al; *Res Rev* 85: 17-28 (1983) (4) Serjeant EP, Dempsey B; *Ionisation Constants of Organic Acids in Aqueous Solution*. International Union of Pure and Applied Chemistry (IUPAC). IUPAC Chemical Data Series No. 23. New York, NY: Pergamon Press, Inc. (1979) (5) Doucette WJ; pp. 141-188 in *Handbook of Property Estimation Methods for Chemicals*. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.9 Volatilization from Water / Soil



The Henry's Law constant for saccharin is estimated as 1.2X10⁻⁹ atm-cu m/mole(SRC) using a fragment constant estimation method(1). This Henry's Law constant indicates that saccharin is expected to be essentially nonvolatile from water and moist soil surfaces(2). Saccharin is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 1.0X10⁻⁷ mm Hg(SRC), determined from a fragment constant method(3).

(1) Meylan WM, Howard PH; *Environ Toxicol Chem* 10: 1283-93 (1991) (2) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (3) Lyman WJ; p. 31 in *Environmental Exposure From Chemicals Vol I*, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.10 Environmental Water Concentrations



GROUNDWATER: Saccharin was not detected in groundwater sampled in Zurich Switzerland, sampled between August and November 2008(1).

(1) Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

SURFACE WATER: Eight lakes were sampled in February and March 2008, resulting in saccharin concentrations ranging from below the detection limit in a remote mountain lake to 0.18 ug/L in the Greifensee, which is within

a densely populated catchment area(1).

(1) Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.11 Effluent Concentrations



Saccharin concentrations in untreated and treated wastewater from the Canton of Zurich, Switzerland, collected in 2008(1).

Location	Sample Date (2008)	Throughput (cu m/day)	Influent (ug/L)	Effluent (ug/L)
Gossau	September 30	2560	18	not detected
Horgen	June 18	9700	3.9	0.27
Maennedorf	May 7	3850	7.1	0.50
Meilen	June 23	10400	7.1	3.2
Regensdorf	September 17	5730	14	0.42
Richterswil	June 24	4150	10	0.33
Uster	September 30	15250	18	0.68
Waedenswil	April 28	10160	4.8	1.5
Wetzikon	September 30	7610	16	1.8
Zurich	September 24	150100	12	0.51

(1) Buerge IJ et al; *Environ Sci Technol* 43: 4381-4385 (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.12 Probable Routes of Human Exposure



According to the 2006 [TSCA](#) Inventory Update Reporting data, the number of persons reasonably likely to be exposed in the industrial manufacturing, processing, and use of saccharin is 100 to 999; the data may be greatly underestimated(1).

(1) US EPA; *Inventory Update Reporting (IUR). Non-confidential 2006 IUR Records by Chemical, including Manufacturing, Processing and Use Information*. Washington, DC: U.S. Environmental Protection Agency. Available from, as of June 1, 2011: <https://cfpub.epa.gov/iursearch/index.cfm>

► [Hazardous Substances Data Bank \(HSDB\)](#)

NIOSH (NOES Survey 1981-1983) has statistically estimated that 225,094 workers (97,727 of these were female) were potentially exposed to saccharin in the US(1). Occupational exposure to saccharin may occur through inhalation and dermal contact with this compound at workplaces where saccharin is produced or used. Monitoring and use data indicate that the general population may be exposed to saccharin via ingestion and contaminated drinking [water](#), and consumer products containing saccharin(SRC).

(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available from, as of June 1, 2011: <https://www.cdc.gov/noes/>

► [Hazardous Substances Data Bank \(HSDB\)](#)

14.2.13 Average Daily Intake



The average daily intake of saccharin through food for the Finnish population was estimated to be 15 mg, based on a survey of the population of Finland(1).

[PMID:6545288](#)

(1) Hemminki K, Vainio H; IARC Sci Publ 59: 37-45 (1984)

► [Hazardous Substances Data Bank \(HSDB\)](#)

15 Associated Disorders and Diseases



17 items

Disease	Evidence Type	Evidence PMID
Adenocarcinoma	marker/mechanism	6468837
Urinary Bladder Neoplasms	marker/mechanism	2004360
		3731063
		3764937
		3779637
		4040099
		...
Urinary Bladder Diseases	marker/mechanism	25891526
Carcinoma	marker/mechanism	3779637
Gastritis	marker/mechanism	3731063

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► [Comparative Toxicogenomics Database \(CTD\)](#)

Disease	References
Colorectal cancer	PubMed: 7482520 , 22148915 , 19006102 , 23940645 , 24424155 , 20156336 , 19678709 , 25105552 , 21773981 , 25037050 , 27015276 , 27107423 , 27275383 , 28587349

Silke Matysik, Caroline Ivanne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984>

► [Human Metabolome Database \(HMDB\)](#)

16 Literature



16.1 Consolidated References



15,802 items

SORT BY **Publication Date - Most Recent** ▼

[Effect of artificial sweetener saccharin on lysozyme aggregation: A combined spectroscopic and in silico approach](#)
Publication Name: Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy
Publication Date: 2023-04-05
PMID: [36566534](#) DOI: [10.1016/j.saa.2022.122269](#)

[Activation of TrkB in Parvalbumin interneurons is required for the promotion of reversal learning in spatial and fear memory by antidepressants](#)
Publication Name: Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology
Publication Date: 2023-03-21
PMID: [36944718](#) DOI: [10.1038/s41386-023-01562-y](#)

[Groundwater characterization of the eastern Minesing Wetlands in support of the endangered Hine's emerald dragonfly \(Somatochlora hineana\)](#)
Publication Name: Wetlands Ecology and Management
Publication Date: 2023-03-15
DOI: [10.1007/s11273-023-09918-3](#)

[Sensory evaluation of the bitterness of asenapine using D-sorbitol pretreatment: single-blind, placebo-controlled, crossover trial](#)
Publication Name: BMC Psychiatry
Publication Date: 2023-03-14
PMID: [36918838](#) DOI: [10.1186/s12888-023-04664-5](#)

[Taste-odor association learning alters the dynamics of intra-oral odor responses in the posterior piriform cortex of awake rats](#)
Publication Name: eneuro
Publication Date: 2023-03-10
PMID: [36898831](#) DOI: [10.1523/eneuro.0010-23.2023](#)

