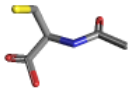
PubChem

COMPOUND SUMMARY

Acetylcysteine

PubChem CID	12035
Structure	 2D  3D  Crystal Find Similar Structures
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_5H_9NO_3S$
Synonyms	N-Acetyl-L-cysteine acetylcysteine 616-91-1 N-Acetylcysteine mercapturic acid More...
Molecular Weight	163.20
Dates	Modify 2022-10-07 Create 2004-09-16

Acetylcysteine is a synthetic N-acetyl derivative and prodrug of the endogenous amino acid L-cysteine, a precursor of the antioxidant glutathione (GSH), with mucolytic, antioxidant, and potential cytoprotective, cancer-preventive, and anti-inflammatory activities. Upon administration, acetylcysteine exerts its mucolytic activity by reducing disulfide bonds in mucoproteins, resulting in liquification of mucus and reducing its viscosity. It is also used for the treatment of acetaminophen overdose as it can restore the depleted GSH reserves in the hepatocytes during the process of detoxification. The antioxidant activity is attributed to the ability of GSH to scavenge reactive oxygen species (ROS), thereby preventing ROS-mediated cell damage, decreasing oxidative stress, protecting cells against the damaging effects of free radicals and preventing apoptosis in these cells. In addition, this may inhibit tumor cell proliferation, progression and survival, in susceptible tumor cells that rely on ROS-mediated signaling for their proliferation and malignant behavior. Under certain circumstances, acetylcysteine is able to induce apoptosis in susceptible cells, including certain tumor cells, via the intrinsic mitochondria-dependent pathway but not involving endoplasmic reticulum stress. Also, acetylcysteine may also be able to degrade Notch2, thereby preventing proliferation, migration, and invasion in Notch2-overexpressing glioblastoma cells. In addition, acetylcysteine may inhibit viral stimulation by reactive oxygen intermediates, thereby producing antiviral activity in HIV patients. Acetylcysteine also possesses anti-inflammatory activity through modulation of the nuclear factor-kappa B (NF-kB) pathway and the modulation of cytokine synthesis.

▸ NCI Thesaurus (NCIt)

Acetylcysteine, also known as N-acetylcysteine (NAC), is a modified amino acid that is used as an antidote for acetaminophen overdose to prevent hepatic injury. Acetylcysteine is a hepatoprotective agent and has not been linked to significant serum enzyme elevations during therapy or to instances of clinically apparent acute liver injury.

▸ LiverTox

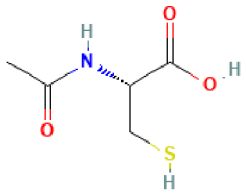
Acetylcysteine is an antioxidant and glutathione inducer indicated for mucolytic therapy and the treatment of [acetaminophen] overdose. Acetylcysteine has also been studied for a wide variety of off-label indications with mixed results. Acetylcysteine was granted FDA approval on 14 September 1963.

▸ DrugBank

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

1.3 Crystal Structures

Showing 1 of 7 View More

CCDC Number	868554
Crystal Structure Data	DOI:10.5517/ccy4swq
Crystal Structure Depiction	
Associated Article	DOI:10.1039/c2ce25241d

The Cambridge Structural Database

2 Biologic Description

SVG Image	
IUPAC Condensed	Ac-Cys-OH
Sequence	C
PLN	[acetyl]-C-OH
HELM	PEPTIDE1{[ac].C}$$$$
IUPAC	N-acetyl-L-cysteine

PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

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

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

3.1.2 InChI

InChI=1S/C5H9NO3S/c1-3(7)6-4(2-10)5(8)9/h4,10H,2H2,1H3,(H,6,7)(H,8,9)/t4-/m0/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.3 InChIKey

PWKSKIMOESPYIA-BYPYZUCNSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.4 Canonical SMILES

CC(=O)NC(CS)C(=O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.1.5 Isomeric SMILES

CC(=O)N[C@@H](CS)C(=O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.2 Molecular Formula

C5H9NO3S

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

3.3 Other Identifiers

3.3.1 CAS

616-91-1

CAS Common Chemistry; ChemIDplus; DrugBank; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); Hazardous Substances Data Bank (HSDB); Human Metabolome Database (HMDB)

3.3.2 Related CAS

18829-79-3 (hydrochloride)

19542-74-6 (mono-hydrochloride salt)

63664-54-0 (hydrochloride salt)

ChemIDplus

3.3.3 Deprecated CAS

7696-05-1, 1261105-20-7

ChemIDplus

1261105-20-7, 7696-05-1

EPA DSSTox

3.3.4 European Community (EC) Number

210-498-3

European Chemicals Agency (ECHA)

3.3.5 UNII

WYQ7N0BPYC

FDA/SPL Indexing Data

3.3.6 DSSTox Substance ID

DTXSID5020021

EPA DSSTox

3.3.7 Wikidata

Q375613

Wikidata

3.3.8 NCI Thesaurus Code

C200

NCI Thesaurus (NCIt)

3.3.9 RXCUI

197

NLM RxNorm Terminology

3.4 Synonyms

3.4.1 MeSH Entry Terms

Acétylcystéine GNR	Acetylcysteine Sodium	Azubronchin	durabronchal	Ilube	Monosodium Salt Acetylcysteine	N-Acetyl-L-c
acebraus	Acetylcysteine Zinc	Bisolvon NAC	Eurespiran	Jenacystein	MPectil	N-Acetylcyst
Acemuc	Acetylcysteine, (D)-Isomer	Bromuc	Exomuc	Jenapharm	Muciteran	NAC AL
Acetabs	Acetylcysteine, (DL)-Isomer	Broncho Fips	Fabrol	Lantamed	Muco Sanigen	NAC Zambo
Acetylcystein AL	Acetylcysteine, Monoammonium Salt	Broncho-Fips	Fluimucil	Larylin NAC	Mucomyst	NAC, Bisolvc
Acetylcystein Atid	Acetylcysteine, Monosodium Salt	BronchoFips	Fluprowit	Lindocetyl	Mucopect, Dampo	Optipect Hu
Acetylcystein Heumann	Acetylin	Broncholysin	Frekatuss	M Pectil	Mucosil	Sanigen, Mu
Acetylcystein Trom	Acetyst	Broncoclar	Genac	M-Pectil	Mucosol	Siccoral
Acetylcystein, mentopin	Acid, Mercapturic	Codotussyl	Hoestil	mentopin Acetylcystein	Mucosolvin	Siran
Acetylcysteine	Airbron	Cystamucil	Hustengetränk, Optipect	Mercapturic Acid	N Acetyl L cysteine	Sodium, Ace
Acetylcysteine Hydrochloride	Alveolex	Dampo Mucopect	Hydrochloride, Acetylcysteine	Monoammonium Salt Acetylcysteine	N Acetylcysteine	Solmucol

Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms

N-Acetyl-L-cysteine	N-Acetyl-cysteine	Fluimicil Infantil	Acetyl-L-cysteine	(2R)-2-acetamido-3-sulfanylpropanoic acid	(2R)-2-Acetamido-3-sulfanyl-propanoic
acetylcysteine	Fluimucetin	Acetilcisteina	N-Acetyl cysteine	component of Naxid	L-alpha-Acetamido-beta-mercaptoprop
616-91-1	Fluprowit	Acetylcysteinum	Mucolyticum	Mercapturic acid, (R)-	NSC 111180
N-Acetylcysteine	Acetein	Lysomucil	LNAC	Cysteine, N-acetyl-, L-	Mucolyticum-Lappe
mercapturic acid	Airbron	Mucofilin	Syntemucol	cysteine, N-acetyl-	WYQ7N0BPYC
Acetadote	Fabrol	Exomuc	acetyl cysteine	L-Cysteine, N-acetyl-	MFCD00004880
L-Acetylcysteine	Flumucetin	Inspir	N-Acetyl-3-mercaptoalanine	(R)-mercapturic acid	MLS000028419
Broncholysin	Mucosolvin	Ac-Cys-OH	Tixair	Fluatox	CHEBI:28939
Mucomyst	Mucosil	Mucolyticum Lappe	N-Acetyl-L-(+)-cysteine	Mucolator	NSC-111180
Fluimucil	Respaire	Mucolytikum Lappe	Neo-fluimucil	Mucret	RK-0202
Parvolex	Brunac	(R)-2-Acetamido-3-mercaptopropanoic acid	NAC-TB	UNII-WYQ7N0BPYC	NCGC00022304-05

PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	163.20	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	0.4	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	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	163.03031432	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	163.03031432	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	67.4 Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	10	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	148	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

Solid

Human Metabolome Database (HMDB)

4.2.2 Color/Form

Crystals from water

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 17

Hazardous Substances Data Bank (HSDB)

WHITE, CRYSTALLINE POWDER

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

4.2.3 Odor

SLIGHT ACETIC ODOR

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

4.2.4 Taste

CHARACTERISTIC SOUR TASTE

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

4.2.5 Boiling Point

407.00 to 408.00 °C. @ 760.00 mm Hg (est)

The Good Scents Company Information System

Human Metabolome Database (HMDB)

4.2.6 Melting Point

109-110

Martin, T.A. and Waller, C.W.; US. Patent 3,184,505; May 18, 1965; assigned to Mead Johnson & Company.

