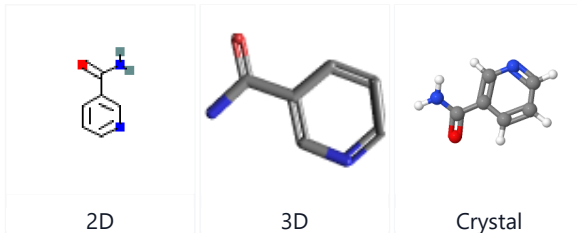


COMPOUND SUMMARY

Nicotinamide

PubChem CID

936

Structure**Chemical Safety**

Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)**Molecular Formula**C₆H₆N₂O**Synonyms**

nicotinamide
niacinamide
98-92-0
3-Pyridinecarboxamide
Nicotinic acid amide

[View More...](#)**Molecular Weight**

122.12 g/mol

*Computed by PubChem 2.1 (PubChem release 2021.05.07)***Dates**

Create: Modify:

2004-09-16 2023-08-12

Description

Nicotinamide is a white powder. (NTP, 1992)

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

► [CAMEO Chemicals](#)

Nicotinamide is a [pyridinecarboxamide](#) that is [pyridine](#) in which the [hydrogen](#) at position 3 is replaced by a carboxamide group. It has a role as an EC 2.4.2.30 ([NAD\(+\) ADP-ribosyltransferase](#)) inhibitor, a metabolite, a cofactor, an antioxidant, a neuroprotective agent, an EC 3.5.1.98 (histone deacetylase) inhibitor, an anti-inflammatory agent, a Sir2 inhibitor, a *Saccharomyces cerevisiae* metabolite, an *Escherichia coli* metabolite, a mouse metabolite, a human urinary metabolite and a geroprotector. It is a [vitamin B3](#), a [pyridinecarboxamide](#) and a pyridine alkaloid. It is functionally related to a [nicotinic acid](#).

► [ChEBI](#)

An important compound functioning as a component of the coenzyme [NAD](#). Its primary significance is in the prevention and/or cure of blacktongue and pellagra. Most animals cannot manufacture this compound in amounts sufficient to prevent nutritional deficiency and it therefore must be supplemented through dietary intake.

► [DrugBank](#)

[View More...](#)

Contents

Title and Summary

1 Structures



2 Names and Identifiers



3 Chemical and Physical Properties



4 Spectral Information



5 Related Records



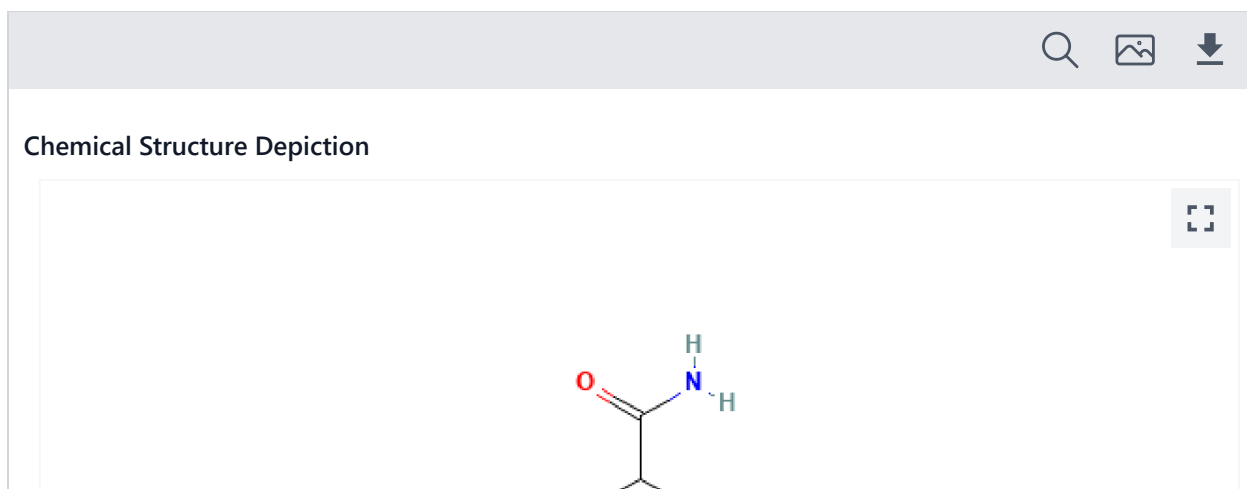
6 Chemical Vendors

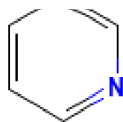
7 Drug and Medication Information	▼
8 Food Additives and Ingredients	▼
9 Pharmacology and Biochemistry	▼
10 Use and Manufacturing	▼
11 Identification	▼
12 Safety and Hazards	▼
13 Toxicity	▼
14 Associated Disorders and Diseases	
15 Literature	▼
16 Patents	▼
17 Interactions and Pathways	▼
18 Biological Test Results	▼
19 Taxonomy	
20 Classification	▼
21 Information Sources	

1 Structures



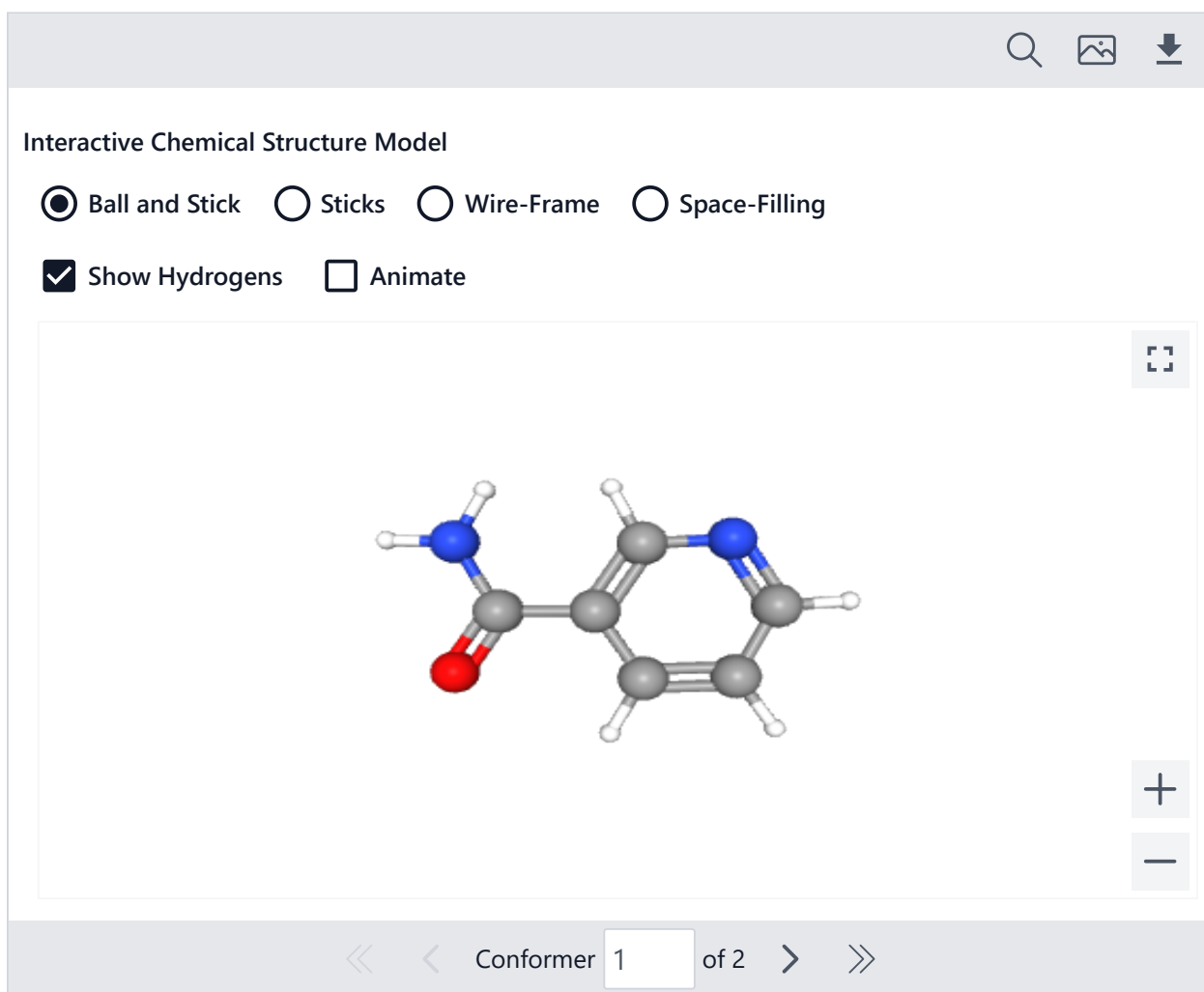
1.1 2D Structure





► PubChem

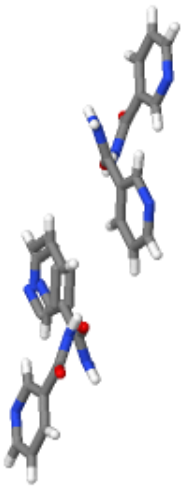
1.2 3D Conformer



► PubChem

1.3 Crystal Structures



1 of 7	View All 
CCDC Number	131756
Associated Article	DOI:10.1107/S0108768198007848
Crystal Structure Data	DOI:10.5517/cc4f36v
Crystal Structure Depiction	

► [The Cambridge Structural Database](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



pyridine-3-carboxamide

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

► [PubChem](#)

2.1.2 InChI



InChI=1S/C₆H₆N₂O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

► [PubChem](#)

2.1.3 InChIKey



DFPAKSUCGFBDDF-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

► [PubChem](#)

2.1.4 Canonical SMILES



C1=CC(=CN=C1)C(=O)N

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

► [PubChem](#)

2.2 Molecular Formula



C₆H₆N₂O

Computed by PubChem 2.1 (PubChem release 2021.05.07)

► [CAMEO Chemicals](#); [Wikipedia](#); [PubChem](#)

C₆H₆N₂O

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

2.3 Other Identifiers



2.3.1 CAS



98-92-0

► CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals un...

11032-50-1

► European Chemicals Agency (ECHA)

2.3.2 Deprecated CAS



123574-63-0, 37321-14-5, 78731-47-2

► ChemIDplus

123574-63-0, 78731-47-2

► EPA DSSTox

2.3.3 European Community (EC) Number



202-713-4

► European Chemicals Agency (ECHA)

234-265-0

► European Chemicals Agency (ECHA)

2.3.4 ICSC Number



1703

► ILO-WHO International Chemical Safety Cards (ICSCs)

2.3.5 NSC Number



759115

► DTP/NCI

27452

► DTP/NCI

13128

► DTP/NCI

2.3.6 UNII



25X51I8RD4

► FDA Global Substance Registration System (GSRS)

2.3.7 DSSTox Substance ID



DTXSID2020929

► EPA DSSTox

2.3.8 Nikkaji Number



J3.988H

► Japan Chemical Substance Dictionary (Nikkaji)

2.3.9 Wikipedia



Nicotinamide

► Wikipedia

2.3.10 Wikidata



Q192423

► Wikidata

2.3.11 NCI Thesaurus Code



C2327

► [NCI Thesaurus \(NCIt\)](#)

2.3.12 RXCUI



7405

► [NLM RxNorm Terminology](#)

2.3.13 Metabolomics Workbench ID



37778

► [Metabolomics Workbench](#)

2.3.14 ChEMBL ID



CHEMBL1140

► [ChEMBL](#)

2.4 Synonyms



2.4.1 MeSH Entry Terms



3 Pyridinecarboxamide	Vitamin B 3
3-Pyridinecarboxamide	Vitamin B3
B 3, Vitamin	Vitamin PP
B3, Vitamin	
Enduramide	
Jenapharm, Nicotinsäureamid	
Niacinamide	
Nicobion	
Nicotinamide	
Nicotinsäureamid Jenapharm	
Papulex	

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

2.4.2 Depositor-Supplied Synonyms



nicotinamide	Nicobion	Delonin amide	Nicamina	Niamide	Pyridine-3-carboxamide
niacinamide	Nicotylamide	Pelonin amide	Nicamindon	Nicasir	Vitamin B3
98-92-0	Nikotinamid	Vi-Nicotyl	Nicofort	Nicogen	Nicotinic acid amide
3-Pyridinecarboxamide	Savacotyl	Austrovit PP	Nicomidol	Nicota	pyridine-3-carboxamide
Nicotinic acid amide	Benicot	Inovitan PP	Nicotamide	Nicotol	vitamin PP
pyridine-3-carboxamide	Dipegyl	Nicosylamide	Nicovitina	Nicovit	Papulex
vitamin PP	Endobion	Nicotilamide	Nicovitol	Niko-tamin	Aminicotin
Papulex	Hansamid	Nicotililamido	Nicozymin	3-Carbamoylpyridine	Amixicotyn
Aminicotin	Pelmine	Amnicotin	Niocinamide	Nicotine acid amide	
Amixicotyn	Nicotinic amide	Niacevit	Niozymin	Nandervit-N	

► PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name Molecular Weight	Property Value 122.12 g/mol	Reference Computed by PubChem 2.1 (PubChem release 2021.05.07)
Property Name XLogP3	Property Value -0.4	Reference Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Property Name Hydrogen Bond Donor Count	Property Value 1	

Reference Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Property Name Hydrogen Bond Acceptor Count
Property Value 2
Reference Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Property Name Rotatable Bond Count
Property Value 1
Reference Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Property Name Exact Mass
Property Value 122.048012819 g/mol
Reference Computed by PubChem 2.1 (PubChem release 2021.05.07)
Property Name Monoisotopic Mass
Property Value 122.048012819 g/mol
Reference Computed by PubChem 2.1 (PubChem release 2021.05.07)
Property Name Topological Polar Surface Area
Property Value 56Å ²
Reference Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Property Name Heavy Atom Count
Property Value

9
Reference Computed by PubChem
Property Name Formal Charge
Property Value 0
Reference Computed by PubChem
Property Name Complexity
Property Value 114
Reference Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Property Name Isotope Atom Count
Property Value 0
Reference Computed by PubChem
Property Name Defined Atom Stereocenter Count
Property Value 0
Reference Computed by PubChem
Property Name Undefined Atom Stereocenter Count
Property Value 0
Reference Computed by PubChem
Property Name Defined Bond Stereocenter Count

Property Value 0
Reference Computed by PubChem
Property Name Undefined Bond Stereocenter Count
Property Value 0
Reference Computed by PubChem
Property Name Covalently-Bonded Unit Count
Property Value 1
Reference Computed by PubChem
Property Name Compound Is Canonicalized
Property Value Yes
Reference Computed by PubChem (release 2021.05.07)

► [PubChem](#)

3.2 Experimental Properties



3.2.1 Physical Description



Nicotinamide is a white powder. (NTP, 1992)

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

► [CAMEO Chemicals](#)

Dry Powder; Other Solid

► [EPA Chemicals under the TSCA](#)

Colorless needles or white crystalline powder. Bitter taste.

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

Solid

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

WHITE CRYSTALLINE POWDER.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

3.2.2 Color / Form



White, powder, needles from [benzene](#)

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-474

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

Colorless crystalline solid

Van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

White, crystalline powder

Chase et al; Remington's Pharmaceutical Sciences 14th ed. Mack Publ Co. Easton, PA p. 1039 (1970)

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

Colorless needles

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 966

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

3.2.3 Odor



Odorless

Osol, A. and J.E. Hoover, et al. (eds.). *Remington's Pharmaceutical Sciences*. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 950

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

3.2.4 Taste



Bitter taste

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; *Hawley's Condensed Chemical Dictionary 16th Edition*. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 966

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

3.2.5 Boiling Point



302 to 320 °F at 760 mmHg (NTP, 1992)

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

► [CAMEO Chemicals](#)

157°C at 5.00E-04 mm Hg

PhysProp

► [DrugBank](#)

BP: 157 °C at 5X10⁻⁴ atm

Haynes, W.M. (ed.). *CRC Handbook of Chemistry and Physics*. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-474

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

BP: 150-160 at 0.67 Pa. Sublimation range 80-100 °C

Van Arnum SD; *Niacin, Nicotinamide, and Nicotinic Acid*. *Kirk-Othmer Encyclopedia of Chemical Technology*. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

3.2.6 Melting Point



264 to 268 °F (NTP, 1992)

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

► [CAMEO Chemicals](#)

130°C

PhysProp

► [DrugBank](#)

128.8 °C

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-474

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

130 °C

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

127-131 °C

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

3.2.7 Flash Point



182 °C

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

3.2.8 Solubility



2.8 [ug/mL] (The mean of the results at pH 7.4)

► [Burnham Center for Chemical Genomics](#)

greater than or equal to 100 mg/mL at 70 °F (NTP, 1992)

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

► [CAMEO Chemicals](#)

500000mg/L (at 25 °C)

MERCK INDEX (1996)

► [DrugBank](#)

In [water](#), 5X10+5 mg/L at 25 °C

Budavari, S. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1114

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

Very soluble in [water](#); 1 g is soluble in 1 mL [water](#)

Van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. *Kirk-Othmer Encyclopedia of Chemical Technology*. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

1 g dissolves in about 1 mL [water](#), in 10 mL [glycerol](#), in about 1.5 mL alcohol

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1214

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

Soluble in [butanol](#), [chloroform](#)

Furia, T.E. (ed.). *CRC Handbook of Food Additives*. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 89

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

For more Solubility (Complete) data for Nicotinamide (6 total), please visit the [HSDB record page](#).

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

500 mg/mL at 25 °C

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

Solubility in [water](#), g/100ml at 20 °C: 100 (very good)

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

3.2.9 Density



1.4 (NTP, 1992)

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

► CAMEO Chemicals

1.400 g/cu cm at 25 °C

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-474

► Hazardous Substances Data Bank (HSDB)

Specific heat = solid, 55 °C: 1.30 kJ/kg; heat of solution in **water**: -148 kJ/kg; heat of fusion: 381 kJ/kg; density of melt, at 150 °C: 1.19 g/cu cm

Van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

► Hazardous Substances Data Bank (HSDB)

1.4 g/cm³

► ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.10 Vapor Density



Relative vapor density (air = 1): 4.2

► ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.11 Vapor Pressure



4.2X10⁻⁴ mm Hg at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools>

► Hazardous Substances Data Bank (HSDB)

Vapor pressure, kPa at 35 °C: 3.1

► ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.12 LogP



-0.37

HANSCH, C ET AL. (1995)

► [DrugBank](#)

log Kow = -0.37

Hansch, C., Leo, A., D. Hoekman. *Exploring QSAR - Hydrophobic, Electronic, and Steric Constants*. Washington, DC: American Chemical Society, 1995., p. 19

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

-0.37

HANSCH, C ET AL. (1995)

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

-0.38

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

3.2.13 LogS



0.61

ADME Research, USCD

► [DrugBank](#)

3.2.14 Henry's Law Constant



Henry's Law constant = 2.90X10⁻¹² atm-cu m/mol at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsc-screening-tools>

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

3.2.15 Stability / Shelf Life



Stable under recommended storage conditions.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

... Nicotinamide is incompatible with alkalis and strong acids.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

3.2.16 Autoignition Temperature



480 °C

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

3.2.17 Decomposition



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

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2623

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

3.2.18 pH



10% "wt in vol" solution in [water](#) is neutral to litmus

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1213

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

3.2.19 Ionization Efficiency



Ionization mode Positive
logIE 2.6
pH 2.7

Instrument Agilent XCT
Ion source Electrospray ionization
Additive formic acid (5.3nM)
Organic modifier MeCN (80%)
Reference DOI: 10.1038/s41598-020-62573-z

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

3.2.20 Refractive Index



Index of refraction: 1.466 at 25 °C/D

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-474

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

Max absorption (alcohol): 255 nm (log e = 3.4); 262.5 nm (log e = 3.4); Index of refraction: 1.466; Sadtler reference number: 860 (IR, prism); 8106 (IR, grating)

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, FL: CRC Press Inc., 1994-1995., p. 3-298

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

3.2.21 Dissociation Constants



pKa

3.35 (at 20 °C)

PERRIN,DD (1965)

► [DrugBank](#)

pKa = 3.35 (conjugate acid)

Perrin DD; *Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chemical Data Series, Butterworth: London (1965)*

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

kb1 = 2.24X10⁻¹¹; kb2 = 3.16X10⁻¹⁴

Van Arnum SD; *Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000*

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

3.2.22 Collision Cross Section



125.3 Å² [M+H]⁺ [CCS Type: DT, Method: single field calibrated with Agilent tune mix (Agilent)]

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

► [CCSbase](#)

129.32 Å² [M+H]⁺ [CCS Type: DT, Method: stepped-field]

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

► [CCSbase](#)

137.3 Å² [M+Na]⁺ [CCS Type: DT, Method: stepped-field]

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

► [CCSbase](#)

118 Å² [M+H]⁺ [CCS Type: TW, Method: calibrated with polyalanine]

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

► [CCSbase](#)

125.3 Å² [M+H]⁺ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

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

► [CCSbase](#)

121.7 Å² [M+H]⁺ [CCS Type: TW, Method: calibrated with polyalanine and drug standards]

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.7b01709>

► [CCSbase](#)

125.2 Å² [M+H]⁺ [CCS Type: DT, Method: single field calibrated]

<https://pubs.rsc.org/en/content/articlelanding/2018/ay/c7ay02808c>

► [CCSbase](#)

136.4 Å² [M+Na]⁺

126.7 Å² [M+H]⁺

S50 | CCSCOMPEND | *The Unified Collision Cross Section (CCS) Compendium* |
[DOI:10.5281/zenodo.2658162](https://doi.org/10.5281/zenodo.2658162)

► [NORMAN Suspect List Exchange](#)

3.2.23 Kovats Retention Index



Semi-standard non-polar
1426

► [NIST Mass Spectrometry Data Center](#)

3.2.24 Other Experimental Properties



Readily hydrolyzed to free acid by heating in acid or alkaline solution

Osol, A. and J.E. Hoover, et al. (eds.). *Remington's Pharmaceutical Sciences*. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 950

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

Forms crystalline salts with acids

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1213

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

Hydroxyl radical reaction rate constant = 2.34X10⁻¹² cu cm/molec sec at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018:
<https://www2.epa.gov/tsca-screening-tools>

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

3.2.25 Chemical Classes



Biological Agents -> Vitamins and Derivatives

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

3.3 SpringerMaterials Properties



Schoenflies notation	Magnetic susceptibility	Unit cell parameter
Boiling point	Melting temperature	Vapor pressure
Chemical bond	Molecular structure	
Crystal structure	Nuclear quadrupole resonance spectroscopy	
Density	Phase transition	
Diamagnetic susceptibility	Point group	
Electric dipole moment	Quadrupole coupling	
Formula unit	Rotational excitation cross section	
Fusion temperature	Space group	
Heat of sublimation	Transition enthalpy	
Internuclear distance	Unit cell	

► [SpringerMaterials](#)

4 Spectral Information



4.1 1D NMR Spectra



1 of 2

1D NMR Spectra

¹H NMR: 453 (Varian Associates NMR Spectra Catalogue)

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

2 of 2

1D NMR Spectra

[NMRShiftDB Link](#)

► [NMRShiftDB](#)

4.1.1 ¹H NMR Spectra

1 of 5

View All

Spectra ID

1700

Instrument Type

Varian

Frequency

600 MHz

Solvent

Water

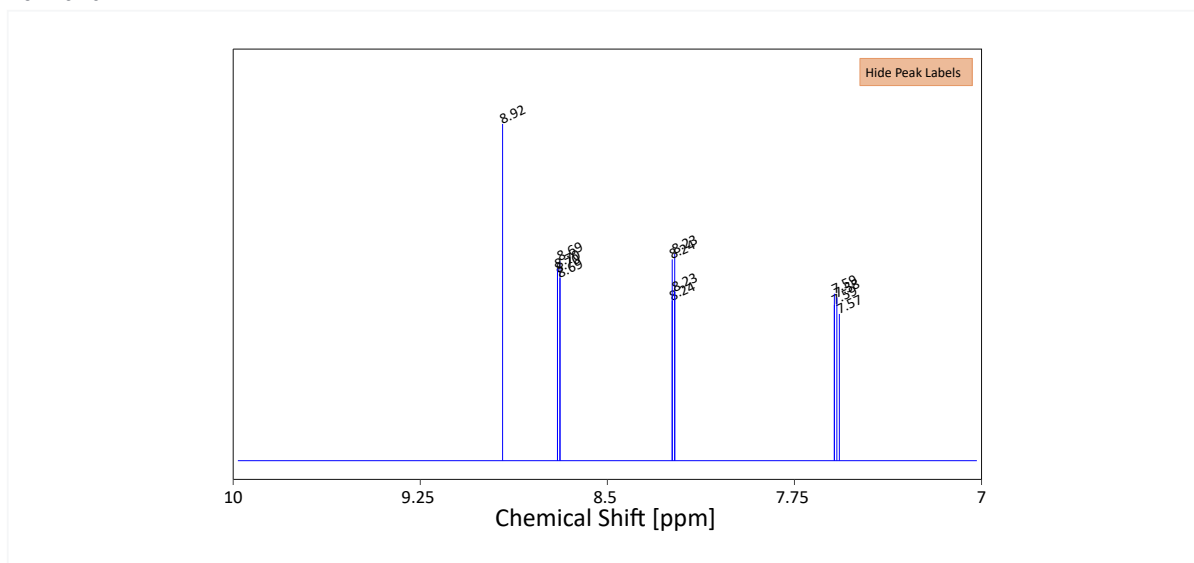
pH

7.00

Shifts [ppm]:Intensity

8.69:59.23, 8.24:47.53, 7.59:46.28, 8.23:61.52, 8.92:100.00, 8.69:54.22, 7.57:43.57, 8.24:59.80, 8.70:55.72, 7.58:48.45, 7.59:49.58, 8.70:57.06, 8.23:50.08