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► [PubChem](#)

16.2 NLM Curated PubMed Citations



All NLM Curated PubMed Citations



administration and dosage	immunology	urine
adverse effects	isolation and purification	
analogues and derivatives	metabolism	
analysis	pharmacokinetics	
antagonists and inhibitors	pharmacology	
blood	physiology	
chemical synthesis	poisoning	
chemistry	radiation effects	
classification	standards	
economics	supply and distribution	
genetics	therapeutic use	
history	toxicity	

► PubChem

16.3 Springer Nature References



6,243 items



SORT BY Publication Date - Oldest



[Effects of alcohol dependence on discrete choice between alcohol and saccharin](#)

PMID: [29875449](#)

Publication Date: 2018

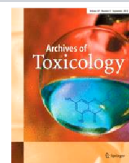
Publication Name: Neuropsychopharmacology



[Real-time co-crystal screening and formation between indomethacin and saccharin via DSC analytical technique or DSC-FTIR microspectroscopy](#)

Publication Date: 2014

Publication Name: Journal of Thermal Analysis and Calorimetry



[Effects on mouse embryos of in utero exposure to saccharin: teratogenic and chromosome effects](#)

Publication Date: 1985

Publication Name: Archives of Toxicology



[Spectroscopic and thermal approaches to investigate the formation mechanism of piroxicam-saccharin co-crystal induced by liquid-assisted grinding or thermal stress](#)

Publication Date: 2015

Publication Name: Journal of Thermal Analysis and Calorimetry

[High-Performance Thin-Layer Chromatography Analysis of Saccharin in Foods and Beverages](#)

Publication Date: 2010

Publication Name: JPC – Journal of Planar Chromatography – Modern TLC

[▶ Springer Nature](#)

16.4 Thieme References



35 items

SORT BY Publication Date - Most Recent

[Organic Isocyanates and Isothiocyanates: Versatile Intermediates in Agrochemistry](#)
DOI: [10.1055/a-1678-8528](#)
Publication Date: 2022
Publication Name: Synthesis

[Organic Nitrating Reagents](#)
DOI: [10.1055/s-0040-1719905](#)
Publication Date: 2022
Publication Name: Synthesis

[Recent Advances in the Transition-Metal-Free Arylation of Heteroarenes](#)
DOI: [10.1055/a-1543-3743](#)
Publication Date: 2021
Publication Name: Synthesis

[Chiral Brønsted Acids Catalyze Asymmetric Additions to Substrates that Are Already Protonated: Highly Enantioselective Disulfonimide-Catalyzed Hantzsch Ester Reductions of NH-Imine Hydrochloride Salts](#)
DOI: [10.1055/s-0040-1706413](#)
Publication Date: 2020
Publication Name: Synlett

[DMSO-Mediated Synthesis of Methylene-Bridged Unsymmetrical Bisamides in the Presence of AcOH](#)
DOI: [10.1055/s-0039-1690031](#)
Publication Date: 2020
Publication Name: Synthesis

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[▶ Thieme Chemistry](#)

16.5 Wiley References



6 items

SORT BY Publication Date - Most Recent

[Novel 1-Aminomethylisatins: Peculiarities of the Synthesis and the Reaction with Tris\(diethylamino\)phosphine](#)

DOI: [10.1002/jhet.2011](#)

Publication Date: 2014

Publication Name: J. Heterocyclic Chem.

[Synthesis, characterization and cytotoxicity of Pt\(II\), Pd\(II\), Cu\(II\) and Zn\(II\) complexes with 4'-substituted terpyridine](#)

DOI: [10.1002/aoc.2988](#)

Publication Date: 2013

Publication Name: Applied Organometallic Chemistry

[Triclabendazole: An Intriguing Case of Co-existence of Conformational and Tautomeric Polymorphism](#)

DOI: [10.1002/asia.201100638](#)

Publication Date: 2012

Publication Name: Chem. Asian J.

[Nanoindentation as a Probe for Mechanically-Induced Molecular Migration in Layered Organic Donor-Acceptor Complexes](#)

DOI: [10.1002/asia.201200224](#)

Publication Date: 2012

Publication Name: Chem. Asian J.

[Acidities of strong neutral Brønsted acids in different media](#)

DOI: [10.1002/poc.2946](#)

Publication Date: 2012

Publication Name: J. Phys. Org. Chem.

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► Wiley

16.6 Depositor Provided PubMed Citations



7,314 items



Q Search

SORT BY Publication Date - Most Recent ▼

Blends of Non-caloric Sweeteners Saccharin and Cyclamate Show Reduced Off-Taste due to TAS2R Bitter Receptor Inhibition

PMID: [28919036](#)

Publication Date: 2017-10-19

Journal: Cell chemical biology

Saccharin induced liver inflammation in mice by altering the gut microbiota and its metabolic functions

PMID: [28472674](#)

Publication Date: 2017-09-01

Journal: Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association

Phenotypic and biomarker evaluation of zebrafish larvae as an alternative model to predict mammalian hepatotoxicity

PMID: [26946349](#)

Publication Date: 2016-09-01

Journal: Journal of applied toxicology : JAT

RNA transcripts for the quantification of differentiation allow marked improvements in the performance of embryonic stem cell test (EST)

PMID: [26272751](#)

Publication Date: 2015-11-04

Journal: Toxicology letters

Evaluation of early changes induced by diuron in the rat urinary bladder using different processing methods for scanning electron microscopy

PMID: [25891526](#)

Publication Date: 2015-07-03

Journal: Toxicology

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► PubChem

16.7 Metabolite References



16 items 	
 Search	SORT BY PMID - Increasing ▼
PMID	Reference
7482520	Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. <i>Tohoku J Exp Med.</i> 1995 May;176(1):61-8.
22148915	Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. <i>J Proteome Res.</i> 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28.
19006102	Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. <i>NMR Biomed.</i> 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345.
23940645	Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. <i>PLoS One.</i> 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013.
24424155	Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. <i>Cancer Biol Ther.</i> 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14.
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[▶ Human Metabolome Database \(HMDB\)](#)

16.8 General References

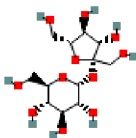


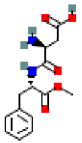
Dulcaryl (saccharin) effervescent tablets (User Guide)

