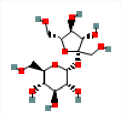
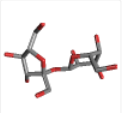
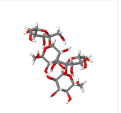
PubChem

COMPOUND SUMMARY

Sucrose

PubChem CID	5988
Structure	 2D  3D  Crystal Find Similar Structures
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{12}H_{22}O_{11}$
Synonyms	sucrose 57-50-1 saccharose Table sugar Cane sugar More...
Molecular Weight	342.30
Dates	Modify 2022-11-12 Create 2004-09-16

Sucrose appears as white odorless crystalline or powdery solid. Denser than water.

- CAMEO Chemicals

Sucrose is a glycosyl glycoside formed by glucose and fructose units joined by an acetal oxygen bridge from hemiacetal of glucose to the hemiketal of the fructose. It has a role as an osmolyte, a sweetening agent, a human metabolite, an algal metabolite, a Saccharomyces cerevisiae metabolite, an Escherichia coli metabolite and a mouse metabolite.

- ChEBI

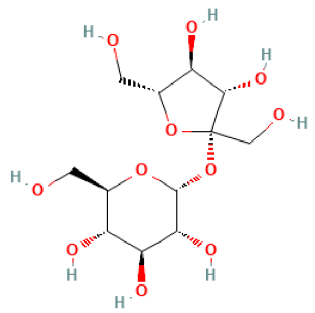
Sucrose is a metabolite found in the aging mouse brain.

- West Coast Metabolomics Center-UC Davis

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

1.3 Crystal Structures

Showing 1 of 29 View More

CCDC Number	156796
Crystal Structure Data	DOI:10.5517/cc584yh

Crystal Structure Depiction

The Cambridge Structural Database

2 Biologic Description

SVG Image	
IUPAC Condensed	Glc(a1-2b)Fruf
LINUCS	[][a-D-Glcp]{}
IUPAC	beta-D-arabino-hex-2-ulofuranosyl alpha-D-gluco-hexopyranoside
WURCS	WURCS=2.0/2,2,1/[a2122h-1a_1-5][ha122h-2b_2-5]/1-2/a1-b2

PubChem

GlyCosmos Monoisotopic Mass	342.12
GlyCosmos Subsumption	Linkage defined saccharide

GlyCosmos Glycoscience Portal

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(2*R*,3*R*,4*S*,5*S*,6*R*)-2-[(2*S*,3*S*,4*S*,5*R*)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

3.1.2 InChI

InChI=1S/C12H22O11/c13-1-4-6(16)8(18)9(19)11(21-4)23-12(3-15)10(20)7(17)5(2-14)22-12/h4-11,13-20H,1-3H2/t4-,5-,6-,7-,8+,9-,10+,11-,12+/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.3 InChIKey

CZMRCDWAGMRECN-UGDNZRGBSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.4 Canonical SMILES

C(C1C(C(C(C(O1)OC2(C(C(C(O2)CO)O)O)CO)O)O)O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.1.5 Isomeric SMILES

C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@]2([C@H]([C@@H]([C@H](O2)CO)O)O)CO)O)O)O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.2 Molecular Formula

C12H22O11

CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC); PubChem

3.3 Other Identifiers

3.3.1 CAS

57-50-1

CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS); Hazardous Substances Data Bank (HSDB); Human Metabolome Database (HMDB); ILO Internatic

92004-84-7

European Chemicals Agency (ECHA)

3.3.2 Related CAS

25702-74-3

Compound: Polysucrose

- CAS Common Chemistry

3.3.3 Deprecated CAS

100405-08-1, 104242-10-6, 131932-12-2, 146054-35-5, 146187-04-4, 151756-02-4, 220376-22-7, 29253-78-9, 29764-06-5, 30027-72-6, 47167-52-2, 47185-09-1, 47257-91-0, 50857-68-6, 51909-69-4, 64533-66-0, 65545-99-5, 75398-84-4, 76056-38-7, 78654-77-0, 80165-03-3, 8027-47-2, 8030-20-4, 85456-51-5, 86101-30-6, 87430-66-8, 92004-84-7, 635681-90-2, 786702-63-4, 12040-73-2, 1159795-78-4, 1206156-82-2, 880257-62-5, 1192061-43-0, 1481578-88-4, 1566560-95-9, 2169316-40-7

- ChemIDplus

100405-08-1, 104242-10-6, 1159795-78-4, 12040-73-2, 1206156-82-2, 131932-12-2, 146054-35-5, 146187-04-4, 151756-02-4, 220376-22-7, 29253-78-9, 29764-06-5, 30027-72-6, 47167-52-2, 47185-09-1, 47257-91-0, 50857-68-6, 51909-69-4, 635681-90-2, 64533-66-0, 65545-99-5, 75398-84-4, 76056-38-7, 78654-77-0, 786702-63-4, 80165-03-3, 8027-47-2, 8030-20-4, 85456-51-5, 86101-30-6, 87430-66-8, 880257-62-5, 92004-84-7

- EPA DSSTox

3.3.4 European Community (EC) Number

200-334-9

- European Chemicals Agency (ECHA)

618-806-1

- European Chemicals Agency (ECHA)

3.3.5 ICSC Number

1507

- ILO International Chemical Safety Cards (ICSC)

3.3.6 RTECS Number

WN6500000

- The National Institute for Occupational Safety and Health (NIOSH)

3.3.7 UNII

C151H8M554

- FDA Global Substance Registration System (GSRS)

3.3.8 DSSTox Substance ID

DTXSID2021288

- EPA DSSTox

3.3.9 Wikidata

Q4027534

- Wikidata

3.3.10 GlyTouCan Accession

G05551OP

- GlyCosmos Glycoscience Portal; GlyTouCan Project

G78152OD

- GlyTouCan Project

G44791DH

- GlyTouCan Project

3.3.11 NCI Thesaurus Code

C68477

- NCI Thesaurus (NCIt)

3.3.12 RXCUI

10159

- NLM RxNorm Terminology

3.4 Synonyms

3.4.1 MeSH Entry Terms

Saccharose
Sucrose

- Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms

sucrose	Granulated sugar	Sucraloxum [INN-Latin]	(+)-Sucrose	DSSTox_CID_1288
57-50-1	Rock candy	beta-D-Fructofuranosyl-alpha-D-glucopyranoside	alpha-D-Glucopyranoside, beta-D-fructofuranosyl-	NSC 406942
saccharose	Amerfand	D-(+)-Saccharose	NCI-C56597	DSSTox_RID_76060
Table sugar	Amerfond	CCRIS 2120	GNE-410	DSSTox_GSID_21288
Cane sugar	Confectioner's sugar	HSDB 500	S-67F	Polysucrose
White sugar	D(+)-Sucrose	Sacharose	1-alpha-D-glucopyranosyl-2-beta-D-fructofuranoside	(2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3,
D-Sucrose	Sucrose, dust	alpha-D-Glucopyranosyl beta-D-fructofuranoside	alpha-D-Glucopyranoside, beta-D-fructofuranosyl	Sucrose [USAN:JAN]
Saccharum	Sucrose, pure	CHEBI:17992	C151H8M554	D-Saccharose
sugar	D(+)-Saccharose	AI3-09085	NSC-406942	MFCD00006626
Rohrzucker	sacarosa	(alpha-D-Glucosido)-beta-D-fructofuranoside	beta-D-Fruf-(2<->1)-alpha-D-Glcp	CAS-57-50-1
Microse	D-(+)-Sucrose	Fructofuranoside, alpha-D-glucopyranosyl, beta-D	NCGC00164248-01	(2R,3R,4S,5S,6R)-2-{[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy}-6-(hydroxymethyl)oxane-3
Beet sugar	beta-D-Fructofuranosyl alpha-D-glucopyranoside	Glucopyranoside, beta-D-fructofuranosyl, alpha-D	Sucraloxum	Sucrose [JAN:NF]

- PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	342.30	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	-3.7	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	8	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	11	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	342.11621151	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	342.11621151	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	190 $Å^2$	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	23	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	395	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	9	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 2021.05.07)

PubChem

4.2 Experimental Properties

4.2.1 Physical Description

Sucrose appears as white odorless crystalline or powdery solid. Denser than water.

CAMEO Chemicals

Liquid; OtherSolid; OtherSolid, Liquid; PelletsLargeCrystals; WetSolid

EPA Chemicals under the TSCA

Hard, white, odorless crystals, lumps, or powder. [Note: May have a characteristic, caramel odor when heated.]; [NIOSH]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Solid

Human Metabolome Database (HMDB)

WHITE SOLID IN VARIOUS FORMS.

ILO International Chemical Safety Cards (ICSC)

Hard, white, odorless crystals, lumps, or powder.

Occupational Safety and Health Administration (OSHA)

Hard, white, odorless crystals, lumps, or powder. [Note: May have a characteristic, caramel odor when heated.]

- The National Institute for Occupational Safety and Health (NIOSH)

4.2.2 Color/Form

Monoclinic sphenoidal crystals, crystalline masses, blocks, or powder

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1517

- Hazardous Substances Data Bank (HSDB)

Hard, white ... crystals, lumps, or powder ...

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

- Hazardous Substances Data Bank (HSDB)

4.2.3 Odor

Characteristic caramel

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

- Hazardous Substances Data Bank (HSDB)

... Odorless ... [Note: May have a characteristic caramel odor when heated].