Thumbnail

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

2 of 5

View All

Spectra ID

2742

Instrument Type

JEOL

Frequency

400 MHz

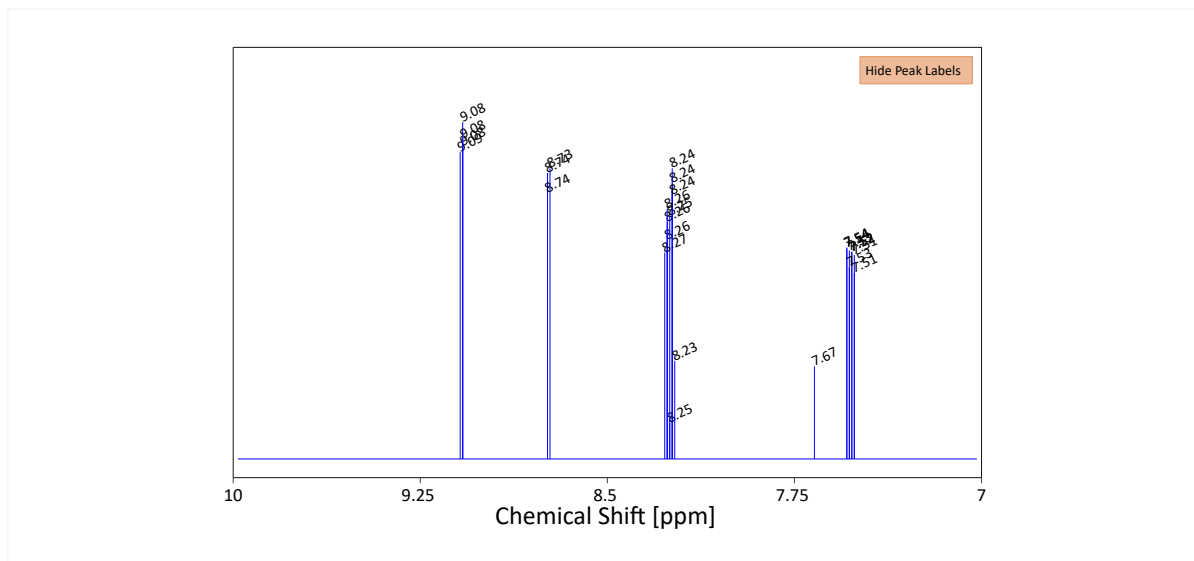
Solvent

DMSO-d₆

Shifts [ppm]:Intensity

7.52:616.00, 7.67:275.00, 8.24:820.00, 8.25:107.00, 7.53:619.00, 8.74:849.00, 8.26:649.00, 8.74:791.00, 8.26:704.00, 7.54:625.00, 7.54:628.00, 8.73:863.00, 7.52:614.00, 8.24:863.00, 8.25:722.00, 7.51:552.00, 9.08:929.00, 8.27:613.00, 9.09:911.00, 8.24:785.00, 9.08:1000.00, 8.23:291.00, 7.51:606.00, 9.08:951.00, 7.53:569.00, 8.26:742.00

Thumbnail



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

4.1.2 ¹³C NMR Spectra

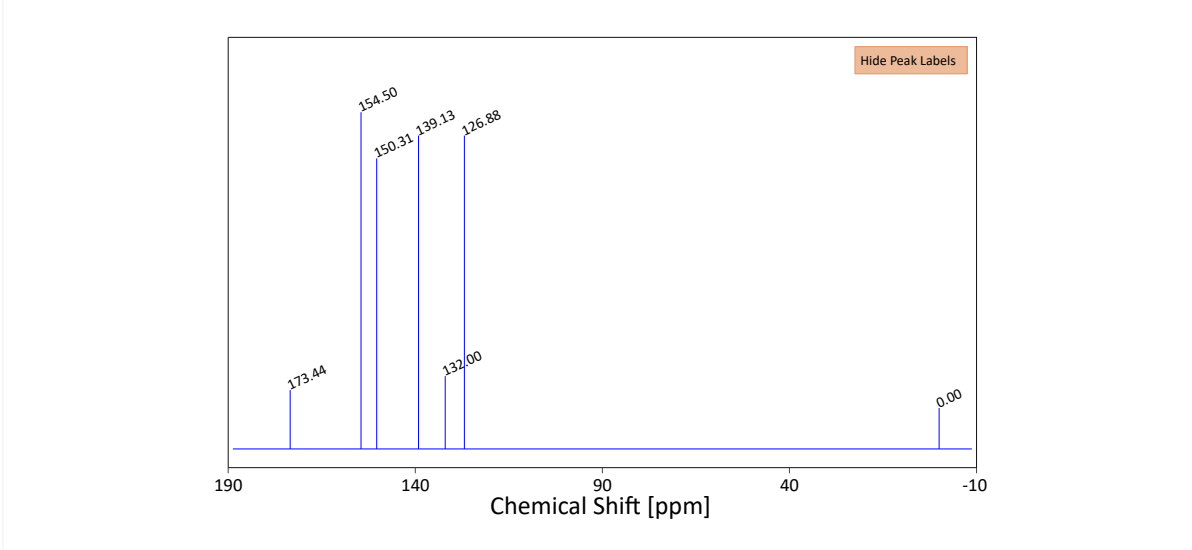
1 of 7

View All

¹³C NMR Spectra

¹³C NMR: 259 (Johnson and Jankowski, [Carbon-13 NMR for Organic Chemists](#), John Wiley & Sons, New York)

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

2 of 7		View All 
Spectra ID 1299		
Instrument Type Bruker		
Frequency 125 MHz		
Solvent Water		
pH 7.00		
Shifts [ppm]:Intensity 173.44:3.32, 139.13:17.68, 150.31:16.39, 154.50:19.00, 132.00:4.11, 126.88:17.68, 0.00:2.31		
Thumbnail 		

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

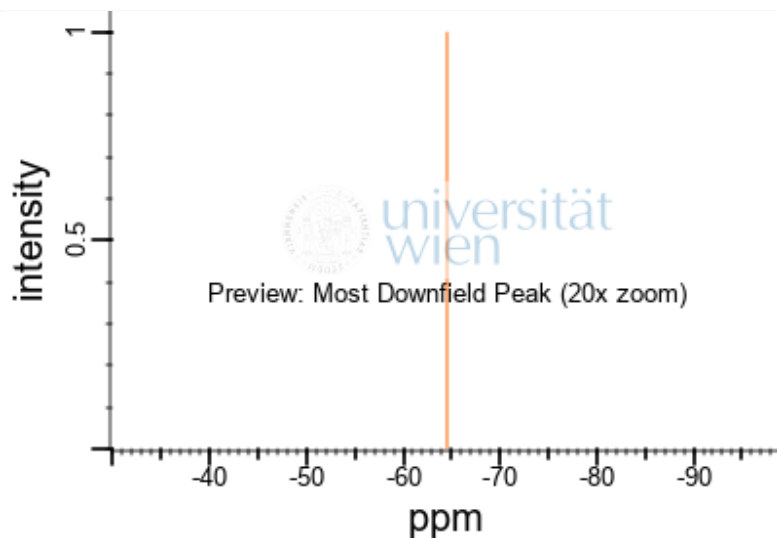
4.1.3 ¹⁵N NMR Spectra



1 of 2

Copyright

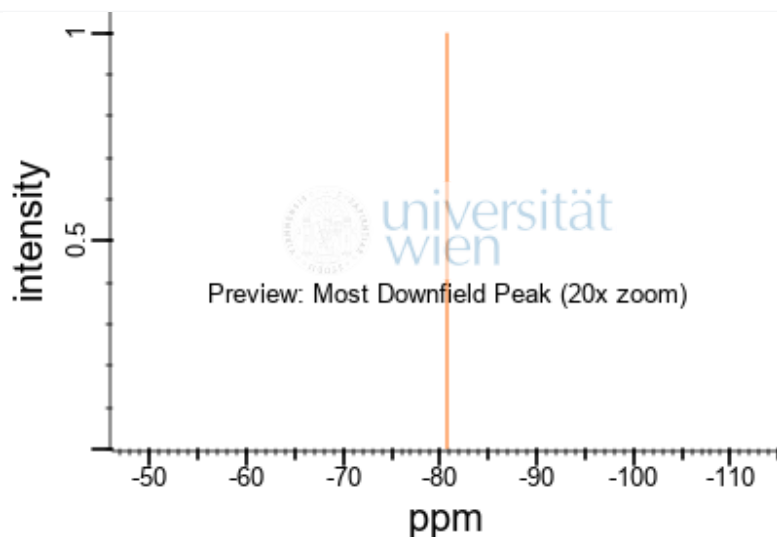
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Thumbnail[► SpectraBase](#)

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Thumbnail

► SpectraBase

4.2 2D NMR Spectra



4.2.1 ¹H-¹H NMR Spectra



2D NMR Spectra Type

1H-1H TOCSY

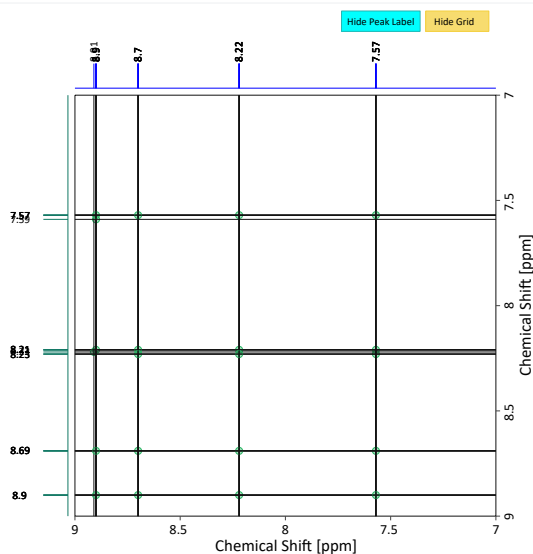
Spectra ID

1068

Shifts [ppm] (F2:F1)

7.57:8.23, 8.90:8.21, 7.57:8.21, 8.70:8.69, 8.22:8.21, 8.22:8.90, 8.90:7.59, 8.22:7.57, 8.70:8.90, 8.91:8.22, 8.90:8.90, 7.57:8.69, 8.90:7.57, 7.57:7.57, 7.57:8.90, 8.70:8.21, 8.22:8.69, 8.70:7.57, 8.70:8.23, 8.90:8.69, 8.22:8.23

Thumbnail



► Human Metabolome Database (HMDB)