[▶ DrugBank](#)

16.9 Chemical Co-Occurrences in Literature

Showing 3 of 25 [View More](#)

Chemical	Selected evidence
 Sucrose CID 5988	809 articles View All Selective pressure on a saccharin intake phenotype and its correlates: A replication study PMID 37387468; DOI 10.1093/chemse/bjad021; Chemical senses 2023 Jun; ?(?): Name matches: sucrose <i>saccharin</i> Long-term aspartame and saccharin intakes are related to greater volumes of visceral, intermuscular, and subcutaneous adipose tissue: the CARDIA study PMID 37443272; DOI 10.1038/s41366-023-01336-y; International journal of obesity (2005) 2023 Jul; ?(?): Name matches: sugar <i>saccharin</i> Artificial sugar saccharin and its derivatives: role as a catalyst PMID 35517977; DOI 10.1039/d0ra05974a; RSC advances 2020 Oct; 10(60):36571-36608 (Review Article) Name matches: sugar <i>saccharin</i>; <i>sodium saccharin</i>
 Water CID 962	1,257 articles View All Untreated wastewater impact and environmental risk assessment of artificial sweeteners in river water and sediments of the Danube River Basin in Serbia PMID 37368207; DOI 10.1007/s11356-023-28348-5; Environmental science and pollution research international 2023 Jun; ?(?): Name matches: water <i>saccharin</i> Emerging contaminants in wastewater, stormwater runoff, and surface water: Application as chemical markers for diffuse sources PMID 31048157; DOI 10.1016/j.scitotenv.2019.04.160; The Science of the total environment 2019 Aug; 676(?):252-267 Name matches: water <i>saccharin</i> Removal of pharmaceutical compounds, artificial sweeteners, and perfluoroalkyl substances from water using a passive treatment system containing zero-valent iron and biochar PMID 31319253; DOI 10.1016/j.scitotenv.2019.06.450; The Science of the total environment 2019 Nov; 691(?):165-177 Name matches: water <i>saccharin</i>

 Aspartame CID 134601	327 articles View All
	Long-term aspartame and saccharin intakes are related to greater volumes of visceral, intermuscular, and subcutaneous adipose tissue: the CARDIA study PMID 37443272; DOI 10.1038/s41366-023-01336-y; International journal of obesity (2005) 2023 Jul; ?(?): Name matches: aspartame <i>saccharin</i>
	Chronic intake of nutritive sweeteners and saccharin increases levels of glycolytic and lipogenic enzymes in rat liver PMID 35708269; DOI 10.1080/09637486.2022.2088705; International journal of food sciences and nutrition 2022 Nov; 73(7):927-939 Name matches: aspartame <i>saccharin</i>
	Saccharin and Sucralose Protect the Glomerular Microvasculature In Vitro against VEGF-Induced Permeability PMID 34444906; DOI 10.3390/nu13082746; Nutrients 2021 Aug; 13(8): Name matches: aspartame <i>saccharin</i>

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16.10 Chemical-Gene Co-Occurrences in Literature



Showing 3 of 100 View More		
Gene/Protein/Enzyme	Selected evidence	
tas1r3	87 articles View All	
	Saccharin and Sucralose Protect the Glomerular Microvasculature In Vitro against VEGF-Induced Permeability PMID 34444906; DOI 10.3390/nu13082746; Nutrients 2021 Aug; 13(8): Name matches: t1r3; taste receptor <i>saccharin</i>	
	Multiple interaction modes between saccharin and sweet taste receptors determine a species-dependent response to saccharin PMID 34932896; DOI 10.1002/2211-5463.13355; FEBS open bio 2022 02; 12(2):494-499 Name matches: t1r3; taste receptor <i>saccharin</i>	
	Saccharin Stimulates Insulin Secretion Dependent on Sweet Taste Receptor-Induced Activation of PLC Signaling Axis PMID 35052799; DOI 10.3390/biomedicines10010120; Biomedicines 2022 Jan; 10(1): Name matches: taste receptor <i>saccharin</i>	
fos	69 articles View All	
	c-Fos activity in the insular cortex, nucleus accumbens and basolateral amygdala following the intraperitoneal injection of saccharin and lithium chloride PMID 28323090; DOI 10.1016/j.neulet.2017.03.025; Neuroscience letters 2017 04; 647(?):32-37 Name matches: c-fos <i>saccharin</i>	
	c-Fos expression in rat brainstem following intake of sucrose or saccharin PMID 21964712; DOI 10.1007/s11684-011-0144-8; Frontiers of medicine 2011 Sep; 5(3):294-301 Name matches: c-fos <i>saccharin</i>	
	Cocaine-induced c-Fos expression in rats selectively bred for high or low saccharin intake and in rats selected for high or low impulsivity PMID 22613730; DOI 10.1016/j.bbr.2012.05.021; Behavioural brain research 2012 Aug; 233(2):271-9	

Name matches: *c-fos saccharin*

35 articles

View All 

tas1r2

[Multiple interaction modes between saccharin and sweet taste receptors determine a species-dependent response to saccharin](#)

PMID 34932896; DOI 10.1002/2211-5463.13355; FEBS open bio 2022 02; 12(2):494-499

Name matches: *t1r2 saccharin*

[High-dose saccharin supplementation does not induce gut microbiota changes or glucose intolerance in healthy humans and mice](#)

PMID 33431052; DOI 10.1186/s40168-020-00976-w; Microbiome 2021 01; 9(1):11

Name matches: *t1r2 saccharin*

[Drinking Non-nutritive Sweetness Solution of Sodium Saccharin or Rebaudioside a for Guinea Pigs: Influence on Histologic Change and Expression of Sweet Taste Receptors in Testis and Epididymis](#)

PMID 34422887; DOI 10.3389/fnut.2021.720889; Frontiers in nutrition 2021; 8(?):720889

Name matches: *t1r2 saccharin sodium; sodium saccharin* PubChem

16.11 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 25 View More 

Disease

Selected evidence

Alcoholism

203 articles

View All 

[Dissecting operant alcohol self-administration using saccharin-fading procedure](#)

PMID 36727594; DOI 10.1002/npr2.12289; Neuropsychopharmacology reports 2023 Feb; ?(?):