DrugBank

109.5 °C

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

4.2.7 Solubility

> [ug/mL]

Burnham Center for Chemical Genomics

1 G IN 5 ML WATER, 4 ML ALC; PRACTICALLY INSOL IN CHLOROFORM & ETHER

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

Soluble in water, alcohol, hot isopropyl alcohol, methyl acetate, and ethyl acetate

Osol A (ed); Remington's Pharmaceutical Sciences. 14th ed. Easton, PA: Mack Publishing Co, p. 871 (1970)

Hazardous Substances Data Bank (HSDB)

2.429e+005 mg/L @ 25 °C (est)

The Good Scents Company Information System

Human Metabolome Database (HMDB)

4.2.8 Vapor Pressure

1.1X10-5 mm Hg at 25 °C /Estimated/

US EPA; Estimation Programs Interface (EPI). ver. 3.11. U.S. EPA version for Windows. Washington, DC: U.S. EPA (2003). Available from, as of Feb. 18, 2005: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

Hazardous Substances Data Bank (HSDB)

4.2.9 LogP

log Kow = -0.66 /Estimated/

US EPA; Estimation Programs Interface (EPI). ver. 3.11. U.S. EPA version for Windows. Washington, DC: U.S. EPA (2003). Available from, as of Feb. 18, 2005: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

Hazardous Substances Data Bank (HSDB)

-0.696 (est)

The Good Scents Company Information System

Human Metabolome Database (HMDB)

4.2.10 Henry's Law Constant

Henry's Law constant = 1.7X10-13 atm-cu m/mole at 25 °C /Estimated/

US EPA; Estimation Programs Interface (EPI). ver. 3.11. U.S. EPA version for Windows. Washington, DC: U.S. EPA (2003). Available from, as of Feb. 18, 2005: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

Hazardous Substances Data Bank (HSDB)

4.2.11 Stability/Shelf Life

Stable in ordinary light; stable at temp up to 120 °C; nonhygroscopic (oxidizes in moist air)

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

4.2.12 Optical Rotation

Specific optical rotation: +5 deg at 20 °C (concn = 3 g/100 mL water)

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA2 83

Hazardous Substances Data Bank (HSDB)

4.2.13 pH

2 TO 2.75 (1 IN 100 ML)

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

4.2.14 Dissociation Constants

pKa

9.52 (at 25 °C)

SERJEANT & DEMPSEY (1979)

DrugBank

pKa= 3.24 (carboxylic acid moiety)

Osol, A. (ed.). Remington's Pharmaceutical Sciences. 16th ed. Easton, Pennsylvania: Mack Publishing Co., 1980., p. 805

Hazardous Substances Data Bank (HSDB)

pKa = 9.52 (SH group)

Serjeant, E.P, Dempsey B.; Ionisation Constants of Organic Acids in Aqueous Solution. International Union of Pure and Applied Chemistry (IUPAC). IUPAC Chemical Data Series No. 23, 1979. New York, New York: Pergamon Press, Inc., p. 154

Hazardous Substances Data Bank (HSDB)

4.2.15 Collision Cross Section

140.9 Å^2 [M+Na]$^+$ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322

CCSbase

140.9 Å^2 [M+Na]$^+$

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

NORMAN Suspect List Exchange

4.2.16 Kovats Retention Index

Standard non-polar	1547, 1547

NIST Mass Spectrometry Data Center

4.2.17 Other Experimental Properties

It is stable in ordinary light, nonhygroscopic (oxidizes in moist air), and stable at temperatures up to 120 °C

Osol A (ed); Remington's Pharmaceutical Sciences. 14th ed. Easton, PA: Mack Publishing Co, p. 871 (1970)

Hazardous Substances Data Bank (HSDB)

Hydroxyl radical reaction rate constant = 5.5X10-11 cu cm/molec-sec at 25 °C /Estimated/

US EPA; Estimation Programs Interface (EPI). ver. 3.11. U.S. EPA version for Windows. Washington, DC: U.S. EPA (2003). Available from, as of Feb. 18, 2005: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

Hazardous Substances Data Bank (HSDB)

4.3 SpringerMaterials Properties

Nuclear quadrupole resonance spectroscopy
Quadrupole coupling

SpringerMaterials

5 Spectral Information

5.1 1D NMR Spectra

1D NMR Spectra	NMRShiftDB Link

NMRShiftDB

5.1.1 1H NMR Spectra

Spectra ID	1783
Instrument Type	Bruker
Frequency	600 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	2.06:100.00, 2.89:2.27, 2.90:1.99, 2.91:14.28, 2.92:17.57, 2.93:16.79, 2.94:2.26, 2.95:1.86, 4.36:3.20, 4.37:4.34, 4.37:4.65, 4.38:4.57, 4.39:2.96
Thumbnail	

Human Metabolome Database (HMDB)

Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	138061
Copyright	Copyright © 2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.1.2 13C NMR Spectra

Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	138061
Copyright	Copyright © 2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.2 2D NMR Spectra

5.2.1 1H-13C NMR Spectra

2D NMR Spectra Type	1H-13C HSQC
Spectra ID	1723
Instrument Type	Bruker
Frequency	600 MHz
Solvent	Water
pH	7.00
Shifts [ppm] (F2:F1):Intensity	2.06:24.68:1.00, 2.92:29.01:0.69, 4.37:59.52:0.35
Thumbnail	

Human Metabolome Database (HMDB)

5.3 Mass Spectrometry

5.3.1 GC-MS

Showing 2 of 9 View More

Spectra ID	29920
Instrument Type	EI-B
Ionization Mode	positive
SPLASH	splash10-01ox-9000000000-192b8907b32f1e180c72
Top 5 Peaks	43.0 99.99 60.0 79.69 74.0 32.63 76.0 31 28.0 18.27
Thumbnail	

Notes	instrument=HITACHI M-2500

Human Metabolome Database (HMDB)

Spectra ID	31365
Instrument Type	GC-MS
SPLASH	splash10-0i00-2970000000-d817070e3a42f5e63ec5
Top 5 Peaks	100.0 1 218.0 0.86 260.0 0.47 116.0 0.27 262.0 0.19
Thumbnail	

Human Metabolome Database (HMDB)

5.3.2 MS-MS

Showing 2 of 6 View More

Spectra ID	1795
Instrument Type	Quattro_QQQ
Ionization Mode	Positive
SPLASH	splash10-00di-0900000000-b0d92bfcc2536077a6fc
Top 5 Peaks	121.992 100 76.107 13.16 118.01 8.92 163.929 8.73 145.986 4.90
Thumbnail	
Notes	delivery=Flow_Injectionanalyzer=Triple_Quad

Human Metabolome Database (HMDB)

Spectra ID	1796
Instrument Type	Quattro_QQQ
Ionization Mode	Positive
SPLASH	splash10-004i-9000000000-f305286cee84e6ae992b

Top 5 Peaks	76.091 100 59.173 39.52 43.301 39.52 87.037 24.55 104.971 12.13
Thumbnail	
Notes	delivery=Flow_Injectionanalyzer=Triple_Quad

Human Metabolome Database (HMDB)

5.3.3 LC-MS

Showing 2 of 5 View More

MoNA ID	MoNA019177
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	164.03759765625
Instrument	Agilent 6550 iFunnel
Instrument Type	LC-ESI-QTOF
Ionization Mode	positive
Top 5 Peaks	122.02974 100 76.02121 33.24 100.0212 23.88 122.05389 11.52 60.04397 7.71
SPLASH	splash10-00di-2900000000-66ff0b9c20dc1e5615fd
Thumbnail	
Submitter	romanas chaleckis, gunma university

MassBank of North America (MoNA)

MoNA ID	MoNA019178
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	164.03759765625

Instrument	Agilent 6550 iFunnel
Instrument Type	LC-ESI-QTOF
Ionization Mode	positive
Top 5 Peaks	76.02121 100 44.04868 75.70 90.05463 63.88 58.99485 51.47 100.0212 39.55
SPLASH	splash10-054o-9100000000-524ab6fae76f6a75c02b
Thumbnail	
Submitter	romanas chaleckis, gunma university

MassBank of North America (MoNA)

5.3.4 Other MS

Showing 2 of 3 View More

Other MS	MASS: 75327 (NIST/EPA/MSDC Mass Specral Database 1990 Version)

Hazardous Substances Data Bank (HSDB)

MoNA ID	CCMSLIB00005464114
MS Category	Experimental
MS Level	MS2
Precursor Type	[M-H]-
Precursor m/z	162.023
Instrument	Orbitrap
Ionization Mode	negative
Top 5 Peaks	84.044022 100 162.892654 28.09 162.021805 9.05 161.892792 6.60 57.033173 6.32
SPLASH	splash10-001i-9400000000-7f512d75af735386f549
Thumbnail	
Submitter	GNPS Team, University of California, San Diego

MassBank of North America (MoNA)

5.4 IR Spectra

5.4.1 FTIR Spectra

Technique	Mull
Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Aldrich
Catalog Number	138061
Copyright	Copyright © 2018-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.4.2 ATR-IR Spectra

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Calbiochem, EMD Chemicals, Inc., an Affiliate of Merck KGaA, Darmstadt, Germany
Catalog Number	106425
Lot Number	200329
Copyright	Copyright © 2012-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Source of Sample	Aldrich
Catalog Number	138061
Copyright	Copyright © 2018-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.5 Raman Spectra

Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Calbiochem, EMD Chemicals, Inc., an Affiliate of Merck KGaA, Darmstadt, Germany
Catalog Number	106425
Lot Number	200329
Copyright	Copyright © 2012-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

SpectraBase

Catalog Number	138061
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Thumbnail

SpectraBase

6 Related Records

6.1 Related Compounds with Annotation

PubChem

6.2 Related Compounds

Same Connectivity	14 Records
Same Stereo	8 Records
Same Isotope	3 Records
Same Parent, Connectivity	161 Records
Same Parent, Stereo	87 Records
Same Parent, Isotope	148 Records
Same Parent, Exact	78 Records
Mixtures, Components, and Neutralized Forms	334 Records
Similar Compounds	293 Records
Similar Conformers	2,039 Records

PubChem

6.3 Substances

6.3.1 Related Substances

All	938 Records
Same	301 Records
Mixture	637 Records

PubChem

6.3.2 Substances by Category

PubChem

6.4 Entrez Crosslinks

PubMed	11,243 Records
Protein Structures	4 Records
Taxonomy	29 Records
OMIM	10 Records
Gene	1,391 Records

PubChem

6.5 NCBI LinkOut

NCBI

7 Chemical Vendors

PubChem

8 Drug and Medication Information

8.1 Drug Indication

Acetylcysteine is indicated for mucolytic therapy and in the management of [acetaminophen] overdose.

▸ DrugBank

FDA Label

▸ DrugBank

8.2 LiverTox Summary

Acetylcysteine, also known as N-acetylcysteine (NAC), is a modified amino acid that is used as an antidote for acetaminophen overdose to prevent hepatic injury. Acetylcysteine is a hepatoprotective agent and has not been linked to significant serum enzyme elevations during therapy or to instances of clinically apparent acute liver injury.