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

- Hazardous Substances Data Bank (HSDB)

4.2.4 Taste

Sweet

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1517

- Hazardous Substances Data Bank (HSDB)

4.2.5 Boiling Point

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

decomposes

- Occupational Safety and Health Administration (OSHA)

Decomposes

- The National Institute for Occupational Safety and Health (NIOSH)

4.2.6 Melting Point

320 to 367 °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

185.5 °C

PhysProp

- DrugBank

185.5 °C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999., p. 3-172

- Hazardous Substances Data Bank (HSDB); Human Metabolome Database (HMDB)

320-367 °F (decomposes)

- Occupational Safety and Health Administration (OSHA)

320-367 °F (Decomposes)

- The National Institute for Occupational Safety and Health (NIOSH)

4.2.7 Solubility

greater than or equal to 100 mg/mL at 66 °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

2100000 mg/L (at 25 °C)

YALKOWSKY,SH & DANNENFELSER,RM (1992)

- DrugBank

1 g dissolves in 0.5 ml water, 170 ml alcohol, about 100 ml methanol. Moderately sol in glycerol, pyridine.

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

- Hazardous Substances Data Bank (HSDB)

Very soluble in water, methanol; slightly soluble in ethanol; insoluble in ethyl ether.

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999., p. 3-172

- Hazardous Substances Data Bank (HSDB)

water solubility = 2.12X10+6 mg/l @ 25 °C

Yalkowsky SH, Dannenfelser RM; The AQUASOL dATAbASE of Aqueous Solubility. Fifth Ed, Tucson, AZ: Univ Az, College of Pharmacy (1992)

- Hazardous Substances Data Bank (HSDB)

2100.0 mg/mL

- Human Metabolome Database (HMDB)

Solubility in water, g/100ml at 25 °C: 200

- ILO International Chemical Safety Cards (ICSC)

200%

- The National Institute for Occupational Safety and Health (NIOSH)

4.2.8 Density

1.59 at 68 °F (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

- CAMEO Chemicals

1.5805 g/cu cm @ 17 °C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999., p. 3-172

- Hazardous Substances Data Bank (HSDB)

1.6 g/cm³

- ILO International Chemical Safety Cards (ICSC)

1.59

- Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

4.2.9 Vapor Pressure

0 mmHg (approx) (NIOSH, 2022)

- CAMEO Chemicals

0 mmHg (approx)

- Occupational Safety and Health Administration (OSHA); The National Institute for Occupational Safety and Health (NIOSH)

4.2.10 LogP

-3.7

HANSCH,C ET AL. (1995)

- DrugBank

log Kow = -3.70

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 107

- Hazardous Substances Data Bank (HSDB)

-3.70

HANSCH,C ET AL. (1995)

- Human Metabolome Database (HMDB)

-3.67

- ILO International Chemical Safety Cards (ICSC)

4.2.11 Stability/Shelf Life

STABLE IN AIR

The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 1149

- Hazardous Substances Data Bank (HSDB)

4.2.12 Decomposition

When heated to decomposition it emits acrid smoke and fumes.

Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2478

- Hazardous Substances Data Bank (HSDB)

186 °C

- ILO International Chemical Safety Cards (ICSC)

4.2.13 Heat of Combustion

-1.35X10+6 cal/mol

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V21 867

Hazardous Substances Data Bank (HSDB)

4.2.14 pH

Soln are neutral to litmus

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057

Hazardous Substances Data Bank (HSDB)

4.2.15 Surface Tension

71-75 mN/m @ 1-0.6 mol/l

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VB1 (90) 6-54

Hazardous Substances Data Bank (HSDB)

4.2.16 Refractive Index

INDEX OF REFRACTION: 1.5376; SADTLER REFERENCE NUMBER: 8659 (IR, PRISM), 563 (IR, GRATING); SPECIFIC OPTICAL ROTATION: +66.37 @ 20 °C/D (WATER)

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-503

Hazardous Substances Data Bank (HSDB)

4.2.17 Caco2 Permeability

-5.77

ADME Research, USCD

DrugBank

4.2.18 Dissociation Constants

pKa

12.6

MERCK INDEX (1996)

DrugBank

pKa= 12.62

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

Hazardous Substances Data Bank (HSDB)

4.2.19 Collision Cross Section

174 Å^2 $[M+Na]^+$ [CCS Type: DT, Method: single field calibrated with Agilent tune mix (Agilent)]

https://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b03091

CCSbase

173.93 Å^2 $[M+Na]^+$ [CCS Type: DT, Method: stepped-field]

https://pubs.rsc.org/en/content/articlelanding/2017/sc/c7sc03464d

CCSbase

168.47 Å^2 [M-H]$^-$ [CCS Type: DT, Method: stepped-field]
https://pubs.rsc.org/en/content/articlelanding/2017/sc/c7sc03464d

CCSbase

170 Å^2 [M+Na]$^+$ [CCS Type: TW, Method: calibrated with polyalanine]
https://pubs.acs.org/doi/abs/10.1021/ac500405x

CCSbase

175.4 Å^2 [M+K]$^+$ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]
https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322

CCSbase

173.9 Å^2 [M+Na]$^+$ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]
https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322

CCSbase

168.2 Å^2 [M-H]$^-$ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]
https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322

CCSbase

168.2 Å^2 [M-H]$^-$

173.9 Å^2 [M+Na]$^+$

175.5 Å^2 [M+K]$^+$

S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium | DOI:10.5281/zenodo.2658162

NORMAN Suspect List Exchange

4.2.20 Other Experimental Properties

Decomp @ 160-186 °C; does not reduce Fehling's soln, form osazone, or show mutarotation; hydrolyzed to glucose and fructose by dil acids and by invertase, a yeast enzyme; upon hydrolysis optical rotation falls and is negative when hydrolysis is complete.

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

Hazardous Substances Data Bank (HSDB)

Surface tension of aqueous solution (0.1-0.6 mol/l) = 71-75 mN/m

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VB1 6-54

Hazardous Substances Data Bank (HSDB)

Enthalpy of formation = 86 cal/mol-deg K

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. V21 867

Hazardous Substances Data Bank (HSDB)

4.2.21 Chemical Classes

Biological Agents -> Disaccharides

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4.3 SpringerMaterials Properties

Chemical diffusion
Crystal structure
Density
Sound absorption
Sound propagation
Sound velocity

Diamagnetic susceptibility
Diffusion
Diffusive flux
Fluorescence
Formula unit
Formula weight
Kinetic properties
Magnetic anisotropy
Magnetic susceptibility
Space group
Unit cell
Unit cell parameter

SpringerMaterials

5 Spectral Information

5.1 1D NMR Spectra

1D NMR Spectra	NMR: 6242 (Sadtler Research Laboratories Spectral Collection)

Hazardous Substances Data Bank (HSDB)

5.1.1 1H NMR Spectra

Showing 2 of 5 View More

Spectra ID	1293
Instrument Type	Varian
Frequency	500 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	3.45:14.34, 3.46:32.94, 3.48:19.73, 3.54:19.67, 3.54:19.93, 3.56:23.56, 3.56:24.20, 3.67:100.00, 3.73:22.02, 3.75:29.84, 3.77:15.98, 3.80:23.93, 3.81:84.56, 3.81:93.51, 3.83:13.15, 3.84:12.88, 3.85:5.07, 3.86:10.19, 3.87:8.15, 3.87:9.80, 3.88:13.29, 3.88:13.36, 3.88:8.83, 3.89:8.78, 3.90:7.79, 4.02:14.45, 4.04:27.23, 4.06:15.18, 4.20:28.93, 4.22:22.97, 5.39:18.49, 5.40:19.11
Thumbnail	

Human Metabolome Database (HMDB)

Spectra ID	3910
Instrument Type	JEOL
Frequency	400 MHz
Solvent	D2O
Shifts [ppm]:Intensity	3.45:136.00, 3.47:279.00, 3.50:200.00, 3.54:187.00, 3.56:183.00, 3.57:228.00, 3.58:235.00, 3.68:1000.00, 3.74:231.00, 3.76:267.00, 3.79:181.00, 3.80:55.00, 3.81:550.00, 3.82:854.00, 3.83:862.00, 3.84:98.00, 3.85:140.00, 3.85:99.00, 3.86:149.00, 3.87:138.00, 3.88:135.00, 3.89:140.00, 3.89:97.00, 3.90:166.00, 3.90:84.00, 3.91:96.00, 3.92:80.00, 4.03:198.00, 4.05:344.00, 4.08:207.00, 4.21:506.00, 4.23:391.00, 5.41:314.00, 5.42:308.00
Thumbnail	

Human Metabolome Database (HMDB)

5.1.2 13C NMR Spectra

Showing 2 of 5 View More

Spectra ID	1220
Instrument Type	Bruker
Frequency	125 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	0.00:1.45, 106.36:14.24, 62.89:15.61, 64.14:14.09, 65.08:18.49, 71.98:20.85, 73.80:22.62, 75.10:22.60, 75.33:21.72, 76.78:18.90, 79.24:16.27, 84.05:22.63, 94.85:21.82
Thumbnail	

Human Metabolome Database (HMDB)

Spectra ID	166519
Frequency	400 MHz
Solvent	H2O
Shifts [ppm]	106.36, 62.89, 64.14, 65.08, 71.98, 73.80, 75.10, 75.33, 76.78, 79.24, 84.05, 94.85
Thumbnail	

Human Metabolome Database (HMDB)