Name matches: *alcohol use disorder saccharin*

[Innate and Acquired Quinine-Resistant Alcohol, but not Saccharin, Drinking in Crossed High-Alcohol-Preferring Mice](#)

PMID 31509609; DOI 10.1111/acer.14196; Alcoholism, clinical and experimental research 2019 11; 43(11):2421-2430

Name matches: *alcoholism saccharin*

[Effects of alcohol dependence on discrete choice between alcohol and saccharin](#)

PMID 29875449; DOI 10.1038/s41386-018-0101-1; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2018 08; 43(9):1859-1866

Name matches: *alcohol dependence saccharin*

Substance-Related Disorders

187 articles

View All 

[Greater avoidance of a saccharin cue paired with passive delivery of heroin is associated with a select increase in expression of CRFR2 and CRFbp in the hippocampus in rats](#)

PMID 36228871; DOI 10.1016/j.brainresbull.2022.10.009; Brain research bulletin 2022 12; 191(?):48-60

Name matches: *drug of abuse saccharin*

[Sucrose and saccharin differentially modulate depression and anxiety-like behavior in diabetic mice: exposures and withdrawal effects](#)

PMID 31073738; DOI 10.1007/s00213-019-05259-3; Psychopharmacology 2019 Nov; 236(11):3095-3110

Name matches: *addictive potential saccharin*

Activation of G-protein coupled estradiol receptor 1 in the dorsolateral striatum attenuates preference for cocaine and saccharin in male but not female rats

PMID 33609527; DOI 10.1016/j.yhbeh.2021.104949; Hormones and behavior 2021 04; 130(?):104949

Name matches: **drug seeking** *saccharin*

323 articles

View All **Infections****Delta-opioid receptor blockade in the ventral pallidum increases perceived palatability and consumption of saccharin solution in rats**

PMID 24739358; DOI 10.1016/j.bbr.2014.04.005; Behavioural brain research 2014 Aug; 269(?):20-7

Name matches: **infections** *saccharin***Intra-nucleus accumbens shell injections of R(+)- and S(-)-baclofen bidirectionally alter binge-like ethanol, but not saccharin, intake in C57BL/6J mice**

PMID 25026094; DOI 10.1016/j.bbr.2014.07.011; Behavioural brain research 2014 Oct; 272(?):238-47

Name matches: **infections** *saccharin***Ceftriaxone attenuates acquisition and facilitates extinction of cocaine-induced suppression of saccharin intake in C57BL/6J mice**

PMID 26066719; DOI 10.1016/j.physbeh.2015.06.009; Physiology & behavior 2015 Oct; 149(?):174-80

Name matches: **infections** *saccharin* PubChem

17 Patents



17.1 Depositor-Supplied Patent Identifiers



143,665 items

 SearchSORT BY Priority Date - Most Recent **Novel mixtures and uses of (2e)-3-(1,3-benzodioxol-5-yl)-n-phenyl-n-(tetrahydro-3-furanyl)-2-propenamide**Publication Number: **WO-202207944-A9**

Priority Date: 2022-07-11

Methods of treating glutathione deficiencies and deficiencies in glutathione synthetase activityPublication Number: **US-11491141-B1**

Priority Date: 2022-01-06 Grant Date: 2022-11-08

Specific conjugation of an antibodyPublication Number: **WO-2022078524-A2**

Priority Date: 2021-11-03

Specific conjugation of an antibodyPublication Number: **WO-2022078524-A4**

Priority Date: 2021-11-03

Pharmaceutical compositions and methods for treatment of psychiatric disordersPublication Number: **US-11351179-B1**

Priority Date: 2021-08-05 Grant Date: 2022-06-07

► PubChem

[Link to all deposited patent identifiers](#)

► PubChem

17.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=CVHZOJJKTDOEJC-UHFFFAOYSA-N>

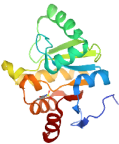
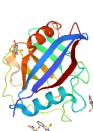
► PATENTSCOPE (WIPO)

18 Interactions and Pathways



18.1 Protein Bound 3D Structures



8 items		↓
Search		SORT BY Resolution - Increasing ▾
	PanDDA analysis group deposition -- Crystal structure of SARS-CoV-2 NSP3 macrodomain in complex with ZINC000002560357 PDB Code: 5RSP Resolution: 1.02 Å	
	A Carbonic Anhydrase IX Mimic in Complex with Saccharin PDB Code: 4RIV Resolution: 1.631 Å	
	Carbonic Anhydrase II in Complex with Saccharin PDB Code: 2Q1B Resolution: 1.7 Å	
	Crystal structure of human liver FBPase complexed with an covalent inhibitor PDB Code: 7WJV Resolution: 1.724 Å	
	Structure of Cyclophilin A in complex with Saccharin. PDB Code: 4N1O Resolution: 1.75 Å	

[► RCSB Protein Data Bank \(RCSB PDB\)](#)[View 7 proteins in NCBI Structure](#)[► PubChem](#)

18.1.1 Ligands from Protein Bound 3D Structures



PDBe Ligand Code

LSA

PDBe Conformer

Interactive Chemical Structure Model

☒ Ball and Stick

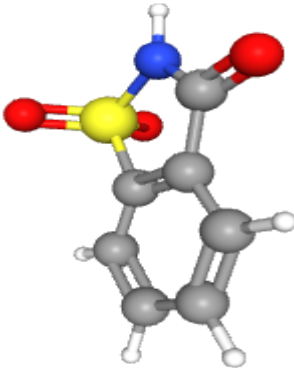
☐ Sticks

☐ Wire-Frame

☐ Space-Filling

☒ Show Hydrogens

☐ Animate



[► Protein Data Bank in Europe \(PDBe\)](#)

18.2 Chemical-Target Interactions



56 items

↓

Q Search

SORT BY

Data Source - A to Z ▾

Structure	Protein	Gene	Taxonomy	Action ⓘ	Evidence IDs	ⓘ Data Source
-----------	---------	------	----------	----------	--------------	---------------