▸ LiverTox

8.3 Drug Classes

Antidotes, Toxicological Emergency

▸ LiverTox

8.4 Drug Effects during Lactation

Summary	No information is available on the use of acetylcysteine during breastfeeding. To avoid infant exposure, nursing mothers may consider pumping and discarding their milk for 30 hours after administration. Acetylcysteine is very minimally absorbed after inhalation, so breastfeeding can be continued and no special precautions are required.
PubMed	29999990
NCBI Books	NBK500931

▸ Drugs and Lactation Database (LactMed)

8.5 WHO Essential Medicines

Drug	Drug Classes	Formulation	Indication
Acetylcysteine	Antidotes and other substances used in poisonings -> Specific	(1) Parenteral - General injections - IV: 200 mg per mL in 10 mL ampoule; (2) Oral - Liquid: 10%; 20%	(1) Exposure to or harmful effects of undetermined intent of analgesics, antipyretics or nonsteroidal anti-inflammatory drugs [co-prescribed with V03AB23]; (2) Acute or subacute hepatic failure [co-prescribed with V03AB23]

▸ WHO Model Lists of Essential Medicines

8.6 FDA Orange Book

▸ FDA Orange Book

8.7 FDA National Drug Code Directory

National Drug Code (NDC) Directory

ACETYLCYSTEINE is an active ingredient in the products 'ANTI AGE STRESS' and ACETYLCYSTEINE.

National Drug Code (NDC) Directory

8.8 Drug Labels for Ingredients

Label Information	Total 25 labels
Drug Ingredient	ACETYLCYSTEINE
NDC Code(s)	0409-3307-03, 0409-3307-11, 0409-3308-03, 0409-3308-11, 0517-7504-25, 0517-7510-03, 0517-7604-25, 0517-7610-03, 0517-7630-03, 0574-0805-30 ... total 43.
Packagers	Akorn; American Regent, Inc.; AuroMedics Pharma LLC; CROWN GENERAL AGENCY INC; Cadila Healthcare Limited; Cardinal Health; Cumberland Pharmaceuticals Inc.; Exela Pharma Sciences, LLC; Fresenius Kabi USA, LLC; Guna spa; Hospira, Inc.; Indoco Remedies Limited; Innovative Apothecary Solutions, LLC; Nextmune AB; Padagis US LLC; Physicians Total Care, Inc.; Sagent Pharmaceuticals; Truemed Group LLC; VIRTUS PHARMACEUTICALS LLC; Zydus Pharmaceuticals (USA) Inc.

DailyMed

8.9 Clinical Trials

8.9.1 ClinicalTrials.gov

ClinicalTrials.gov

8.9.2 EU Clinical Trials Register

EU Clinical Trials Register

8.10 Therapeutic Uses

Antiviral Agents; Expectorants; Free Radical Scavengers

National Library of Medicine's Medical Subject Headings online file (MeSH, 1999)

Hazardous Substances Data Bank (HSDB)

... 113 patients entered into the study were reported to be pregnant at the time of /acetaminophen/ overdose. Follow up including appropriate laboratory and pregnancy data outcome data, was available in 60 cases. Of these, 19 overdosed during the first trimester, 22 during the second trimester and 19 during the third trimester of pregnancy. Of the 24 patients with acetaminophen levels above the acetaminophen overdose nomogram line, 10 were treated with N-acetylcysteine within 10 hr postingestion; eight delivered normal infants, two had elective abortions. Of ten patients treated with N-acetylcysteine 10-16 hr postingestion, five delivered viable infants, two had elective abortions, and three had spontaneous abortions. Of four women treated with N-acetylcysteine 16-24 hr postingestion, one mother died, and there was one spontaneous abortion, one stillbirth, one elective abortion, and one delivery. ...

PMID:2748061

Riggs BS et al; Obstet Gynecol 74 (2): 247-53 (1989)

Hazardous Substances Data Bank (HSDB)

Acetylcysteine is indicated in the treatment of acetaminophen overdose to protect against hepatotoxicity . /Included in US product labeling/

Thomson.Micromedex. Drug Information for the Health Care Professional. 24th ed. Volume 1. Plus Updates. Content Reviewed by the United States Pharmacopeial Convention, Inc. Greenwood Village, CO. 2004.

Hazardous Substances Data Bank (HSDB)

Acetylcysteine is used in current medical practice in conjunction with chest physiotherapy as mucolytic in patients who have viscid or thickened airway mucus. When administered via direct instillation, it is used to loosen impacted mucus plugs during bronchoscopy. Acetylcysteine can irritate the airways and induce bronchospasm when given by inhalation; therefore, it should be administered simultaneously with or following administration of an inhaled beta-adrenergic bronchodilator. /NOT included in US product labeling/

Thomson.Micromedex. Drug Information for the Health Care Professional. 24th ed. Volume 1. Plus Updates. Content Reviewed by the United States Pharmacopeial Convention, Inc. Greenwood Village, CO. 2004., p. 19

Hazardous Substances Data Bank (HSDB)

To evaluate the effectiveness and safety of N-acetylcysteine (NAC) in treating chronic hepatitis B patients, 144 patients with chronic hepatitis B (total bilirubin, TBil>170 mmol/L) from several centers were chosen for a randomized and double blind clinical trial. The patients were divided into a NAC group and a placebo group and all of them were treated with an injection containing the same standardized therapeutic drugs. A daily dose of 8 microgram NAC was added to the injection of the NAC group. The trial lasted 45 days. Hepatic function and other biochemistry parameters were checked at the experimental day 0 and days 15, 30, 45. Each group consisted of 72 patients of similar demology and disease characteristics. During the trial, 28 cases of the 144 patients dropped out. In the NAC group, at day 0 and day 30, the TBil were401.7 vs. 149.2 and 160.1+/-160.6. In the placebo group, the TBil on the corresponding days were 384.1+/-134.0 and 216.3+/-199.9. Its decrease in the NAC group was 62% and 42% in the placebo group. At day 0 and day 45 of treatment, the effective PTa increase rate was 72% in the NAC group and 54% in the placebo group. The total effective rate (TBil + PTa) was 90% in the NAC group and 69% in the placebo group. The parameters of the two groups showed a remarkable difference. The rate of side effects was 14% in the NAC and 5% in the placebo groups. NAC can decrease the level of serum TBil, increase the PTa and reduce the time of hospitalization. NAC showed no serious adverse effects during the period of our treatment. We find that NCA is effective and secure in treating chronic hepatitis B patients.

PMID:15670485

Shi XF et al; Zhonghua Gan Zang Bing Za Zhi 13 (1): 20-3 (2005)

Hazardous Substances Data Bank (HSDB)

8.11 Drug Warnings

... /Acetylcysteine/ should be used during pregnancy only when clearly needed. ... Since it is not known if acetylcysteine is distributed into human milk, the drug should be used with caution in nursing women.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

Hazardous Substances Data Bank (HSDB)

Anaphylactoid reactions (i.e., acute hypersensitivity reactions such as rash, hypotension, wheezing, and/or dyspnea) have been reported in patients receiving IV acetylcysteine for the treatment of acetaminophen overdosage; in some cases, the anaphylactoid reactions were serious, including death in a patient with asthma. Rash, urticaria, and pruritus are the most frequently reported adverse reactions in patients receiving IV acetylcysteine. Acute flushing and erythema also have occurred; these reactions generally occur 30-60 minutes after initiating the infusion and resolve despite infusion of the drug. Reactions to acetylcysteine that involve manifestations other than flushing and erythema should be considered anaphylactoid reactions and treated as such.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3564

Hazardous Substances Data Bank (HSDB)

Chest tightness and bronchoconstriction have been reported with acetylcysteine. Clinically overt acetylcysteine-induced bronchospasm occurs rarely and unpredictably, even in patients with asthmatic bronchitis or bronchitis complicating bronchial asthma. Occasionally, patients receiving oral inhalation of acetylcysteine develop increased airway obstruction of varying and unpredictable severity. Patients who have had such reactions to previous therapy with acetylcysteine may not react during subsequent therapy with the drug, and patients who have had inhalation treatments with acetylcysteine without incident may react to subsequent therapy.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3564

Hazardous Substances Data Bank (HSDB)

Nausea, vomiting, and other GI symptoms may occur following oral administration of acetylcysteine in the treatment of acetaminophen overdosage. The drug may also aggravate vomiting associated with acetaminophen overdosage. Administration of dilute acetylcysteine solutions may minimize the tendency of the drug to aggravate vomiting.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3564

Hazardous Substances Data Bank (HSDB)

For more Drug Warnings (Complete) data for N-ACETYLCYSTEINE (15 total), please visit the HSDB record page.

Hazardous Substances Data Bank (HSDB)

8.12 Reported Fatal Dose

2. 2= Slightly toxic. Probable oral lethal dose (human) 5-15 g/kg; for 70 kg person (150 lb) between 1 pint and 1 quart.

Gosselin, R.E., R.P. Smith, H.C. Hodge. Clinical Toxicology of Commercial Products. 5th ed. Baltimore: Williams and Wilkins, 1984., p. II-380

- Hazardous Substances Data Bank (HSDB)

9 Pharmacology and Biochemistry

9.1 Pharmacodynamics

Acetylcysteine is indicated for mucolytic therapy and in the management of acetaminophen overdose. It has a short duration of action as it is given every 1-8 hours depending on route of administration, and has a wide therapeutic window. Patients should be counselled regarding diluting oral solutions in cola for taste masking, the risk of hypersensitivity, and the risk of upper gastrointestinal hemorrhage.

▸ DrugBank

9.2 MeSH Pharmacological Classification

Antiviral Agents

Agents used in the prophylaxis or therapy of VIRUS DISEASES. Some of the ways they may act include preventing viral replication by inhibiting viral DNA polymerase; binding to specific cell-surface receptors and inhibiting viral penetration or uncoating; inhibiting viral protein synthesis; or blocking late stages of virus assembly. (See all compounds classified as Antiviral Agents.)

▸ Medical Subject Headings (MeSH)

Free Radical Scavengers

Substances that eliminate free radicals. Among other effects, they protect PANCREATIC ISLETS against damage by CYTOKINES and prevent myocardial and pulmonary REPERFUSION INJURY. (See all compounds classified as Free Radical Scavengers.)

▸ Medical Subject Headings (MeSH)

Expectorants

Agents that increase mucous excretion. Mucolytic agents, that is drugs that liquefy mucous secretions, are also included here. (See all compounds classified as Expectorants.)

▸ Medical Subject Headings (MeSH)

9.3 FDA Pharmacological Classification

FDA UNII	WYQ7N0BPYC
Active Moiety	ACETYLCYSTEINE
Pharmacological Classes	Established Pharmacologic Class [EPC] - Antidote
Pharmacological Classes	Established Pharmacologic Class [EPC] - Antidote for Acetaminophen Overdose
Pharmacological Classes	Physiologic Effects [PE] - Decreased Respiratory Secretion Viscosity
Pharmacological Classes	Physiologic Effects [PE] - Increased Glutathione Concentration
Pharmacological Classes	Established Pharmacologic Class [EPC] - Mucolytic
Pharmacological Classes	Mechanisms of Action [MoA] - Reduction Activity
FDA Pharmacology Summary	Acetylcysteine is an Antidote, and Antidote for Acetaminophen Overdose, and Mucolytic. The mechanism of action of acetylcysteine is as a Reduction Activity. The physiologic effect of acetylcysteine is by means of Decreased Respiratory Secretion Viscosity, and Increased Glutathione Concentration.