5.2 2D NMR Spectra

5.2.1 1H-1H NMR Spectra

2D NMR Spectra Type	1H-1H TOCSY
Spectra ID	1009
Shifts [ppm] (F2:F1)	3.30:3.66, 3.39:3.66, 3.42:3.66, 3.43:3.49, 3.44:5.40, 3.46:3.43, 3.46:3.46, 3.46:3.54, 3.46:3.66, 3.46:3.73, 3.46:3.75, 3.46:3.81, 3.46:3.85, 3.47:3.78, 3.48:5.40, 3.50:3.49, 3.52:3.66, 3.53:5.40, 3.54:3.66, 3.55:3.46, 3.55:3.47, 3.55:3.54, 3.55:3.56, 3.55:3.73, 3.55:3.75, 3.55:3.78, 3.55:3.81, 3.55:3.85, 3.56:5.40, 3.58:3.66, 3.61:3.66, 3.67:3.67, 3.71:3.67, 3.71:3.72, 3.72:3.80, 3.74:3.66, 3.74:3.78, 3.75:3.43, 3.75:3.46, 3.75:3.49, 3.75:3.54, 3.75:3.55, 3.75:3.75, 3.75:3.84, 3.75:5.40, 3.80:3.72, 3.81:3.43, 3.81:3.46, 3.81:3.48, 3.81:3.53, 3.81:3.56, 3.81:3.81, 3.81:3.85, 3.81:3.88, 3.81:3.90, 3.81:4.02, 3.81:4.20, 3.81:4.22, 3.82:4.04, 3.82:4.07, 3.83:3.73, 3.83:3.75, 3.83:5.40, 3.88:3.72, 3.88:3.87, 3.88:3.89, 3.88:4.02, 3.88:4.04, 3.88:4.06, 3.88:4.19, 3.88:4.22, 3.89:3.77, 3.90:3.66, 3.94:3.66, 3.98:3.98, 4.01:3.66, 4.01:3.80, 4.02:4.07, 4.03:3.83, 4.03:4.01, 4.04:3.81, 4.04:3.88, 4.04:4.04, 4.04:4.20, 4.04:4.21, 4.06:4.01, 4.06:4.07, 4.14:3.80, 4.18:3.91, 4.20:3.77, 4.20:3.87, 4.20:3.89, 4.20:4.04, 4.20:4.19, 4.20:4.22, 4.21:3.81, 4.21:4.02, 4.21:4.06, 4.23:3.91, 4.78:4.78, 5.40:3.43, 5.40:3.48, 5.40:3.53, 5.40:3.56, 5.40:3.73, 5.40:3.75, 5.40:3.78, 5.40:3.81, 5.40:3.84, 5.40:5.40
Thumbnail	

Human Metabolome Database (HMDB)

5.2.2 1H-13C NMR Spectra

2D NMR Spectra Type	1H-13C HSQC
Spectra ID	1243
Instrument Type	Bruker
Frequency	600 MHz
Solvent	Water
pH	7.00
Shifts [ppm] (F2:F1):Intensity	3.47:71.97:0.17, 3.55:73.78:0.26, 3.66:64.07:1.00, 3.74:75.30:0.16, 3.81:62.76:0.88, 3.81:65.05:0.79, 3.83:75.16:0.25, 3.88:84.14:0.30, 4.04:76.75:0.26, 4.21:79.22:0.22, 5.40:94.80:0.68
Thumbnail	

Human Metabolome Database (HMDB)

5.3 Mass Spectrometry

5.3.1 GC-MS

Showing 2 of 14 View More

Spectra ID	30233
Instrument Type	GC-EI-TOF
Ionization Mode	positive
SPLASH	splash10-0gba-0930000000-594ae5d59d217235e6c7
Top 5 Peaks	103.0 100 147.0 88.29 217.0 61.76 129.0 56.46 169.0 42.64
Thumbnail	
Notes	instrument=Pegasus III TOF-MS system, Leco; GC 6890, Agilent Technologies

Human Metabolome Database (HMDB)

Spectra ID	30697
Instrument Type	GC-EI-TOF
Ionization Mode	positive
SPLASH	splash10-02ta-0932000000-8fa2c23f886fb0c63312
Top 5 Peaks	147.0 100 103.0 94.79 217.0 91.39 361.0 86.29 129.0 66.87
Thumbnail	

Notes	instrument=Pegasus III TOF-MS system, Leco; GC 6890, Agilent Technologies

Human Metabolome Database (HMDB)

5.3.2 MS-MS

Showing 2 of 6 View More

Spectra ID	2227157
Ionization Mode	Negative
SPLASH	splash10-000i-9500000000-292e67f588f0d531ef65
Top 5 Peaks	89.02496 100 119.0361 45.60 59.01422 29.10 71.01436 28.40 113.02558 16.60
Thumbnail	

Human Metabolome Database (HMDB)

Spectra ID	2227566
Ionization Mode	Negative
SPLASH	splash10-0006-2709000000-0e3c703e04384a1e3293
Top 5 Peaks	341.11018 100 179.0559 42.90 89.02527 21.10 119.03527 17.20 161.04558 9.10
Thumbnail	

Human Metabolome Database (HMDB)

5.3.3 LC-MS

Showing 2 of 6 View More

Accession ID	MSBNK-RIKEN-PR100500
Authors	Matsuda F, Suzuki M, Sawada Y, Plant Science Center, RIKEN.
Instrument	UPLC Q-Tof Premier, Waters
Instrument Type	LC-ESI-QTOF
MS Level	MS2
Ionization Mode	NEGATIVE
Ionization	ESI
Collision Energy	Ramp 5-60 V
Precursor m/z	341.10841
Precursor Adduct	[M-H]-
Top 5 Peaks	341.1084 999 71.0149 800 89.0247 687 101.0245 569 179.0558 490
SPLASH	splash10-0fdx-9804000000-018a029ba3843a8db2bd
Thumbnail	
License	CC BY-SA

MassBank Europe

MoNA ID	MoNA018317

MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+Na]+
Precursor m/z	365.105438232422
Instrument	Agilent 6550 iFunnel
Instrument Type	LC-ESI-QTOF
Ionization Mode	positive
Top 5 Peaks	365.10651 24.90 272.08096 13.10
SPLASH	splash10-01b9-0049000000-aa5a4558dd60c39c28d4
Thumbnail	
Submitter	romanas chaleckis, gunma university

MassBank of North America (MoNA)

5.3.4 Other MS

Showing 2 of 6 View More

Other MS	MASS: 4955 (National Bureau of Standards EPA-NIH Mass Spectra Data Base, NSRDS-NBS-63)

Hazardous Substances Data Bank (HSDB)

MoNA ID	CCMSLIB00000479739
MS Category	Experimental
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	343.1
Instrument	Orbitrap
Ionization Mode	positive
Top 5 Peaks	127.045181 100 85.030952 95.71 145.056595 55.18 97.031975 32.84 69.035049 15
SPLASH	splash10-004s-8900000000-f71100adbafa5209fee1
Thumbnail	

Submitter	GNPS Team, University of California, San Diego

MassBank of North America (MoNA)

5.4 IR Spectra

IR Spectra	IR: 3335 (Coblentz Society Spectral Collection)

Hazardous Substances Data Bank (HSDB)

5.4.1 FTIR Spectra

Technique	KBr (2/400)
Source of Spectrum	SPECTRA AND PROPERTIES PROVIDED BY PROFESSOR DOCTOR DIETER O. HUMMEL
Source of Sample	Commercial Cube Sugar
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Technique	KBr WAFER
Source of Sample	Merck & Company, Inc.
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.4.2 ATR-IR Spectra

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	USB Biochemicals, Affymetrix, Inc.
Catalog Number	Ultrapure MB Grade
Lot Number	117034
Copyright	Copyright © 2014-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Source of Sample	Aldrich
Catalog Number	247618
Copyright	Copyright © 2018-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.5 Raman Spectra

Instrument Name	Thermo Nicolet FT-Raman 960
Technique	FT-Raman
Copyright	Copyright © 2003-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Catalog Number	179949
Copyright	Copyright © 2017-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2017-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

6 Related Records

6.1 Related Compounds with Annotation

PubChem

6.2 Related Compounds

Same Connectivity	180 Records
Same Stereo	20 Records
Same Isotope	151 Records
Same Parent, Connectivity	362 Records
Same Parent, Stereo	165 Records
Same Parent, Isotope	333 Records
Same Parent, Exact	146 Records
Mixtures, Components, and Neutralized Forms	364 Records
Similar Compounds	5,425 Records
Similar Conformers	92 Records

PubChem

6.3 Substances

6.3.1 Related Substances

All	961 Records
Same	454 Records
Mixture	507 Records

PubChem

6.3.2 Substances by Category

PubChem

6.4 Entrez Crosslinks

PubMed	54,232 Records
Protein Structures	220 Records
Taxonomy	5 Records
OMIM	5 Records
Gene	1,455 Records

PubChem

7 Chemical Vendors

PubChem

8 Drug and Medication Information

8.1 FDA National Drug Code Directory

- National Drug Code (NDC) Directory

SUCROSE is an active ingredient in 35 products including: '2 TRANSFORM', 'ALLER-CHORD F', and 'ANISE PYRITE'.

- National Drug Code (NDC) Directory

8.2 Clinical Trials

8.2.1 ClinicalTrials.gov

- ClinicalTrials.gov

8.2.2 NIPH Clinical Trials Search of Japan

NIPH Clinical Trials Search of Japan

8.3 Therapeutic Uses

MEDICATION (VET): ITS ORAL USE IN ACETONEMIA OF CATTLE IS CONTROVERSIAL BUT STILL POPULAR. IT IS OFTEN USED ORALLY WITH **VINEGAR**...IN EMERGENCY TREATMENT OF ACUTE **UREA** TOXICITY IN CATTLE. DAILY ORAL USE CAN OCCASIONALLY REDUCE INCIDENCE OF BLOAT IN CATTLE ON SPRING PASTURE LOW IN CARBOHYDRATES.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 561

Hazardous Substances Data Bank (HSDB)

MEDICATION (VET): 20% ORAL SOLN CAUSE REFLEX CLOSURE OF ESOPHAGEAL GROOVE. ... SUGAR IS OCCASIONALLY USED...TO FACILITATE REDN OF EDEMA & EASE OF REPLACEMENT OF PROLAPSED UTERI IN COWS, EWES, BITCHES, ETC, & HAS BEEN USED LOCALLY ON WOUNDS, FOOT ROT, ETC BY LAYMEN & PROFESSIONALS.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 561

Hazardous Substances Data Bank (HSDB)

IV ADMIN OF HYPERTONIC SOLN OF SUCROSE HAS BEEN EMPLOYED CHIEFLY TO INITIATE OSMOTIC DIURESIS. SUCH PROCEDURE IS NOT COMPLETELY SAFE & RENAL TUBULAR DAMAGE MAY RESULT, PARTICULARLY IN PATIENTS WITH EXISTING RENAL PATHOLOGY. SAFER & MORE EFFECTIVE DIURETICS ARE AVAILABLE. /FORMER USE/

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 1235

Hazardous Substances Data Bank (HSDB)

8.4 Drug Warnings

VET: ORAL ADMIN TO YOUNG ANIMALS UNABLE TO DIGEST IT WILL CAUSE OR ACCENT DIARRHEAS.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 562

Hazardous Substances Data Bank (HSDB)

8.5 Reported Fatal Dose

1. 1= PRACTICALLY NONTOXIC: PROBABLE ORAL LETHAL DOSE (HUMAN) ABOVE 15 G/KG, MORE THAN 1 QUART (2.2 LB) FOR 70 KG PERSON (150 LB).

Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-151

Hazardous Substances Data Bank (HSDB)

9 Food Additives and Ingredients

9.1 FDA Substances Added to Food

Substance	SUCROSE
Used for (Technical Effect)	NUTRITIVE SWEETENER
Document Number (21 CFR)	73.85 172.810 172.816 172.859 172.861 172.880 172.884 173.145 184.1854

FDA Center for Food Safety and Applied Nutrition (CFSAN)

10 Agrochemical Information

10.1 Agrochemical Category

Pesticide active substances

- EU Pesticides Database

10.2 EU Pesticides Data

Active Substance	sucrose
Status	Approved [Reg. (EC) No 1107/2009]
Legislation	Reg. (EU) No 916/2014

- EU Pesticides Database

11 Pharmacology and Biochemistry

11.1 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)

11.2 Human Metabolite Information

11.2.1 Tissue Locations

Adipose Tissue
Bladder
Epidermis
Fibroblasts
Intestine
Kidney
Neuron
Placenta
Platelet
Prostate
Skeletal Muscle
Spleen
Testis

- Human Metabolome Database (HMDB)

11.2.2 Cellular Locations

Extracellular

- Human Metabolome Database (HMDB)

11.2.3 Metabolite Pathways

Galactose Metabolism
Galactosemia
Glycogen synthetase deficiency
Glycogenosis, Type III. Cori disease, Debrancher glycogenosis
Glycogenosis, Type IV. Amylopectinosis, Anderson disease
Glycogenosis, Type VI. Hers disease
Mucopolysaccharidosis VI. Sly syndrome
Starch and Sucrose Metabolism
Sucrase-isomaltase deficiency

- Human Metabolome Database (HMDB)

11.3 Biochemical Reactions

- Rhea - Annotated Reactions Database

- PubChem

12 Use and Manufacturing

12.1 Uses

EPA CPDat Chemical and Product Categories

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

Obtained from cane sugar, sugar beet, and sorghum; Used as a sweetener; [ChemIDplus]

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

For Sucrose (USEPA/OPP Pesticide Code: 000023) there are 0 labels match. /SRP: Not registered for current use in the U.S., but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently approved uses./

U.S. Environmental Protection Agency/Office of Pesticide Program's Chemical Ingredients Database on Sucrose (57-50-1). Available from, as of Sept 8, 2000: https://npirspublic.ceris.purdue.edu/ppis/

- Hazardous Substances Data Bank (HSDB)

FLAVOR BLENDER, ACCENTUATOR, MODIFIER & DISPERSING AGENT, SWEETENING, TEXTURE & BODYING AGENT FOR FOODS & BEVERAGES; RAW MATERIAL FOR NUMEROUS ORG CHEM & YEAST PRODN; LUBRICANT IN FOODS

SRI

- Hazardous Substances Data Bank (HSDB)

Sweetener in foods and soft drinks, manufacture of syrups, source of invert sugar, confectionary, preserves and jams, demulcent, pharmaceutical products, caramel, chemical intermediate for detergents, emulsifying agents, and other sucrose derivatives.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1058

- Hazardous Substances Data Bank (HSDB)

Sweetening agent and food. Starting material in fermentative prodn of ethanol, butanol, glycerol, citric and levulinic acids. Used in pharmaceuticals as a flavor, as a preservative, as antioxidant (in form of invert sugar), as demulcent, as substitute for glycerol, as granulation agent and excipient for tablets, as coating for tablets. In plastics and cellulose industry, in rigid polyurethane foams, manuf of ink and of transparent soaps.

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

- Hazardous Substances Data Bank (HSDB)

For more Uses (Complete) data for SUCROSE (9 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

12.1.1 Use Classification

EPA Safer Chemical Functional Use Classes -> Processing Aids and Additives

- EPA Safer Choice

Safer Chemical Classes -> Green circle - The chemical has been verified to be of low concern

EPA Safer Choice

Agrochemicals -> Pesticides

EU Pesticides Database

Cosmetics -> Humectant; Skin conditioning; Soothing

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

NORMAN Suspect List Exchange

12.1.2 Industry Uses

Adhesives and sealant chemicals
Intermediates

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

EPA Chemicals under the TSCA

12.1.3 Consumer Uses

Cleaning and furnishing care products
Furniture and furnishings not covered elsewhere

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

EPA Chemicals under the TSCA

12.1.4 Household Products

Household & Commercial/Institutional Products

Information on 73 consumer products that contain Sucrose in the following categories is provided:

- Inside the Home
- Personal Care
- Pesticides
- Pet Care

Consumer Product Information Database (CPID)

12.2 Methods of Manufacturing

Obtained from sugar cane (Saccharum officinarum L, Gramineae) and sugar beet (Beta valgaris L, Chenopodiaceae). Sugar cane contains from 15-20% and sugar beet form 10-17% sucrose. Structure: Avery et al, J Chem Soc 1927, 2308; Beevers, Cochrane, Proc Roy Soc 190a, 257 (1947).

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

Hazardous Substances Data Bank (HSDB)

By crushing and extraction of sugarcane (Saccharum officinarum) with water or extraction of the sugar beet (Beta vulgaris) with water, evaporating, and purifying with lime, carbon, and various liquids. Also obtainable from sorghum by conventional methods.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057

Hazardous Substances Data Bank (HSDB)

Sucrose is extracted commercially from sugar maple

KIRK-OTHMER CONDENSED ENCYC CHEM TECH 1985 p.1118

Hazardous Substances Data Bank (HSDB)

12.3 Formulations/Preparations

USEPA/OPP Pesticide Code 000023; Trade Names: None.

U.S. Environmental Protection Agency/Office of Pesticide Program's Chemical Ingredients Database on Sucrose (57-50-1). Available from, as of Sept 8, 2000: https://npirspublic.ceris.purdue.edu/ppis/

Hazardous Substances Data Bank (HSDB)

Grade: Reagent, USP, technical, refined.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057

Hazardous Substances Data Bank (HSDB)

Also sold as syrup .. liquid sugar

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA4 (85) 65

Hazardous Substances Data Bank (HSDB)

12.4 Consumption Patterns

(DELIVERIES OF REFINED SUGAR): 35% WAS CONSUMED DIRECTLY FOR SWEETENING FOODS & BEVERAGES; THE REMAINING 65% WAS USED INDUSTRIALLY IN BEVERAGES (22%); IN BAKERY & CEREAL PRODUCTS (12%); IN CONFECTIONS (9%); IN CANNED, BOTTLED, & FROZEN FOODS (6%); IN ICE CREAM & DAIRY PRODUCTS (5%); IN MISC FOODS (5%); & IN NON-FOOD & UNSPECIFIED USES (6%) (1976)

SRI

Hazardous Substances Data Bank (HSDB)

12.5 U.S. Production

Aggregated Product Volume (EPA CDR 2016)

1,000,000,000 - 5,000,000,000 lb

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

EPA Chemicals under the TSCA

(1972) 5.01X10+13 G (CANE & BEET SUGAR)

SRI

Hazardous Substances Data Bank (HSDB)

(1975) 5.19X10+13 G (CANE AND BEET SUGAR)

SRI

Hazardous Substances Data Bank (HSDB)

12.6 U.S. Imports

(1972) 4.77X10+12 G (CANE/BEET SUGAR & SYRUP)

SRI

Hazardous Substances Data Bank (HSDB)

(1975) 3.62X10+12 G

SRI

Hazardous Substances Data Bank (HSDB)

(1984) 3.28X10+12 g /Cane or beet sugars, syrups, molasses, NSPF (Raw Value)/

BUREAU OF THE CENSUS. U.S. IMPORTS FOR CONSUMPTION AND GENERAL IMPORTS 1984 p.1-41

Hazardous Substances Data Bank (HSDB)

12.7 U.S. Exports

(1972) 7.06X10+8 G (CANE/BEET, RAW & REFINED)
SRI

Hazardous Substances Data Bank (HSDB)

(1975) 1.87X10+11 G
SRI

Hazardous Substances Data Bank (HSDB)

(1984) 2.79X10+10 g /Sugar cane, beet, crystalline structure or dry amorphous form, refined/
BUREAU OF THE CENSUS. U.S. EXPORTS, SCHEDULE E, 1984 p.2-25

Hazardous Substances Data Bank (HSDB)

12.8 General Manufacturing Information

Industry Processing Sectors

Furniture and related product manufacturing
Wood product manufacturing

EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

.alpha.-D-Glucopyranoside, .beta.-D-fructofuranosyl: ACTIVE
https://www.epa.gov/tsca-inventory

EPA Chemicals under the TSCA

CARBOHYDRATE (QV) PRODUCT OF PHOTOSYNTHESIS COMPRISED OF 1, 2, OR MORE SACCHAROSE GROUPS. ... SUGAR IS IMPORTANT SOURCE OF METABOLIC ENERGY IN FOODS, & ITS FORMATION IN PLANTS IS ESSENTIAL FACTOR IN LIFE PROCESS.
Hawley, G.G. The Condensed Chemical Dictionary. 9th ed. New York: Van Nostrand Reinhold Co., 1977., p. 823

Hazardous Substances Data Bank (HSDB)

Sucrose is the most important industrial sugar
KIRK-OTHMER CONDENSED ENCYC CHEM TECH 1985 p.202

Hazardous Substances Data Bank (HSDB)

Sucrose was first synthesized enzymatically in the laboratory from potassium D-glucosyl-1-phosphate and D-fructose. The first chemical synthesis was accomplished by reaction of 3,4,6-tri-O-acetyl-1,2-anhydro-alpha-D-glucopyranose with 1,3,4,6-tetra-O-acetyl-D-fructofuranose
Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V21 865

Hazardous Substances Data Bank (HSDB)

Traditionally, the standard /sweetening agent/ is sucrose, both in terms of quality of taste and taste profile
Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V22 448

Hazardous Substances Data Bank (HSDB)

For more General Manufacturing Information (Complete) data for SUCROSE (6 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

13 Identification

13.1 Analytic Laboratory Methods

SUGARS & SUGAR PRODUCTS BY POLARIMETRIC METHODS.