	Carbonic anhydrase 3	CA3	Homo sapiens (human)	Inhibitor	PMID:17826101	DrugBank
		HELLS	Mus musculus (house mouse)	Saccharin results in increased expression of HELLs mRNA	PMID:19000923	Comparative Toxicogenomics Database (CTD)
		IL1RL1	Mus musculus (house mouse)	Saccharin results in increased expression of IL1RL1 mRNA	PMID:19000923	Comparative Toxicogenomics Database (CTD)
		AFP	Mus musculus (house mouse)	Saccharin results in increased expression of AFP mRNA	PMID:26272751	Comparative Toxicogenomics Database (CTD)
		CA3	Homo sapiens (human)	Saccharin binds to and results in decreased activity of CA3 protein	PMID:17826101	Comparative Toxicogenomics Database (CTD)

[« First](#)
[< Previous](#)
Page **1**
[of 12 Next >](#)
[Last »](#)

► [BindingDB](#); [Comparative Toxicogenomics Database \(CTD\)](#); [DrugBank](#); [IUPHAR/BPS Guide to PHARMACOLOGY](#); [Thera...](#)

19 Biological Test Results



19.1 BioAssay Results



1,778 items


SORT BY
Activity Value - Increasing




A quantitative high throughput screen for small molecules that induce DNA re-replication in SW480 colon adenocarcinoma cells.

Activity: **Inconclusive** Activity Type: Potency Activity Value: 0.0008 µM

BioAssay AID: [624297](#)

Substance SID: [26753733](#) Compound CID: [5143](#)

	qHTS assay to identify small molecule antagonists of the androgen receptor (AR) signaling pathway using the MDA cell line Activity: Inconclusive Activity Type: Potency Activity Value: 0.0017 µM BioAssay AID: 743042 Substance SID: 144204911 Compound CID: 5143
	qHTS assay for small molecule agonists of thyroid hormone receptor beta signaling Activity: Inconclusive Activity Type: Potency Activity Value: 0.0025 µM BioAssay AID: 588545 Substance SID: 26753733 Compound CID: 5143
	qHTS Assay for Modulators of Lamin A Splicing Activity: Inconclusive Activity Type: Potency Activity Value: 0.0056 µM BioAssay AID: 1487 Substance SID: 26753733 Compound CID: 5143
	qHTS assay for small molecule agonists of vitamin D receptor signaling Activity: Inconclusive Activity Type: Potency Activity Value: 0.0056 µM

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[► PubChem](#)

20 Taxonomy



2 items 			
Structure	Taxonomy	Evidence IDs 	Data Source
	Homo sapiens (human)		Human Metabolome Database (HMDB)
	Homo sapiens (human)	PMID:22308371	Natural Product Activity and Species Source (NPASS)

[► Natural Product Activity and Species Source \(NPASS\)](#)

21 Classification



21.1 MeSH Tree



1 item

View in Classification Browser 

MeSH Tree > Technology and Food and Beverages Category > Food and Beverages > Food > Food Ingredients > Food Additives > Flavoring Agents

[Saccharin](#)

Flavoring agent and non-nutritive sweetener.

[▶ Medical Subject Headings \(MeSH\)](#)

21.2 NCI Thesaurus Tree



1 item

View in Classification Browser 

NCI Thesaurus Tree > Drug, Food, Chemical or Biomedical Material > Food or Food Product > Food Component

[Saccharin](#)[▶ NCI Thesaurus \(NCIt\)](#)

21.3 ChEBI Ontology



1 item

View in Classification Browser 

ChEBI Ontology > chemical entity > molecular entity > main group molecular entity > p-block molecular entity > carbon group molecular entity > organic molecular entity > heteroorganic entity > organic heterocyclic compound > organic heteropolycyclic compound > organic heterobicyclic compound > benzothiazoles

[saccharin](#)

A 1,2-benzisothiazole having a keto-group at the 3-position and two oxo substituents at the 1-position. It is used as an artificial sweetening agent.

[▶ ChEBI](#)

21.4 KEGG: JP15



1 item

View in Classification Browser 

Drugs listed in the Japanese Pharmacopoeia

[Saccharin](#)[▶ KEGG](#)

21.5 ChemIDplus



56 items

View in Classification Browser 

ChemIDplus Chemical Information Classification

[CAMEO](#)

Computer-Aided Management of Emergency Operation - CAMEO Chemicals is a library of datasheets containing response-related information and recommendations for hazardous materials that are commonly transported, used, or stored in the United States

ChemIDplus Chemical Information Classification

CTD

Comparative Toxicogenomics Database - CTD selects and organizes gene, sequence, chemical, reference, and taxonomic data about gene-chemical interactions. It is hosted at North Carolina State University (NCSU).

ChemIDplus Chemical Information Classification

ChEBI

Chemical Entities of Biological Interest - Dictionary of molecular entities focused on "small" chemical compounds. ChEBI is part of the EMBL-European Bioinformatics Institute.

ChemIDplus Chemical Information Classification

ClinicalTrials.gov

ClinicalTrials.gov - ClinicalTrials.gov offers up-to-date information for locating federally and privately supported clinical trials for a wide range of diseases and conditions

ChemIDplus Chemical Information Classification

DSL

Domestic Substance List of Canada - The DSL list is an inventory of substances manufactured in, imported into or used in Canada on a commercial scale

« First < Previous Page 1 of 12 Next > Last »

► [ChemIDplus](#)

21.6 CAMEO Chemicals



4 items

[View in Classification Browser](#)

Amides and Imides

Reactive group: Amides and Imides

Amines, Phosphines, and Pyridines

Reactive group: Amines, Phosphines, and Pyridines

Salts, Basic

Reactive group: Salts, Basic

Sulfonates, Phosphonates, and Thiophosphonates, Organic

Reactive group: Sulfonates, Phosphonates, and Thiophosphonates, Organic

► [CAMEO Chemicals](#)

21.7 IUPHAR / BPS Guide to PHARMACOLOGY Target Classification



1 item

[View in Classification Browser](#)

Guide to Pharmacology Target Classification > Receptors > G protein-coupled receptors

Taste 2 receptors

Taste 2 receptors or Bitter taste receptors (TAS2Rs) are G protein-coupled receptors expressed in oral sensory cells and a variety of non-gustatory tissues. The ~25 human TAS2Rs share low amino acid sequence identities with other GPCR families and are classified as broadly tuned "generalist"

receptors with numerous, chemically diverse bitter agonists, as narrowly tuned "specialist" receptors with very few activators, as intermediately tuned receptors with an average number of agonists, or receptors specialized to interact with chemically defined activators. The number of functional bitter taste receptor genes varies among species and orthologues might not be functionally conserved. Due to their expression in various tissues, the signal transduction of TAS2Rs is complex. Some TAS2Rs interact with drugs such as analgesic, anti-inflammatory, and antibacterial compounds. The specialist database BitterDB contains additional information on bitter compounds and receptors.

