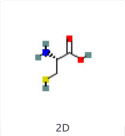
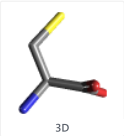
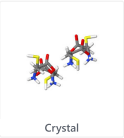
PubChem

COMPOUND SUMMARY

Cysteine

Cite Download

PubChem CID	5862
Structure	 2D  3D  Crystal Find Similar Structures
Chemical Safety	Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_3H_7NO_2S$
Synonyms	L-cysteine cysteine 52-90-4 Thioserine (R)-2-Amino-3-mercaptopropanoic acid More...
Molecular Weight	121.16
Dates	Modify 2022-11-05 Create 2004-09-16

Cysteine is a non-essential sulfur-containing amino acid in humans, related to cystine, Cysteine is important for protein synthesis, detoxification, and diverse metabolic functions. Found in beta-keratin, the main protein in nails, skin, and hair, Cysteine is important in collagen production, as well as skin elasticity and texture. Also required in the manufacture of amino acid taurine, Cysteine is a component of the antioxidant glutathione, and plays a role in the metabolism of essential biochemicals such as coenzyme A, heparin, and biotin. (NCI04)

NCI Thesaurus (NCIt)

L-cysteine is an optically active form of cysteine having L-configuration. It has a role as a flour treatment agent, a human metabolite and an EC 4.3.1.3 (histidine ammonia-lyase) inhibitor. It is a serine family amino acid, a proteinogenic amino acid, a cysteine and a L-alpha-amino acid. It is a conjugate base of a L-cysteinium. It is a conjugate acid of a L-cysteinate(1-). It is an enantiomer of a D-cysteine. It is a tautomer of a L-cysteine zwitterion.

ChEBI

Cysteine is a metabolite found in the aging mouse brain.

West Coast Metabolomics Center-UC Davis

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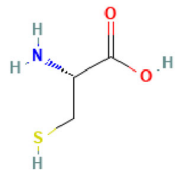
1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

1.3 Crystal Structures

Showing 1 of 16 View More

CCDC Number	126977
Crystal Structure Data	DOI:10.5517/cc4841k
Crystal Structure Depiction	
Associated Article	DOI:10.1107/S0108270196003952

The Cambridge Structural Database

2 Biologic Description

SVG Image	
IUPAC Condensed	H-Cys-OH
Sequence	C
PLN	H-C-OH
HELM	PEPTIDE1{C}$$$$
IUPAC	L-cysteine

PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(2*R*)-2-amino-3-sulfanylpropanoic acid

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

3.1.2 InChI

InChI=1S/C3H7NO2S/c4-2(1-7)3(5)6/h2,7H,1,4H2,(H,5,6)/t2-/m0/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.3 InChIKey

XUJNEKJLAYXESH-REOHCLBHSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.4 Canonical SMILES

C(C(C(=O)O)N)S

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.1.5 Isomeric SMILES

C([C@@H](C(=O)O)N)S

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.2 Molecular Formula

C3H7NO2S

Wikipedia; PubChem

3.3 Other Identifiers

3.3.1 CAS

52-90-4

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 (HSDI

3.3.2 Related CAS

7048-04-6 (Hydrochloride)

ChemIDplus

3.3.3 Deprecated CAS

4371-52-2, 154605-72-8, 1404190-35-7

ChemIDplus

154605-72-8, 4371-52-2

EPA DSSTox

3.3.4 European Community (EC) Number

200-158-2

European Chemicals Agency (ECHA)

3.3.5 UNII

K848JZ4886

- FDA Global Substance Registration System (GSRS)

3.3.6 JECFA Number

1419

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

3.3.7 FEMA Number

3263

- Flavor and Extract Manufacturers Association (FEMA); Joint FAO/WHO Expert Committee on Food Additives (JECFA)

3.3.8 DSSTox Substance ID

DTXSID8022876

- EPA DSSTox

3.3.9 Wikipedia

Cysteine

- Wikipedia

3.3.10 Wikidata

Q186474

- Wikidata

3.3.11 NCI Thesaurus Code

C29609

- NCI Thesaurus (NCIt)

3.3.12 RXCUI

3024

- NLM RxNorm Terminology

3.4 Synonyms

3.4.1 MeSH Entry Terms

Cysteine
Cysteine Hydrochloride
Half Cystine
Half-Cystine
L Cysteine
L-Cysteine
Zinc Cysteinate

- Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms

L-cysteine	beta-Mercaptoalanine	L Cysteine	CCRIS 912	CHEMBL863	3
cysteine	Half cystine	L-Zystein	CHEBI:17561	E920	2
52-90-4	FREE CYSTEINE	alpha-Amino-beta-thiolpropionic acid	HSDB 2109	E 920	E
Thioserine	Cysteine, L-	L-2-Amino-3-mercaptopropanoic acid	alpha-Amino-beta-thiolpropionic acid, L-	MFCD00064306	I-
(R)-2-Amino-3-mercaptopropanoic acid	Cysteinum	L-2-Amino-3-mercaptopropionic acid	AI3-26559	K848JZ4886	r
Cystein	L-Cys	Cysteinum [INN-Latin]	alpha-Amino-beta-mercaptopropanoic acid, L-	(+)-2-Amino-3-mercaptopropionic acid	2
Half-cystine	L-Alanine, 3-mercapto-	FEMA No. 3263	alpha-Amino-beta-mercaptopropionic acid, L-	4371-52-2	L
(R)-Cysteine	Cisteinum [Latin]	Cisteina [INN-Spanish]	Propanoic acid, 2-amino-3-mercapto-, (R)-	Polycysteine	1
L-(+)-Cysteine	Cisteina [Spanish]	beta-Mercaptoalanine, L-	2-Amino-3-mercaptopropanoic acid, (R)-	Cysteine [INN]	E
L-Cystein	cisteina	(2R)-2-amino-3-mercaptopropanoic acid	Cysteine HCl	b-Mercaptoalanine	L
(2R)-2-amino-3-sulfanylpropanoic acid	Cisteinum	NSC-8746	(R)-(+)-Cysteine	(2R)-2-amino-3-mercaptopropanoate	.I
H-Cys-OH	(R)-2-Amino-3-mercaptopropionic acid	2-Amino-3-mercaptopropionic acid	Cys	(2R)-2-amino-3-sulfanylpropanoate	(

PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	121.16	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	-2.5	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	121.01974964	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	121.01974964	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	64.3 $Å^2$	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	7	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	75.3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	1	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

DryPowder

EPA Chemicals under the TSCA

Colorless or white solid; [HSDB] Colorless crystalline solid; [Sigma-Aldrich MSDS]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Solid

Human Metabolome Database (HMDB)

White crystals; Sulferous aroma

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

4.2.2 Color/Form

Colorless crystals

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 329

Hazardous Substances Data Bank (HSDB)

White crystals

Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 255

Hazardous Substances Data Bank (HSDB)

4.2.3 Melting Point

240 dec °C

PhysProp

DrugBank

260 °C decomposes

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-140

Hazardous Substances Data Bank (HSDB)

220 °C

Human Metabolome Database (HMDB)

4.2.4 Solubility

277000 mg/L (at 25 °C)

BEILSTEIN

DrugBank

Freely soluble in water

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

Freely soluble in alcohol, acetic acid, ammonia water; insoluble in ether, acetone, ethyl acetate, benzene, carbon disulfide, carbon tetrachloride

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

Water solubility (per g/100 g H2O): 28 g/100 mL of solution at 25 °C; 16 g/100 mL of solution at 20 °C

Drauz K et al; Amino Acids. Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (1999-2016). New York, NY: John Wiley & Sons. Online Posting Date: 15 Apr 2007

Hazardous Substances Data Bank (HSDB)

277 mg/mL at 25 °C

BEILSTEIN

Human Metabolome Database (HMDB)

Very soluble in water and acetic acid; Insoluble in ether, acetone and benzene

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Soluble (in ethanol)

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

4.2.5 Vapor Pressure

0.00000207 [mmHg]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

6.73X10-7 mm Hg at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of July 12, 2016: https://www2.epa.gov/tsca-screening-tools

Hazardous Substances Data Bank (HSDB)

4.2.6 LogP

-2.49

HANSCH,C ET AL. (1995)

DrugBank

log Kow = -2.49

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 6

Hazardous Substances Data Bank (HSDB)

-2.49

HANSCH,C ET AL. (1995)

Human Metabolome Database (HMDB)

4.2.7 Henry's Law Constant

Henry's Law constant = 5.30X10-11 atm-cu m/mol at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of July 12, 2016: https://www2.epa.gov/tsca-screening-tools

Hazardous Substances Data Bank (HSDB)

4.2.8 Stability/Shelf Life

Stable under recommended storage conditions.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

In neutral or slightly alkaline aq solns it is oxidized to cystine by air. More stable in acidic solns.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 497

Hazardous Substances Data Bank (HSDB)

4.2.9 Optical Rotation

Decomposes 175-178 °C; soluble in water, alcohol, acetone; the aqueous solution is acid; decomposes and oxidizes slowly; hygroscopic. Specific optical rotation: +5.0 °C (5 N HCl) at 25 °C/D; +10.0 °C at 25 °C/D (glacial acetic acid) /Cysteine hydrochloride/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

Specific optical rotation: +6.5 deg at 25 °C/D (5 N HCl); +13.0 deg at 25 °C/D (glacial acetic acid)

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

Specific optical rotation: +9.7 deg (c = 8 in 1M HCl) at 25 °C/D

Drauz K et al; Amino Acids. Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (1999-2016). New York, NY: John Wiley & Sons. Online Posting Date: 15 Apr 2007

Hazardous Substances Data Bank (HSDB)

4.2.10 Decomposition

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

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1059

Hazardous Substances Data Bank (HSDB)

4.2.11 Dissociation Constants

pKa

1.71

MERCK INDEX (1996); pK1

DrugBank

pK1 1.71 /carboxylic/; pK2 8.33 /amine/; pK3 10.78 /sulfide/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