▸ FDA Pharm Classes

Non-Proprietary Name	ACETYLCYSTEINE
Pharmacological Classes	Antidote for Acetaminophen Overdose [EPC]; Decreased Respiratory Secretion Viscosity [PE]; Increased Glutathione Concentration [PE]; Mucolytic [EPC]; Reduction Activity [MoA]; Antidote [EPC]

▸ National Drug Code (NDC) Directory

9.4 ATC Code

R05CB01

*S76 | LUXPHARMA | Pharmaceuticals Marketed in Luxembourg | Pharmaceuticals marketed in Luxembourg, as published by d'Gesondheetskeess (CNS, la caisse nationale de sante, www.cns.lu), mapped by name to structures using CompTox by R. Singh et al. (in prep.). List downloaded from **https://cns.public.lu/en/legislations/textes-coordonnes/liste-med-comm.html**. Dataset **DOI:10.5281/zenodo.4587355***

▸ NORMAN Suspect List Exchange

R - Respiratory system

R05 - Cough and cold preparations

R05C - Expectorants, excl. combinations with cough suppressants

R05CB - Mucolytics

R05CB01 - Acetylcysteine

▸ WHO Anatomical Therapeutic Chemical (ATC) Classification

S - Sensory organs

S01 - Ophthalmologicals

S01X - Other ophthalmologicals

S01XA - Other ophthalmologicals

S01XA08 - Acetylcysteine

▸ WHO Anatomical Therapeutic Chemical (ATC) Classification

V - Various

V03 - All other therapeutic products

V03A - All other therapeutic products

V03AB - Antidotes

V03AB23 - Acetylcysteine

▸ WHO Anatomical Therapeutic Chemical (ATC) Classification

9.5 Absorption, Distribution and Excretion

Absorption

An 11 g dose in the form of an effervescent tablet for solution reaches a mean C_{max} of 26.5 µg/mL, with a T_{max} of 2 hours, and an AUC of 186 µg*h/mL.

▸ DrugBank

Route of Elimination

An oral dose of radiolabelled acetylcysteine is 13-38% recovered in the urine in the first 24 hours, while 3% is recovered in the feces.

▸ DrugBank

Volume of Distribution

The volume of distribution of acetylcysteine is 0.47 L/kg.

▸ DrugBank

Clearance

Acetylcysteine has a mean clearance of 0.11 L/hr/kg.

▸ DrugBank

Following oral administration (e.g., when used as an antidote for acetaminophen overdosage), acetylcysteine is absorbed from the GI tract.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

Oral acetylcysteine is rapidly absorbed, but the bioavailability is low (10-30%) due to significant first-pass metabolism. Intact acetylcysteine has a relatively small volume of distribution (0.5 L/kg). Serum concentrations after intravenous administration of an initial loading dose of 150 mg/kg over 15 minutes are about 500 mg/L. A steady state plasma concentration of 35 mg/L (10-90 mg/L) was reached in about 12 hours following the loading dose with a continuous infusion of 50 mg/kg over 4 hours and 100 mg/kg over the next 16 hours.

Goldfrank, L.R., Flomenbaum, N.E., Lewin, N.A., Weisman, R.S., Howland, M.A., Hoffman, R.S., Goldfrank's Toxicologic Emergencies 6th Ed. (1998)., McGraw-Hill, New York, N.Y., p. 566

▸ Hazardous Substances Data Bank (HSDB)

9.6 Metabolism/Metabolites

Acetylcysteine can be deacetylated by aminoacylase 1 or other undefined deacetylases before undergoing the normal metabolism of cysteine.

▸ DrugBank

Following oral inhalation or intratracheal instillation, most of the administered drug appears to participate in the sulfhydryl-disulfide reaction; the remainder is absorbed from the pulmonary epithelium, deacetylated by the liver to cysteine, and subsequently metabolized.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

Acetylcysteine undergoes rapid deacetylation in vivo to yield cysteine or oxidation to yield diacetylcystine.

Thomson.Micromedex. Drug Information for the Health Care Professional. 24th ed. Volume 1. Plus Updates. Content Reviewed by the United States Pharmacopeial Convention, Inc. Greenwood Village, CO. 2004., p. 19

▸ Hazardous Substances Data Bank (HSDB)

9.7 Biological Half-Life

The mean terminal half life of acetylcysteine in adults is 5.6 hours and in pre-term neonates is 11 hours.

▸ DrugBank

Following IV administration of acetylcysteine, mean elimination half lives of 5.6 and 11 hours have been reported in adults and in neonates, respectively. The mean elimination half life was increased by 80% in patients with severe liver damage (i.e., alcoholic cirrhosis (Child-Pugh score of 7-13) or primary and/or secondary biliary cirrhosis (Child-Pugh score of 5-11)).

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

9.8 Mechanism of Action

A number of possible mechanisms for the mucolytic activity of acetylcysteine have been proposed. Acetylcysteine's sulfhydryl groups may hydrolize disulfide bonds within mucin, breaking down the oligomers, and making the mucin less viscous. Acetylcysteine has also been shown to reduce mucin secretion in rat models. It is an antioxidant in its own right but is also deacetylated to **cysteine**, which participates in the synthesis of the antioxidant **glutathione**. The antioxidant activity may also alter intracellular redox reactions, decreasing phosphorylation of EGFR and MAPK, which decrease transcription of the gene MUC5AC which produces mucin. In the case of **acetaminophen** overdoses, a portion of the drug is metabolized by CYP2E1 to form the potentially toxic metabolite **N-acetyl-p-benzoquinone imine** (**NAPQI**). The amount of **NAPQI** produced in an overdose saturates and depletes **glutathione** stores. The free **NAPQI** promiscuously binds to proteins in hepatocytes, leading to cellular necrosis. Acetylcysteine can directly conjugate **NAPQI** or provide **cysteine** for **glutathione** production and **NAPQI** conjugation.

▸ DrugBank

Acetylcysteine exerts its mucolytic action through its free sulfhydryl group, which opens the disulfide bonds and lower the viscosity of the mucus. This action increases with increasing pH and is most significant at pH 7 to 9. The mucolytic action of acetylcysteine is not affected by the presence of DNA.

Thomson.Micromedex. Drug Information for the Health Care Professional. 24th ed. Volume 1. Plus Updates. Content Reviewed by the United States Pharmacopeial Convention, Inc. Greenwood Village, CO. 2004., p. 19

▸ Hazardous Substances Data Bank (HSDB)

Acetylcysteine may protect against **acetaminophen** overdose-induced hepatotoxicity by maintaining or restoring hepatic concentrations of **glutathione**. **Glutathione** is required to inactivate an intermediate metabolite of **acetaminophen** that is thought to be hepatotoxic. In **acetaminophen** overdose, excessive quantities of this metabolite are formed because the primary metabolic (glucuronide and **sulfate** conjugation) pathways become saturated. Acetylcysteine may act by reducing the metabolite to the parent compound and/or by providing sulfhydryl for conjugation of the metabolite. Experimental evidence also suggests that a sulfhydryl-containing compound such as acetylcysteine may directly inactivate the metabolite.

Thomson.Micromedex. Drug Information for the Health Care Professional. 24th ed. Volume 1. Plus Updates. Content Reviewed by the United States Pharmacopeial Convention, Inc. Greenwood Village, CO. 2004.

▸ Hazardous Substances Data Bank (HSDB)

9.9 Human Metabolite Information

9.9.1 Tissue Locations

Fibroblasts
Intestine
Kidney
Liver
Neuron
Placenta

▸ Human Metabolome Database (HMDB)

9.9.2 Cellular Locations

Cytoplasm

▸ Human Metabolome Database (HMDB)

9.10 Biochemical Reactions

▸ PubChem

10 Use and Manufacturing

10.1 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)**

MUCOLYTIC AGENT (ADJUVANT) FOR BRONCHOPULMONARY DISORDERS

SRI

▸ **Hazardous Substances Data Bank (HSDB)**

Medicine, biochemical research

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Rheinhold Co., 1993, p. 12

▸ **Hazardous Substances Data Bank (HSDB)**

Mucolytic; corneal vulnerary; antidote to **acetaminophen** poisoning

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 17

▸ **Hazardous Substances Data Bank (HSDB)**

Secretolytic agent

Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA2 83

▸ **Hazardous Substances Data Bank (HSDB)**

For more Uses (Complete) data for N-ACETYLCYSTEINE (6 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

10.1.1 Use Classification

Human Drugs -> FDA Approved Drug Products with Therapeutic Equivalence Evaluations (Orange Book) -> Active Ingredients

▸ **FDA Orange Book**

Cosmetics -> Antioxidant

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

▸ **NORMAN Suspect List Exchange**

10.2 Methods of Manufacturing

Direct acetylation of naturally occurring **L-cysteine**

SRI

▸ **Hazardous Substances Data Bank (HSDB)**

... Made by acylating **L-cysteine hydrochloride hydrate** with **acetic anhydride** in the presence of **sodium acetate**.

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V9 626 (2003)

▸ **Hazardous Substances Data Bank (HSDB)**

Preparation and use in treatment of respiratory diseases: Martin, Waller, US 3184505 (1965 to Mead Johnson)

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 17

▸ **Hazardous Substances Data Bank (HSDB)**

10.3 Formulations/Preparations

Parenteral: For injection concentrate, for IV infusion: 200 mg/mL Acetadote (Cumberland).