Association of Official Analytical Chemists. Official Methods of Analysis. 10th ed. and supplements. Washington, DC: Association of Official Analytical Chemists, 1965. New editions through 13th ed. plus supplements, 1982., p. 12/567 31.020

Hazardous Substances Data Bank (HSDB)

DETERMINATION IN FOODSTUFF BY SPECTROPHOTMETRY @ 340, 334, OR 365 NM.

Bergmeyer, H.W. (ed.). Methods of Enzymatic Analysis. 2nd English ed. New York City: Academic Press, 1974., p. 1176

Hazardous Substances Data Bank (HSDB)

14 Safety and Hazards

14.1 Hazards Identification

14.1.1 GHS Classification

GHS Hazard Statements	Not Classified Reported as not meeting GHS hazard criteria by 410 of 425 companies (only ~ 3.5% companies provided GHS information). For more detailed information, please visit ECHA C&L website.

European Chemicals Agency (ECHA)

14.1.2 EPA Safer Chemical

Chemical: Sucrose

Green circle - The chemical has been verified to be of low concern based on experimental and modeled data.

EPA Safer Choice

14.1.3 Health Hazards

None (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

CAMEO Chemicals

14.1.4 Fire Hazards

Special Hazards of Combustion Products: Irritating fumes may form in fires. Behavior in Fire: Melts and chars (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

CAMEO Chemicals

Combustible. Finely dispersed particles form explosive mixtures in air.

ILO International Chemical Safety Cards (ICSC)

14.1.5 Hazards Summary

May cause mechanical irritation.; [ICSC]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

14.2 Safety and Hazard Properties

14.2.1 Flammable Limits

Flammability

Noncombustible Solid, but fine airborne dust may explode.

The National Institute for Occupational Safety and Health (NIOSH)

14.2.2 Lower Explosive Limit (LEL)

0.045 g/L (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

0.045 g/L

Occupational Safety and Health Administration (OSHA)

14.2.3 Physical Dangers

Dust explosion possible if in powder or granular form, mixed with air.

ILO International Chemical Safety Cards (ICSC)

14.2.4 OSHA Standards

Permissible Exposure Limit: Table Z-1 8-hr Time Weighted Avg: 15 mg/cu m. /Total dust/

29 CFR 1910.1000 (7/1/2000)

Hazardous Substances Data Bank (HSDB)

Permissible Exposure Limit: Table Z-1 8-hr Time Weighted Avg: 5 mg/cu m. /Respirable fraction/

29 CFR 1910.1000 (7/1/2000)

Hazardous Substances Data Bank (HSDB)

14.2.5 NIOSH Recommendations

Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 10 mg/cu m (total).

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

Hazardous Substances Data Bank (HSDB)

Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 5 mg/cu m (resp).

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

Hazardous Substances Data Bank (HSDB)

14.3 First Aid Measures

14.3.1 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. If symptoms (such as redness or irritation) develop, immediately transport the victim to a hospital. 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. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. 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. (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

(See procedures)

Eye: Irrigate immediately - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.

Breathing: Fresh air

The National Institute for Occupational Safety and Health (NIOSH)

14.3.2 Inhalation First Aid

Fresh air, rest.

- ILO International Chemical Safety Cards (ICSC)

14.3.3 Skin First Aid

Rinse skin with plenty of water or shower.

- ILO International Chemical Safety Cards (ICSC)

14.3.4 Eye First Aid

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

- ILO International Chemical Safety Cards (ICSC)

14.4 Fire Fighting

Fire Extinguishing Agents: Water (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

- CAMEO Chemicals

Use water spray, powder, alcohol-resistant foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

- ILO International Chemical Safety Cards (ICSC)

14.4.1 Fire Fighting Procedures

Water

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

- Hazardous Substances Data Bank (HSDB)

14.4.2 Firefighting Hazards

Irritating fumes may form in fires.

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

- Hazardous Substances Data Bank (HSDB)

14.5 Accidental Release Measures

14.5.1 Spillage Disposal

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting.

- ILO International Chemical Safety Cards (ICSC)

14.5.2 Disposal Methods

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

- Hazardous Substances Data Bank (HSDB)

14.6 Handling and Storage

14.6.1 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 material under ambient temperatures. (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

14.6.2 Safe Storage

Separated from strong oxidants.

- ILO International Chemical Safety Cards (ICSC)

14.7 Exposure Control and Personal Protection

14.7.1 Recommended Exposure Limit (REL)

REL-TWA (Time Weighted Average)

10 mg/m^3 (total), 5 mg/m^3 (resp)

- Occupational Safety and Health Administration (OSHA)

TWA 10 mg/m^3 (total) TWA 5 mg/m^3 (resp)

- The National Institute for Occupational Safety and Health (NIOSH)

14.7.2 Permissible Exposure Limit (PEL)

15.0 [mg/m3](total dust), 5 mg/m3(respirable fraction)

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

PEL-TWA (8-Hour Time Weighted Average)

15 mg/m^3 (total dust), 5 mg/m^3 (respirable fraction)

- Occupational Safety and Health Administration (OSHA)

TWA 15 mg/m^3 (total) TWA 5 mg/m^3 (resp)

- The National Institute for Occupational Safety and Health (NIOSH)

14.7.3 Immediately Dangerous to Life or Health (IDLH)

N.D.

See: IDLH INDEX

- The National Institute for Occupational Safety and Health (NIOSH)

14.7.4 Threshold Limit Values (TLV)

10.0 [mg/m3]

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

8 hr Time Weighted Avg (TWA): 10 mg/cu m

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 53

- Hazardous Substances Data Bank (HSDB)

Excursion Limit Recommendation: Excursions in worker exposure levels may exceed 3 times the TLV-TWA for no more than a total of 30 minutes during a work day, and under no circumstances should they exceed 5 times the TLV-TWA, provided that the TLV-TWA is not exceeded.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 5

- Hazardous Substances Data Bank (HSDB)

A4: Not classifiable as a human carcinogen.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 53

- Hazardous Substances Data Bank (HSDB)

10 mg/m3, as TWA; A4 (not classifiable as a human carcinogen)

- ILO International Chemical Safety Cards (ICSC)

TLV-TWA (Time Weighted Average)

10 mg/m^3 [1992]

- Occupational Safety and Health Administration (OSHA)

14.7.5 Effects of Short Term Exposure

May cause mechanical irritation.

- ILO International Chemical Safety Cards (ICSC)

14.7.6 Effects of Long Term Exposure

The substance may have effects on the teeth. This may result in dental caries. Repeated or prolonged contact with skin may cause dermatitis.

- ILO International Chemical Safety Cards (ICSC)

14.7.7 Allowable Tolerances

Residues of sucrose are exempted from the requirement of a tolerance when used as a solid diluent, carrier or safener in accordance with good agricultural practices as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

40 CFR 180.1001(c) (7/1/2000)

- Hazardous Substances Data Bank (HSDB)

Sucrose is exempted from the requirement of a tolerance when used as a solid diluent or carrier in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

40 CFR 180.1001(e) (7/1/2000)

- Hazardous Substances Data Bank (HSDB)

14.7.8 Personal Protective Equipment (PPE)

Excerpt from NIOSH Pocket Guide for Sucrose: Skin: No recommendation is made specifying the need for personal protective equipment for the body. Eyes: No recommendation is made specifying the need for eye protection. Wash skin: No recommendation is made specifying the need for washing the substance from the skin (either immediately or at the end of the work shift). Remove: No recommendation is made specifying the need for removing clothing that becomes wet or contaminated. Change: No recommendation is made specifying the need for the worker to change clothing after the workshift. (NIOSH, 2022)

- CAMEO Chemicals

/NIOSH approved respirator/ and goggles or face shield.

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

- Hazardous Substances Data Bank (HSDB)

(See protection codes)

Skin: No recommendation

Eyes: No recommendation

Wash skin: No recommendation

Remove: No recommendation

Change: No recommendation

- The National Institute for Occupational Safety and Health (NIOSH)

14.7.9 Respirator Recommendations

Important additional information about respirator selection

- The National Institute for Occupational Safety and Health (NIOSH)

14.7.10 Fire Prevention

NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust.

- ILO International Chemical Safety Cards (ICSC)

14.7.11 Inhalation Prevention

Use local exhaust or breathing protection.

- ILO International Chemical Safety Cards (ICSC)

14.7.12 Skin Prevention

Protective gloves.

- ILO International Chemical Safety Cards (ICSC)

14.7.13 Eye Prevention

Wear safety goggles.

- ILO International Chemical Safety Cards (ICSC)

14.8 Stability and Reactivity

14.8.1 Air and Water Reactions

Water soluble. Sugar dust explosion is possibility.