4.2.12 Collision Cross Section

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

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

CCSbase

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

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

CCSbase

144.47 Å^2 $[M-H]^-$ [CCS Type: DT, Method: stepped-field]

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

CCSbase

113 Å^2 $[M+H]^+$ [CCS Type: TW, Method: calibrated with polyalanine]

https://pubs.acs.org/doi/abs/10.1021/ac500405x

CCSbase

144 Å^2 $[M-H]^-$

148.6 Å^2 $[M+H]^+$

150.4 Å^2 $[M+Na]^+$

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

NORMAN Suspect List Exchange

4.2.13 Other Experimental Properties

Readily oxidizes to form a dimeric amino acid, cystine, in which the two cysteines are linked via a disulfide bridge, a common structural feature in proteins. Amino Acids and Proteins, D.M. Greenberg, Ed. (Charles C. Thomas, Springfield, IL, 1951) 950 pp.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

In neutral or slightly alkaline aqueous solution it is oxidized to cystine by air. More stable in acidic solutions.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

Hazardous Substances Data Bank (HSDB)

MP (anhydrous): 178 °C (decomposes). Specific optical rotation: +6.53 deg at 25 °C/D (calculated as cysteine) (c = 2 in 5M HCl); solubility >100 (20 °C) g/100 g H2O / L-Cysteine hydrochloride monohydrate/

Drauz K et al; Amino Acids. Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (1999-2016). New York, NY: John Wiley & Sons. Online Posting Date: 15 Apr 2007

- Hazardous Substances Data Bank (HSDB)

Hydroxyl radical reaction rate constant = 7.96X10-11cu cm/molecule-sec at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of July 12, 2016: https://www2.epa.gov/tsca-screening-tools

- Hazardous Substances Data Bank (HSDB)

4.2.14 Chemical Classes

Biological Agents -> Amino Acids and Derivatives

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

5 Spectral Information

5.1 1D NMR Spectra

1D NMR Spectra	1H NMR: SAD 16992 (Sadtler Research Laboratories spectral collection)

Hazardous Substances Data Bank (HSDB)

1D NMR Spectra	NMRShiftDB Link

NMRShiftDB

5.1.1 1H NMR Spectra

Showing 2 of 4 View More

Spectra ID	1426
Instrument Type	Varian
Frequency	500 MHz
Solvent	Water
pH	5.00
Shifts [ppm]:Intensity	3.00:43.43, 3.01:45.61, 3.03:100.00, 3.04:98.88, 3.08:92.22, 3.09:93.74, 3.11:40.74, 3.12:42.42, 3.96:71.83, 3.97:82.72, 3.97:85.99, 3.98:67.50
Thumbnail	

Human Metabolome Database (HMDB)

Spectra ID	4743
Instrument Type	Bruker
Solvent	D2O
pH	7.4
Shifts [ppm]:Intensity	3.00:7.07, 3.00:7.27, 3.02:15.00, 3.03:14.61, 3.06:14.31, 3.07:14.49, 3.09:6.76, 3.10:6.95, 3.95:10.70, 3.95:12.43, 3.96:10.26, 3.96:12.10
Thumbnail	

Human Metabolome Database (HMDB)

5.1.2 13C NMR Spectra

Showing 2 of 4 View More

Spectra ID	1241
Instrument Type	Bruker
Frequency	125 MHz
Solvent	Water

pH	7.00
Shifts [ppm]:Intensity	-0.00:1.58, 175.39:2.64, 27.80:19.00, 58.80:12.68
Thumbnail	

Human Metabolome Database (HMDB)

Spectra ID	166443
Frequency	400 MHz
Solvent	H2O
Shifts [ppm]	175.39, 27.80, 58.80
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	1024
Shifts [ppm] (F2:F1)	3.03:2.99, 3.04:3.06, 3.04:3.94, 3.05:3.03, 3.05:3.05, 3.06:3.10, 3.95:3.00, 3.95:3.03, 3.95:3.05, 3.95:3.06, 3.95:3.09, 3.95:3.10, 3.95:3.93, 3.95:3.96
Thumbnail	

Human Metabolome Database (HMDB)

5.2.2 1H-13C NMR Spectra

2D NMR Spectra Type	1H-13C HSQC
Spectra ID	1371

Instrument Type	Bruker
Frequency	600 MHz
Solvent	Water
pH	7.00
Shifts [ppm] (F2:F1):Intensity	3.05:27.79:0.01, 3.95:58.88:1.00
Thumbnail	

Human Metabolome Database (HMDB)

5.3 Mass Spectrometry

5.3.1 GC-MS

Showing 2 of 20 View More

Spectra ID	30101
Instrument Type	EI-B
Ionization Mode	positive
SPLASH	splash10-014j-0690100000-0aeb88fd507505e6b718
Top 5 Peaks	218.1 100 146.1 59.84 266.15 31.93 147.15 30.14 100.1 28.86
Thumbnail	
Notes	instrument=GCMS-2010 Plus, Shimadzu

Human Metabolome Database (HMDB)

Spectra ID	30201
Instrument Type	GC-EI-TOF
Ionization Mode	positive
SPLASH	splash10-00kb-0950000000-df7e91c95b610ff21c79
Top 5 Peaks	218.0 100 146.0 91.99 100.0 52.05 147.0 51.25 148.0 20.72
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	1471148
Instrument Type	QqQ
Ionization Mode	negative
SPLASH	splash10-001i-9000000000-5dc69d3b59bd15290aef
Top 5 Peaks	33.0 100
Thumbnail	
Notes	adduct_type [M-H]- original_collision_energy -14 CannabisDB spectra from MoNa 2020 June API 2000 ReSpect

Human Metabolome Database (HMDB)

Spectra ID	2226479
Ionization Mode	Positive
SPLASH	splash10-0a6r-9100000000-ed3c9c47ed98679090ab
Top 5 Peaks	76.02084 100 58.99469 97 86.98946 30.67 105.00021 21.56 122.02696 16.60
Thumbnail	

Human Metabolome Database (HMDB)

5.3.3 LC-MS

Showing 2 of 7 View More

Accession ID	MSBNK-BGC_Munich-RP001801
Authors	BGC, Helmholtz Zentrum Muenchen
Instrument	maXis plus UHR-ToF-MS, Bruker Daltonics
Instrument Type	LC-ESI-QTOF
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	10
Fragmentation Mode	CID
Column Name	BEH C18 1.7um, 2.1x100mm, Waters
Retention Time	0.604 min
Precursor m/z	122.027
Precursor Adduct	[M+H]+
Top 5 Peaks	76.0208 999 86.9894 167 105 137 122.0264 75 125.0257 1
SPLASH	splash10-004i-9100000000-42fd929d985bfd416ebf
Thumbnail	
License	CC BY

MassBank Europe

Accession ID	MSBNK-BGC_Munich-RP001802
Authors	BGC, Helmholtz Zentrum Muenchen
Instrument	maXis plus UHR-ToF-MS, Bruker Daltonics
Instrument Type	LC-ESI-QTOF
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	20
Fragmentation Mode	CID
Column Name	BEH C18 1.7um, 2.1x100mm, Waters
Retention Time	0.604 min
Precursor m/z	122.027
Precursor Adduct	[M+H]+
Top 5 Peaks	76.0209 999 86.9895 128 104.9997 19 77.0237 13 62.9893 7
SPLASH	splash10-004i-9000000000-d4e5b9ec1a14314a822e
Thumbnail	

License	CC BY

MassBank Europe

5.3.4 Other MS

Showing 2 of 8 View More

Other MS	MASS: NIST 63547 (NIST/EPA/MCDC Mass Spectral Database 1990 version)

Hazardous Substances Data Bank (HSDB)

Accession ID	MSBNK-GL_Sciences_Inc-GLS00103
Authors	Miyagawa H, Akimoto S, Yamasaki K, GL Sciences Inc.
Instrument	GCMS-2010 Plus, Shimadzu
Instrument Type	EI-B
MS Level	MS
Ionization Mode	POSITIVE
Column Name	InertCap 5MS/NP 0.25 mmI.D. x 30 m, df=0.25 um
Retention Time	941.58
Top 5 Peaks	218.1 999 146.1 598 266.15 319 147.15 301 100.1 288
SPLASH	splash10-014j-0690100000-0aeb88fd507505e6b718
Thumbnail	
License	CC BY-SA

MassBank Europe

5.4 UV Spectra

UV: OES 2-10 (Phillip et al; Organic Electronic Spectral Data. NT, NY: John Wiley and Sons)

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. V3: 2407

Hazardous Substances Data Bank (HSDB)

5.5 IR Spectra

IR Spectra	IR: SADP 13419 (Sadtler Research Laboratories IR prism collection)

Hazardous Substances Data Bank (HSDB)

5.5.1 FTIR Spectra

Technique	KBr WAFER
Source of Sample	Fluka Chemie AG, Buchs, Switzerland
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Technique	KBr WAFER
Source of Sample	Fluka Chemie AG, Buchs, Switzerland
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.5.2 ATR-IR Spectra

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Sigma-Aldrich Company Llc
Catalog Number	C7755
Lot Number	38C-0297
Copyright	Copyright © 2014-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Source of Sample	Aldrich
Catalog Number	168149
Copyright	Copyright © 2018-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.6 Raman Spectra

Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Sigma-Aldrich Inc.
Catalog Number	C7755
Lot Number	38C-0297
Copyright	Copyright © 2012-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Catalog Number	168149
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	50 Records
Same Stereo	33 Records
Same Isotope	3 Records
Same Parent, Connectivity	359 Records
Same Parent, Stereo	180 Records
Same Parent, Isotope	309 Records
Same Parent, Exact	147 Records
Mixtures, Components, and Neutralized Forms	891 Records
Similar Compounds	214 Records
Similar Conformers	3,870 Records

PubChem

6.3 Substances

6.3.1 Related Substances

All	2,006 Records
Same	340 Records
Mixture	1,666 Records

PubChem

6.3.2 Substances by Category

PubChem

6.4 Entrez Crosslinks

PubMed	44,777 Records
Protein Structures	107 Records

Taxonomy	5 Records
OMIM	25 Records
Gene	69 Records

PubChem

6.5 Associated Chemicals

(+)-Cysteine; 921-01-7

Hazardous Substances Data Bank (HSDB)

(+-)-Cysteine; 3374-22-9

Hazardous Substances Data Bank (HSDB)

Cysteine hydrochloride; 52-89-1

Hazardous Substances Data Bank (HSDB)

6.6 NCBI LinkOut

NCBI

7 Chemical Vendors

PubChem

8 Drug and Medication Information

8.1 Drug Indication

For the prevention of liver damage and kidney damage associated with overdoses of acetaminophen

- DrugBank

8.2 FDA National Drug Code Directory

CYSTEINE is an active ingredient in 28 products including: 'B COMPLEX MIX SYSTEM FORMULA', 'BIO CO-ENZYME PHASE', and 'DIATHESIS V 2'.