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

Oral inhalation, intratracheal instillation, and oral: Solution: 100 mg (of acetylcysteine) per mL (10%), **Acetylcysteine Sodium** Solution, (Abbott, American Regent, Bedford, Dey, Mayne, Roxane); Mucomyst (Sandoz); 200 mg (of acetylcysteine) per mL (20%) **Acetylcysteine Sodium** Solution (Abbott, American Regent, Bedford, Dey, Mayne, Roxane); Mucomyst (Sandoz). /**Acetylcysteine sodium**/

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

10.4 Consumption Patterns

ESSENTIALLY 100% AS A MUCOLYTIC AGENT

SRI

▸ Hazardous Substances Data Bank (HSDB)

10.5 U.S. Production

(1976) PROBABLY GREATER THAN 4.54X10+5 GRAMS

SRI

▸ Hazardous Substances Data Bank (HSDB)

(1979) NOT PRODUCED COMMERCIALLY IN US

SRI

▸ Hazardous Substances Data Bank (HSDB)

10.6 General Manufacturing Information

EPA TSCA Commercial Activity Status

L-Cysteine, N-acetyl-: ACTIVE

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

▸ EPA Chemicals under the TSCA

Information available in 2005 indicated that Acetylcysteine was used in the manufacture of pharmaceutical preparations in the following countries: Algeria, Argentina, Australia, Austria, Belgium, Brazil, Canada, Chile, Colombia, Croatia, Czech Republic, Denmark, Ecuador, Finland, France, Germany, Greece, Hong Kong, Hungary, India, Indonesia, Ireland, Israel, Italy, Japan, Luxembourg, Malaysia, Monaco, Netherlands, New Zealand, Norway, Poland, Portugal, Romania, Russian Federation, Singapore, Slovenia, South Africa, Spain, Sweden, Switzerland, Thailand, Turkey, United Kingdom, United States, Yugoslavia (1,2)

(1) Swiss Pharmaceutical Society, ed. (2005) Index Nominum: International Drug Directory, 18th Ed., Medpharm Scientific Publishers, Stuttgart, Germany; (2) Royal Pharmaceutical Society of Great Britain (2005) Martindale, The Complete Drug Reference, 34th Ed., The Pharmaceutical Press, London, England

▸ Hazardous Substances Data Bank (HSDB)

Information available in 2005 indicated that **Acetylcysteine sodium** was used in the manufacture of pharmaceutical preparations in the following countries: Australia, Germany, Netherlands, Norway, Poland, Romania, Russian Federation, Switzerland, United States (1,2) /**Acetylcysteine Sodium**/

(1) Swiss Pharmaceutical Society, ed. (2005) Index Nominum: International Drug Directory, 18th Ed., Medpharm Scientific Publishers, Stuttgart, Germany (2) Royal Pharmaceutical Society of Great Britain (2005) Martindale, The Complete Drug Reference, 34th Ed., The Pharmaceutical Press, London, England

▸ Hazardous Substances Data Bank (HSDB)

11 Identification

11.1 Analytic Laboratory Methods

THREE N-SUBSTITUTED MALEIMIDES, INCLUDING ACETYLCYSTEINE, WERE TESTED AS DERIVATIZING REAGENTS. N-ACETYLCYSTEINE WAS READILY CONVERTED INTO THE ADDUCT WITH **N-(4-ANILINOPHENYL)MALEIMIDE**. PICROGRAM LEVELS WERE SEPARATED & QUANTIFIED.

SHIMADA K ET AL; SENSITIVE DERIVATIZATION REAGENTS FOR THIOL COMPOUNDS IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY WITH ELECTROCHEMICAL DETECTION; ANAL CHIM ACTA 147: 375 (1983)

▸ **Hazardous Substances Data Bank (HSDB)**

The following methods have been developed for the analysis of free amino acids in blood, food, and feedstocks: (1) Protein hydrolysis, (2) Chromatographic methods that include high performance liquid chromatography (HPLC), gas chromatography (GC) and thin-layer chromatography (TLC), (3) Colorimetric and Fluorimetric Analysis, (4) Spectrometric Analysis, and (5) Enzymatic Determination and Microbial Assay /amino acids/

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V2 531-4

▸ **Hazardous Substances Data Bank (HSDB)**

Analyte: acetylcysteine; matrix: chemical identification; procedure: infrared absorption spectrophotometry with comparison to standards

U.S. Pharmacopeia. The United States Pharmacopeia, USP 28/The National Formulary, NF 23; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p46 (2005)

▸ **Hazardous Substances Data Bank (HSDB)**

Analyte: acetylcysteine; matrix: chemical purity; procedure: liquid chromatography with detection at 214 nm and comparison to standards

U.S. Pharmacopeia. The United States Pharmacopeia, USP 28/The National Formulary, NF 23; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p46 (2005)

▸ **Hazardous Substances Data Bank (HSDB)**

For more Analytic Laboratory Methods (Complete) data for N-ACETYLCYSTEINE (6 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

12 Safety and Hazards

12.1 Hazards Identification

12.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	**Warning**
GHS Hazard Statements	H315 (58.62%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (96.55%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H335 (58.62%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	P261, P264, P264+P265, P271, P280, P302+P352, P304+P340, P305+P351+P338, P319, P321, 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 57 companies from 9 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 28 of 57 companies. For more detailed information, please visit ECHA C&L website.* *Of the 8 notification(s) provided by 29 of 57 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)

12.1.2 Hazard Classes and Categories

Skin Irrit. 2 (58.62%)

Eye Irrit. 2 (96.55%)

STOT SE 3 (58.62%)

▸ European Chemicals Agency (ECHA)

12.2 Accidental Release Measures

12.2.1 Disposal Methods

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

▸ Hazardous Substances Data Bank (HSDB)

12.3 Handling and Storage

12.3.1 Storage Conditions

Unopened vials of acetylcysteine sodium solution should be stored at 15-30 °C. Following exposure to air, solutions should be stored at 2-8 °C to retard oxidation and should be used within 96 hr.

McEvoy, G.K. (ed.). American Hospital Formulary Service--Drug Information 94. Bethesda, MD: American Society of Hospital Pharmacists, Inc. 1994 (Plus Supplements)., p. 1762

▸ Hazardous Substances Data Bank (HSDB)

Unopened vials of acetylcysteine sodium solution should be stored at 15-30 °C. Following exposure to air, oral and oral inhalation solutions should be stored at 2-8 °C to retard oxidation and should be used within 96 hours.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

Acetylcysteine solution does not contain an antimicrobial agent; therefore, care must be taken to minimize contamination of the sterile solution. After opening, the vial should be stored in the refrigerator; the opened vial should be discarded after 96 hours.

Thomson.Micromedex. Drug Information for the Health Care Professional. 24th ed. Volume 1. Plus Updates. Content Reviewed by the United States Pharmacopeial Convention, Inc. Greenwood Village, CO. 2004., p. 20

▸ Hazardous Substances Data Bank (HSDB)

12.4 Stability and Reactivity

12.4.1 Hazardous Reactivities and Incompatibilities

Acetylcysteine is a reducing agent and is incompatible with oxidizing agents. Solutions of acetylcysteine become discolored and liberate hydrogen sulfide upon contact with rubber, some metals, particularly iron and copper, and/or when subjected to autoclaving. ... Solutions containing amphotericin B, tetracyclines, erythromycin lactobionate, or ampicillin sodium. ...

Acetylcysteine solutions are also physically imcompatible with iodized oil, trypsin, hydrogen peroxide.

McEvoy, G.K. (ed.). American Hospital Formulary Service--Drug Information 94. Bethesda, MD: American Society of Hospital Pharmacists, Inc. 1994 (Plus Supplements)., p. 1762

- Hazardous Substances Data Bank (HSDB)

12.5 Regulatory Information

12.5.1 FDA Requirements

The Approved Drug Products with Therapeutic Equivalence Evaluations List identifies currently marketed prescription drug products, incl acetylcysteine, approved on the basis of safety and effectiveness by FDA under sections 505 of the Federal Food, Drug, and Cosmetic Act.

*DHHS/FDA; Electronic Orange Book-Approved Drug Products with Therapeutic Equivalence Evaluations. Available from, as of March 15, 2005: **https://www.fda.gov/cder/ob/***

- Hazardous Substances Data Bank (HSDB)

12.6 Other Safety Information

12.6.1 Special Reports

A REVIEW WITH 55 REFERENCES ON THE BIOCHEMISTRY & PHARMACOLOGY OF ACETYLCYSTEINE.[MCKINNEY GR, SISSON GM; ACETYLCYSTEINE; PHARMACOL BIOCHEM PROP DRUG SUBST 2: 479 (1979)]

- Hazardous Substances Data Bank (HSDB)

A REVIEW WITH 28 REFERENCES OF THE EFFECT OF N-ACETYLCYSTEINE ON THE ANTITUMOR ACTIVITY OF DOXORUBICIN & THE LATTER'S CARDIOTOXICITY.[OLSON RD ET AL; INFLUENCE OF N-ACETYLCYSTEINE ON THE ANTITUMOR ACTIVITY OF DOXORUBICIN; SEMIN ONCOL 10(1) 29 (1983)]

- Hazardous Substances Data Bank (HSDB)

Haddad LM, Winchester JF; Clinical Management of Poisoning and Drug Over Dose 2nd ed (1990). Acetaminophen and the use of N-acetylcysteine in treatment of overdose (review). pp 893-908.

- Hazardous Substances Data Bank (HSDB)

13 Toxicity

13.1 Toxicological Information

13.1.1 Toxicity Summary

Patients experiencing an overdose may present with vomiting, nausea, bronchospasm, periorbital angioedema, and hypotension. Treat patients with symptomatic and supportive measures. Hemodialysis may remove some acetylcysteine from circulation as it is somewhat protein bound.

▸ DrugBank

13.1.2 Hepatotoxicity

Acetylcysteine is a simple modified amino acid and appears to be hepatoprotective. In the many studies of acetylcysteine use with **acetaminophen** overdose as well as with other conditions such as contrast media nephropathy, pulmonary fibrosis, cystic fibrosis and ulcerative colitis, it has not been associated with serum enzyme elevations during therapy or with episodes of clinically apparent liver injury. Since approval of the oral and intravenous forms of acetylcysteine, there have been no published reports of hepatotoxicity and the product label does not mention liver injury as an adverse event. Indeed, acetylcysteine may be beneficial in treating liver diseases in general, although its current indications are limited to **acetaminophen** overdose or **acetaminophen** related acute liver injury.

Likelihood score: E (unlikely cause of clinically apparent liver injury).

▸ LiverTox

13.1.3 Drug Induced Liver Injury

Compound	acetylcysteine
DILI Annotation	No-DILI-Concern
Label Section	No match
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

13.1.4 Acute Effects

▸ ChemIDplus

13.1.5 Interactions

Guinea pigs were treated with daily drug injections as follows: 1 group received 200 mg **kanamycin**/kg, sc, 1 group received n-acetylcysteine (300 mg/kg, ip) & the 3rd group received n-acetylcysteine followed by **kanamycin** 1 hr later. After 7-day recovery, thresholds for detection of the compound action potential were measured. N-acetylcysteine alone had no detectable effect on hearing thresholds. **Kanamycin** alone produced a moderate (10-20 db) hearing loss below 10 khz & a more severe loss above 10 khz. Animals receiving both n-acetylcysteine & **kanamycin** had severe hearing losses (40-60 db) at all frequencies between 3 & 30 khz. These data indicate that n-acetylcysteine exerts a strong synergistic effect on **kanamycin** in producing severe hearing loss & cochlear damage.