4.2.2 ^1H - ^{13}C NMR Spectra



2D NMR Spectra Type

1H-13C HSQC

Spectra ID

1641

Instrument Type

Bruker

Frequency

600 MHz

Solvent

Water

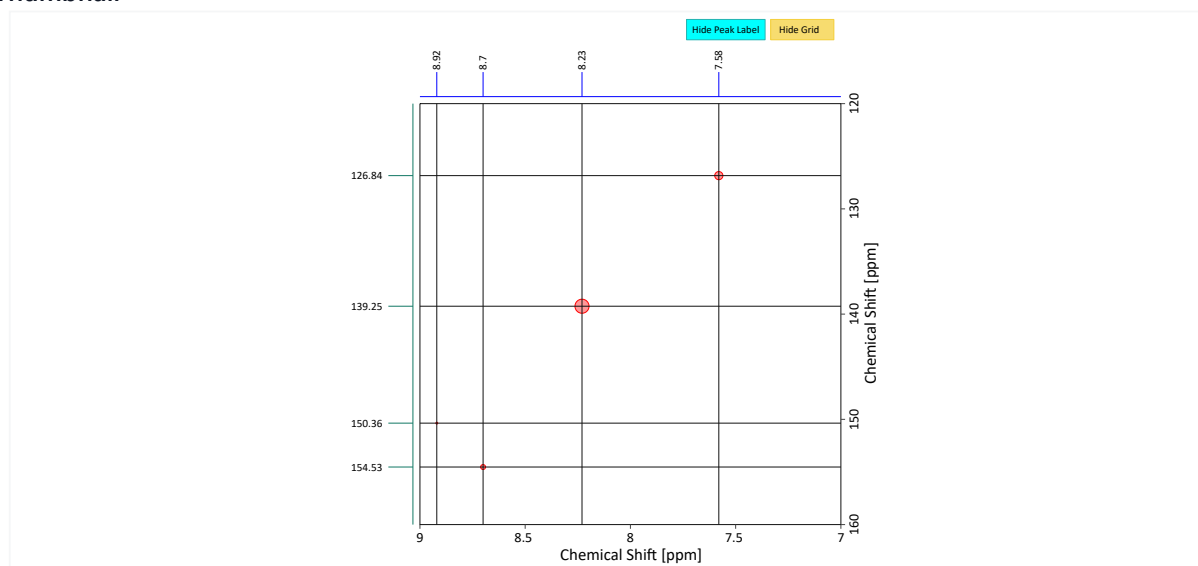
pH

7.00

Shifts [ppm] (F2:F1):Intensity

7.58:126.84:0.58, 8.92:150.36:0.13, 8.23:139.25:1.00, 8.70:154.53:0.35

Thumbnail

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

4.3 Mass Spectrometry



4.3.1 GC-MS



1 of 20

[View All](#)

Spectra ID

1161

Instrument Type

GC-MS

SPLASH

[splash10-0udi-2910000000-d760b65bb76d6464038e](#)

Top 5 Peaks

151.0 1

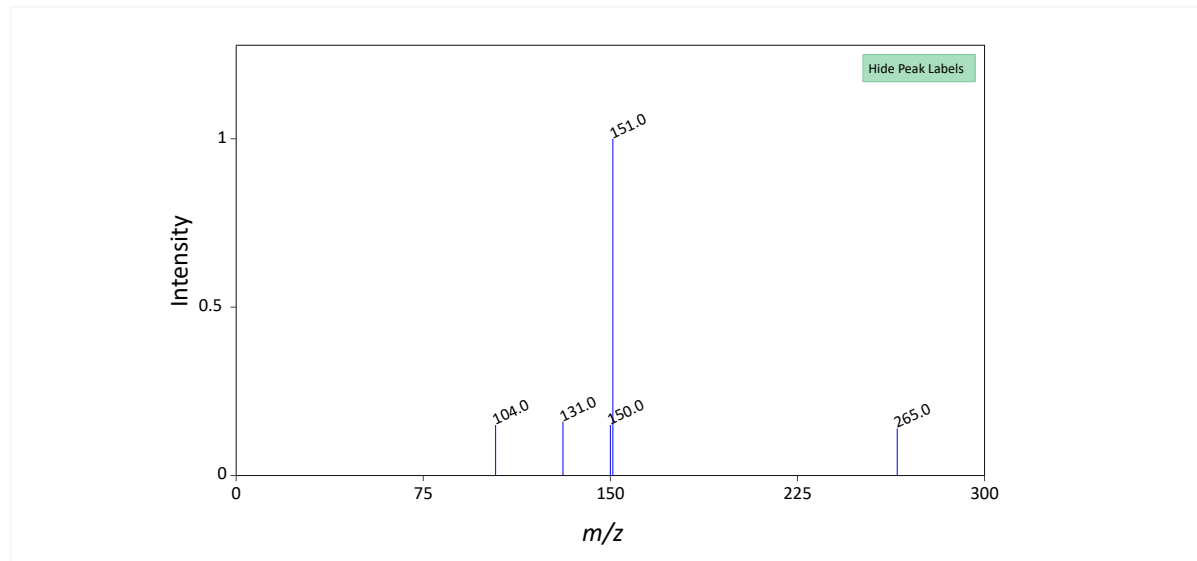
131.0 0.16

104.0 0.15

150.0 0.15

265.0 0.14

Thumbnail

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

2 of 20

[View All](#)

Spectra ID

1185

Instrument Type

GC-MS

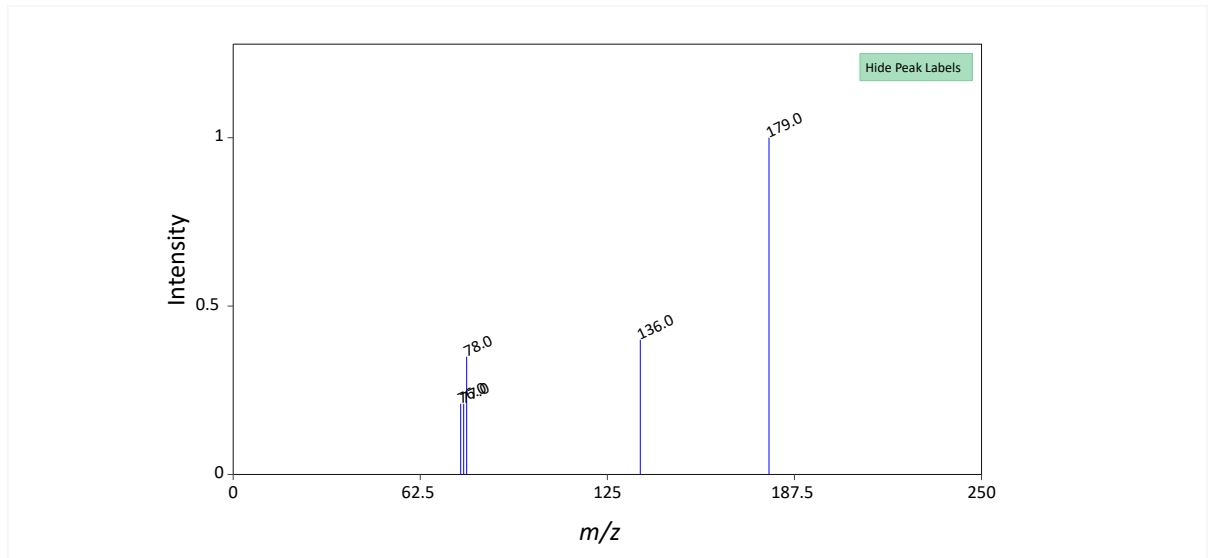
SPLASH

[splash10-004i-4900000000-47c6f72d1bb5465c1376](#)

Top 5 Peaks

179.0 1
136.0 0.40
78.0 0.35
77.0 0.21
76.0 0.21

Thumbnail



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

4.3.2 MS-MS



1 of 7

[View All](#)

Spectra ID

1559

Instrument Type

Quattro_QQQ

Ionization Mode

Positive

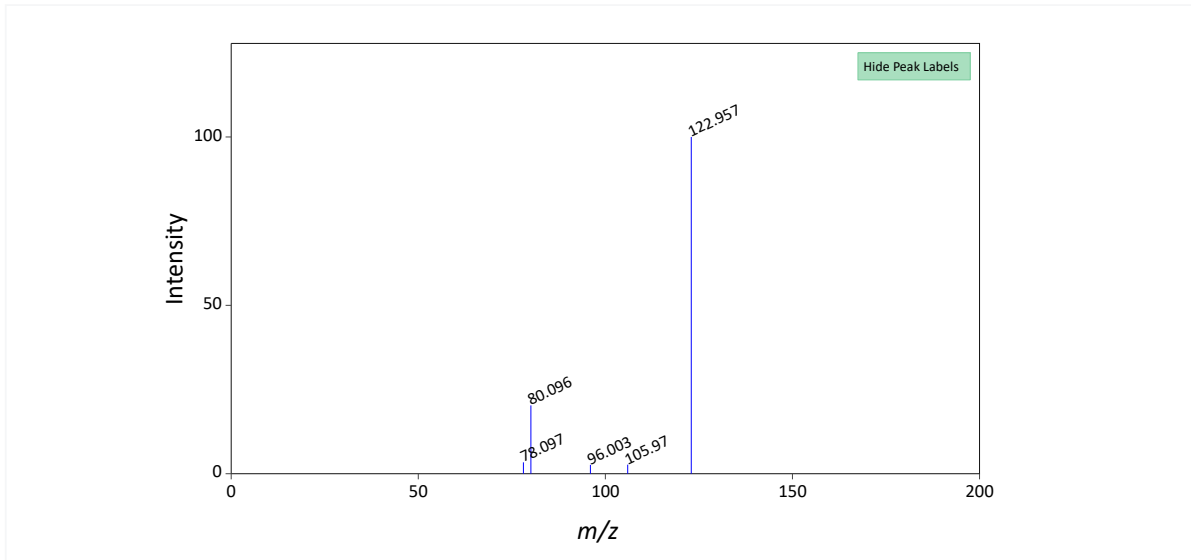
SPLASH

[splash10-00di-2900000000-72a7c92eb2667f5b6c3f](#)

Top 5 Peaks

122.957 100
80.096 20.29
78.097 3.38
105.97 2.70
96.003 2.62

Thumbnail



Notes

delivery=Flow_Injectionanalyzer=Triple_Quad

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

2 of 7

[View All](#) ↗

Spectra ID
[1560](#)

Instrument Type
Quattro_QQQ

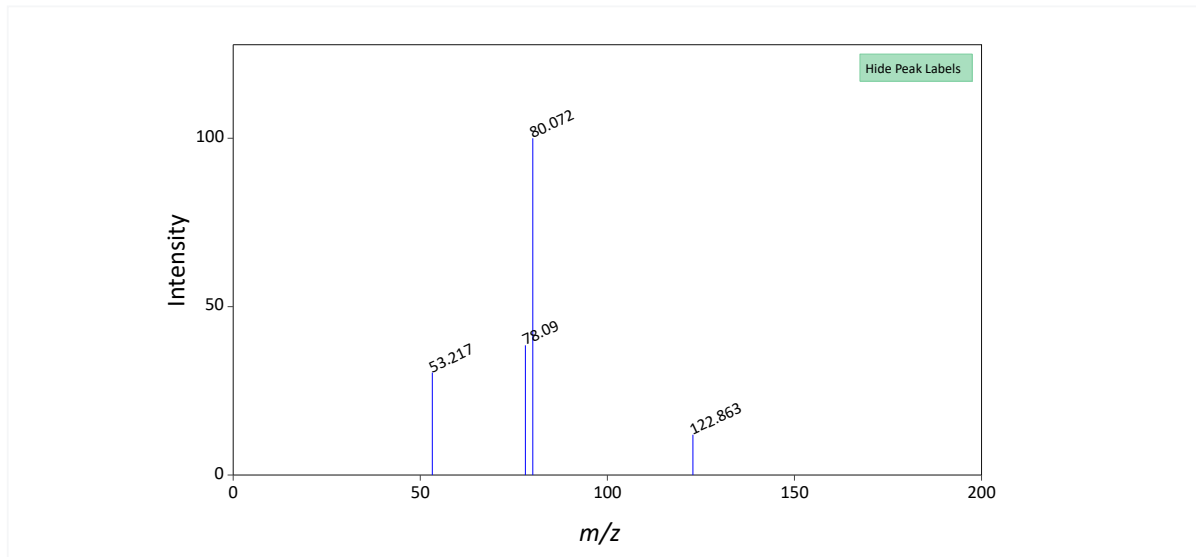
Ionization Mode
Positive

SPLASH
[splash10-001i-9000000000-6486d230a4a2fd4bab0e](#)

Top 5 Peaks
80.072 100
78.09 38.51

53.217 30.43
122.863 11.96

Thumbnail



Notes

delivery=Flow_Injectionanalyzer=Triple_Quad

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

4.3.3 LC-MS



1 of 39

[View All](#)

Accession ID

[MSBNK-BGC_Munich-RP022301](#)