- National Drug Code (NDC) Directory

- National Drug Code (NDC) Directory

8.3 Clinical Trials

8.3.1 ClinicalTrials.gov

- ClinicalTrials.gov

8.3.2 NIPH Clinical Trials Search of Japan

- NIPH Clinical Trials Search of Japan

8.4 Therapeutic Uses

/EXPL THER/ Acetaminophen-cysteine adducts (APAP-CYS) are a serum biomarker of acetaminophen exposure, formed when the oxidative metabolite of acetaminophen binds to cysteine residues of hepatic proteins. APAP-CYS adducts become elevated in cases of acute liver failure following acetaminophen overdose and have been proposed as a diagnostic tool to identify acetaminophen-induced acute liver failure when standard testing is inconclusive.

PMID:25896948
Full text: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4469719
Frey SM et al; J Med Toxicol 11 (2): 218-22 (2015)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ Lead is a toxic heavy metal that adversely affects nervous tissues; it often occurs as an environmental pollutant. We investigated histological changes in the cerebral cortex, hippocampus and cerebellum of adult albino mice following exposure to lead acetate. We also studied the possible ameliorative effect of the chelating agent, L-cysteine, on lead-induced neurotoxicity. We divided albino mice into six groups: 1) vehicle-only control, 2) L-cysteine control, 3 and 4) treated for 7 days with 20 and 40 mg/kg lead acetate, respectively, and 5 and 6) treated for 7 days with 20 and 40 mg/kg lead acetate, respectively, followed by 50 mg/kg L-cysteine for 7 days. Lead acetate administration caused disorganization of cell layers, neuronal loss and degeneration, and neuropil vacuolization. Brain sections from lead-intoxicated mice treated with L-cysteine showed fewer pathological changes; the neuropil showed less vacuolization and the neurons appeared less damaged. L-cysteine at the dose we used only marginally alleviated lead-induced toxicity.

PMID:27045382
Mahmoud YI, Sayed SS; Biotech Histochem 1-6 (2016) (Epub ahead of print)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ In hamster lung cell cultures addn of l-Cysteine or vit C to media protects against or reverses abnormal growth & malignant transformation in aged controls (1-2 yr old) or young (3-6 mo) after repeated exposure to smoke of tobacco or marijuana cigarettes.

Leuchtenberger C; Br J Exp Pathol 58 (6): 625-34 (1977)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ L-Cysteine admin orally or ip to rats protected against acute toxicity of methylmercury chloride, reducing mercury content in kidney & brain but not in liver.

Sugiyama et al; Toho Igakkai Zasshi 22 (1): 78-85 (1975)

Hazardous Substances Data Bank (HSDB)

For more Therapeutic Uses (Complete) data for CYSTEINE (7 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

8.5 Biomarker Information

MarkerDB

9 Food Additives and Ingredients

9.1 Food Additive Classes

Flavoring Agents

- EU Food Improvement Agents; Joint FAO/WHO Expert Committee on Food Additives (JECFA)

JECFA Functional Classes

Flavouring Agent -> FLAVOURING_AGENT;

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

9.2 FEMA Flavor Profile

Savory

- Flavor and Extract Manufacturers Association (FEMA)

9.3 FDA Substances Added to Food

Substance	L-CYSTEINE
Used for (Technical Effect)	NUTRIENT SUPPLEMENT
Document Number (21 CFR)	172.320 184.1271

- FDA Center for Food Safety and Applied Nutrition (CFSAN)

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

Chemical Name	L-CYSTEINE
Evaluation Year	2004
ADI	No safety concern at current levels of intake when used as a flavouring agent
Comments	Not evaluated using the Procedure for the Safety Evaluation of Flavouring Agents; the substance is a macronutrient and a normal component of protein and, as such, human exposure through food is orders of magnitude higher than the anticipated level of exposure from use as a flavouring agent
Report	TRS 928-JECFA 63/98
Tox Monograph	FAS 54-JECFA 63/435

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

10 Agrochemical Information

10.1 Agrochemical Category

Pesticide active substances

- EU Pesticides Database

10.2 EU Pesticides Data

Active Substance	l-cysteine
Status	Approved [Reg. (EC) No 1107/2009]
Legislation	Reg. (EU) 2020/642

- EU Pesticides Database

11 Pharmacology and Biochemistry

11.1 Pharmacodynamics

Due to this ability to undergo redox reactions, cysteine has antioxidant properties. Cysteine is an important source of sulfur in human metabolism, and although it is classified as a non-essential amino acid, cysteine may be essential for infants, the elderly, and individuals with certain metabolic disease or who suffer from malabsorption syndromes. Cysteine may at some point be recognized as an essential or conditionally essential amino acid.

DrugBank

11.2 Bionecessity

L-Cysteine is the central compound in sulfur metabolism in the human body. In proteins the formation of disulfide bonds between the thiol groups of cysteine plays an important role for tertiary structure and enzymatic activity ... .

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

Hazardous Substances Data Bank (HSDB)

Amino acid catabolism is essential for adjusting pool sizes of free amino acids and takes part in energy production as well as nutrient remobilization. The carbon skeletons are generally converted to precursors or intermediates of the tricarboxylic acid cycle. In the case of cysteine, the reduced sulfur derived from the thiol group also has to be oxidized in order to prevent accumulation to toxic concentrations. ...

PMID:27105581
Hofler S et al; Physiol Plant doi: 10.1111/ppl.12454 (2016) (Epub ahead of print)

Hazardous Substances Data Bank (HSDB)

11.3 Metabolism/Metabolites

L-Cysteine is the central compound in sulfur metabolism in the human body. In proteins the formation of disulfide bonds between the thiol groups of cysteine plays an important role for tertiary structure and enzymatic activity; cysteine is however always incorporated in the polypeptide chain as cysteine. L-Cysteine is degraded to pyruvate in two steps: one is removal of sulfur and the other is a transamination. Cysteine can be metabolized to form taurine and carbon dioxide through the cysteinsulfinate pathway, where the initial step is oxidation of cysteine to cysteine sulfinate. This step is catalyzed by cysteine dioxygenase. Cysteine sulfinate may then be decarboxylated to form taurine or it may be metabolized via the putative intermediate beta-sulfinylpyruvate to pyruvate and sulfite and then to carbon dioxide and sulfate.

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

Hazardous Substances Data Bank (HSDB)

Amino acid catabolism is essential for adjusting pool sizes of free amino acids and takes part in energy production as well as nutrient remobilization. The carbon skeletons are generally converted to precursors or intermediates of the tricarboxylic acid cycle. In the case of cysteine, the reduced sulfur derived from the thiol group also has to be oxidized in order to prevent accumulation to toxic concentrations. Here we present a mitochondrial sulfur catabolic pathway catalyzing the complete oxidation of L-cysteine to pyruvate and thiosulfate. After transamination to 3-mercaptopyruvate the sulfhydryl group from L-cysteine is transferred to glutathione by sulfurtransferase 1 and oxidized to sulfite by the sulfur dioxygenase ETHE1. Sulfite is then converted to thiosulfate by addition of a second persulfide group by sulfurtransferase 1. This pathway is most relevant during early embryo development and for vegetative growth under light limiting conditions. Characterization of a double mutant produced from Arabidopsis thaliana T-DNA insertion lines for ETHE1 and sulfurtransferase 1 revealed that an intermediate of the ETHE1 dependent pathway, most likely a persulfide, interferes with amino acid catabolism and induces early senescence.

PMID:27105581
Hofler S et al; Physiol Plant doi: 10.1111/ppl.12454 (2016) (Epub ahead of print)

Hazardous Substances Data Bank (HSDB)

11.4 Mechanism of Action

Cysteine can usually be synthesized by the human body under normal physiological conditions if a sufficient quantity of methionine is available. Cysteine is typically synthesized in the human body when there is sufficient methionine available. Cysteine exhibits antioxidant properties and participates in redox reactions. Cysteine's antioxidant properties are typically expressed in the tripeptide glutathione, which occurs in humans as well as other organisms. Glutathione (GSH) typically requires biosynthesis from its constituent amino acids, cysteine, glycine, and glutamic acid, due to its limited systemic availability. Glutamic acid and glycine are readily available in the diets of most industrialized countries, but the availability of cysteine can be the limiting substrate. In human metabolism, cysteine is also involved in the generation of sulfide present in iron-sulfur clusters and nitrogenase by acting as a precursor. In a 1994 report released by five top cigarette companies, cysteine is one of the 599 additives to cigarettes. Its use or purpose, however, is unknown, like most cigarette additives. Its inclusion in cigarettes could offer two benefits: Acting as an expectorant, since smoking increases mucus production in the lungs; and increasing the beneficial antioxidant glutathione (which is diminished in smokers).