PMID:6841282
Bock Gr et al; Hear Res 9 (3): 255 (1983)

▸ Hazardous Substances Data Bank (HSDB)

The major side effect of photodynamic therapy (PDT) using photofrin enhanced skin sensitivity for sunlight which persists for 3-8 weeks after injection. Formation of **singlet oxygen** and radicals is believed to be involved in the basic mechanism of inducing skin damage. Reducing this side effect would make PDT more widely acceptable particularly for palliative use. Hairless dorsal skin patches of mice injected with 10 mg/kg photofrin ip 24 hr before illumination were used to evaluate the effect of increasing light doses. The light was obtained from a halogen lamp and transmitted via a fiber optic to illuminate a field of 2.5 sq cm. After establishing a dose response relationship for single or fractionated light dose illumination of the skin, drugs known to scavenge radicals, quench **singlet oxygen** or interfere with **histamine** release were tested for their protective effect. N-Acetylcysteine, a radical scavenger admin ip (1,000 and 2,000 mg/kg) 1 hr before illumination produced a significant decr in skin damage at light doses > 50 J sq cm (protection factor of 1.3-1.8). When N-acetylcysteine was administered in a dose of 500

mg/kg no protection was observed. Fractionated illumination experiments in combination with multiple injections of N-acetylcysteine (1000 mg/kg) also failed to show any protection. The addition of ranitidine, a histamine blocking agent (25-100 mg/kg) given prior to illumination resulted in a limited protection at higher light doses. From this study /results suggest/ that N-acetylcysteine could be of value in amelioration of the photosensitivity in patients with PDT.

PMID:8022887

Baas P et al; Photochem Photobiol 59 (4): 448-54 (1994)

Hazardous Substances Data Bank (HSDB)

The influence of acetylcysteine on cisplatin nephrotoxicity was investigated in female Wistar rats. Admin of 0.6 mg cisplatin/100 mg bw was followed by oliguria and proteinuria, as well as a significant incr of blood urea nitrogen concn. The ip admin of 0.6 mg cisplatin/100 g body wt concomitantly with 100 mg acetylcysteine/100 g body wt sc completely abolished the nephrotoxic effects of cisplatin. However, following this, the platinum concn in the kidney was decr significantly by acetylcysteine treatment. This was caused by a enhanced urinary excretion of platinum. The same effect on cisplatin nephrotoxicity appeared when cisplatin and acetylcysteine were dissolved together in a soln prior to injection. It could be shown that in this soln a ligand exchange reaction of cisplatin by acetylcysteine started immediately, resulting in incr renal excretion and decr platinum concn in the kidney. ... /Results show/ that the protective effect of acetylcysteine on cisplatin nephrotoxicity is based on the formation of a complex unsuitable for tubular resorption. ...

PMID:8326088

Appenroth D et al; J Appl Toxicol 13 (3): 189-92 (1993)

Hazardous Substances Data Bank (HSDB)

... Studies have shown that the in utero admin of alcohol alters the activity of gamma-glutamyl transpeptidase, the major enzyme involved with the break down of glutathione. The implication is that the in utero admin of alcohol interferes with gamma-glutamyl cycle and ultimately alters glutathione levels. ... The in utero admin of alcohol results in a decr in brain and liver glutathione levels in the developing fetus. ... N-Acetylcysteine ... was given to pregnant mothers throughout gestation in a liquid diet concomitantly with a dose of alcohol which produces a decr in body and brain weights. ... N-Acetylcysteine antagonized the effects of alcohol in the developing fetus.

Reyes E et al; Alcohol Clin Exp Res 15 (2): 343 (1991)

Hazardous Substances Data Bank (HSDB)

13.1.6 Antidote and Emergency Treatment

Basic treatment: Establish a patent airway. 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 normal saline 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 ... . /Poison A and B/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 139

Hazardous Substances Data Bank (HSDB)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in respiratory arrest. Positive pressure ventilation techniques with a bag valve mask device may be beneficial. Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start an IV with D5W /SRP: "To keep open", minimal flow rate/. Use lactated Ringer's if signs of hypovolemia are present. Watch for signs of fluid overload. Consider drug therapy for pulmonary edema ... . For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload ... . Treat seizures with diazepam (Valium) ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Poison A and B/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 139

Hazardous Substances Data Bank (HSDB)

13.1.7 Human Toxicity Excerpts

/SIGNS AND SYMPTOMS/ The features of n-acetyl-l-cysteine overdose are similar to the anaphylactoid reactions but more severe. Cardiovascular collapse and death were temporally assocated with the administration of intravenous n-acetyl-l-cysteine in a 4 year old with subtoxic plasma acetaminophen levels. Several fatalities occurred following intravenous n-acetyl-l-cysteine administration, but the contribution of fulminant hepatic failure to mortality limits conclusions about n-acetyl-l-cysteine effects.

Ellenhorn, M.J. and D.G. Barceloux. Medical Toxicology - Diagnosis and Treatment of Human Poisoning. New York, NY: Elsevier Science Publishing Co., Inc. 1988., p. 163

Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ A case of serum sickness like illness assoc with acetylcysteine therapy in a 29 yr old man who was admitted with an acetaminophen overdose is reported. Acetylcysteine was started at 5 g orally every 6 hr. Three days after admission, the patient developed fever, diffuse abdominal tenderness, and bilateral, symmetric swelling of the knee and elbow joints. Had a discrete erythematous maculopapular eruption on the chest, abdomen, back and extremities with a few erythematous macules on the palms and face. The platelet count was 233 x 109/l. Twelve hr after antibiotic admin for suspected intraabdominal abscess, his temperature was 40 °C and he had tender, palpable cervical, axillary and inguinal lymph nodes. a hypersensitivity reaction to acetylcysteine was suspected and the drug was discontinued. ...

Mohammed S et al; Ann Pharmacother 28: 285 (1994)

Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ A healthy 30-month-old girl allegedly ingested acetaminophen at 418 mg/kg. Because the emergency physician feared the time of ingestion might not be accurate, he decided to start the 20.5-hour intravenous N-acetylcysteine protocol 8 hours after ingestion. He mistakenly prescribed the maximum milliliter-per-kilogram volume of the dextrose 5% diluent for the milliliter-per-kilogram volume of N-acetylcysteine 20% to be administered. Five hours after the error was detected (19.5 hours postingestion), the patient started developing myoclonus on the left side of her body, with left eye deviation. This condition persisted intermittently for 3 hours despite treatment with diazepam, lorazepam, and phenytoin. A first computed tomographic scan result was normal. A few hours later, she sustained shorter recurrences of the myoclonus. At 30 hours after ingestion, she started to have irregular breathing and became unresponsive to pain. A repeated computed tomographic scan showed diffuse cerebral edema. A postmortem examination showed the presence of acute anoxic encephalopathy with marked cerebral edema and the beginning of uncal herniation that confirmed the clinical diagnosis of intracranial hypertension and brain death. A cumulative intravenous dose of 2,450 mg/kg of N -acetylcysteine was associated with status epilepticus, intracranial hypertension, and death in a child.

PMID:15459624

Bailey B et al; Ann Emerg Med 44 (4): 401-6 (2004)

Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ Paracetamol overdose is a common reason for presentation to the emergency department and N-acetylcysteine is frequently used in the treatment of toxic paracetamol ingestions. Adverse reactions to N-acetylcysteine are common though usually mild and easily treated. Serious reactions to N-acetylcysteine however, are rare and there have been no previous

reported fatalities with its therapeutic use. This report describes the case of a 40 year old brittle asthmatic patient who died after treatment with intravenous N-acetylcysteine. Asthma is a risk factor for adverse reactions to N-acetylcysteine and special caution should be exercised in its use in brittle asthmatic patients.

PMID:12421803
Full text: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1756296
Appelboam AV et al; Emerg Med J 19 (6): 594-5 (2002)

▸ Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ Marked elevations in liver function test results (eg, AST (SGOT) and ALT (SGPT), occurred on 2 occasions following administration of high doses (total doses: 106 and 250 g over 3-4 days) of acetylcysteine rectally and via nasogastric tube in a 3 year old by with cystic fibrosis; these abnormalities were noted within a few days of initiation of acetylcysteine therapy and resolved gradually following discontinuance of the drug.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3564

▸ Hazardous Substances Data Bank (HSDB)

13.1.8 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ Although adequately tolerated when applied as drops to alkali burned corneas (as a collagenase inhibitor), a 20% solution was severely damaging when injected into the corneal stroma. In rabbits receiving drops, corneal epithelial wound healing was not retarded.

Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 45

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ In the dog, rabbit, & rat, exposure to a chamber atmosphere produced by 30 sec of nebulization of 20% soln of acetylcysteine has been evaluated. These animals were exposed to this atmosphere for 15 min twice daily for 35 consecutive days. Addnl groups of animals were exposed for 1 hr daily, 5 times a wk for 12 wk. No clinical or histophathologic changes were found that could be assoc with the exposure of the animals to acetylcysteine.

Booth, N.H., L.E. McDonald (eds.). Veterinary Pharmacology and Therapeutics. 5th ed. Ames, Iowa: Iowa State University Press, 1982., p. 683

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Chronic Exposure or Carcinogenicity/ No evidence of oncogenic activity was observed in rats given oral acetylcysteine in dosages up to 1000 mg/kg daily (5.2 times the human mucolytic dose) for 12 months. ...

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ A slight reduction in fertility wa observed in a reproductive study in rats given oral acetylcysteine dosages of 500 or 1000 mg/kg daily (2.6 or 5.2 times the human mucolytic dose, respectively.

McEvoy, G.K. (ed.). American Hospital Formulary Service- Drug Information 2005. Bethesda, MD: American Society of Health-System Pharmacists, Inc. 2005 (Plus Supplements)., p. 3565

▸ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for N-ACETYLCYSTEINE (7 total), please visit the **HSDB record page**.