Authors

BGC, Helmholtz Zentrum Muenchen

Instrument

maXis plus UHR-ToF-MS, Bruker Daltonics

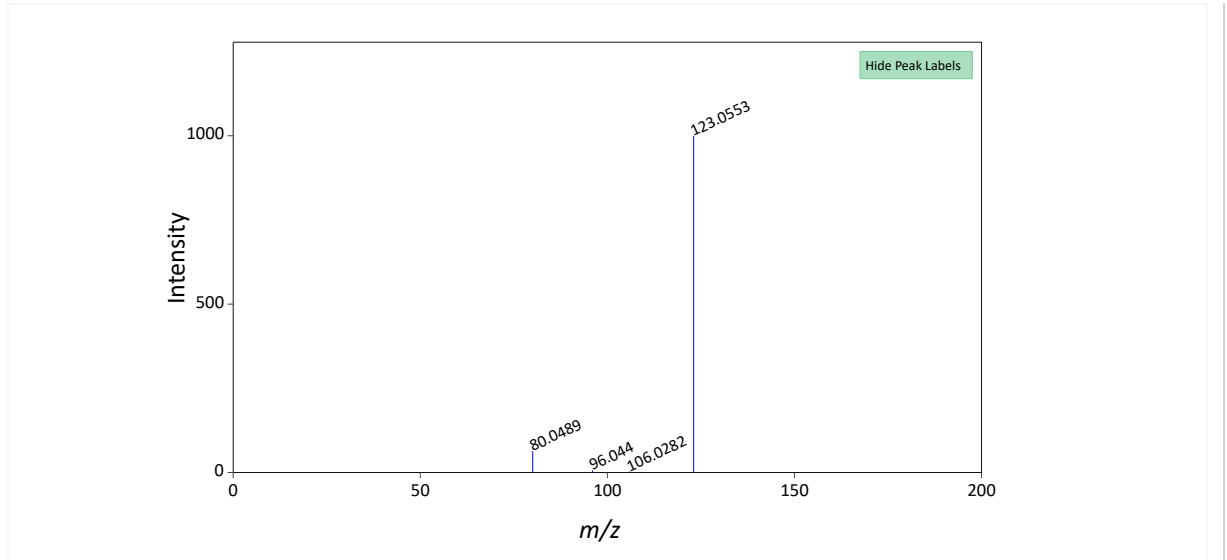
Instrument Type

LC-ESI-QTOF

MS Level

MS2

Ionization Mode POSITIVE
Ionization ESI
Collision Energy 10
Fragmentation Mode CID
Column Name BEH C18 1.7um, 2.1x100mm, Waters
Retention Time 0.698 min
Precursor m/z 123.0553
Precursor Adduct [M+H] ⁺
Top 5 Peaks 123.0553 999 80.0489 63 96.044 6 106.0282 3
SPLASH splash10-00di-0900000000-4b443e8203890ad60aa1
Thumbnail

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2 of 39

[View All](#) **Accession ID**[MSBNK-BGC_Munich-RP022302](#)**Authors**

BGC, Helmholtz Zentrum Muenchen

Instrument

maXis plus UHR-ToF-MS, Bruker Daltonics

Instrument Type

LC-ESI-QTOF

MS Level

MS2

Ionization Mode

POSITIVE

Ionization

ESI

Collision Energy

20

Fragmentation Mode

CID

Column Name

BEH C18 1.7um, 2.1x100mm, Waters

Retention Time

0.698 min

Precursor m/z

123.0553

Precursor Adduct[M+H]⁺**Top 5 Peaks**

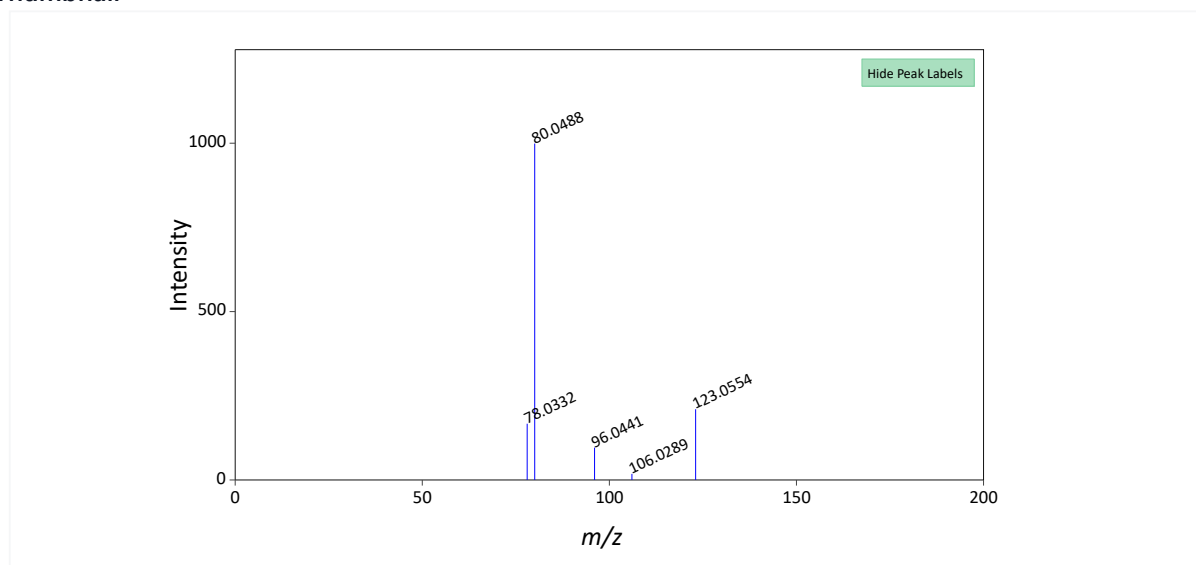
80.0488 999

123.0554 210

78.0332 167

96.0441 96

106.0289 18

SPLASH[splash10-001i-9100000000-321a9a908665a25ffdf9](#)**Thumbnail****License**

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[► MassBank Europe](#)

4.3.4 Other MS



1 of 7

View All

Other MSMASS: 2279 (NIST/EPA/[MSDC](#) Mass Spectral database, 1990 version)[► Hazardous Substances Data Bank \(HSDB\)](#)

2 of 7

View All

Accession ID[MSBNK-Fac_Eng_Univ_Tokyo-JP005706](#)**Authors**

MASS SPECTROSCOPY SOC. OF JAPAN (MSSJ)

Instrument

HITACHI M-80

Instrument Type

EI-B

MS Level

MS

Ionization Mode

POSITIVE

Ionization

ENERGY 70 eV

Top 5 Peaks

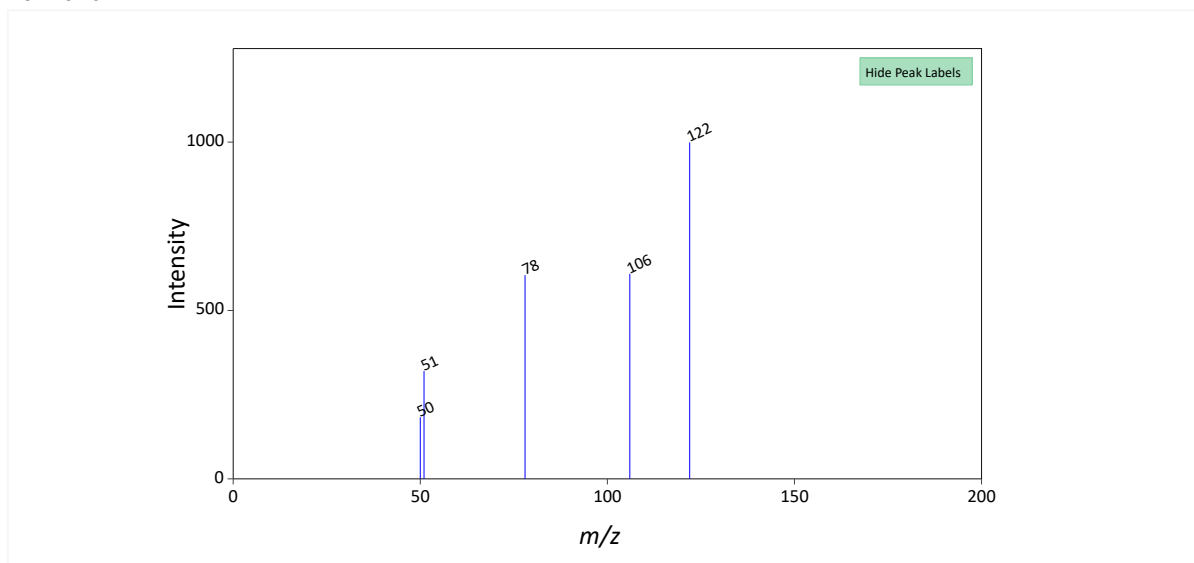
122 999

106 609

78 605

51 320

50 183

SPLASH[splash10-0kor-9800000000-1809e537780b814af0c9](#)**Thumbnail****License**

CC BY-NC-SA

[► MassBank Europe](#)

4.4 UV Spectra



UV: 261 (Sadtlar Research Laboratories Spectral Collection)

lide, D.R., G.W.A. Milne (eds.). *Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V5: 4683*

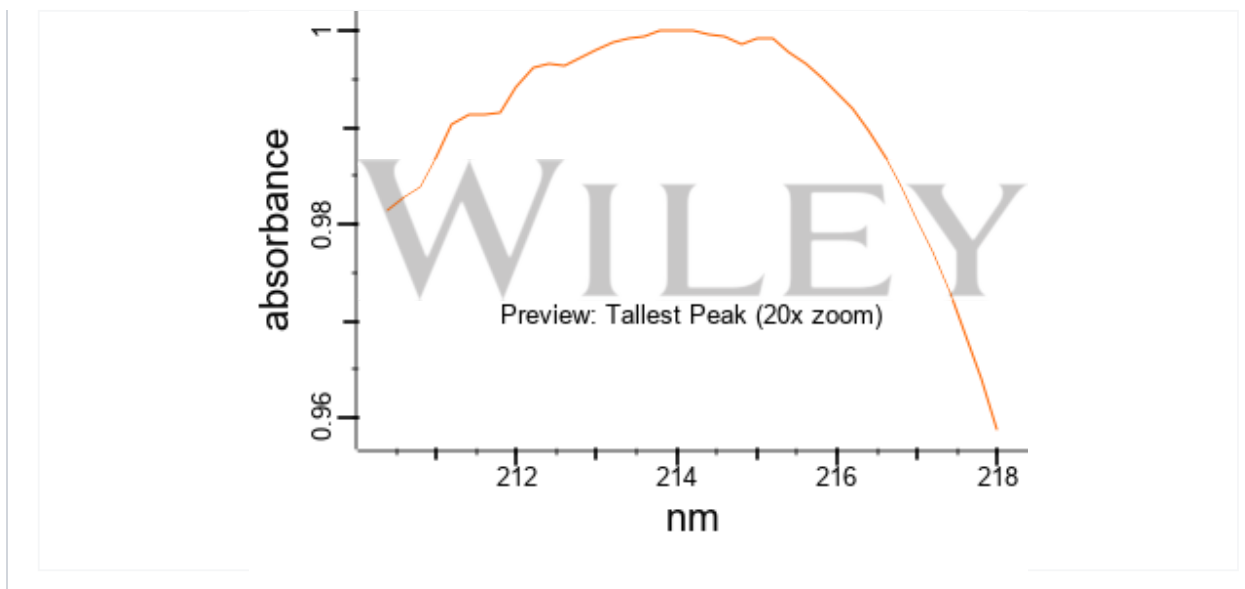
[► Hazardous Substances Data Bank \(HSDB\)](#)

4.4.1 UV-VIS Spectra

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4.5 IR Spectra



IR Spectra

IR: 5080 (Coblentz Society Spectral Collection)