DrugBank

11.5 Human Metabolite Information

11.5.1 Tissue Locations

Adrenal Cortex	Thyroid Gland
Epidermis	
Fibroblasts	
Intestine	
Kidney	
Liver	
Neuron	
Placenta	
Platelet	
Prostate	
Skeletal Muscle	
Spleen	
Testis	

Human Metabolome Database (HMDB)

11.5.2 Cellular Locations

Cytoplasm
Extracellular
Mitochondria

Human Metabolome Database (HMDB)

11.5.3 Metabolite Pathways

2-Hydroxyglutric Aciduria (D And L Form)
3-Phosphoglycerate dehydrogenase deficiency
4-Hydroxybutyric Aciduria/Succinic Semialdehyde Dehydrogenase Deficiency
5-oxoprolinase deficiency
5-Oxoprolinuria
Amiloride Action Pathway
Bendroflumethiazide Action Pathway
Beta-mercaptolactate-cysteine disulfiduria
Blue diaper syndrome
Bumetanide Action Pathway
Total 65 pathways, visit the HMDB page for details

Human Metabolome Database (HMDB)

11.6 Biochemical Reactions

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

Cysteine is a non-essential amino acid that has been used as a dough conditioner and veterinary detoxicant; [Merck Index] Used as a flavoring agent, dough strengthener, nutritional supplement, and flour treating agent for foods; [FDA] Used for biochemical and nutritional research and as a medication; [HSDB]

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

Reported uses (ppm):

Table: Reported uses (ppm): (Flavor and Extract Manufacturers' Association, 1994)

Food Category	Usual	Max.
Breakfast cereals	100.00	100.00
Condiments, relishes	100.00	100.00
Meat products	100.00	100.00
Milk products	100.00	100.00

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 370

- Hazardous Substances Data Bank (HSDB)

Biochemical and nutrition research, reducing agent in bread doughs (up to 90 ppm).

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 408

- Hazardous Substances Data Bank (HSDB)

MEDICATION

- Hazardous Substances Data Bank (HSDB)

MEDICATION (VET)

- Hazardous Substances Data Bank (HSDB)

Treatment with cysteine reduced seedling injury caused by gamma-irradiation of sorghum seed. Cysteine effects were most pronounced in primary root elongation.

Reddy CS, JD Smith; Environ Exp Bot 18 (4): 241-3 (1978)

- Hazardous Substances Data Bank (HSDB)

12.1.1 Use Classification

Food additives -> Flavoring Agents

- EU Food Improvement Agents

Agrochemicals -> Pesticides

- EU Pesticides Database

Flavouring Agent -> FLAVOURING_AGENT; -> JECFA Functional Classes

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Flavoring Agents -> JECFA Flavorings Index

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Cosmetics -> Antioxidant; Antistatic; Hair conditioning; Reducing

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

nutritional supplement

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

EPA Chemicals under the TSCA

12.1.3 Consumer Uses

nutritional supplement

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

EPA Chemicals under the TSCA

12.1.4 Household Products

Household & Commercial/Institutional Products

Information on 3 consumer products that contain Cysteine in the following categories is provided:

• Personal Care

Consumer Product Information Database (CPID)

12.2 Methods of Manufacturing

By addition of a thiol compound to an unsaturated amino acid derivative; by hydrolysis of proteins in the presence of carbon dioxide; by treating in HCl hydrolysis of proteins in the presence of carbon dioxide; by treating an HCl hydrolysate of hair with CuO2, followed by the decomposition of the resulting copper-cysteine complex with hydrogen sulfide; by the addition of thioacetic acid to alpha-acetamido acrylic acid; by treatment of a keratine HCl hydrolysate with zinc to reduce the cystine present to cysteine; by electrolytic reduction of cystine.

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 370

Hazardous Substances Data Bank (HSDB)

L-Cysteine used to be produced almost exclusively by hydrolysis of hair or other keratins. The amino acid isolated was l-cystine, which was reduced electrolytically to l-cysteine. L-Cysteine has also been prepared from beta-chloro-d,l-alanine and sodium sulfide with cysteine desulfhydrase, an enzyme obtained from, e.g., Citrobacterium freundii. Today, however, the main processes for cysteine production are biological. A direct fermentation process has been developed for the manufacture of l-cystine, using a modified Escherichia coli bacterium. The technology has been extended to prepare other modified l-cysteine analogues. An enzymatic process for l-cysteine has been successfully developed using microorganisms capable to hydrolyze 2-amino-delta2-thiazoline 4-carboxylic acid (ATC) which is readily available from methyl alpha-chloroacrylate and thiourea. A mutant of Pseudomonas thiazolinophilum converts d,l-ATC to l-cysteine in 95% molar yield at product concentrations higher than 30 g/L.

Drauz K et al; Amino Acids. Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2016). NY, NY: John Wiley & Sons. Online Posting Date: April 15, 2007

Hazardous Substances Data Bank (HSDB)

12.3 Formulations/Preparations

Available commercially as L(+)-cysteine hydrochloride.

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 408

Hazardous Substances Data Bank (HSDB)

12.4 U.S. Production

Aggregated Product Volume (EPA CDR 2016)

25,000 - 100,000 lb

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

EPA Chemicals under the TSCA

Non-confidential 2012 Chemical Data Reporting (CDR) information on the production and use of chemicals manufactured or imported into the United States. Chemical: L-Cysteine. National Production Volume: 28,660 lb/yr.

USEPA/Pollution Prevention and Toxics; 2012 Chemical Data Reporting Database. L-Cysteine (52-90-4). Available from, as of July 12, 2016: https://java.epa.gov/oppt_chemical_search/

Hazardous Substances Data Bank (HSDB)

12.5 General Manufacturing Information

Industry Processing Sectors

Food, beverage, and tobacco product manufacturing

EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

L-Cysteine: ACTIVE

https://www.epa.gov/tsca-inventory

- EPA Chemicals under the TSCA

A non-essential amino acid in human development.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 486

- Hazardous Substances Data Bank (HSDB)

An amino acid derived from cystine, occurring naturally in the L-form ...

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. V2: 1292

- Hazardous Substances Data Bank (HSDB)

13 Identification

13.1 Analytic Laboratory Methods

The near-infrared (NIR) fluorescence sensor for rapid, selective, and sensitive detection of cysteine (Cys) is of great importance in both biological and environmental sciences. Herein, we report a specific probe with turn-on fluorescence property, visible color change with naked-eye, and large wavelength shift on UV spectra for highly selective detection of Cys over homocysteine (Hcy) and glutathione (GSH) in both HEPES buffer (10 mM, pH 7.4) and diluted human serum. The probe based on the conjugate addition-cyclization reaction has a low limit of detection to Cys (0.16 uM as NIR fluorescence sensor and 0.13 uM as UV sensor). Kinetic study indicated that the probe has a very rapid response to Cys, owing to the much higher pseudo-first-order reaction constant with Cys (299/M/s) than with Hcy (1.29/M/s) or GSH (0.53/M/s). Upon addition of Cys to a solution of the probe, the color changed from purple to cyan, with the maximum wavelength shifting from 582 to 674 nm in the UV spectrum and a fluorescence emission at 697 nm appearing. It has been successfully applied for determination of Cys in diluted serum and bioimaging of Cys in living cells with low cell toxicity.

PMID:25875053
Zhang J et al; Anal Chem 87 (9): 4856-63 (2015)

Hazardous Substances Data Bank (HSDB)

Gold nanoparticles (AuNPs) were synthesized at room temperature following a simple, rapid, and green route using fresh-squeezed apple juice as a reducing reagent. The optimal AuNPs, based on the particle color, stability, and color change suitable for colorimetric detection of cysteine (Cys), are synthesized using 5 mL of 10% apple juice, 1 mL of 10 mM gold precursor solution, and 1 mL of 0.1 M NaOH. Under this set of parameters, the AuNPs are synthesized within 30 min at room temperature. The average size (11.1 +/- 3.2 nm) and zeta potential (-36.5 mV) of the AuNPs synthesized were similar to those of AuNPs prepared via the conventional citrate-reduction method. In the presence of Cys, unlike with any other amino acid, the AuNPs aggregated, possibly due to the gold-sulfur covalent interaction, yielding red-to-purple color change of the sample solution. The red-shift of the localized surface plasmon resonance peak of the AuNPs responsible for the color change was recorded by UV-vis spectrometer. The effect of other potential interferents such as glucose, ascorbic acid, K(+) , Na(+) , Ca(2+) , Zn(2+) , Ag(+) , Ni(2+) , Cu(2+) , Co(2+) , and Hg(2+) were also examined. The results show that AuNPs can be used to selectively detect and measure Cys with a linear dependency in the range of 2 to 100 uM and a limit of detection (signal-to-noise ratio > 3) of 50 nM. The results suggest that the green-synthesized AuNPs are useful for simple, rapid, and sensitive colorimetric detection of Cys, which is an essential amino acid in food and biological systems.

PMID:26239641
Bagci PO et al; J Food Sci 80 (9): N2071-8 (2015)

Hazardous Substances Data Bank (HSDB)

13.2 Clinical Laboratory Methods

A new fluorescent probe based on an ensemble of gold nanoclusters (AuNCs) and polymer protected gold nanoparticles (AuNPs) for turn-on sensing of L-cysteine was designed and prepared. The AuNCs were protected by bovine serum albumin and had strong fluorescence. The polymer protected AuNPs were synthesized by a facile in situ strategy at room temperature and could quench the fluorescence of AuNCs due to the Forster resonance energy transfer. Interestingly, it has been observed that the quenched fluorescence of AuNCs was recovered by L-cysteine, which could induce the aggregation of polymer protected AuNPs by sulfur group. Then the prepared fluorescent probe was successfully used for determination of L-Cys in human urines ... .