► [IUPHAR/BPS Guide to PHARMACOLOGY](#)

21.8 ChEMBL Target Tree



11 items	View in Classification Browser
Enzyme Biological molecules that possess catalytic activity. They may occur naturally or be synthetically created. Enzymes are usually proteins, however CATALYTIC RNA and CATALYTIC DNA molecules have also been identified. [MESH:D004798]	
Membrane receptor Cell surface proteins that bind signalling molecules external to the cell with high affinity and convert this extracellular event into one or more intracellular signals that alter the behavior of the target cell (From Alberts, Molecular Biology of the Cell, 2nd ed, pp693-5). Cell surface receptors, unlike enzymes, do not chemically alter their ligands. [MESH:D011956]	
ChEMBL Protein Target Tree > Ion channel > Voltage-gated ion channel Voltage-gated potassium channel Potassium channel whose permeability to ions is extremely sensitive to the transmembrane potential difference. The opening of these channels is induced by the membrane depolarization of the ACTION POTENTIAL. [MESH:D024642]	
Unclassified protein ChEMBL Protein Target Tree > Membrane receptor Taste receptor (family C GPCR)	
<< First < Previous Page 1 of 3 Next > Last >>	

► [ChEMBL](#)

21.9 UN GHS Classification



1 item	View in Classification Browser
Not Classified No hazards have been classified (by majority companies[ECHA] or information source)	

► [UN Globally Harmonized System of Classification and Labelling of Chemicals \(GHS\)](#)

21.10 EPA CPDat Classification



19 items	View in Classification Browser
EPA CPDat Classification > Functional Use	

flavoring and nutrient

EPA CPDat Classification > Functional Use

fragrance

EPA CPDat Classification > Functional Use

no specific technical function

EPA CPDat Classification > Functional Use

artificial sweeteners

EPA CPDat Classification > Functional Use

artificial sweetener

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[▶ EPA Chemical and Products Database \(CPDat\)](#)

21.11 NORMAN Suspect List Exchange Classification



52 items

[View in Classification Browser](#)

NORMAN Suspect List Exchange Classification

Pesticide transformation products (TPs, metabolites, successors)

These are pesticide transformation products (TPs, metabolites, successors) documented to occur in environmental transformations.

NORMAN Suspect List Exchange Classification

Masking

NORMAN Suspect List Exchange Classification

Oral care

NORMAN Suspect List Exchange Classification > S36 | UBAPMT | Potential Persistent, Mobile and Toxic (PMT) substances

Toxic

This substance is classified as Toxic (T)

NORMAN Suspect List Exchange Classification > S36 | UBAPMT | Potential Persistent, Mobile and Toxic (PMT) substances

PBT/vPvB mandated

This indicates that the substance is mandated for a PBT/vPvB (Persistent, Bioaccumulative and Toxic / very Persistent, very Bioaccumulative) assessment based on Article 14 (i.e. non-intermediate uses and volumes over 10 tonnes/year)

<< First < Previous Page 1 of 11 Next > Last >>

[▶ NORMAN Suspect List Exchange](#)

21.12 EPA DSSTox Classification



86 items

[View in Classification Browser](#)

CompTox Chemicals Dashboard Chemical Lists

[BLOODEXPOSOME] LIST: BLOODEXPOSOME Chemicals identified as part of the blood exposome

Short_Description: Chemicals identified as part of the blood exposome

Long_Description: Barupal et al report on Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach. The database can be used for prioritizing chemicals for systematic reviews, developing target assays in exposome research, identifying compounds in untargeted mass spectrometry, and biological interpretation in metabolomics data. (Last remapped February 17th 2023)

CompTox Chemicals Dashboard Chemical Lists

[CANADADSL] Canadian Domestic Substances List 2019

Short_Description: The domestic substances list (DSL) is the sole standard against which a substance is judged to be "new" to Canada.

Long_Description: On May 4, 1994, Environment and Climate Change Canada published the domestic substances list (DSL) in Part II of the Canada Gazette. The DSL is an inventory of approximately 23 000 substances manufactured in, imported into or used in Canada on a commercial scale. It is based on substances present in Canada, under certain conditions, between January 1, 1984 and December 31, 1986. The DSL is the sole standard against which a substance is judged to be "new" to Canada. With few exemptions, all substances not on this list are considered new and must be reported prior to importation or manufacture in order that they can be assessed to determine if they are toxic or could become toxic to the environment or human health.

CompTox Chemicals Dashboard Chemical Lists

[CECSCREEN] METABOLITES: HBM4EU CECscreen: Screening List for Chemicals of Emerging Concern

Short_Description: HBM4EU CECscreen is a suspect screening list for Chemicals of Emerging Concern (CECs) plus metadata and predicted Phase 1 metabolites

Long_Description: HBM4EU CECscreen is a suspect screening list for Chemicals of Emerging Concern (CECs) plus metadata and predicted Phase 1 metabolites; this list contains the CECs only. CECscreen is part of the HBM4EU project (coord. UBA) > WP16 "emerging chemicals" (lead INRA, JP Antignac/L Debrauwer) > Task 16.1 (lead IRAS, J Vlanderen / R Vermeulen) > Main contributor (J Meijer) > Involved Partners (M Lamoree, T Hamers, S Hutinet, A, Covaci, C Huber, M Krauss, DI Walker, EL Schymanski) and hosted on the NORMAN Suspect List Exchange. Further details in Meijer et al (2021) DOI: 10.1016/j.envint.2021.106511. Dataset DOI: 10.5281/zenodo.3956586.

CompTox Chemicals Dashboard Chemical Lists

[CERAPP] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)

Short_Description: CERAPP uses predictive computational models trained on HTS data to evaluate thousands of chemicals for ER-related activity.