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

4.5.1 FTIR Spectra



1 of 2

Instrument Name

Bio-Rad FTS

Technique

KBr0

Source of Spectrum

Forensic Spectral Research

Source of Sample

Supelco, Sigma-Aldrich Company LLC

Catalog Number

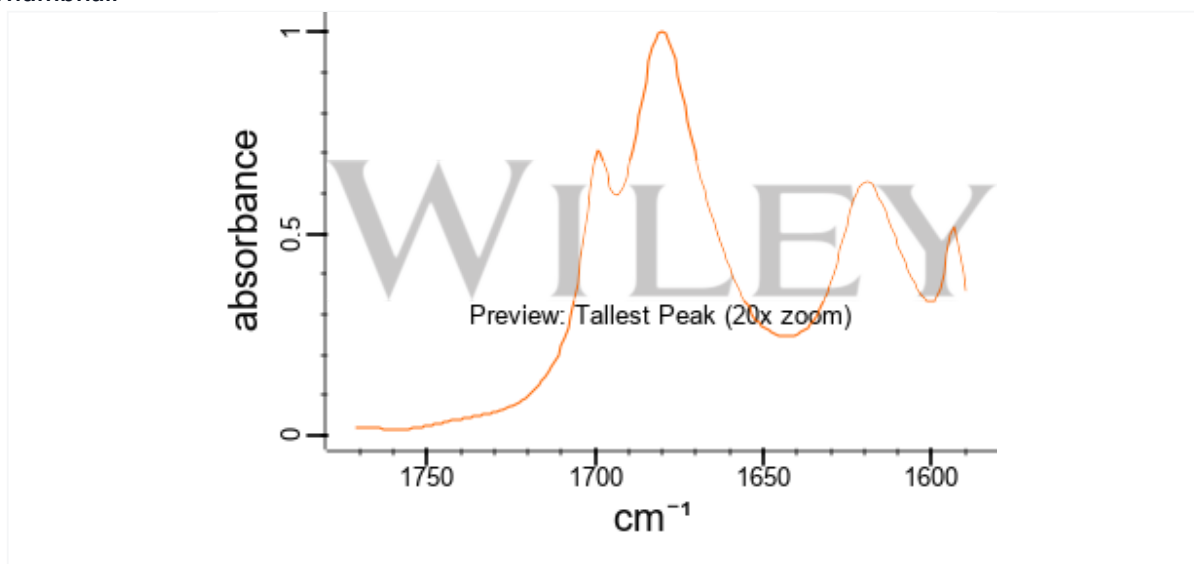
47865-U

Lot Number

LB60593

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2 of 2

Instrument Name

Bruker IFS 85

Technique

KBr-Pellet

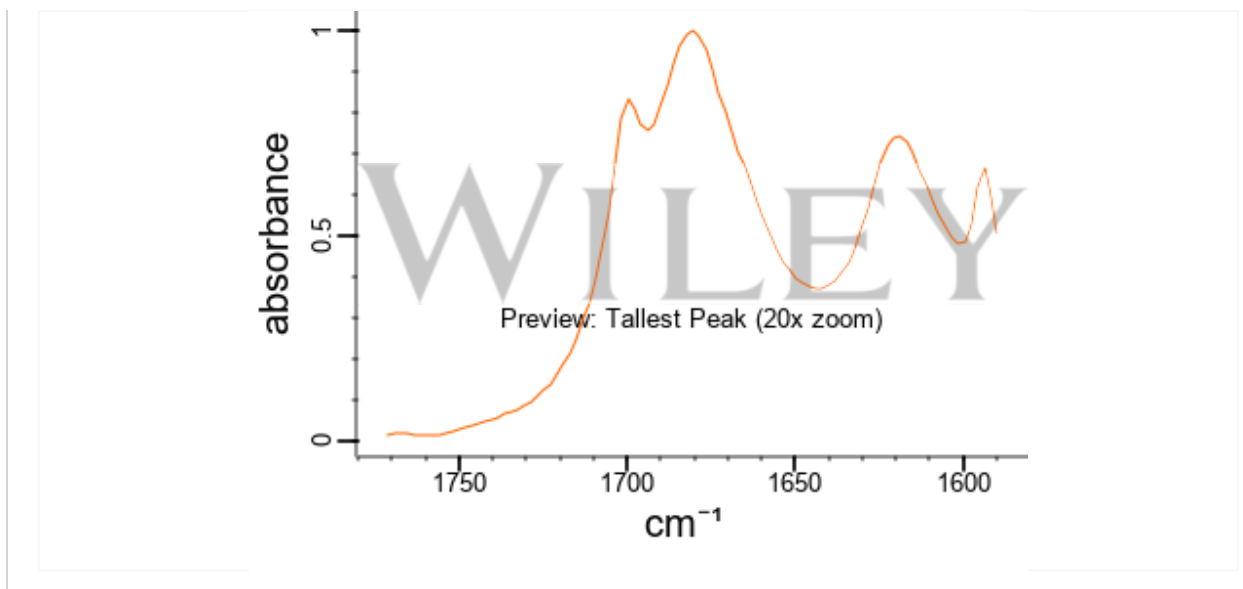
Source of Sample

E. Merck AG, Darmstadt

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► SpectraBase

4.5.2 ATR-IR Spectra



1 of 2

Instrument Name

Bio-Rad FTS

Technique

ATR-Neat (DuraSamplIR II) ground

Source of Spectrum

Forensic Spectral Research

Source of Sample

Supelco, Sigma-Aldrich Inc.

Catalog Number

47865-U

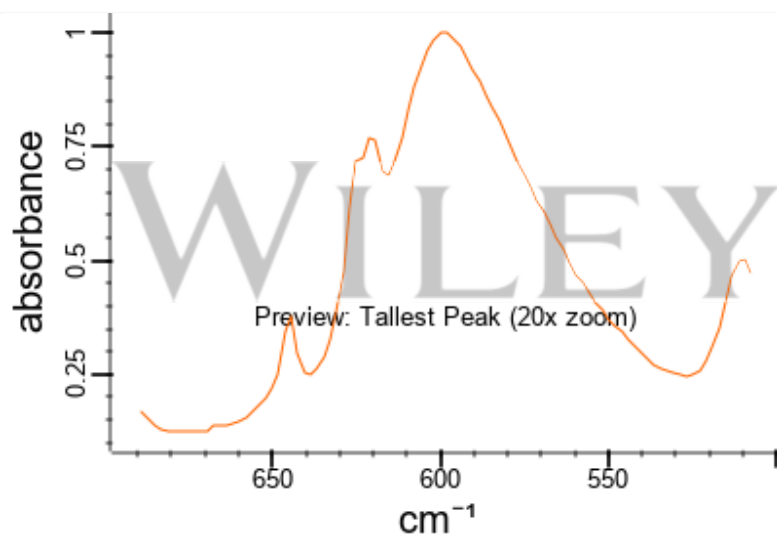
Lot Number

LB60593

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► SpectraBase

2 of 2

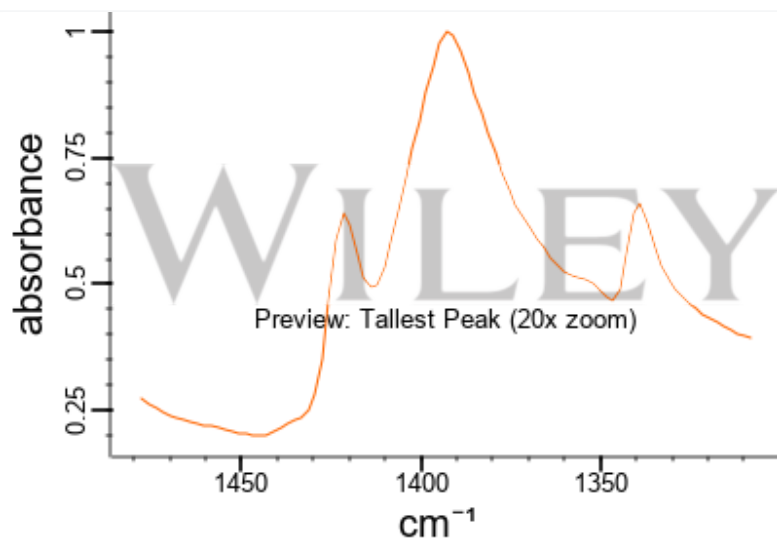
Source of Sample
Aldrich

Catalog Number
240206

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[► SpectraBase](#)

4.5.3 Vapor Phase IR Spectra

**Instrument Name**

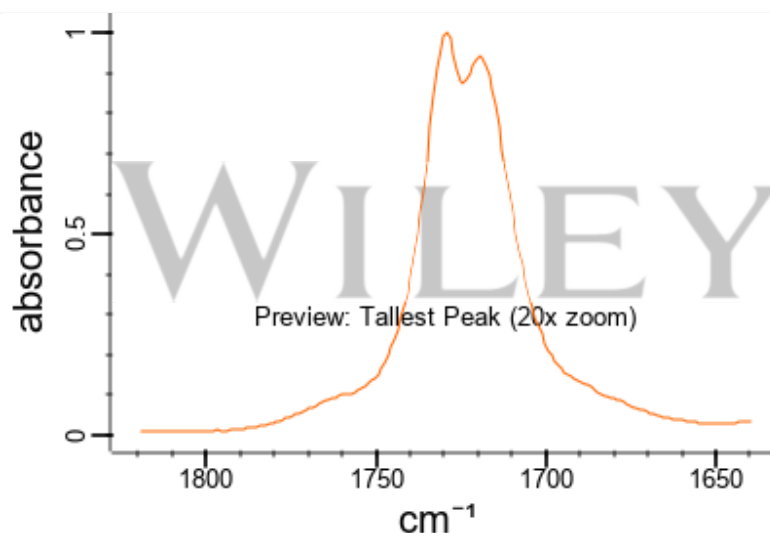
DIGILAB FTS-14

Technique

Vapor Phase

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Thumbnail[► SpectraBase](#)

4.6 Raman Spectra

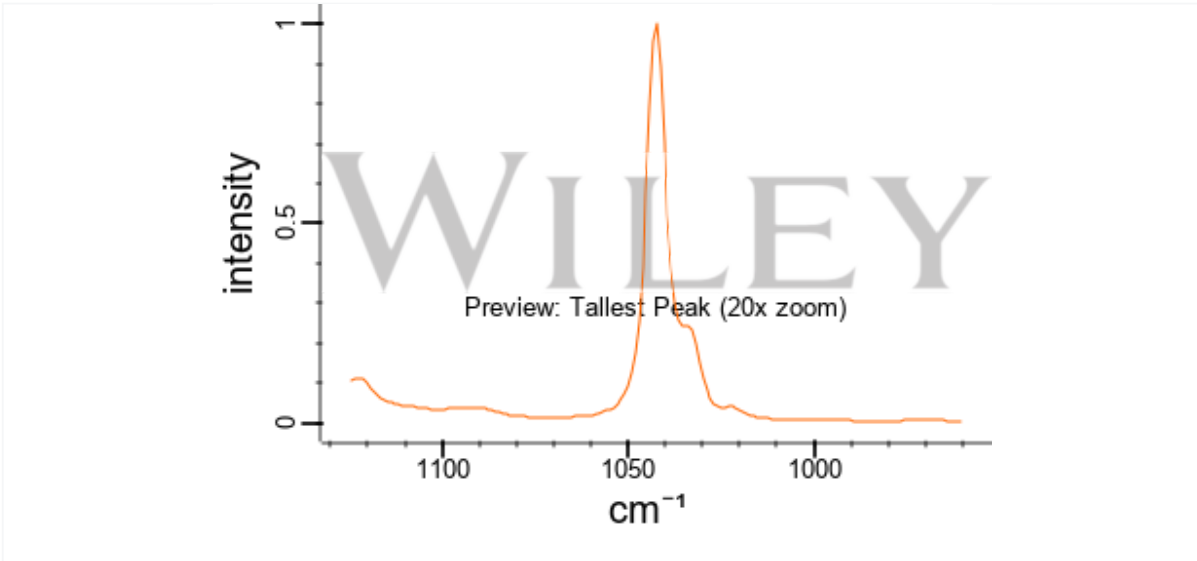


1 of 3

[View All](#)**Raman Spectra**

Raman: 518 (Sadtler Research Laboratories spectral collection)

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

2 of 3	View All ↗
Technique FT-Raman	
Source of Spectrum Forensic Spectral Research	
Source of Sample Supelco, Sigma-Aldrich	
Catalog Number 47865-U	
Lot Number LB60593	
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Thumbnail	

► [SpectraBase](#)

4.7 Other Spectra



Intense mass spectral peaks: 78 m/z, 106 m/z, 122 m/z

Pfleger, K., H. Maurer and A. Weber. Mass Spectral and GC Data of Drugs, Poisons and their Metabolites. Parts I and II. Mass Spectra Indexes. Weinheim, Federal Republic of Germany. 1985., p. 155

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

5 Related Records



5.1 Related Compounds with Annotation



7,535 items

SORT BY Neighbor Type - A to Z

1-methylnicotinamide, Trigonellinamide, N(1)-Methylnicotinamide, Trigonellamide, 3106-60-3, ...
Compound CID: [457](#)
Neighbor Type: 2D+3D
Annotation Types Count: 11

3-pyridine aldoxime, N-[(pyridin-3-yl)methylidene]hydroxylamine, pyridine-3-carbaldehyde oxime, 3-formylpyridine oxime, CHEBI:86555, ...
Compound CID: [694](#)
Neighbor Type: 2D+3D
Annotation Types Count: 5

nicotinamide, niacinamide, 98-92-0, 3-Pyridinecarboxamide, Nicotinic acid amide, ...