▸ Hazardous Substances Data Bank (HSDB)

13.1.9 Non-Human Toxicity Values

LD50 Dog oral 1 g/kg

Booth, N.H., L.E. McDonald (eds.). Veterinary Pharmacology and Therapeutics. 5th ed. Ames, Iowa: Iowa State University Press, 1982., p. 683

▸ Hazardous Substances Data Bank (HSDB)

LD50 Rat oral 3 g/kg

Booth, N.H., L.E. McDonald (eds.). Veterinary Pharmacology and Therapeutics. 5th ed. Ames, Iowa: Iowa State University Press, 1982., p. 683

▸ Hazardous Substances Data Bank (HSDB)

LD50 Mouse oral > 3 g/kg

Gosselin, R.E., R.P. Smith, H.C. Hodge. Clinical Toxicology of Commercial Products. 5th ed. Baltimore: Williams and Wilkins, 1984., p. II-380

▸ Hazardous Substances Data Bank (HSDB)

LD50 Rat oral > 6 g/kg

Gosselin, R.E., R.P. Smith, H.C. Hodge. Clinical Toxicology of Commercial Products. 5th ed. Baltimore: Williams and Wilkins, 1984., p. II-380

▸ Hazardous Substances Data Bank (HSDB)

LD50 Dog ip 700 mg/kg

Booth, N.H., L.E. McDonald (eds.). Veterinary Pharmacology and Therapeutics. 5th ed. Ames, Iowa: Iowa State University Press, 1982., p. 683

▸ Hazardous Substances Data Bank (HSDB)

13.1.10 Ongoing Test Status

The following link will take the user to the National Toxicology Program (NTP) Test Agent Search Results page, which tabulates all of the "Standard Toxicology & Carcinogenesis Studies", "Developmental Studies", and "Genetic Toxicity Studies" performed with this chemical. Clicking on the "Testing Status" link will take the user to the status (i.e., in review, in progress, in preparation, on test, completed, etc.) and results of all the studies that the NTP has done on this chemical. [http://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm?fuseaction=ntpsearch.searchresults&searchterm=616-91-1]

Available from: ***https://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm?fuseaction=ntpsearch.searchresults&searchterm=616-91-1***

▸ Hazardous Substances Data Bank (HSDB)

13.1.11 Populations at Special Risk

Asthma is a risk factor for adverse reactions to N-acetylcysteine and special caution should be exercised in its use in brittle asthmatic patients.

PMID:12421803
Full text: ***https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1756296***
Appelboam AV et al; Emerg Med J 19 (6): 594-5 (2002)

▸ Hazardous Substances Data Bank (HSDB)

13.1.12 Protein Binding

Acetylcysteine is 66-97% protein bound in serum, usually to albumin.

▸ DrugBank

13.2 Ecological Information

13.2.1 Environmental Fate/Exposure Summary

Acetylcysteine's production and use as a mucolytic, in the treatment of chronic bronchitis, cancer, **paracetamol** intoxication, **acetaminophen** overdose, corneal damage, and in veterinary applications as an expectorant may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 1.1X10-5 mm Hg at 25 °C indicates acetylcysteine will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase acetylcysteine 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 7 hours. Particulate-phase acetylcysteine will be removed from the atmosphere by wet and dry deposition. Acetycysteine does not contain chromophores that absorb UV light at wavelengths >290 nm; therefore, acetylcysteine is not expected to be susceptible to photolysis. If released to soil, acetylcysteine is expected to have very high mobility based upon an estimated Koc of 10. Growth of 10 different bacteria strains were inhibited by acetylcysteine, suggesting that biodegradation is not an important environmental fate process. The pKa of the thiol group is 9.52 and the pKa of carboxylic acid moiety of acetylcysteine is 3.24, indicating that this compound will primarily exist as an anion in the environment and will not volatilize from moist soil surfaces. Acetylcysteine is not expected to volatilize from dry soil surfaces based upon its vapor pressure. If released into **water**, acetylcysteine is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from **water** surfaces is not expected to be an important fate process because this compound will exist as a anion in aqueous conditions. An estimated BCF of 3.2 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. Occupational exposure to acetylcysteine may occur through inhalation and dermal contact with this compound at workplaces where acetylcysteine is produced or used. Exposure to the drug among the general population may be limited to those administered acetylcysteine (a mucolytic). (SRC)

▸ Hazardous Substances Data Bank (HSDB)

13.2.2 Artificial Pollution Sources

Acetylcysteine's production and use as a mucolytic, in the treatment of chronic bronchitis(1), cancer(1), **paracetamol** intoxication(1), **acetaminophen** overdose(2), corneal damage(2), and in veterinary application as an expectorant(2) may result in its release to the environment through various waste streams(SRC).

(1) Olofsson AC et al; Appl Environ Microbiol 69: 4814-22 (2003) (2) O'Neil MJ, ed; The Merck Index. 13th ed. Whitehouse Station, NJ: Merck and Co., Inc., p. 17 (2001)

▸ Hazardous Substances Data Bank (HSDB)

13.2.3 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 10(SRC), determined from a structure estimation method(2), indicates that acetylcysteine is expected to have very high mobility in soil(SRC). The pKa of the thiol group is 9.52(3) and the pKa of carboxylic acid moiety of acetylcysteine is 3.24(4), indicating that this compound will primarily exist as an anion in the environment and will not volatilize from moist soil surfaces. Acetylcysteine is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 1.1X10-5 mm Hg(SRC), determined from a fragment constant method(5). Growth of 10 different bacteria strains were inhibited by acetylcysteine(6), suggesting that biodegradation is not an important environmental fate process in soil(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (3) Serjeant EP, Dempsey B; Ionisation constants of organic acids in aqueous solution. IUPAC Chem Data Ser No.23. NY, NY: Pergamon pp. 989 (1979) (4) Osol A, ed; Remington's Pharmaceutical Sciences. 16th ed. Easton, PA: Mack Publishing Co., (1980) (5) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985) (6) Olofsson AC et al; Appl Environ Microbiol 69: 4814-22 (2003)

▸ Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 10(SRC), determined from a structure estimation method(2), indicates that acetylcysteine is not expected to adsorb to suspended solids and sediment(SRC). The pKa of the thiol group is 9.52(3) and the pKa of carboxylic acid moiety of acetylcysteine is 3.24(4), indicating that this compound will primarily exist as an anion in the environment and anions will not volatilize from **water** surfaces. According to a classification scheme(6), an estimated BCF of 3.2(SRC), from an estimated log Kow of -0.66(7) and a regression derived equation(8), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Growth of 10 different bacteria strains were inhibited by acetylcysteine(9), suggesting that biodegradation is not an important environmental fate process in **water**(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (3) Serjeant EP, Dempsey B; Ionisation constants of organic acids in aqueous solution. IUPAC Chem Data Ser No.23. NY, NY: Pergamon pp. 989 (1979) (4) Osol A, ed; Remington's Pharmaceutical Sciences. 16th ed. Easton, PA: Mack Publishing Co., (1980) (5) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (6) Franke C et al; Chemosphere 29: 1501-14 (1994) (7) Meylan WM, Howard PH; J Pharm Sci 84: 83-92 (1995) (8) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (9) Olofsson AC et al; Appl Environ Microbiol 69: 4814-22 (2003)

▸ Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), acetylcysteine, which has an estimated vapor pressure of 1.1X10-5 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 acetylcysteine 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 7 hours(SRC), calculated from its rate constant of 5.5X10-11 cu cm/molec-sec at 25 °C(SRC) that was derived using a structure estimation method(3). Particulate-phase acetylcysteine may be removed from the air by wet and dry deposition(SRC). Acetycysteine does not absorb UV light at wavelengths >290 nm; therefore, acetylcysteine is not expected to be susceptible to photolysis(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

▸ Hazardous Substances Data Bank (HSDB)

13.2.4 Environmental Biodegradation

Growth of 10 different bacteria strains isolated from Swedish paper mills were inhibited by acetylcysteine at concentrations of 0.5 mg/mL(1). Also application of acetylcysteine decreased the production of extracellular polysaccarides in all of the bacteria at concentration of 0.25 mg/mL(1). This suggests that biodegradation is not an important environmental fate process.

PMID:12902275
Full text: ***https://www.ncbi.nlm.nih.gov/pmc/articles/PMC169071***
(1) Olofsson AC et al; Appl Environ Microbiol 69: 4814-22 (2003)

▸ Hazardous Substances Data Bank (HSDB)

13.2.5 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of acetylcysteine with photochemically-produced hydroxyl radicals has been estimated as 5.5X10-11 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 7 hours at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions(2). Acetycysteine does not absorb UV light at wavelengths >290 nm; therefore, acetylcysteine is not expected to be susceptible to photolysis(SRC).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5 (1990)

▸ Hazardous Substances Data Bank (HSDB)

13.2.6 Environmental Bioconcentration

An estimated BCF of 3.2 was calculated for acetylcysteine(SRC), using an estimated log Kow of -0.66(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) Meylan WM, Howard PH; J Pharm Sci 84: 83-92 (1995) (2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

▸ Hazardous Substances Data Bank (HSDB)

13.2.7 Soil Adsorption/Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc for acetylcysteine can be estimated to be 10(SRC). According to a classification scheme(2), this estimated Koc value suggests that acetylcysteine is expected to have very high mobility in soil. The pKa of acetylcysteine is 3.24(3), indicating that this compound will primarily exist as an anion in the environment anions generally do not adsorb more strongly to organic **carbon** and clay than their neutral counterparts(4).

(1) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) Osol A, ed; Remington's Pharmaceutical Sciences. 16th ed. Easton, PA: Mack Publishing Co., (1980) (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)

13.2.8 Volatilization from Water/Soil

The pKa of the carboxylic acid moiety of acetylcysteine is 3.24(1), indicating that this compound will primarily exist as an anion in the environment and will not volatilize from moist soil or **water** surfaces. Acetylcysteine is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 1.1X10-5 mm Hg(SRC), determined from a fragment constant method(2).

(1) Osol A, ed; Remington's Pharmaceutical Sciences. 16th ed. Easton, PA: Mack Publishing Co., (1980) (2) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985)

▸ Hazardous Substances Data Bank (HSDB)

13.2.9 Probable Routes of Human Exposure

Occupational exposure to acetylcysteine may occur through inhalation and dermal contact with this compound at workplaces where acetylcysteine is produced or used. Exposure to the drug among the general population may be limited to those administered the acetylcysteine (a mucolytic). (SRC)

▸ Hazardous Substances Data Bank (HSDB)

14 Associated Disorders and Diseases

- Comparative Toxicogenomics Database (CTD)

15 Literature

15.1 Coronavirus Studies

PubChem

15.2 NLM Curated PubMed Citations

PubChem

15.3 Springer Nature References

Springer Nature

15.4 Thieme References

Thieme Chemistry

15.5 Wiley References

Wiley

15.6 Depositor Provided PubMed Citations

PubChem

15.7 Synthesis References

Rolf-Dieter Juch, Gerd Birrenbach, Christian Pflugshaupt, "Solid, fast-soluble pharmaceutical preparation containing S-(carboxymethyl)-L-cysteine and/or N-acetylcysteine." U.S. Patent US5401514, issued November, 1990.