PMID:26002483
Xu X et al; Anal Chim Acta 879: 97-103 (2015)

Hazardous Substances Data Bank (HSDB)

A chlorinated coumarin-aldehyde was developed as a colorimetric and ratiometric fluorescent probe for distinguishing glutathione (GSH), cysteine (Cys) and homocysteine (Hcy). The GSH-induced substitution-cyclization and Cys/Hcy-induced substitution-rearrangement cascades lead to the corresponding thiol-coumarin-iminium cation and amino-coumarin-aldehyde with distinct photophysical properties. The probe can be used to simultaneously detect GSH and Cys/Hcy by visual determination based on distinct different colors - red and pale-yellow in PBS buffer solution by two reaction sites. From the linear relationship of fluorescence intensity and biothiols concentrations, it was determined that the limits of detection for GSH, Hcy and Cys are 0.08, 0.09 and 0.18 uM, respectively. Furthermore, the probe was successfully used in living cell imaging with low cell toxicity.

PMID:26572845
Dai X et al; Anal Chim Acta 900: 103-10 (2015)

Hazardous Substances Data Bank (HSDB)

A highly sensitive and selective turn on fluorescent probe P-acid-aldehyde (P-CHO) is developed for the determination of cysteine (Cys) and homocysteine (Hcy). The probe is designed and synthesized by incorporating the specific functional group aldehyde group for thiols into a stable ?-conjugated material 4,4'-(2,5-dimethoxy-1,4-phenylene) bis(ethyne-2,1-diyl) dibenzoic acid (P-acid). The probe fluorescence is quenched through donor photoinduced electron transfer (d-PET) between the fluorophore (P-acid) and the recognition group (aldehyde group). In the presence of thiols, Cys and Hcy can selectively react with aldehyde group of the probe because the inhibition of d-PET between fluorophore and recognition group. Therefore, a turn-on fluorescent sensor was established for the fluorescence recovery. Under the optimized conditions, the fluorescence response of probe is directly proportional to the concentration of Cys in the range of 4-95 nM/L, with a detection limit 3.0 nM. In addition, the sensing system exhibits good selectively toward Cys and Hcy in the presence of other amino acids. It has been successfully applied for bioimaging of Cys and Hcy in living cells with low cell toxicity.

PMID:26802748
Yang C et al; Biosens Bioelectron 80: 17-23 (2016)

Hazardous Substances Data Bank (HSDB)

14 Safety and Hazards

14.1 Hazards Identification

14.1.1 GHS Classification

Showing 1 of 2 View More

Pictogram(s)	Irritant
Signal	Warning
GHS Hazard Statements	H302 (82.76%): Harmful if swallowed [Warning Acute toxicity, oral] H315 (18.5%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (18.5%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H335 (29.78%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	P261, P264, P264+P265, P270, P271, P280, P301+P317, P302+P352, P304+P340, P305+P351+P338, P319, P321, P330, P332+P317, P337+P317, P362+P364, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 416 companies from 13 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 97 of 416 companies. For more detailed information, please visit ECHA C&L website.* *Of the 11 notification(s) provided by 319 of 416 companies with hazard statement code(s).* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

- European Chemicals Agency (ECHA)

14.1.2 Hazard Classes and Categories

Acute Tox. 4 (82.76%)

Skin Irrit. 2 (18.5%)

Eye Irrit. 2 (18.5%)

STOT SE 3 (29.78%)

- European Chemicals Agency (ECHA)

Acute toxicity (Oral) - Category 4

- NITE-CMC

14.1.3 Hazards Summary

Safe when used as a flavoring agent in food; [JECFA] May cause irritation; Harmful by ingestion; [Sigma-Aldrich MSDS]

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

14.1.4 Skin, Eye, and Respiratory Irritations

... A single ocular application of the test item L-Cysteine to rabbits at a dose of 0.1 g produced slight irritant effects, which were fully reversible within 48 hours. ...

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

- Hazardous Substances Data Bank (HSDB)

... The single dermal application of the test item L-Cysteine to three rabbits at a dose of 0.5 g showed neither irritant nor corrosive effects. ...

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

- Hazardous Substances Data Bank (HSDB)

... Single dermal application of the test item L-Cysteine to rats at a dose of 2000 mg/kg body weight was associated with neither mortality nor signs of toxicity but signs of irritation. ...

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

- Hazardous Substances Data Bank (HSDB)

14.2 Fire Fighting

14.2.1 Fire Fighting Procedures

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

- Hazardous Substances Data Bank (HSDB)

Advice for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

14.3 Accidental Release Measures

14.3.1 Cleanup Methods

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Avoid breathing dust. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

14.3.2 Disposal Methods

SRP: 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 air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

Hazardous Substances Data Bank (HSDB)

Product: Offer surplus and non-recyclable solutions to a licensed disposal company; Contaminated packaging: Dispose of as unused product.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

14.3.3 Preventive Measures

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Avoid breathing dust. Environmental precautions: Do not let product enter drains.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

Precautions for safe handling: Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs. Provide appropriate exhaust ventilation at places where dust is formed.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

Hazardous Substances Data Bank (HSDB)

14.4 Handling and Storage

14.4.1 Storage Conditions

Keep container tightly closed in a dry and well-ventilated place. Store under inert gas. Air sensitive. Storage class (TRGS 510): Non Combustible Solids.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

14.5 Exposure Control and Personal Protection

14.5.1 Allowable Tolerances

Residues of cysteine are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only. Use: Synergist. Limit: Maximum of 0.5% of formulation.

40 CFR 180.920 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 12, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

14.5.2 Personal Protective Equipment (PPE)

Eye/face protection: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

Skin protection: Handle with gloves.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

Body Protection: Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

Respiratory protection: Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

14.6 Stability and Reactivity

14.6.1 Hazardous Reactivities and Incompatibilities

Incompatible materials: Strong oxidizing agents.

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

14.7 Regulatory Information

14.7.1 FIFRA Requirements

Residues of cysteine are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only. Use: Synergist. Limit: Maximum of 0.5% of formulation.

40 CFR 180.920 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 12, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

14.7.2 FDA Requirements

Cysteine used as a nutrient and/or dietary supplement in animal drugs, feeds, and related products is generally recognized as safe when used in accordance with good manufacturing or feeding practice.

21 CFR 582.5271 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 12, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

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

21 CFR 184.1271 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 12, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

The food additive amino acids may be safely used as nutrients added to foods in accordance with the following conditions: (a) The food additive consists of one or more of the following individual amino acids in the free, hydrated, or anhydrous form, or as the hydrochloride, sodium, or potassium salts. L-Cysteine is included on this list.

21 CFR 172.320 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 12, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

14.8 Other Safety Information

14.8.1 Toxic Combustion Products

Special hazards arising from the substance or mixture: Carbon oxides, nitrogen oxides (NOx), sulphur oxides

Sigma-Aldrich; Safety Data Sheet for L-Cysteine. Product Number: 168149, Version 4.5 (Revision Date 08/26/2015). Available from, as of May 18, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

15 Toxicity

15.1 Toxicological Information

15.1.1 Toxicity Summary

IDENTIFICATION AND USE: Cysteine forms white or colorless crystals. It is used in biochemical and nutrition research, as a reducing agent in bread doughs (up to 90 ppm). It is also used as flavor enhancer and medication, including veterinary medication. HUMAN EXPOSURE AND TOXICITY: Cysteine solution (3%) was not irritating for human eyes. ANIMAL STUDIES: A single ocular application of L-cysteine to rabbits at a dose of 0.1 g produced slight irritant effects, which were fully reversible within 48 hours. The single dermal application of L-cysteine to three rabbits at a dose of 0.5 g showed neither irritant nor corrosive effects. Decreased litter size observed in rats receiving high-dose cysteine, which was related to the degeneration and/or death of ovulated unfertilized oocytes and embryos with changes in the zona pellucida, which was already affected in the ovary. Pregnant mice and rats were treated s.c. with 1.2 mg per g on the last day of pregnancy and brain degeneration was observed one day later in the fetus. L-Cysteine is considered to be non-mutagenic in the HPRT locus using V79 cells of the Chinese Hamster. L-Cysteine did not induce structural chromosomal aberrations in the V79 Chinese hamster cell line. ECOTOXICITY STUDIES: The objective of the study was to determine the effects of cysteine on postthaw sperm motility, duration of sperm motility, DNA damage, and fertility in the common carp (Cyprinus carpio). Supplementation with cysteine increased the fertilization and hatching rate and decreased DNA damage.

Hazardous Substances Data Bank (HSDB)

15.1.2 Drug Induced Liver Injury

Compound	l-cysteine
DILI Annotation	Ambiguous DILI-concern
Severity Grade	3
Label Section	Warnings and precautions
References	M Chen, V Vijay, Q Shi, Z Liu, H Fang, W Tong. FDA-Approved Drug Labeling for the Study of Drug-Induced Liver Injury, Drug Discovery Today, 16(15-16):697-703, 2011. PMID:21624500 DOI:10.1016/j.drudis.2011.05.007 M Chen, A Suzuki, S Thakkar, K Yu, C Hu, W Tong. DILIrank: the largest reference drug list ranked by the risk for developing drug-induced liver injury in humans. Drug Discov Today 2016, 21(4): 648-653. PMID:26948801 DOI:10.1016/j.drudis.2016.02.015

Drug Induced Liver Injury Rank (DILIrank) Dataset

15.1.3 Acute Effects

ChemIDplus

15.1.4 Antidote and Emergency Treatment

/SRP:/ 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 revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160

Hazardous Substances Data Bank (HSDB)

/SRP:/ 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 revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160

Hazardous Substances Data Bank (HSDB)

/SRP:/ 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 TKO /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) 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 revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160-1

Hazardous Substances Data Bank (HSDB)

15.1.5 Human Toxicity Excerpts

/HUMAN EXPOSURE STUDIES/ ... Applied as a 3% near-neutral soln to ... human eyes ... no adverse effect is reported.

Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 300

Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ A 26-year-old female with history of unexplained, severe hepatitis presented with a second episode of severe hepatitis including coagulopathy and transaminase levels >10,000 U/L. The patient reported ingesting "only a couple" of acetaminophen tablets several days prior to her presentation. An acetaminophen concentration of 14 ug/mL at presentation aroused suspicion that acetaminophen might have caused the patient's liver failure, despite her adamant denial of overdose. ...

PMID:25896948
Full text: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4469719
Frey SM et al; J Med Toxicol 11 (2): 218-22 (2015)

Hazardous Substances Data Bank (HSDB)

15.1.6 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ An eye irritation study according to OECD Guideline 405 was performed with L-Cysteine. 0.1 g of the pure test substance was administered into the conjunctival sac of the eye of three New Zealand White rabbits. The eyes were not rinsed after the application. After the application into the eyes of three female NZW rabbits the test item produced slight irritant but no corrosive ocular effects. Upon fluorescein examinations at the end of the observation period of 72 hours no corneal lesions were found in any animal. Conjunctival redness was observed in all animals, discharge in one animal. There were no significant body weight changes during the observation period. Under the conditions of the present study, a single ocular application of the test item L-Cysteine to rabbits at a dose of 0.1 g produced slight irritant effects, which were fully reversible within 48 hours. Neither mortalities nor significant clinical signs of toxicity were observed.

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ ... The single dermal application of the test item L-Cysteine to three rabbits at a dose of 0.5 g showed neither irritant nor corrosive effects. Neither mortalities nor significant clinical signs of toxicity were observed. ...

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ An actute dermal toxicity study was performed with L-Cysteine according to OECD Guideline 402. The substance was administered at a single dose, uniformly over an area which was approximately 10% of the total body surface. The test item was held in contact with the skin by a dressing throughout a 24-hour period. The dressing consisted of a gauze-dressing and non-irritating tape. Under the conditions of the present study, single dermal application of the test item L-Cysteine to rats at a dose of 2000 mg/kg body weight was associated with neither mortality nor signs of toxicity but signs of irritation. The dermal LD50 was determined to be > 2000 mg L-Cysteine/kg body weight. No clear signs of toxicity were observed.

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ L-Cysteine (CySH) is widely distributed throughout the body. A decrease in litter size was observed in female rats that received high-dose CySH before mating. The oocytes were assessed morphologically to investigate the cause of this effect of CySH. Ten-week-old female SD rats received CySH intravenously at a dosage of 1000 mg/kg/day for more than 1 week before mating. Rats in the control group received no treatment. The ovaries were stained with PAS and examined by light microscopy (n = 6) and an antral follicle exhibiting the effects of CySH was examined by electron microscopy (n = 1). Unfertilized oocytes (n = 10) collected from the ampulla of the uterine tube after ovulation and embryos (n = 10 to 13) collected from the oviduct on gestational day 2 (GD 2) were examined by stereomicroscopy. In light microscopic examination of the ovary in the CySH group, the zona pellucida (ZP) of follicles in almost all stages was thinned or indistinct. In addition, outflow of the ZP between the corona radiata (CR) and disarrangement of the CR were occasionally observed in the developing antral follicles. Electron microscopic examination of the antral follicles in the CySH group confirmed these findings, but no lesions were observed except for those related to the ZP. Fewer unfertilized oocytes were collected from the ampulla of the uterine tube in the CySH group than in the control group. Interestingly, ZP-lacking or partially ZPlacking oocytes were observed in the CySH group. On GD 2, embryos with changes in the ZP as well as unfertilized oocytes were observed, and most of the embryos were degenerative. It is known that the ZP plays several important roles in early embryogenesis. The oocytes in which the ZP was affected by CySH treatment were abnormal or nonviable. In conclusion, the findings of this study suggest that the decreased litter size observed in rats receiving high-dose CySH was related to the degeneration and/or death of ovulated unfertilized oocytes and embryos with changes in the ZP, which was already affected in the ovary.

Harada M et al; Congenit Anom Kyoto 42 (3): 271-2 (2002)

Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for CYSTEINE (10 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

15.1.7 Non-Human Toxicity Values

LD50 Rat dermal >2000 mg/kg body weight

European Chemicals Agency (ECHA); Registered Substances, L-cysteine (CAS Number: 52-90-4) (EC Number: 200-158-2) (Last updated: May 17, 2016). Available from, as of May 24, 2016: https://echa.europa.eu/

Hazardous Substances Data Bank (HSDB)

LD50 Rat oral 1890 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1059

Hazardous Substances Data Bank (HSDB)

LD50 Rat ip 1620 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1059

Hazardous Substances Data Bank (HSDB)

LD50 Rat sc 1550 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1059

Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Values (Complete) data for CYSTEINE (7 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

15.1.8 Ecotoxicity Values

LD50; Species: Oncorhynchus mykiss (Rainbow trout) weight 30 g; Conditions: freshwater, 15 °C, ip injection; Concentration: 4.5 mmol/kg bw for 4 hr (95% confidence interval: 3.7-5.3 mmol/kg bw) /formulation/

Yokoyama M, Sakaguchi M; Fish Sci 62 (4): 660-661 (1996)

Hazardous Substances Data Bank (HSDB)

LD50; Species: Oncorhynchus mykiss (Rainbow trout) weight 30 g; Conditions: freshwater, 15 °C, ip injection; Concentration: 4.8 mmol/kg bw for 3 hr (95% confidence interval: 4.5-5.7 mmol/kg bw) /formulation/

Yokoyama M, Sakaguchi M; Fish Sci 62 (4): 660-661 (1996)

Hazardous Substances Data Bank (HSDB)

LD50; Species: Oncorhynchus mykiss (Rainbow trout) weight 30 g; Conditions: freshwater, 15 °C, ip injection; Concentration: 7.5 mmol/kg bw for 2 hr (95% confidence interval: 6.3-9.6 mmol/kg bw) /formulation/

Yokoyama M, Sakaguchi M; Fish Sci 62 (4): 660-661 (1996)

Hazardous Substances Data Bank (HSDB)

15.2 Ecological Information

15.2.1 Environmental Fate/Exposure Summary

Cysteine's production and use as a dough enhancer and in biochemical and nutritional research may result in its release to the environment through various waste streams. Cysteine is a non-essential amino acid for humans and also occurs in many plants. If released to air, an estimated vapor pressure of 6.7X10-7 mm Hg at 25 °C indicates cysteine will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase cysteine 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 1.6 hours. Particulate-phase cysteine will be removed from the atmosphere by wet and dry deposition. Cysteine does not contain chromophores that absorb at wavelengths >290 nm and, therefore, is not expected to be susceptible to direct photolysis by sunlight. If released to soil, cysteine is expected to have very high mobility based upon a an estimated Koc of 3. The pKa values of cysteine are 1.71, 8.33 and 10.78, indicating that this compound will exist as a zwitterion in the environment and zwitterions generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil is not expected because the compound exists as an ion and ions do not volatilize. Cysteine is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Utilizing the Warburg test, 4.7% of the Theoretical BOD was reached in 24 hours indicating that biodegradation is not an important environmental fate process in soil and water. If released into water, cysteine is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. The pKa values indicate cysteine will exist almost entirely as a zwitterion at pH values of 5 to 9 and, therefore, volatilization from water surfaces is not expected to be an important fate process. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions (pH 5 to 9). Occupational exposure to cysteine may occur through inhalation and dermal contact with this compound at workplaces where cysteine is produced or used. Monitoring data indicate that the general population may be exposed to cysteine via ingestion of food. (SRC)

Hazardous Substances Data Bank (HSDB)

15.2.2 Natural Pollution Sources

Cysteine is a non-essential amino acid for human development(1). Cysteine also occurs in many plants(2).

*(1) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry, p. 486 (2013) (2) US Dept Agric; US Dept Agric, Agric Res Service. 1992-2016. Dr. Duke's Phytochemical and Ethnobotanical Databases. Cysteine. Available from, as of Sept 28, 2016: **https://phytochem.nal.usda.gov/phytochem/search***

Hazardous Substances Data Bank (HSDB)

15.2.3 Artificial Pollution Sources

Cysteine's production and use as a dough enhancer(1) and in biochemical and nutritional research(2) may result in its release to the environment through various waste streams(SRC).

(1) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry, p. 486 (2013) (2) Larranaga MD et al; Hawley's Condensed Chemical Dictionary 16th ed., Hoboken, NJ: John Wiley & Sons, Inc. p. 408 (2016)

Hazardous Substances Data Bank (HSDB)

15.2.4 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 3(SRC), determined from a structure estimation method(2), indicates that cysteine is expected to have very high mobility in soil(SRC). The pKa values of cysteine are 1.71, 8.33 and 10.78(3), indicating that this compound will exist as a zwitterion in the environment and zwitterions generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4). Volatilization from moist soil is not expected because the compound exists as an ion and ions do not volatilize. Cysteine is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 6.7X10-7 mm Hg at 25 °C(SRC), determined from a fragment constant method(2). Utilizing the Warburg test, 4.7% of the Theoretical BOD was reached in 24 hours(5) indicating that biodegradation is not an important environmental fate process in soil(SRC).

*(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Jul 13, 2016: **https://www2.epa.gov/tsca-screening-tools** (3) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry p. 486 (2013) (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (5) Malaney GW, Gerhold RM; J Water Pollut Control Fed 41: R18-R33 (1969)*

Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 3(SRC), determined from a structure estimation method(2), indicates that cysteine is not expected to adsorb to suspended solids and sediment(SRC). The pKa values of 1.71, 8.33 and 10.78(3) indicates cysteine will exist as a zwitterion at pH values of 5 to 9 and, therefore, volatilization from water surfaces is not expected to be an important fate process(SRC). According to a classification scheme(4), an estimated BCF of 3(SRC), from its log Kow of -2.49(5) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Utilizing the Warburg test, 4.7% of the Theoretical BOD was reached in 24 hours(6) indicating that biodegradation is not an important environmental fate process in water(SRC).