- CAMEO Chemicals

14.8.2 Reactive Group

Alcohols and Polyols

- CAMEO Chemicals

14.8.3 Reactivity Profile

SUCROSE is a reducing agent. Can react explosively with oxidizing agents such as chlorates and perchlorates. Is hydrolyzed by dilute acids and by invertase (a yeast enzyme) (NTP, 1992). Chars rapidly and exothermically when mixed with concentrated sulfuric acid.

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

14.8.4 Hazardous Reactivities and Incompatibilities

Oxidizers, sulfuric acid, nitric acid.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

- Hazardous Substances Data Bank (HSDB)

14.9 Regulatory Information

14.9.1 FIFRA Requirements

Residues of sucrose are exempted from the requirement of a tolerance when used as a solid diluent, carrier or safener in accordance with good agricultural practices as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

40 CFR 180.1001(c) (7/1/2000)

- Hazardous Substances Data Bank (HSDB)

Sucrose is exempted from the requirement of a tolerance when used as a solid diluent or carrier in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

40 CFR 180.1001(e) (7/1/2000)

- Hazardous Substances Data Bank (HSDB)

14.9.2 FDA Requirements

Substance added directly to human food affirmed as generally recognized as safe (GRAS).

21 CFR 184.1854 (4/1/2000)

- Hazardous Substances Data Bank (HSDB)

14.10 Other Safety Information

14.10.1 Special Reports

INFORMATICS INC; SCIENTIFIC LITERATURE REVIEWS ON GENERALLY RECOGNIZED AS SAFE (GRAS) FOOD INGREDIENTS: SUCROSE; US NTIS PB REPORT PB-228 548, 202 PP. (1973). LITERATURE REVIEW OF SUCROSE AND ITS USE IN FOOD PRODUCTS.

- Hazardous Substances Data Bank (HSDB)

15 Toxicity

15.1 Toxicological Information

15.1.1 NIOSH Toxicity Data

- The National Institute for Occupational Safety and Health (NIOSH)

15.1.2 Evidence for Carcinogenicity

A4: Not classifiable as a human carcinogen.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 53

- Hazardous Substances Data Bank (HSDB)

15.1.3 Exposure Routes

The substance can be absorbed into the body by inhalation and by ingestion.

- ILO International Chemical Safety Cards (ICSC)

inhalation, skin and/or eye contact

- The National Institute for Occupational Safety and Health (NIOSH)

15.1.4 Symptoms

irritation eyes, skin, upper respiratory system; cough

- The National Institute for Occupational Safety and Health (NIOSH)

15.1.5 Inhalation Symptoms

Cough.

- ILO International Chemical Safety Cards (ICSC)

15.1.6 Skin Symptoms

Redness. Roughness.

- ILO International Chemical Safety Cards (ICSC)

15.1.7 Eye Symptoms

Redness.

- ILO International Chemical Safety Cards (ICSC)

15.1.8 Target Organs

Eyes, respiratory system

- The National Institute for Occupational Safety and Health (NIOSH)

15.1.9 Adverse Effects

ACGIH Carcinogen - Not Classifiable.

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

15.1.10 Acute Effects

- ChemIDplus

15.1.11 Human Toxicity Excerpts

Liquid medicines, particularly those intended for children, often formulated as syrups, usually based on sucrose. Total sugar content may be up to 80% (w/v). Complicated diabetes management. Increased dental caries especially in chronically sick children (eg, asthmatics or epileptics) who frequently take liquid medicine.

Ellenhorn, M.J. and D.G. Barceloux. Medical Toxicology - Diagnosis and Treatment of Human Poisoning. New York, NY: Elsevier Science Publishing Co., Inc. 1988., p. 527

- Hazardous Substances Data Bank (HSDB)

Sucrose is reported to be capable of producing dermatoses in bakers, candy makers, and related occupations. It is well established that uncontrolled **glucose** conc in maternal blood are associated with elevated embryonic and fetal death and increased neonatal morbidity and mortality.

American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1450

- Hazardous Substances Data Bank (HSDB)

15.1.12 Non-Human Toxicity Excerpts

EVIDENCE EXISTS THAT HIGHLY CONCN SOLN ARE LETHAL TO NEMATODES IN SOIL.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 562

Hazardous Substances Data Bank (HSDB)

DIFFUSE PATHOLOGICAL CHANGES /IN POISONED ANIMALS/ INCL SHRINKAGE, SWELLING & NECROSIS OF RENAL TUBULAR EPITHELIUM, ARTERIOLITIS, MILD HEPATITIS, MYOCARDITIS, CONGESTIVE ENCEPHALITIS & SOME ADRENAL HYPERTROPHY.

Gosselin, R.E., R.P. Smith, H.C. Hodge. Clinical Toxicology of Commercial Products. 5th ed. Baltimore: Williams and Wilkins, 1984., p. II-227

Hazardous Substances Data Bank (HSDB)

SUCROSE HAS SHOWN NO TOXICITY TO CORNEAS OF RABBITS WHEN APPLIED FOR 3 TO 7 HR IN NEUTRAL AQ SOLN...

Grant, W. M. Toxicology of the Eye. 2nd ed. Springfield, Illinois: Charles C. Thomas, 1974., p. 949

Hazardous Substances Data Bank (HSDB)

...CANE SUGAR...OBSERVED TO CAUSE DIARRHEA, COLIC, INFLAMMATION OF KIDNEYS &...PETECHIAL HEMORRHAGES IN SPINAL DURA MATER OF HORSES.

Clarke, E.G., and M. L. Clarke. Veterinary Toxicology. Baltimore, Maryland: The Williams and Wilkins Company, 1975., p. 284

Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for SUCROSE (14 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

15.1.13 Non-Human Toxicity Values

LD50 Rat oral 29,700 mg/kg

Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2478

Hazardous Substances Data Bank (HSDB)

15.1.14 Populations at Special Risk

Patients with severe malabsorption secondary to disease or resection ... may have deficiency of other disaccharidases and large amounts of sucrose should be avoided /in enteral formulations/.

American Medical Association, Council on Drugs. AMA Drug Evaluations Annual 1994. Chicago, IL: American Medical Association, 1994., p. 2195

Hazardous Substances Data Bank (HSDB)

15.2 Ecological Information

15.2.1 Natural Pollution Sources

Occurs in low percentages in honey and maple sap

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057

Hazardous Substances Data Bank (HSDB)

Sugar cane contains from 15-20% and sugar beet from 10-17% sucrose

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1517

Hazardous Substances Data Bank (HSDB)

The quantity of sucrose synthesized by all plants on earth is estimated to be 150X10+9 t/a.

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA 5 (86) 83

Hazardous Substances Data Bank (HSDB)

16 Associated Disorders and Diseases

Comparative Toxicogenomics Database (CTD)

Disease	References
Colorectal cancer	PubMed: 7482520, 19006102, 23940645, 24424155, 20156336, 19678709, 22148915, 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
Crohn's disease	PubMed: 16440420, 11418788, 8723414, 19491857, 17269711, 23516449, 23867873, 24811995, 25598765, 26806034, 26848182, 27609529, 28842642
Ulcerative colitis	PubMed: 21059682, 1740537, 17269711, 17314143, 21761941, 23516449, 23867873, 24811995, 25598765, 26806034, 26848182, 27609529, 28842642
Sepsis	PubMed: 9141546, 19034423, 28701177
Attachment loss	PubMed: 31026179
Periodontal Probing Depth	PubMed: 31026179
Lung Cancer	PubMed: 22157537, 18953024, 25961003
Autosomal dominant polycystic kidney disease	PubMed: 18215696, 21389975
Eosinophilic esophagitis	Mordechai, Hien, and David S. Wishart

Human Metabolome Database (HMDB)

17 Literature

17.1 Coronavirus Studies

PubChem

17.2 NLM Curated PubMed Citations

PubChem

17.3 Springer Nature References

- Springer Nature

17.4 Thieme References

- Thieme Chemistry

17.5 Depositor Provided PubMed Citations

- PubChem

17.6 Synthesis References

Francois B. Paul, Pierre F. Monsan, Magali M. C. Remaud, Vincent P. Pelenc, "Process for the enzymatic preparation from sucrose of a mixture of sugars having a high content of isomaltose, and products obtained." U.S. Patent US4861381, issued April, 1956.

- DrugBank

Fitremann, Juliette; Queneau, Yves; Maitre, Jean-Paul; Bouchu, Alain. Co-melting of solid sucrose and multivalent cation soaps for solvent-free synthesis of sucrose esters. Tetrahedron Letters (2007), 48(23), 4111-4114.

- Human Metabolome Database (HMDB)

17.7 Metabolite References

Human Metabolome Database (HMDB)

17.8 General References

1. Ten S, Maclaren N: Insulin resistance syndrome in children. J Clin Endocrinol Metab. 2004 Jun;89(6):2526-39. [PMID:15181020]
2. Aguilera AA, Diaz GH, Barcelata ML, Guerrero OA, Ros RM: Effects of fish oil on hypertension, plasma lipids, and tumor necrosis factor-alpha in rats with sucrose-induced metabolic syndrome. J Nutr Biochem. 2004 Jun;15(6):350-7. [PMID:15157941]
3. Fukuchi S, Hamaguchi K, Seike M, Himeno K, Sakata T, Yoshimatsu H: Role of fatty acid composition in the development of metabolic disorders in sucrose-induced obese rats. Exp Biol Med (Maywood). 2004 Jun;229(6):486-93. [PMID:15169967]
4. Lombardo YB, Drago S, Chicco A, Fainstein-Day P, Gutman R, Gagliardino JJ, Gomez Dumm CL: Long-term administration of a sucrose-rich diet to normal rats: relationship between metabolic and hormonal profiles and morphological changes in the endocrine pancreas. Metabolism. 1996 Dec;45(12):1527-32. [PMID:8969287]

DrugBank

17.9 Chemical Co-Occurrences in Literature

PubChem

17.10 Chemical-Gene Co-Occurrences in Literature

PubChem

17.11 Chemical-Disease Co-Occurrences in Literature

PubChem

18 Patents

18.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

18.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=CZMRCDWAGMRECN-UGDNZRGBSA-N

- PATENTSCOPE (WIPO)

19 Interactions and Pathways

19.1 Protein Bound 3D Structures

View 220 proteins in NCBI Structure

PubChem

19.2 Chemical-Target Interactions

Comparative Toxicogenomics Database (CTD)

DrugBank

- Therapeutic Target Database (TTD)

19.3 Pathways

- PubChem

20 Biological Test Results

20.1 BioAssay Results

PubChem

21 Taxonomy

Sucrose is a metabolite found in or produced by Escherichia coli (strain K12, MG1655).