DrugBank

15.8 Metabolite References

Human Metabolome Database (HMDB)

15.9 General References

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15. Dailymed: Acetylcysteine Intravenous Injection, Solution
16. Health Canada Approved Drug Products: Acetylcysteine USP Solution for Intravenous Injection, Respiratory Inhalation, or Oral Administration
17. FDA Approved Drug Products: Cetylev (Acetylcysteine) Oral Effervescent Tablets for Solution
18. FDA Approved Drug Products: Mucomyst (Acetylcysteine) Oral and Respiratory Solution (Discontinued)

DrugBank

Yoshida et al. Nitric oxide activates TRP channels by cysteine S-nitrosylation Nature Chemical Biology, doi: 10.1038/nchembio821, published online 24 September 2006 http://www.nature.com/naturechemicalbiology

Nature Chemical Biology

Chang et al. Identification of small molecules rescuing fragile X syndrome phenotypes in Drosophila Nature Chemical Biology, doi: 10.1038/nchembio.78, published online 9 March 2008. http://www.nature.com/naturechemicalbiology

Nature Chemical Biology

15.10 Chemical Co-Occurrences in Literature

PubChem

15.11 Chemical-Gene Co-Occurrences in Literature

PubChem

15.12 Chemical-Disease Co-Occurrences in Literature

PubChem

16 Patents

US8399445
US8722738
US8653061
US8148356
US8747894
US9327028
US9427421
US9561204

DrugBank

16.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

16.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

PATENTSCOPE (WIPO)

16.3 FDA Orange Book Patents

Showing 3 of 8 View More

Patent	8148356
Expiration	May 21, 2026
Applicant	CUMBERLAND PHARMS
Drug Application	N021539 (Prescription Drug: ACETADOTE. Ingredients: ACETYLCYSTEINE)

FDA Orange Book

Patent	8399445
Expiration	Aug 24, 2025
Applicant	CUMBERLAND PHARMS
Drug Application	N021539 (Prescription Drug: ACETADOTE. Ingredients: ACETYLCYSTEINE)

FDA Orange Book

Patent	8653061
Expiration	Aug 24, 2025
Applicant	CUMBERLAND PHARMS
Drug Application	N021539 (Prescription Drug: ACETADOTE. Ingredients: ACETYLCYSTEINE)

FDA Orange Book

17 Interactions and Pathways

17.1 Protein Bound 3D Structures

- RCSB Protein Data Bank (RCSB PDB)

View 4 proteins in NCBI Structure

- PubChem

17.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code	SC2
PDBe Structure Code	2J1G
PDBe Conformer	

- Protein Data Bank in Europe (PDBe)

17.2 Drug-Drug Interactions

- DrugBank

17.3 Pathways

PubChem

18 Biological Test Results

18.1 BioAssay Results

PubChem

19 Taxonomy

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

- LOTUS - the natural products occurrence database

20 Classification

20.1 MeSH Tree

- Medical Subject Headings (MeSH)

20.2 NCI Thesaurus Tree

- NCI Thesaurus (NCIt)

20.3 ChEBI Ontology

- ChEBI

20.4 KEGG: Drug

KEGG

20.5 KEGG: USP

KEGG

20.6 KEGG: ATC

KEGG

20.7 KEGG: JP15

KEGG

20.8 WHO ATC Classification System

- WHO Anatomical Therapeutic Chemical (ATC) Classification

20.9 FDA Pharm Classes

- FDA Pharm Classes

20.10 ChemIDplus

- ChemIDplus

20.11 ChEMBL Target Tree

ChEMBL

20.12 UN GHS Classification

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

20.13 EPA CPDat Classification

EPA Chemical and Products Database (CPDat)

20.14 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

20.15 CCSBase Classification

- CCSbase

20.16 EPA DSSTox Classification

- EPA DSSTox

20.17 LOTUS Tree

- LOTUS - the natural products occurrence database

20.18 FDA Drug Type and Pharmacologic Classification

National Drug Code (NDC) Directory

21 Information Sources

FILTER BY SOURCE ALL SOURCES

1. **Burnham Center for Chemical Genomics**

   SID56423146
   https://pubchem.ncbi.nlm.nih.gov/bioassay/1996#section=Data-Table

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

   N-ACETYLCYSTEINE
   https://pubchem.ncbi.nlm.nih.gov/source/hsdb/3003

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

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   Acetylcysteine
   http://www.hmdb.ca/metabolites/HMDB0001890

   HMDB0001890_cms_29920
   https://hmdb.ca/metabolites/HMDB0001890#spectra

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   N-Acetyl-L-cysteine
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   Acetylcysteine [USAN:USP:INN:BAN:JAN]
   https://chem.nlm.nih.gov/chemidplus/sid/0000616911

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

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   Acetylcysteine
   https://www.drugbank.ca/drugs/DB06151

7. **EPA Chemicals under the TSCA**

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   L-Cysteine, N-acetyl-
   https://www.epa.gov/chemicals-under-tsca

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   N-Acetyl-L-cysteine
   https://comptox.epa.gov/dashboard/DTXSID5020021

   CompTox Chemicals Dashboard Chemical Lists
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   Acetylcysteine
   https://echa.europa.eu/substance-information/-/substanceinfo/100.009.545

   Acetylcysteine
   https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/17156

10. **CCSbase**

    N-ACETYLCYSTEINE

    CCSbase Classification
    https://ccsbase.net/

11. **NORMAN Suspect List Exchange**

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    N-Acetylcysteine

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

12. ## ChEBI

N-acetyl-L-cysteine
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:28939

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

13. ## FDA Pharm Classes

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ACETYLCYSTEINE
https://dailymed.nlm.nih.gov/dailymed/browse-drug-classes.cfm

FDA Pharmacological Classification
https://www.fda.gov/ForIndustry/DataStandards/StructuredProductLabeling/ucm162549.htm

14. ## LiverTox

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Acetylcysteine
https://www.ncbi.nlm.nih.gov/books/n/livertox/Acetylcysteine/

15. ## LOTUS - the natural products occurrence database

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https://lotus.nprod.net/

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

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NCI Thesaurus Tree
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20. ## DailyMed

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

22. ## Nature Chemical Biology

https://pubchem.ncbi.nlm.nih.gov/substance/14717147
https://pubchem.ncbi.nlm.nih.gov/substance/47213192

23. ## Drugs and Lactation Database (LactMed)

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Acetylcysteine
https://www.ncbi.nlm.nih.gov/books/NBK500931/

24. ## EPA Chemical and Products Database (CPDat)

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https://comptox.epa.gov/dashboard/DTXSID5020021#exposure

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

25. **EU Clinical Trials Register**
https://www.clinicaltrialsregister.eu/

26. **FDA Orange Book**

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Patent:8148356
https://www.fda.gov/drugs/drug-approvals-and-databases/approved-drug-products-therapeutic-equivalence-evaluations-orange-book

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

30. **NIST Mass Spectrometry Data Center**

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> https://www.nist.gov/srd/public-law

L-Cysteine, N-acetyl-
http://www.nist.gov/srd/nist1a.cfm

31. **SpectraBase**

Acetylcysteine
https://spectrabase.com/spectrum/EvlxlOPzYg4

Acetylcysteine
https://spectrabase.com/spectrum/KXQ5b2wwHhY

N-acetyl-L-cysteine
https://spectrabase.com/spectrum/6zBgnB26fFM

N-alpha-Acetyl-L-cysteine
https://spectrabase.com/spectrum/kkp1i8f1n2

N-acetyl-L-cysteine
https://spectrabase.com/spectrum/ImYGWeVGRHA

N-alpha-Acetyl-L-cysteine
https://spectrabase.com/spectrum/Vn8A1sBIag

N-acetyl-L-cysteine
https://spectrabase.com/spectrum/DTNw0cEAjXN

N-acetyl-L-cysteine
https://spectrabase.com/spectrum/KfOErclckoQ

N-acetyl-L-cysteine
https://spectrabase.com/spectrum/BMa1Mfv4Z5H

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

https://rxnav.nlm.nih.gov/id/rxnorm/197

33. **NMRShiftDB**
https://pubchem.ncbi.nlm.nih.gov/substance/594019

34. **WHO Anatomical Therapeutic Chemical (ATC) Classification**

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ATC Code
https://www.whocc.no/atc_ddd_index/

35. **Protein Data Bank in Europe (PDBe)**
http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/SC2

36. **PubChem**

https://pubchem.ncbi.nlm.nih.gov

37. ## RCSB Protein Data Bank (RCSB PDB)

https://www.rcsb.org/

38. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=10043227-554453248
https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=10043227-554429613

39. ## SpringerMaterials

L-Cysteine, N-acetyl-
https://materials.springer.com/substanceprofile/docs/smsid_qddbosuturvjfjpt

40. ## The Cambridge Structural Database

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=868554
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=868555
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=868556
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=868557
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=868558
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=939816
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=939817

41. ## Thieme Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=10043227-554429613
https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=10043227-554453248

42. ## WHO Model Lists of Essential Medicines

Acetylcysteine
https://list.essentialmeds.org/medicines/36

43. ## Wikidata

Acetylcysteine
https://www.wikidata.org/wiki/Q375613

44. ## Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=118579

45. ## Medical Subject Headings (MeSH)

Acetylcysteine
https://www.ncbi.nlm.nih.gov/mesh/68000111

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

Antiviral Agents
https://www.ncbi.nlm.nih.gov/mesh/68000998

Free Radical Scavengers
https://www.ncbi.nlm.nih.gov/mesh/68016166

Expectorants
https://www.ncbi.nlm.nih.gov/mesh/68005100

46. ## KEGG

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

USP drug classification
http://www.genome.jp/kegg-bin/get_htext?br08302.keg

Anatomical Therapeutic Chemical (ATC) classification
http://www.genome.jp/kegg-bin/get_htext?br08303.keg

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

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

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

48. ## ChEMBL

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

49. **PATENTSCOPE (WIPO)**

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https://pubchem.ncbi.nlm.nih.gov/substance/403032911

50. **NCBI**

https://www.ncbi.nlm.nih.gov/projects/linkout