Long_Description: CERAPP (Collaborative Estrogen Receptor Activity Prediction Project) is a large-scale modeling project demonstrate the efficacy of using predictive computational models trained on high-throughput screening data to evaluate thousands of chemicals for ER-related activity and prioritize them for further testing. CERAPP combined multiple models developed in collaboration with 17 groups in the United States and Europe to predict ER activity of a common set of 32,464 chemical structures. Quantitative structure-activity relationship models and docking approaches were employed, mostly using a common training set of 1,677 chemical structures provided by the U.S. EPA, to build a total of 40 categorical and 8 continuous models for binding, agonist, and antagonist ER activity. All predictions were evaluated on a set of 7,522 chemicals curated from the literature. To overcome the limitations of single models, a consensus was built by weighting models on scores based on their evaluated accuracies. The work is described in this peer-reviewed publication: <https://ehp.niehs.nih.gov/doi/10.1289/ehp.1510267>

CompTox Chemicals Dashboard Chemical Lists

[CHEMINV] EPA|CHEMINV: EPA Chemical Inventory for ToxCast (20170203)

Short_Description: CHEMINV is full list of unique DSSTox substances mapped to historical chemical inventory of physical samples registered by EPA's ToxCast Chemical Contractor (Evotec) since launch of ToxCast program in 2007.

Long_Description: CHEMINV consists of the full list of unique DSSTox substance records mapped to the historical chemical inventory of physical samples registered by EPA's ToxCast Chemical Contractor (Evotec) in their sample tracking database since the launch of the ToxCast program in 2007. The CHEMINV file includes all chemical samples procured by Evotec for possible inclusion in EPA's ToxCast program since the start of the program in 2007, as well as a relatively small set of donated or EPA-supplied samples that were shipped to Evotec to be included in EPA's physical sample library. The list includes all samples received and registered by Evotec, but all samples were not necessarily solubilized or plated for testing, i.e., the full list includes volatiles, DMSO insolubles, depleted chemicals, and discarded chemicals deemed too dangerous for storage and handling. All physical samples plated for screening in the ToxCast program (TOXCAST), which includes EPA's full contribution to the Tox21 screening program (TOX21SL), are included as a subset of CHEMINV, as is the full list of samples currently available for ToxCast plating. Hence, the CHEMINV inventory file is a snapshot of all past and present samples. The CHEMINV file provides a complete historical record of chemicals that were prioritized for inclusion in EPA's ToxCast and Tox21 screening programs based on multiple criteria (toxicity data, exposure potential, use, etc.), and that were successfully procured by (or provided to) EPA's ToxCast Chemical Contractor (Evotec) for possible inclusion in those programs. The CHEMINV file is a subset of EPA's ChemTrack database (CHEMTRACK), the latter including all chemicals for which ToxCast or Tox21 screening data have been generated. CHEMTRACK additionally includes reference chemicals for which data were provided by ToxCast collaborators, as well as Tox21 chemicals not in EPA's physical inventory that were separately provided by Tox21 federal testing partners (the National Institutes of Health's National Toxicology Program and National Center for Advancing Translational Sciences). A detailed description of EPA's chemical management system and the DSSTox curation associated with chemical registration and mapping of the CHEMINV file is provided in the published document available for download at: <https://www.epa.gov/chemical-research/toxcast-chemicals-data-management-and-quality-considerations-overview> For more information on EPA's ToxCast program, see: <https://www.epa.gov/chemical-research/toxicity-forecasting> <https://www.epa.gov/chemical-research/toxicity-forecasting>

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► EPA DSSTox

21.13 International Agency for Research on Cancer (IARC) Classification



1 item

View in Classification Browser

Group 3: Not classifiable as to its carcinogenicity to humans

This category is used most commonly when the evidence of carcinogenicity in humans is inadequate, the evidence of carcinogenicity in experimental animals is limited (or inadequate), and the mechanistic evidence is limited (or inadequate). Limited evidence of carcinogenicity in experimental animals means that the available information suggests a carcinogenic effect but is not conclusive.

► International Agency for Research on Cancer (IARC)

21.14 Consumer Product Information Database Classification



4 items

View in Classification Browser

Home Maintenance

Inside the Home

Personal Care

Pet Care

► Consumer Product Information Database (CPID)

21.15 EPA Substance Registry Services Tree



29 items

View in Classification Browser

EPA SRS List Classification

2012 Chemical Data Reporting

2012 CDR :: This list contains chemicals that were reported to EPA's 2012 Chemical Data Reporting (CDR). Companies that manufacture (including import) certain chemicals at certain volumes in the U.S. must report to EPA every four years through its CDR. The vast majority of chemicals on this

2012 CDR list needed to be reported, but some of these chemicals were not required to be reported. EPA uses the CDR data to support many health, safety, and environmental protection activities.

EPA SRS List Classification

CAMEO Chemicals

CAMEO Chemicals is an emergency response and planning tool. This program includes an extensive chemical database with critical response information for thousands of chemicals, as well as a reactivity prediction tool that allows you to see what hazards might occur if chemicals in your collection were mixed together. CAMEO Chemicals is available as a website, mobile website, and a desktop application. CAMEO Chemicals is part of a software suite of programs called CAMEO (Computer-Aided Management of Emergency Operations). The CAMEO suite also includes a hazard modeling tool (ALOHA), a mapping program (MARPLOT), and two database applications (CAMEOfm and Tier2 Submit) designed to assist with the data management requirements under the Emergency Planning and Community Right-to-Know Act (EPCRA, also known as SARA Title III). The CAMEO suite programs can be used (individually or together) to help first responders and emergency planners access and manage crucial chemical property and emergency response information for hazardous chemical releases. The CAMEO programs are developed jointly by EPA's Office of Emergency Management and NOAA's Office of Response and Restoration.

EPA SRS List Classification

Chemicals On Reporting Rules

CORR :: The CORR database contains information on chemical substances, categories, and mixtures that are regulated under specific sections of the Toxic Substances Control Act (TSCA), or section 313 of the Emergency Planning and Community Right-to-Know Act (EPCRA). These chemical substances have been the subject of proposed or final rules issued by the Office of Pollution Prevention and Toxics (OPPT) in the Federal Register (FR). Certain TSCA 5(e) consent order chemicals are also included. The CORR database consists of two parts, a list of chemicals regulated by certain sections of TSCA and EPCRA, and a list of FR citations relevant to the specific regulation of chemical substances. The information on CORR contained in the SRS was derived from the CORR database dated September 30, 2001.