- E. coli Metabolome Database (ECMDB)

WormJam Metabolites Local CSV for MetFrag | *DOI:10.5281/zenodo.3403364*
WormJam: A consensus C. elegans Metabolic Reconstruction and Metabolomics Community and Workshop Series, Worm, 6:2, e1373939, *DOI:10.1080/21624054.2017.1373939*

- ECI Group, LCSB, University of Luxembourg

Zebrafish Pathway Metabolite MetFrag Local CSV (Beta) | *DOI:10.5281/zenodo.3457553*

- ECI Group, LCSB, University of Luxembourg

The LOTUS Initiative for Open Natural Products Research: frozen dataset union wikidata (with metadata) | ***DOI:10.5281/zenodo.5794106***

- **LOTUS - the natural products occurrence database**

Sucrose is a metabolite found in or produced by Saccharomyces cerevisiae.

- **Yeast Metabolome Database (YMDB)**

22 Classification

22.1 MeSH Tree

Medical Subject Headings (MeSH)

22.2 NCI Thesaurus Tree

NCI Thesaurus (NCIt)

22.3 ChEBI Ontology

ChEBI

22.4 KEGG: Metabolite

KEGG

22.5 KEGG: Drug

KEGG

22.6 KEGG: JP15

KEGG

22.7 KEGG: Risk Category of Japanese OTC Drugs

KEGG

22.8 EPA Safer Choice

EPA Safer Choice

22.9 ChemIDplus

ChemIDplus

22.10 CAMEO Chemicals

CAMEO Chemicals

22.11 ChEMBL Target Tree

ChEMBL

22.12 UN GHS Classification

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

22.13 EPA CPDat Classification

- EPA Chemical and Products Database (CPDat)

22.14 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

22.15 CCSBase Classification

- CCSbase

22.16 EPA DSSTox Classification

- EPA DSSTox

22.17 Consumer Product Information Database Classification

- Consumer Product Information Database (CPID)

22.18 LOTUS Tree

- LOTUS - the natural products occurrence database

22.19 FDA Drug Type and Pharmacologic Classification

- National Drug Code (NDC) Directory

22.20 EPA Substance Registry Services Tree

- EPA Substance Registry Services

23 Information Sources

FILTER BY SOURCE ALL SOURCES

1. **CAMEO Chemicals**

   LICENSE

   CAMEO Chemicals and all other CAMEO products are available at no charge to those organizations and individuals (recipients) responsible for the safe handling of chemicals. However, some of the chemical data itself is subject to the copyright restrictions of the companies or organizations that provided the data.

   https://cameochemicals.noaa.gov/help/reference/terms_and_conditions.htm?d_f=false

   SUCROSE
   https://cameochemicals.noaa.gov/chemical/12695

   CAMEO Chemical Reactivity Classification
   https://cameochemicals.noaa.gov/browse/react

2. **CAS Common Chemistry**

   LICENSE

   The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.

   https://creativecommons.org/licenses/by-nc/4.0/

   Sucrose
   https://commonchemistry.cas.org/detail?cas_rn=57-50-1

   Polysucrose
   https://commonchemistry.cas.org/detail?cas_rn=25702-74-3

3. **ChemIDplus**

   LICENSE

   https://www.nlm.nih.gov/copyright.html

   Sucrose [JAN:NF]
   https://chem.nlm.nih.gov/chemidplus/sid/0000057501

   ChemIDplus Chemical Information Classification
   https://chem.nlm.nih.gov/chemidplus/

4. **DrugBank**

   LICENSE

   Creative Common's Attribution-NonCommercial 4.0 International License (http://creativecommons.org/licenses/by-nc/4.0/legalcode)

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

   Sucrose
   https://www.drugbank.ca/drugs/DB02772

5. **EPA Chemicals under the TSCA**

   LICENSE

   https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

   .alpha.-D-Glucopyranoside, .beta.-D-fructofuranosyl
   https://www.epa.gov/chemicals-under-tsca

6. **EPA DSSTox**

   LICENSE

   https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

   Sucrose
   https://comptox.epa.gov/dashboard/DTXSID2021288

   CompTox Chemicals Dashboard Chemical Lists
   https://comptox.epa.gov/dashboard/chemical-lists/

7. **European Chemicals Agency (ECHA)**

   LICENSE

   Use of the information, documents and data from the ECHA website is subject to the terms and conditions of this Legal Notice, and subject to other binding limitations provided for under applicable law, the information, documents and data made available on the ECHA website may be reproduced, distributed and/or used, totally or in part, for non-commercial purposes provided that ECHA is acknowledged as the source: "Source: European Chemicals Agency, http://echa.europa.eu/". Such acknowledgement must be included in each copy of the material. ECHA permits and encourages organisations and individuals to create links to the ECHA website under the following cumulative conditions: Links can only be made to webpages that provide a link to the Legal Notice page.

   https://echa.europa.eu/web/guest/legal-notice

   Sucrose
   https://echa.europa.eu/substance-information/-/substanceinfo/100.000.304

   α-D-Glucopyranoside, β-D-fructofuranosyl
   https://echa.europa.eu/information-on-chemicals

Sucrose
https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/42557

8. **FDA Global Substance Registration System (GSRS)**

LICENSE

Unless otherwise noted, the contents of the FDA website (www.fda.gov), both text and graphics, are not copyrighted. They are in the public domain and may be republished, reprinted and otherwise used freely by anyone without the need to obtain permission from FDA. Credit to the U.S. Food and Drug Administration as the source is appreciated but not required.

https://www.fda.gov/about-fda/about-website/website-policies#linking

SUCROSE
https://gsrs.ncats.nih.gov/ginas/app/beta/substances/C151H8M554

9. **Hazardous Substances Data Bank (HSDB)**

SUCROSE
https://pubchem.ncbi.nlm.nih.gov/source/hsdb/500

10. **Human Metabolome Database (HMDB)**

LICENSE

HMDB is offered to the public as a freely available resource. Use and re-distribution of the data, in whole or in part, for commercial purposes requires explicit permission of the authors and explicit acknowledgment of the source material (HMDB) and the original publication (see the HMDB citing page). We ask that users who download significant portions of the database cite the HMDB paper in any resulting publications.

http://www.hmdb.ca/citing

Sucrose
http://www.hmdb.ca/metabolites/HMDB0000258

HMDB0000258_cms_30233
https://hmdb.ca/metabolites/HMDB0000258#spectra

11. **ILO International Chemical Safety Cards (ICSC)**

LICENSE

The reproduction of ILO material is generally authorized for non-commercial purposes and within established limits. For non-commercial purposes of reproduction of data, any required permission is hereby granted and no further permission must be obtained from the ILO, but acknowledgement to the ILO as the original source must be made.

https://www.ilo.org/global/copyright/request-for-permission/lang--en/index.htm

SUCROSE
https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=1507

12. **Occupational Safety and Health Administration (OSHA)**

LICENSE

Materials created by the federal government are generally part of the public domain and may be used, reproduced and distributed without permission. Therefore, content on this website which is in the public domain may be used without the prior permission of the U.S. Department of Labor (DOL). Warning: Some content - including both images and text - may be the copyrighted property of others and used by the DOL under a license.

https://www.dol.gov/general/aboutdol/copyright

SUCROSE
https://www.osha.gov/chemicaldata/420

13. **The National Institute for Occupational Safety and Health (NIOSH)**

LICENSE

The information provided using CDC Web site is only intended to be general summary information to the public. It is not intended to take the place of either the written law or regulations.

https://www.cdc.gov/Other/disclaimer.html

Sucrose
https://www.cdc.gov/niosh-rtecs/WN632EA0.html

Sucrose
https://www.cdc.gov/niosh/npg/npgd0574.html

14. **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

LICENSE

Copyright (c) 2022 Haz-Map(R). All rights reserved. Unless otherwise indicated, all materials from Haz-Map are copyrighted by Haz-Map(R). No part of these materials, either text or image may be used for any purpose other than for personal use. Therefore, reproduction, modification, storage in a retrieval system or retransmission, in any form or by any means, electronic, mechanical or otherwise, for reasons other than personal use, is strictly prohibited without prior written permission.

https://haz-map.com/About

Sucrose
https://haz-map.com/Agents/633

15. **ChEBI**

Sucrose
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:17992

ChEBI Ontology
http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

16. **E. coli Metabolome Database (ECMDB)**

LICENSE

ECMDB is offered to the public as a freely available resource.

https://ecmdb.ca/citations

https://ecmdb.ca/compounds/M2MDB000109

17. **LOTUS - the natural products occurrence database**

LICENSE
The code for LOTUS is released under the GNU General Public License v3.0.
https://lotus.nprod.net/

LOTUS Tree
https://lotus.naturalproducts.net/

18. **West Coast Metabolomics Center-UC Davis**

Sucrose

19. **Yeast Metabolome Database (YMDB)**

LICENSE
YMDB is offered to the public as a freely available resource.
http://www.ymdb.ca/downloads

http://www.ymdb.ca/compounds/YMDB00906

20. **CCSbase**

Sucrose

CCSbase Classification
https://ccsbase.net/

21. **NORMAN Suspect List Exchange**

LICENSE
Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
https://creativecommons.org/licenses/by/4.0/