Page of 1,507

► [PubChem](#)

5.2 Related Compounds



Same Connectivity Count 16
Same Parent, Connectivity Count 113
Same Parent, Exact Count 97
Mixtures, Components, and Neutralized Forms Count 1037
Similar Compounds Count 1908
Similar Conformers Count 5738

► PubChem

5.3 Substances



5.3.1 Related Substances



All Count 2147
Same Count 411
Mixture Count 1736

► PubChem

5.3.2 Substances by Category



8 categories	↓
Chemical Vendors (123)	+
Curation Efforts (33)	+
Governmental Organizations (98)	+
Journal Publishers (8)	+
NIH Initiatives (15)	+
Research and Development (60)	+
Subscription Services (3)	+
Legacy Depositors (111)	+

► PubChem

5.4 Entrez Crosslinks



PubMed Count 3812
Protein Structures Count 67
Taxonomy Count 9
OMIM Count 18
Gene Count 168

► PubChem

6 Chemical Vendors



74 vendors

**Alichem**

PubChem SID: [377947750](#)
Purchasable Chemical: [029205886](#)

Yick-Vic Chemicals & Pharmaceuticals (HK) Ltd.

PubChem SID: [459144781](#)
Purchasable Chemical: MIS-6143

PubChem SID: [441071408](#)
Purchasable Chemical: PH-0271AA

Acadechem

PubChem SID: [381690714](#)
Purchasable Chemical: [ACDC-066615](#)

PubChem SID: [321906423](#)
Purchasable Chemical: [ACDS-017518](#)

Lan Pharmatech

PubChem SID: [439592343](#)
Purchasable Chemical: LAN-B78990

MedChemexpress MCE

PubChem SID: [210281591](#)
Purchasable Chemical: [HY-B0150](#)

LEAPCHEM

PubChem SID: [439961805](#)
Purchasable Chemical: LP079161

J&H Chemical Co.,Ltd

PubChem SID: [468615109](#)
Purchasable Chemical: [JH21428](#)

TargetMol

PubChem SID: [312695969](#)
Purchasable Chemical: [T0934](#)

Sigma-Aldrich

PubChem SID: [329750553](#)
Purchasable Chemical: [1462006_USP](#)

PubChem SID: [329757343](#)
Purchasable Chemical: [47865-U_SUPELCO](#)

PubChem SID: [57652413](#)
Purchasable Chemical: [72340_SIGMA](#)

Aaron Chemicals LLC

PubChem SID: [406545736](#)
Purchasable Chemical: [AR00IKPC](#)

Alfa Chemistry

PubChem SID: [376089554](#)
Purchasable Chemical: [1255150-40-3](#)

PubChem SID: [438649733](#)
Purchasable Chemical: [ACM98920-1](#)

PubChem SID: [445524962](#)
Purchasable Chemical: [ACM98920-2](#)

Finetech Industry Limited

PubChem SID: [164815311](#)
Purchasable Chemical: [FT-0631517](#)

PubChem SID: [164763313](#)
Purchasable Chemical: [FT-0672696](#)

PubChem SID: [347881686](#)
Purchasable Chemical: [FT-0773644](#)

AA BLOCKS

PubChem SID: [479915801](#)
Purchasable Chemical: [AA0099ZS](#)

PubChem SID: [374225004](#)
Purchasable Chemical: [AA00IJXK](#)

Biosynth

PubChem SID: [459129100](#)
Purchasable Chemical: [BN166252](#)

PubChem SID: [255370431](#)
Purchasable Chemical: [Q-201470](#)

Vitas-M Laboratory

PubChem SID: [125292932](#)
Purchasable Chemical: [STL163867](#)

Santa Cruz Biotechnology, Inc.

PubChem SID: [472958691](#)
Purchasable Chemical: [sc-208096](#)

Win-Win Chemical

PubChem SID: [438510638](#)
Purchasable Chemical: [7035](#)

China MainChem Co., Ltd

PubChem SID: [354339099](#)
Purchasable Chemical: [98-92-0](#)

PubChem SID: [381623080](#)
Purchasable Chemical: [MS98-92-0](#)

AHH Chemical co.,ltd

PubChem SID: [252376008](#)
Purchasable Chemical: [MT-19649](#)

PubChem SID: [381118587](#)

Purchasable Chemical: [NP-1178](#)

VladaChem

PubChem SID: [329734429](#)

Purchasable Chemical: [VL143553](#)

PubChem SID: [381001849](#)

Purchasable Chemical: [VL164029](#)

PubChem SID: [381006868](#)

Purchasable Chemical: [VL261825-100G](#)

Chemenu Inc.

PubChem SID: [443372545](#)

Purchasable Chemical: [CM178071](#)

BenchChem

PubChem SID: [443549843](#)

Purchasable Chemical: [B372718](#)

Sinfoo Biotech

PubChem SID: [404780394](#)

Purchasable Chemical: [S001861](#)

Starshine Chemical

PubChem SID: [464505075](#)

Purchasable Chemical: [starbld0694283](#)

Synblock Inc

PubChem SID: [446878751](#)

Purchasable Chemical: [SB74497](#)

3WAY PHARM INC

PubChem SID: [438522540](#)

Purchasable Chemical: [SWK-00201](#)

BOC Sciences

PubChem SID: [480406573](#)

Purchasable Chemical: [11032-50-1](#)

PubChem SID: [341106653](#)

Purchasable Chemical: [98-92-0](#)

LGC Standards

PubChem SID: [438644830](#)

Purchasable Chemical: [DRE-A15519500AL-10](#)

PubChem SID: [404848214](#)

Purchasable Chemical: [DRE-A15519500ME-100](#)

PubChem SID: [340509944](#)

Purchasable Chemical: [DRE-C15519500](#)

Norris Pharm

PubChem SID: [383232012](#)

Purchasable Chemical: [NSTH-D40278](#)

PubChem SID: [383459379](#)

Purchasable Chemical: NSZB-A269557

Combi-Blocks

PubChem SID: [482704754](#)

Purchasable Chemical: [NA-0257](#)

001Chemical

PubChem SID: [440061140](#)

Purchasable Chemical: [DY583359](#)

CSNpharm

PubChem SID: [384652340](#)

Purchasable Chemical: [CSN16796](#)

Life Chemicals

PubChem SID: [315359022](#)

Purchasable Chemical: [F2173-0513](#)

Clearsynth

PubChem SID: [387196520](#)

Purchasable Chemical: [CS-EB-01471](#)

PubChem SID: [387209617](#)

Purchasable Chemical: [CS-ER-01463](#)

PubChem SID: [313077155](#)

Purchasable Chemical: [CS-O-30679](#)

Chem-Space.com Database

PubChem SID: [434423952](#)

Purchasable Chemical: [CSSB00000162173](#)

abcr GmbH

PubChem SID: [316397008](#)

Purchasable Chemical: [AB118154](#)

AbMole Bioscience

PubChem SID: [348354975](#)

Purchasable Chemical: [M4896](#)

Tocris Bioscience

PubChem SID: [252157789](#)

Purchasable Chemical: [4106](#)

Amadis Chemical

PubChem SID: [171578433](#)

Purchasable Chemical: [205304](#)

PubChem SID: [131331779](#)

Purchasable Chemical: [A845925](#)

Enamine

PubChem SID: [131363165](#)

Purchasable Chemical: [EN300-15612](#)

PubChem SID: [335140755](#)

Purchasable Chemical: [Z33546463](#)

ThoreauChem

PubChem SID: [478172894](#)

Purchasable Chemical: [TH-D40278](#)

A2B Chem

PubChem SID: [480590182](#)

Purchasable Chemical: [AE32756](#)

PubChem SID: [444096291](#)

Purchasable Chemical: [AI65540](#)

Thermo Fisher Scientific

PubChem SID: [459192432](#)

Purchasable Chemical: [GID_900000000080569](#)

PubChem SID: [459192433](#)

Purchasable Chemical: [GID_900000000080670](#)

PubChem SID: [459193397](#)

Purchasable Chemical: [GID_900000000127372](#)

Oakwood Products

PubChem SID: [312604480](#)

Purchasable Chemical: [239905](#)

AstaTech, Inc.

PubChem SID: [445642053](#)

Purchasable Chemical: [11886](#)

Matrix Scientific

PubChem SID: [406715304](#)

Purchasable Chemical: [139707](#)

Smolecule

PubChem SID: [438483373](#)

Purchasable Chemical: [S537140](#)

MuseChem

PubChem SID: [355038905](#)

Purchasable Chemical: [A000452](#)

VWR, Part of Avantor

PubChem SID: [384257668](#)

Purchasable Chemical: [200000-710](#)

PubChem SID: [384256661](#)

Purchasable Chemical: [200013-660](#)

Yuhao Chemical

PubChem SID: [318239132](#)

Purchasable Chemical: [XJ0261](#)

MolPort

PubChem SID: [88826860](#)

Purchasable Chemical: [MolPort-001-783-876](#)

BioCrick

PubChem SID: [382166903](#)

Purchasable Chemical: [BCN1025](#)

BioChemPartner

PubChem SID: [375590497](#)

Purchasable Chemical: [BCP07322](#)

AKos Consulting & Solutions

PubChem SID: [131998477](#)

Purchasable Chemical: [AKOS005715850](#)

3B Scientific (Wuhan) Corp

PubChem SID: [375134367](#)

Purchasable Chemical: [3B1-00061](#)

PubChem SID: [375197950](#)

Purchasable Chemical: [3B3-029729](#)

AvaChem Scientific

PubChem SID: [475549165](#)

Purchasable Chemical: [6975](#)

THE BioTek

PubChem SID: [434301828](#)

Purchasable Chemical: [bt-277049](#)

AbaChemScene

PubChem SID: [210279268](#)

Purchasable Chemical: [CS-1968](#)

BLD Pharm

PubChem SID: [375447638](#)

Purchasable Chemical: [BD42146](#)

Specs

PubChem SID: [16957244](#)

Purchasable Chemical: [AC-907/25014114](#)

Key Organics/BIONET

PubChem SID: [354267784](#)

Purchasable Chemical: [AS-13845](#)

TCI (Tokyo Chemical Industry)

PubChem SID: [87573471](#)

Purchasable Chemical: [N0078](#)

Achemtek

PubChem SID: [381344666](#)

Purchasable Chemical: [0104-014668](#)

Ambeed

PubChem SID: [376146769](#)
Purchasable Chemical: [A187855](#)

Accela ChemBio Inc.

PubChem SID: [442146830](#)
Purchasable Chemical: [SY024804](#)

CymitQuimica

PubChem SID: [470808762](#)
Purchasable Chemical: [CQ_98-92-0](#)

Innovapharm

PubChem SID: [439594538](#)
Purchasable Chemical: [VT-00686232](#)

Selleck Chemicals

PubChem SID: [347912579](#)
Purchasable Chemical: [S1899](#)

ChemFaces

PubChem SID: [274951028](#)
Purchasable Chemical: [CFN99926](#)

Cooke Chemical Co., Ltd

PubChem SID: [478267751](#)
Purchasable Chemical: [A6157512](#)

MolCore BioPharmatech

PubChem SID: [446287108](#)
Purchasable Chemical: [DY583359](#)

PubChem SID: [405514484](#)
Purchasable Chemical: [MC583359](#)

DC Chemicals

PubChem SID: [350090295](#)
Purchasable Chemical: [DCY-061](#)

AbovChem LLC

PubChem SID: [319554746](#)
Purchasable Chemical: [HY-B0150](#)

RR Scientific

PubChem SID: [472459979](#)
Purchasable Chemical: [R002454](#)

► [PubChem](#)

7 Drug and Medication Information



7.1 WHO Essential Medicines

**Drug**[Nicotinamide](#)**Drug Classes**

Vitamins and minerals

Formulation

Oral - Solid: 50 mg

Indication

Pellagra [co-prescribed with A11HA01]

► [WHO Model Lists of Essential Medicines](#)

7.2 FDA Approved Drugs



16 items

SORT BY **Marketing Status - Z to A****Drug**[INFUVITE ADULT](#)**Ingredient(s)**

ALPHA-TOCOPHEROL ACETATE; ASCORBIC ACID; BIOTIN; CHOLECALCIFEROL; CYANOCOBALAMIN; DEXPANTHENOL; FOLIC ACID; NIACINAMIDE; PYRIDOXINE HYDROCHLORIDE; RIBOFLAVIN 5'-PHOSPHATE SODIUM; THIAMINE HYDROCHLORIDE; VITAMIN A PALMITATE; VITAMIN K