*(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Jul 13, 2106: **https://www2.epa.gov/tsca-screening-tools** (3) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry p. 486 (2013) (4) Franke C et al; Chemosphere 29: 1501-14 (1994) (5) 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. 6 (1995) (6) Malaney GW, Gerhold RM; J Water Pollut Control Fed 41: R18-R33 (1969)*

Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), cysteine, which has an estimated vapor pressure of 6.7X10-7 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 cysteine 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 1.6 hours(SRC), calculated from its rate constant of 8.0X10-11 cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(3). Particulate-phase cysteine may be removed from the air by wet and dry deposition(SRC). Cysteine does not contain chromophores that absorb at wavelengths >290 nm(4) and, therefore, is not expected to be susceptible to direct photolysis by sunlight(SRC).

*(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Jul 13, 2016: **https://www2.epa.gov/tsca-screening-tools** (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)

15.2.5 Environmental Biodegradation

AEROBIC: Cysteine, present at 500 mg/L, reached 1.5, 2.4 and 4.7% of its theoretical BOD in 6, 12, and 24 hours, respectively, using an activated sludge inoculum at 2500 mg/L in the Warburg test. It is one of the more resistant of the amino acids(1).

(1) Malaney GW, Gerhold RM; J Water Pollut Control Fed 41: R18-R33 (1969)

Hazardous Substances Data Bank (HSDB)

PURE CULTURE: Alcaligenes faecalis, isolated from activated sludge, was able to oxidize 500 mg/L cysteine, exhibiting an O2 uptake of 575 mg/L in 130 hours in the Warburg test at 20 °C(1).

(1) Marion CV, Malaney GW; J Water Pollut Control Fed 35: 1269-84 (1963)

Hazardous Substances Data Bank (HSDB)

ANAEROBIC: An enrichment culture capable of degrading cysteine was isolated from sediment from a stream in Charleston, WV that received industrial wastewater effluent(1).

(1) Jessee JA et al; Appl Environ Microbiol 45: 97-102 (1983)

Hazardous Substances Data Bank (HSDB)

15.2.6 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of cysteine with photochemically-produced hydroxyl radicals has been estimated as 8.0X10-22 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 1.6 hours at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). The rate constant for the estimated OH radical reaction of cysteine with hydroxyl radicals in aqueous solutions at pH 7 is 3.5X10-10 L/mol-sec(2); this corresponds to an aquatic half-life of 1 hour at an aquatic concentration of 1X10-17 hydroxyl radicals per liter(3). Cysteine is not expected to undergo hydrolysis in the environment due to the lack of functional groups that hydrolyze under environmental conditions(4). Cysteine does not contain chromophores that absorb at wavelengths >290 nm(4) and, therefore, is not expected to be susceptible to direct photolysis by sunlight(SRC).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) Buxton GV et al; J Phys Chem Ref Data 17: 513-882 (1988) (3) Mill T et al; Science 207: 886-887 (1980) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 8-12 (1990)

Hazardous Substances Data Bank (HSDB)

15.2.7 Environmental Bioconcentration

An estimated BCF of 3 was calculated in fish for cysteine(SRC), using a log Kow of -2.49(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).

*(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. 6 (1995) (2)US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Jul 13, 2016: **https://www2.epa.gov/tsca-screening-tools** (3) Franke C et al; Chemosphere 29: 1501-14 (1994)*

Hazardous Substances Data Bank (HSDB)

15.2.8 Soil Adsorption/Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc of cysteine can be estimated to be 3(SRC). According to a classification scheme(2), this estimated Koc value suggests that cysteine is expected to have very high mobility in soil. The pKa values of cysteine are 1.71, 8.33 and 10.78(3) indicating that this compound will exist as a zwitterion in the environment and zwitterions generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4).

*(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Jul 13, 2016: **https://www2.epa.gov/tsca-screening-tools** (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry p. 486 (2013) (4) 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)

15.2.9 Volatilization from Water/Soil

The pKa values of cysteine are 1.71, 8.33 and 10.78(1), indicating that this compound will exist as a zwitterion at pH values of 5 to 9; therefore, volatilization from water surfaces is not expected to be an important fate process. Cysteine is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 6.7X10-7 mm Hg(SRC), determined from a fragment constant method(2).

*(1) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry p. 486 (2013) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Jul 13, 2016: **https://www2.epa.gov/tsca-screening-tools***

Hazardous Substances Data Bank (HSDB)

15.2.10 Environmental Water Concentrations

SURFACE WATER: Cysteine was tested for but not detected in grab samples from the Huron River at the Ann Arbor, Michigan Water Treatment Plant intake, sampled in June 2004(1).

(1) Lee JH et al; Environ Sci Technol 40: 1478-1484 (2006)

Hazardous Substances Data Bank (HSDB)

15.2.11 Effluent Concentrations

Cysteine was present at 5.0, 1.5 and 0.8 nmol/g in three consecutive horizon samples from an active landfill in a low permeability clay soil, located in Conica-Montemarta, Sevilla, Spain; sampling was conducted following 3 years of use(1).

(1) Gonzalez-Vila FJ et al; Chemosphere 31: 2817-25 (1995)

Hazardous Substances Data Bank (HSDB)

15.2.12 Food Survey Values

Cysteine in fruit juices purchased in supermarkets in Davis, CA(1).

Juice	Concn (mg/L juice)
prune, with pulp	4
prune, no pulp	not determined
prune, concentrated extracts of dried	not determined
prune, frozen juice from fresh	76
prune, fresh French	27
plum	55
peach	53
cherry	90
nectarine	86
pear	38
apple	1
grape	23
kiwi fruit	46
strawberry	not detected

(1) van Gorsel H et al; J Agric Food Chem 40: 784-789 (1992)

Hazardous Substances Data Bank (HSDB)

15.2.13 Plant Concentrations

Cysteine has been reported in 30 plants(1).

Genus species	Family	Common name(s)	Part	Concn (ppm)
Helianthus annuus	Asteraceae	Girasol; Sunflower	Seed	16000.0
Glycine max	Fabacaea	Soybean	Seed	6430.0
Citrullus lanatus	Cucurbitaceae	Watermelon	Seed	5742.0
Opuntia ficusindica	Castaceae	Nopal; Indian Fig; Prickly Pear; Nopalito	Seed	5740.0
Cucurbita foetidissima	Cucurbitaceae	Buffalo Gourd	Seed	3080.0
Phaseolus acutifolius	Fabaceae	Tepary Bean	Seed	2920.0
Senna obtusifolia	Fabaceae	Sicklepod	Seed	244.0
Triticum aestivum	Poaceae	Wheat	Seed	1449.0
Phoenix dactylifera	Arecaceae	Date Palm	Fruit	1140.0
Citrullus lanatus	Cucurbitaceaea	Watermelon	Fruit	236.0

(1) US Dept Agric; US Dept Agric, Agric Res Service. 1992-2016. Dr. Duke's Phytochemical and Ethnobotanical Databases. Cysteine. Available from, as of Sept 28, 2016: https://phytochem.nal.usda.gov/phytochem/search

Hazardous Substances Data Bank (HSDB)

15.2.14 Probable Routes of Human Exposure

According to the 2012 TSCA Inventory Update Reporting data, 1 reporting facility estimated the number of persons reasonably likely to be exposed in the manufacturing, processing, or use of cysteine in the United States may be in the range of 25-49 workers per plant; the data may be greatly underestimated due to confidential business information (CBI) or unknown values(1).

(1) US EPA; Chemical Data Reporting (CDR). Non-confidential 2012 Chemical Data Reporting information on chemical production and use in the United States. Available from, as of July 13, 2016: https://java.epa.gov/chemview

Hazardous Substances Data Bank (HSDB)

Occupational exposure to cysteine may occur through inhalation and dermal contact with this compound at workplaces where cysteine is produced or used. Monitoring data indicate that the general population may be exposed to cysteine via ingestion of food. (SRC)

Hazardous Substances Data Bank (HSDB)

16 Associated Disorders and Diseases

Comparative Toxicogenomics Database (CTD)

Therapeutic Target Database (TTD)

Disease	References
AIDS	PubMed: 9071566, 1969014, 11153075, 8748311, 9657528, 1565552, 11418788, 1315794
Alzheimer's disease	PubMed: 17031479, 11959400, 8595727, 15361288, 9693263, 15465626, 15061359, 10494443, 11255442, 12498967, 16227558, 9720975, 12111441, 16244393, 8356878, 12391605, 8478958, 21292280, 20858978, 21474939, 20523031, 11314776, 1716470, 23857558
Uremia	PubMed: 11865086, 10509899, 9607216, 7482520, 6520173, 22626821, 21359215, 2026685, 9573551, 24023812, 15353324, 19309105, 8087979, 17132244, 12675874 Merck Manual of Diagnosis and Therapy. David F. Putnam Composition and Concentrative Properties of Human Urine. NASA Contractor Report. July 1971 Geigy Scientific Tables, 8th Rev edition, pp. 130. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp. Basel, Switzerland c1981-1992. Geigy Scientific Tables, 8th Rev edition, pp. 165-177. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp., Basel, Switzerland c1981-1992. National Health and Nutrition Examination Survey (NHANES Survey) 2013 Geigy Scientific Tables, 8th Rev edition, pp. 80-82. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp., Basel, Switzerland c1981-1992.
Sulfite oxidase deficiency, ISOLATED	PubMed: 10682307, 27289259, 23452914, 15558695 Clinical and Laboratory Barriers to the Timely Diagnosis of Sulphite Oxidase Deficiency. Proceedings of Singapore Healthcare, 19(2), 94-100.
Multiple sclerosis	PubMed: 17611627, 15061359, 15576852, 12938853, 7707089, 17384003, 10609336, 16244395, 11985629, 10577274, 20347721, 20541774, 20374079, 18562510, 16244396
Stroke	PubMed: 15993662, 17384003, 12967724, 17892481
Peripheral neuropathy	PubMed: 17384003, 17157116
Dementia	PubMed: 17384003, 9693263, 11739625, 10577274
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
Autism	PubMed: 20423563, 7687150, 6150139, 15585776, 3410814, 12205654, 24130822
Eosinophilic esophagitis	Mordechai, Hien, and David S. Wishart
Cystinylglycinuria	PubMed: 10384375

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 Wiley References

Wiley

17.6 Depositor Provided PubMed Citations

PubChem

17.7 Synthesis References

Alfred Maierhofer, Hans Wagner, "Process for the production of high purity S-carboxymethyl-L-cysteine." U.S. Patent US4129593, issued May, 1965.