Sucrose

NORMAN Suspect List Exchange Classification
https://www.norman-network.com/nds/SLE/

22. **ClinicalTrials.gov**

LICENSE
The ClinicalTrials.gov data carry an international copyright outside the United States and its Territories or Possessions. Some ClinicalTrials.gov data may be subject to the copyright of third parties; you should consult these entities for any additional terms of use.
https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use

https://clinicaltrials.gov/

23. **Comparative Toxicogenomics Database (CTD)**

LICENSE
It is to be used only for research and educational purposes. Any reproduction or use for commercial purpose is prohibited without the prior express written permission of NC State University.
http://ctdbase.org/about/legal.jsp

https://ctdbase.org/detail.go?type=chem&acc=D013395

24. **Therapeutic Target Database (TTD)**

Sucrose
http://idrblab.net/ttd/data/drug/details/D08TCV

25. **Consumer Product Information Database (CPID)**

LICENSE
Copyright (c) 2021 DeLima Associates. All rights reserved. Unless otherwise indicated, all materials from CPID are copyrighted by DeLima Associates. No part of these materials, either text or image may be used for any purpose other than for personal use. Therefore, reproduction, modification, storage in a retrieval system or retransmission, in any form or by any means, electronic, mechanical or otherwise, for reasons other than personal use, is strictly prohibited without prior written permission.
https://www.whatsinproducts.com/contents/view/1/6

Sucrose
https://www.whatsinproducts.com/chemicals/view/1/1362/000057-50-1

Consumer Products Category Classification
https://www.whatsinproducts.com/

26. **ECI Group, LCSB, University of Luxembourg**

LICENSE
Data: CC-BY 4.0; Code: Artistic-2.0
https://creativecommons.org/licenses/by/4.0/

27. **EPA Chemical and Products Database (CPDat)**

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

https://comptox.epa.gov/dashboard/DTXSID2021288#exposure

EPA CPDat Classification
https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

28. **EPA Safer Choice**

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Sucrose
https://www.epa.gov/saferchoice/safer-ingredients

EPA Safer Chemical Ingredients Classification
https://www.epa.gov/saferchoice

29. **EU Pesticides Database**

Sucrose
https://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/active-substances/?event=as.details&as_id=1206

30. **FDA Center for Food Safety and Applied Nutrition (CFSAN)**

LICENSE
Unless otherwise noted, the contents of the FDA website (www.fda.gov), both text and graphics, are not copyrighted. They are in the public domain and may be republished, reprinted and otherwise used freely by anyone without the need to obtain permission from FDA. Credit to the U.S. Food and Drug Administration as the source is appreciated but not required.
https://www.fda.gov/about-fda/about-website/website-policies#linking

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

31. **GlyCosmos Glycoscience Portal**

LICENSE
All copyrightable parts of the datasets in GlyCosmos are under the Creative Commons Attribution (CC BY 4.0) License.
https://glycosmos.org/license

https://glycosmos.org/glycans/show/G05551OP

32. **GlyTouCan Project**

LICENSE
https://creativecommons.org/licenses/by/4.0/

https://glytoucan.org/Structures/Glycans/G78152OD
https://glytoucan.org/Structures/Glycans/G44791DH
https://glytoucan.org/Structures/Glycans/G05551OP

33. **MassBank of North America (MoNA)**

LICENSE
The content of the MoNA database is licensed under CC BY 4.0.
https://mona.fiehnlab.ucdavis.edu/documentation/license

Sucrose
https://mona.fiehnlab.ucdavis.edu/spectra/browse?query=compound.metaData%3Dq%3D%27name%3D%3D%22InChIKey%22%20and%20value%3D%3D%22CZMRCDWAGMRECN-UGDNZRGBSA-N%22%27

34. **MassBank Europe**

LICENSE
https://github.com/MassBank/MassBank-web/blob/main/MassBank-Project/LICENSE.txt

CZMRCDWAGMRECN-UGDNZRGBSA-N
https://massbank.eu/MassBank/Result.jsp?inchikey=CZMRCDWAGMRECN-UGDNZRGBSA-N

35. **SpectraBase**

Sucrose, 11TMS
https://spectrabase.com/spectrum/9SVwuBC8QiG

SUCROSE
https://spectrabase.com/spectrum/6gS90D0VTLc

Sucrose
https://spectrabase.com/spectrum/GtsxQKBSRHm

sucrose
https://spectrabase.com/spectrum/Ax3PIVXjnO

Sucrose
https://spectrabase.com/spectrum/9QGk0iPtMJk

SUCROSE, GLUCOPYRANOSIDOFRUCTOFURANOSIDE
https://spectrabase.com/spectrum/K0bGhEfFB0z

SUCROSE
https://spectrabase.com/spectrum/BqfxPagae9c

Sugar
https://spectrabase.com/spectrum/7fDKpvl4kiK

Sucrose
https://spectrabase.com/spectrum/34czK6Huovq

Sucrose
https://spectrabase.com/spectrum/AhtrUdzxhX1

Sucrose
https://spectrabase.com/spectrum/2QBQSZO7591

36. ## National Drug Code (NDC) Directory

LICENSE

Unless otherwise noted, the contents of the FDA website (www.fda.gov), both text and graphics, are not copyrighted. They are in the public domain and may be republished, reprinted and otherwise used freely by anyone without the need to obtain permission from FDA. Credit to the U.S. Food and Drug Administration as the source is appreciated but not required.

https://www.fda.gov/about-fda/about-website/website-policies#linking

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

37. ## NCI Thesaurus (NCIt)

LICENSE

Unless otherwise indicated, all text within NCI products is free of copyright and may be reused without our permission. Credit the National Cancer Institute as the source.

https://www.cancer.gov/policies/copyright-reuse

https://ncithesaurus.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=ncit&code=C68477

NCI Thesaurus Tree
https://ncit.nci.nih.gov

38. ## NIPH Clinical Trials Search of Japan
https://rctportal.niph.go.jp/en/

39. ## NLM RxNorm Terminology

LICENSE

The RxNorm Terminology is created by the National Library of Medicine (NLM) and is in the public domain and may be republished, reprinted and otherwise used freely by anyone without the need to obtain permission from NLM. Credit to the U.S. National Library of Medicine as the source is appreciated but not required. The full RxNorm dataset requires a free license.

https://www.nlm.nih.gov/research/umls/rxnorm/docs/termsofservice.html

sucrose
https://rxnav.nlm.nih.gov/id/rxnorm/10159

40. ## PubChem
https://pubchem.ncbi.nlm.nih.gov

41. ## Rhea - Annotated Reactions Database

LICENSE

Rhea has chosen to apply the Creative Commons Attribution License (http://creativecommons.org/licenses/by/4.0/). This means that you are free to copy, distribute, display and make commercial use of the database in all legislations, provided you credit (cite) Rhea.

https://www.rhea-db.org/help/license-disclaimer

https://www.rhea-db.org/rhea?query=CHEBI:17992

42. ## Springer Nature
https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=23053998-26631472

43. ## SpringerMaterials

Rohrzucker
https://materials.springer.com/substanceprofile/docs/smsid_hhdklwmwjrpnejmg

44. ## The Cambridge Structural Database
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=156796
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=207169
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=212775
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=634580
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=763166
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=775215
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835302
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835303
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835304
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835305
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835306
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835307
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835308
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835309

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835310
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835311
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835312
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835313
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835314
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835315
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835316
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835317
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835318
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835319
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835320
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835321
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835322
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835323
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=835324

45. **Thieme Chemistry**

> LICENSE
> The Thieme Chemistry contribution within PubChem is provided under a CC-BY-NC-ND 4.0 license, unless otherwise stated.
> https://creativecommons.org/licenses/by-nc-nd/4.0/

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=23053998-26513100
https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=23053998-26631472

46. **Wikidata**

> LICENSE
> CCZero
> https://creativecommons.org/publicdomain/zero/1.0/

Sucrose
https://www.wikidata.org/wiki/Q4027534

47. **Medical Subject Headings (MeSH)**

> LICENSE
> Works produced by the U.S. government are not subject to copyright protection in the United States. Any such works found on National Library of Medicine (NLM) Web sites may be freely used or reproduced without permission in the U.S.
> https://www.nlm.nih.gov/copyright.html

Sucrose
https://www.ncbi.nlm.nih.gov/mesh/68013395

MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html

Sweetening Agents
https://www.ncbi.nlm.nih.gov/mesh/68013549

48. **KEGG**

> LICENSE
> Academic users may freely use the KEGG website. Non-academic use of KEGG generally requires a commercial license
> https://www.kegg.jp/kegg/legal.html

Compounds with biological roles
http://www.genome.jp/kegg-bin/get_htext?br08001.keg

Therapeutic category of drugs in Japan
http://www.genome.jp/kegg-bin/get_htext?br08301.keg

Drugs listed in the Japanese Pharmacopoeia
http://www.genome.jp/kegg-bin/get_htext?br08311.keg

Risk category of Japanese OTC drugs
http://www.genome.jp/kegg-bin/get_htext?br08312.keg

49. **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

50. **ChEMBL**

> LICENSE
> Access to the web interface of ChEMBL is made under the EBI's Terms of Use (http://www.ebi.ac.uk/Information/termsofuse.html). The ChEMBL data is made available on a Creative Commons Attribution-Share Alike 3.0 Unported License (http://creativecommons.org/licenses/by-sa/3.0/).
> http://www.ebi.ac.uk/Information/termsofuse.html

ChEMBL Protein Target Tree
https://www.ebi.ac.uk/chembl/g/#browse/targets

51. **EPA Substance Registry Services**

> LICENSE

> https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

EPA SRS List Classification
https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

52. **PATENTSCOPE (WIPO)**

SID 403029430
https://pubchem.ncbi.nlm.nih.gov/substance/403029430