EPA SRS List Classification

Ecotoxicology Database

ECOTOX :: Comprehensive database providing adverse effects of single chemical stressors to ecologically relevant aquatic and terrestrial species.

EPA SRS List Classification

Emergency Response Notification System

ERNS :: ERNS is a database used to store information on notifications of oil discharges and hazardous substances releases. The ERNS program is a cooperative data sharing effort encompassing the National Response Center (NRC), operated by the US Coast Guard, EPA HQ and EPA regional offices. ERNS data is used to analyze release notifications, track EPA responses and compliance to environmental laws, support emergency planning efforts, and assist decision-makers in developing spill prevention programs.

« First < Previous Page 1 of 6 Next > Last »

► EPA Substance Registry Services

22 Information Sources



FILTER BY SOURCE

ALL SOURCES

1. BindingDB

LICENSE

All data curated by BindingDB staff are provided under the Creative Commons Attribution 3.0 License (<https://creativecommons.org/licenses/by/3.0/us/>).
<https://www.bindingdb.org/rwd/bind/info.jsp>

CHEMBL310671

<https://www.bindingdb.org/rwd/bind/chemsearch/marvin/MolStructure.jsp?monomerid=29278>

2. Comparative Toxicogenomics Database (CTD)

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<http://ctdbase.org/about/legal.jsp>

Saccharin

<https://ctdbase.org/detail.go?type=chem&acc=D012439>

3. DrugBank

LICENSE

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https://www.drugbank.ca/legal/terms_of_use

Saccharin

<https://www.drugbank.ca/drugs/DB12418>

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Guide to Pharmacology Target Classification

<https://www.guidetopharmacology.org/targets.jsp>

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<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000081072>

ChemIDplus Chemical Information Classification

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1,2-benzisothiazol-3(2H)-one 1,1-dioxide

<https://echa.europa.eu/substance-information/-/substanceinfo/100.001.202>

1,2-benzisothiazol-3(2H)-one 1,1-dioxide

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/17025>

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<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/FST467XS7D>

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<http://www.hmdb.ca/metabolites/HMDB0029723>
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<https://haz-map.com/About>

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<https://haz-map.com/Agents/17165>

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<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:32111>
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<https://www.whatsinproducts.com/contents/view/1/6>

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<https://www.whatsinproducts.com/chemicals/view/1/2293/000081-07-2>

Consumer Products Category Classification

<https://www.whatsinproducts.com/>

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<https://www.crystallography.net/cod/1517163.html>

<https://www.crystallography.net/cod/2206019.html>

<https://www.crystallography.net/cod/2300331.html>

<https://www.crystallography.net/cod/2300332.html>

<https://www.crystallography.net/cod/7226402.html>

22. The Cambridge Structural Database

<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=274592>

<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=814272>

<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=814273>

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<https://dailymed.nlm.nih.gov/dailymed/>

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<https://www.ncbi.nlm.nih.gov/books/n/lactmed/LM630/>

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<https://comptox.epa.gov/dashboard/DTXSID5021251#exposure>

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<https://www.cfsanappsexternal.fda.gov/scripts/fdcc/index.cfm?set=FoodSubstances&id=SACCHARIN>

27. SpectraBase

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<https://spectrabase.com/spectrum/BtfWoTEnkf5>

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<https://spectrabase.com/spectrum/HGKQavTQhzc>

1,2-BENZISOTHIAZOLIN-3-ONE 1,1-DIOXIDE

<https://spectrabase.com/spectrum/3HgLSOZUFJb>

1,2-BENZISOTHIAZOL-3(2H)-ONE, 1,1-DIOXIDE

<https://spectrabase.com/spectrum/E4UE0CTZQZ>

1,2-BENZISOTHIAZOLIN-3-ONE, 1,1-DIOXIDE

<https://spectrabase.com/spectrum/JWqeLBQIZTT>

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<https://spectrabase.com/spectrum/8Kwuvud1AZx>

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<https://spectrabase.com/spectrum/3vRfzCJxDzo>

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<https://spectrabase.com/spectrum/Epikhc7a9O1>

1,2-Benzisothiazol-3(2H)-one, 1,1-dioxide; 1,2-Benzisothiazolin-3-one 1,1-dioxide

<https://spectrabase.com/spectrum/4L4MOmx57Rv>

1,2-BENZISOTHIAZOLIN-3-ONE, 1,1-DIOXIDE

<https://spectrabase.com/spectrum/1OGTzgNI0XF>

1,2-benzisothiazolin-3-one-2-d, 1,1-dioxide

<https://spectrabase.com/spectrum/6IAqMdiLaSv>

1,2-BENZISOTHIAZOLIN-3-ONE, 1,1-DIOXIDE

<https://spectrabase.com/spectrum/53lrZY0N8GG>

1,2-Benzisothiazolin-3-one 1,1-dioxide

<https://spectrabase.com/spectrum/ASCo7EBS4pd>

CVHZOJJKTDOEJC-UHFFFAOYSA-N

<https://spectrabase.com/spectrum/1ry2K1mPROj>

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<https://pubchem.ncbi.nlm.nih.gov/substance/839978>

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CVHZOJJKTDOEJC-UHFFFAOYSA-N

<https://massbank.eu/MassBank/Result.jsp?inchikey=CVHZOJJKTDOEJC-UHFFFAOYSA-N>

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[query=exists\(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27CVHZOJJKTDOEJC-UHFFFAOYSA-N%27\)](https://mona.fiehnlab.ucdavis.edu/spectra/browse?query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27CVHZOJJKTDOEJC-UHFFFAOYSA-N%27))

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NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

36. Kruve Lab, Ionization & Mass Spectrometry, Stockholm University

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<https://www.fda.gov/drugs/drug-approvals-and-databases/national-drug-code-directory>

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NCI Thesaurus Tree

<https://ncit.nci.nih.gov>

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Drugs listed in the Japanese Pharmacopoeia

http://www.genome.jp/kegg-bin/get_htext?br08311.keg

55. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

56. EPA Substance Registry Services

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EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

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SID 403029527

<https://pubchem.ncbi.nlm.nih.gov/substance/403029527>

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