DrugBank

Kumagai, Hidehiko; Tanaka, Hideyuki; Sejima, Shunsuke; Yamada, Hideaki. Elimination and replacement reactions of b-chloro-L-alanine by cysteine desulfhydrase from Aerobacter aerogenes. Agricultural and Biological Chemistry (1977), 41(10), 2071-5.

Human Metabolome Database (HMDB)

17.8 Metabolite References

- Human Metabolome Database (HMDB)

17.9 General References

1. Bulaj G, Kortemme T, Goldenberg DP: Ionization-reactivity relationships for cysteine thiols in polypeptides. Biochemistry. 1998 Jun 23;37(25):8965-72. [PMID:9636038]
2. Baker DH, Czarnecki-Maulden GL: Pharmacologic role of cysteine in ameliorating or exacerbating mineral toxicities. J Nutr. 1987 Jun;117(6):1003-10. [PMID:3298579]

- DrugBank

Jenkins et al. A New Thiamin Salvage Pathway. Nature Chemical Biology, doi: 10.1038/NChemBio.2007.13, published online 8 July 2007. http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Sawa et al. Protein S-guanylation by the biological signal 8-nitroguanosine 3',5'-cyclic monophosphate Nature Chemical Biology, doi: 10.1038/NChemBio.2007.33, published online 30 September 2007. http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Wang et al. Phosphorothioation of DNA in bacteria by dnd genes Nature Chemical Biology, doi: 10.1038/NChemBio.2007.39, published online 14 October 2007. http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Chatterjee et al. Reconstitution of ThiC in thiamine pyrimidine biosynthesis expands the radical SAM superfamily Nature Chemical Biology, doi: 10.1038/nchembio.121, published online 26 October 2008 http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Matsuura et al. Identification of the toxic trigger in mushroom poisoning Nature Chemical Biology, doi: 10.1038/nchembio.179, published online 24 May 2009 http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Geu-Flores et al. Glucosinolate engineering identifies a gamma-glutamyl peptidase Nature Chemical Biology, doi: 10.1038/nchembio.185, published online 31 May 2009 http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Newton et al. Bacillithiol is an antioxidant thiol produced in Bacilli Nature Chemical Biology, doi: 10.1038/nchembio.189, published online 5 July 2009 http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Yan et al. Extracellular redox modulation by regulatory T cells. Nature Chemical Biology, doi: 10.1038/nchembio.212, published online 30 August 2009 http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

Hein et al. A route to enantiopure RNA precursors from nearly racemic starting materials. Nature Chemistry, doi: 10.1038/nchem.1108, published online 7 August 2011 http://www.nature.com/nchem

- Nature Chemistry

17.10 Chemical Co-Occurrences in Literature

- PubChem

17.11 Chemical-Gene Co-Occurrences in Literature

PubChem

17.12 Chemical-Disease Co-Occurrences in Literature

PubChem

18 Patents

US10478453
US10493051
US10543186
US10583155
US10653719
US10702490
US10905714
US10905713
US10912795
US10918662
US10933089
US11045438

DrugBank

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=XUJNEKJLAYXESH-REOHCLBHSA-N

PATENTSCOPE (WIPO)

19 Interactions and Pathways

19.1 Protein Bound 3D Structures

RCSB Protein Data Bank (RCSB PDB)

View 107 proteins in NCBI Structure

PubChem

19.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code	CYS
PDBe Conformer	

Protein Data Bank in Europe (PDBe)

19.2 Chemical-Target Interactions

Comparative Toxicogenomics Database (CTD)

Drug Gene Interaction database (DGIdb)

DrugBank

19.3 Pathways

PubChem

20 Biological Test Results

20.1 BioAssay Results

PubChem

21 Taxonomy

L-Cysteine 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

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 KEGG: OTC drugs

KEGG

22.9 ChemIDplus

ChemIDplus

22.10 ChEMBL Target Tree

ChEMBL

22.11 UN GHS Classification

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

22.12 EPA CPDat Classification

- EPA Chemical and Products Database (CPDat)

22.13 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

22.14 CCSBase Classification

- CCSbase

22.15 EPA DSSTox Classification

- EPA DSSTox

22.16 Consumer Product Information Database Classification

- Consumer Product Information Database (CPID)

22.17 LOTUS Tree

- LOTUS - the natural products occurrence database

22.18 FDA Drug Type and Pharmacologic Classification

- National Drug Code (NDC) Directory

22.19 EPA Substance Registry Services Tree

EPA Substance Registry Services

23 Information Sources

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   https://commonchemistry.cas.org/detail?cas_rn=52-90-4

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   https://chem.nlm.nih.gov/chemidplus/sid/0000052904

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

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   https://www.epa.gov/chemicals-under-tsca

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   L-cysteine
   https://echa.europa.eu/substance-information/-/substanceinfo/100.000.145

   L-cysteine
   https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/7677

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   CYSTEINE
   https://gsrs.ncats.nih.gov/ginas/app/beta/substances/K848JZ4886

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

   CYSTEINE
   https://pubchem.ncbi.nlm.nih.gov/source/hsdb/2109

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

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   http://www.hmdb.ca/citing

   L-Cysteine
   http://www.hmdb.ca/metabolites/HMDB0000574

   HMDB0000574_cms_30101
   https://hmdb.ca/metabolites/HMDB0000574#spectra

10. **CCSbase**

    L-Cysteine

    CCSbase Classification
    https://ccsbase.net/

11. **NORMAN Suspect List Exchange**

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L-Cysteine

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

12. **ChEBI**

L-cysteine
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:17561

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

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

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

Cysteine

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https://clinicaltrials.gov/

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> http://www.dgidb.org/downloads

https://www.dgidb.org/drugs/CYSTEINE

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

L-cysteine
http://idrblab.net/ttd/data/drug/details/D0L4VI

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> https://www.whatsinproducts.com/contents/view/1/6

Cysteine
https://www.whatsinproducts.com/chemicals/view/1/1692/004371-52-2

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

21. **Drug Induced Liver Injury Rank (DILIrank) Dataset**

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

l-cysteine
https://www.fda.gov/science-research/liver-toxicity-knowledge-base-ltkb/drug-induced-liver-injury-rank-dilirank-dataset

22. **Nature Chemical Biology**

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https://pubchem.ncbi.nlm.nih.gov/substance/26683853
https://pubchem.ncbi.nlm.nih.gov/substance/26683899
https://pubchem.ncbi.nlm.nih.gov/substance/56269947
https://pubchem.ncbi.nlm.nih.gov/substance/57643975
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https://pubchem.ncbi.nlm.nih.gov/substance/81049156
https://pubchem.ncbi.nlm.nih.gov/substance/85147453

23. **Nature Chemistry**

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24. **Joint FAO/WHO Expert Committee on Food Additives (JECFA)**

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https://www.fao.org/food/food-safety-quality/scientific-advice/jecfa/jecfa-flav/details/en/c/1409/

L-CYSTEINE
https://apps.who.int/food-additives-contaminants-jecfa-database/Home/Chemical/4381

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

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https://haz-map.com/About

Cysteine
https://haz-map.com/Agents/13558

28. **EU Food Improvement Agents**

L-Cysteine
https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32012R0872

29. **EU Pesticides Database**

L-cysteine
https://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/active-substances/?event=as.details&as_id=1291

30. **NITE-CMC**

L-Cysteine - FY2012
https://www.nite.go.jp/chem/english/ghs/12-mhlw-0020e.html

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

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

32. **Flavor and Extract Manufacturers Association (FEMA)**

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https://www.femaflavor.org/flavor-library/l-cysteine

33. **MassBank Europe**

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35. **NMRShiftDB**

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36. **NIST Mass Spectrometry Data Center**

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http://www.nist.gov/srd/nist1a.cfm

37. **SpectraBase**

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L-Cysteine
https://spectrabase.com/spectrum/ux8iHELNNE

L-(+)-cysteine
https://spectrabase.com/spectrum/9Po2PT620VJ

L-Cysteine
https://spectrabase.com/spectrum/1m4iLE1DEjG

L-(+)-CYSTEINE
https://spectrabase.com/spectrum/HmYcTiHVxPM

L-CYSTEINE
https://spectrabase.com/spectrum/6m6UcyWTNJL

L-Cysteine
https://spectrabase.com/spectrum/6sKJiCoUxKY

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

40. **NIPH Clinical Trials Search of Japan**
https://rctportal.niph.go.jp/en/

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

https://rxnav.nlm.nih.gov/id/rxnorm/3024

42. **Protein Data Bank in Europe (PDBe)**
http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/CYS

43. **PubChem**
https://pubchem.ncbi.nlm.nih.gov

44. **RCSB Protein Data Bank (RCSB PDB)**

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45. **Springer Nature**
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46. **The Cambridge Structural Database**
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=126977
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=282711
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=605633
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49. **Wikipedia**

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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

Classification of Japanese OTC drugs
http://www.genome.jp/kegg-bin/get_htext?br08313.keg

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

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

54. **ChEMBL**

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57. **PATENTSCOPE (WIPO)**

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58. **NCBI**

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