Dosage Form/Route

SOLUTION;INTRAVENOUS

Strength

2 IU/ML;40MG/ML;12MCG/ML;40
IU/ML;1MCG/ML;3MG/ML;120MCG/ML;8MG/ML;1.2MG/ML;0.72MG/ML;1.2MG/ML;660
IU/ML;0.03MG/ML

Marketing Status

Prescription

Company

SANDOZ CANADA INC

Application Number

021163**Production Number**

001

Drug**INFUVITE ADULT****Ingredient(s)**

ALPHA-TOCOPHEROL ACETATE; ASCORBIC ACID; BIOTIN; CHOLECALCIFEROL; CYANOCOBALAMIN;
DEXPANTHENOL; FOLIC ACID; NIACINAMIDE; PYRIDOXINE HYDROCHLORIDE; RIBOFLAVIN 5'-
PHOSPHATE SODIUM; THIAMINE HYDROCHLORIDE; VITAMIN A PALMITATE; VITAMIN K

Dosage Form/Route

SOLUTION;INTRAVENOUS

Strength

2 IU/ML;40MG/ML;12MCG/ML;40
IU/ML;1MCG/ML;3MG/ML;120MCG/ML;8MG/ML;1.2MG/ML;0.72MG/ML;1.2MG/ML;660
IU/ML;30MCG/ML

Marketing Status

Prescription

Company

SANDOZ CANADA INC

Application Number**021163****Production Number**

002

Drug**INFUVITE PEDIATRIC****Ingredient(s)**

ASCORBIC ACID; BIOTIN; CHOLECALCIFEROL; CYANOCOBALAMIN; DEXPANTHENOL; FOLIC ACID;
NIACINAMIDE; PYRIDOXINE; RIBOFLAVIN; THIAMINE; TOCOPHEROL ACETATE; VITAMIN A; VITAMIN K

Dosage Form/Route

INJECTABLE;INTRAVENOUS

Strength

80MG/VIAL;0.02MG/VIAL;400
IU/VIAL;0.001MG/VIAL;5MG/VIAL;0.14MG/VIAL;17MG/VIAL;1MG/VIAL;1.4MG/VIAL;1.2MG/VIAL;7
IU/VIAL;2,300 IU/VIAL;0.2MG/VIAL

Marketing Status

Prescription

Company

SANDOZ CANADA INC

Application Number

[021265](#)

Production Number

001

Drug

[INFUVITE PEDIATRIC \(PHARMACY BULK PACKAGE\)](#)

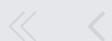
Ingredient(s)

ASCORBIC ACID; BIOTIN; CHOLECALCIFEROL; CYANOCOBALAMIN; DEXPANTHENOL; FOLIC ACID; NIACINAMIDE; PYRIDOXINE; RIBOFLAVIN; THIAMINE; TOCOPHEROL ACETATE; VITAMIN A; VITAMIN K

Dosage Form/Route

INJECTABLE;INTRAVENOUS

Strength

 Page 1 of 4[► Drugs@FDA](#)

7.3 FDA Orange Book



12 items

 Search

SORT BY Trade Name - A to Z



Trade Name

[M.V.I. PEDIATRIC](#)

Marketing Status

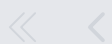
Discontinued

Application Number

[N018920](#)

Applicant

HOSPIRA INC

 Page 1 of 3[► FDA Orange Book](#)

7.4 FDA National Drug Code Directory



236 items	
Search	
SORT BY Start Marketing Date - Most Recent	
Product NDC 83027-0095	
Start Marketing Date 2023-08-14	
Dosage Form LIQUID	
Strength 15 [hp_C]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 8 [hp_X]/mL; 8 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL	
Labeler Nutritional Specialties, Inc.	
Product NDC 43742-2087	
Start Marketing Date 2023-07-18	
Dosage Form LIQUID	
Strength 6 [hp_X]/mL; 6 [hp_X]/mL; 6 [hp_X]/mL; 10 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 12 [hp_X]/mL; 30 [hp_X]/mL; 30 [hp_X]/mL; 30 [hp_X]/mL	
Page 1 of 48	

► [National Drug Code \(NDC\) Directory](#)

7.5 Drug Labels



Drug and label

130 items 

 Search

SORT BY **Date - Most Recent** 

DERMA PELLA FACIAL CLEANSER FOR NORMAL SKIN (NIACINAMIDE) SOLUTION
 Drug: Niacinamide
 Download: [PDF label](#)
 Data File: [XML](#)
 Ingredient (UNII): NIACINAMIDE (UNII:25X51I8RD4)
 Description: This foaming face wash penetrates deep into your pores, scrubbing them from the inside out to eliminate dirt and oils. Rosemary Extract makes the skin feel soft and sparkling by purifying, soothing, hydrating and provides...
 Indication: A mild facial cleanser for normal skin.
 Category: Human over the counter
 Company: Pella Pharmaceuticals Co. Ltd
 Date: 2023-06-19

DERMA PELLA CLEANSER FOR SENSITIVE AND DRY SKIN (NIACINAMIDE) SOLUTION
 Drug: Niacinamide
 Download: [PDF label](#)
 Data File: [XML](#)
 Ingredient (UNII): NIACINAMIDE (UNII:25X51I8RD4)
 Description: A refreshing cleanser for sensitive and dry skin. It cleanses gently without a harsh drying effect, leaving your skin feeling refreshed. A combination of Aloe Vera, Cucumber Extracts, Vitamin B3 and Allantoin make it perfect...
 Indication: A mild facial cleanser for sensitive and dry skin.
 Category: Human over the counter
 Company: Pella Pharmaceuticals Co. Ltd
 Date: 2023-06-19

DR. CELLMO (NIACINAMIDE) SHAMPOO
 Drug: NIACINAMIDE
 Download: [PDF label](#)
 Data File: [XML](#)
 Ingredient (UNII): NIACINAMIDE (UNII:25X51I8RD4)
 Category: Human over the counter
 Company: Pharmacal-International Co. Ltd

<< < Page 1 of 26 > >>

► [DailyMed](#)

Active ingredient and drug

989 items		
 Search		
SORT BY Ingredient - A to Z		
Ingredient DEXPANTHENOL (UNII:1O6C93RI7Z); CYANOCOBALAMIN (UNII:P6YC3EG204); PYRIDOXINE HYDROCHLORIDE (UNII:68Y4CF58BV); RIBOFLAVIN 5'-PHOSPHATE SODIUM (UNII:20RD1DZH99); NIACINAMIDE (UNII:25X51I8RD4); THIAMINE HYDROCHLORIDE (UNII:M572600E5P)		
Drug CYANOCOBALAMIN, NIACINAMIDE, DEXPANTHENOL, PYRIDOXINE HYDROCHLORIDE, RIBOFLAVIN 5 PHOSPHATE SODIUM, THIAMINE HYDROCHLORIDE		
Label Drug PDF label		
Data File XML		
Data SetID 074287f8-e2e8-45c7-acc1-1847f69de1ee		
Ingredient DEXPANTHENOL (UNII:1O6C93RI7Z); CYANOCOBALAMIN (UNII:P6YC3EG204); PYRIDOXINE HYDROCHLORIDE (UNII:68Y4CF58BV); RIBOFLAVIN 5'-PHOSPHATE SODIUM (UNII:20RD1DZH99); NIACINAMIDE (UNII:25X51I8RD4); THIAMINE HYDROCHLORIDE (UNII:M572600E5P)		
Drug CYANOCOBALAMIN, NIACINAMIDE, DEXPANTHENOL, PYRIDOXINE HYDROCHLORIDE, RIBOFLAVIN 5 PHOSPHATE SODIUM, THIAMINE HYDROCHLORIDE		
Label Drug PDF label		
Data File XML		
Data SetID 050e8dc2-3dba-476e-8256-3b9784daa05b		
Ingredient DEXPANTHENOL (UNII:1O6C93RI7Z); CYANOCOBALAMIN (UNII:P6YC3EG204); PYRIDOXINE HYDROCHLORIDE (UNII:68Y4CF58BV); RIBOFLAVIN 5'-PHOSPHATE SODIUM (UNII:20RD1DZH99); NIACINAMIDE (UNII:25X51I8RD4); THIAMINE HYDROCHLORIDE (UNII:M572600E5P)		
Drug CYANOCOBALAMIN, NIACINAMIDE, DEXPANTHENOL, PYRIDOXINE HYDROCHLORIDE, RIBOFLAVIN 5 PHOSPHATE SODIUM, THIAMINE HYDROCHLORIDE		

Label

<< < Page 1 of 198 > >>

► DailyMed

7.6 Clinical Trials



7.6.1 ClinicalTrials.gov



47 items



SORT BY Date - Most Recent



The Glaucoma Nicotinamide Trial

CTID: [NCT05275738](#)

Phase: N/A

Status: Recruiting

Date: 2023-07-27

Nicotinamide Chemoprevention for Keratinocyte Carcinoma in Solid Organ Transplant Recipients - Pivotal Trial

CTID: [NCT05955924](#)

Phase: Phase 3

Status: Not yet recruiting

Date: 2023-07-21

NAD+ Augmentation in Cardiac Surgery Associated Myocardial Injury Trial

CTID: [NCT04750616](#)

Phase: Phase 2

Status: Recruiting

Date: 2023-07-18

Nicotinamide and Glaucoma

CTID: [NCT05916066](#)

Phase: N/A

Status: Completed

Date: 2023-06-23

<< < Page 1 of 10 > >>

► [ClinicalTrials.gov](#)

7.6.2 EU Clinical Trials Register



11 items	
Search	
SORT BY Date - Most Recent	
A phase II randomized, double-blind, active placebo-controlled parallel group trial to examine the efficacy and safety of psilocybin in treatment-resistant EudraCT: 2019-003984-24 Phase: Phase 2 Status: Ongoing Date: 2020-11-17	
Assessing penetration of high dose Nicotinamide (Vitamin B3) in synovial fluid EudraCT: 2018-002245-11 Phase: Phase 1, Phase 2 Status: Ongoing Date: 2019-01-16	
A RANDOMISED, DOUBLE-BLIND, PLACEBO-CONTROLLED, PARALLEL-GROUP, MULTICENTRE STUDY OF THE EFFICACY AND SAFETY OF NICOTINAMIDE IN PATIENTS WITH FRIEDREICH'S ATAXIA (NICOFA) EudraCT: 2017-002163-17 Phase: Phase 2, Phase 3 Status: Ongoing, GB - no longer in EU/EEA, Prematurely Ended Date: 2018-10-25	
Efficacy and tolerability of nicotinamide as add-on therapy compared to placebo in dialysis-dependent patients with hyperphosphatemia EudraCT: 2013-000488-95 Phase: Phase 3 Status: Completed, Prematurely Ended Date: 2013-08-28	
A placebo controlled evaluation of a developmental gel for the treatment of atopic eczema	
<< < Page 1 of 3 > >>	

► [EU Clinical Trials Register](#)

7.6.3 NIPH Clinical Trials Search of Japan



2 items	Download
Measurement of NAD ⁺ metabolites in blood after oral intake of Vitamin B3 CTID: jRCTs041190107 Status: Complete Date: 2020-01-20	
Pharmacokinetics of orally-administered Nicotinamide Powder 10% Zonne and its NAD ⁺ pathway metabolites CTID: UMIN000031610 Phase: Phase I Status: Complete: follow-up complete	

► [NIPH Clinical Trials Search of Japan](#)

7.7 Therapeutic Uses



Vitamin B Complex

National Library of Medicine's Medical Subject Headings. Niacinamide. Online file (MeSH, 2018). Available from, as of June 1, 2018: https://www.nlm.nih.gov/mesh/2017/mesh_browser/MBrowser.html

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

/CLINICAL TRIALS/ ClinicalTrials.gov is a registry and results database of publicly and privately supported clinical studies of human participants conducted around the world. The Web site is maintained by the National Library of Medicine (NLM) and the National Institutes of Health (NIH). Each ClinicalTrials.gov record presents summary information about a study protocol and includes the following: Disease or condition; Intervention (for example, the medical product, behavior, or procedure being studied); Title, description, and design of the study; Requirements for participation (eligibility criteria); Locations where the study is being conducted; Contact information for the study locations; and Links to relevant information on other health Web sites, such as NLM's MedlinePlus for patient health information and PubMed for citations and abstracts for scholarly articles in the field of medicine. Nicotinamide is included in the database.

NIH/NLM; ClinicalTrials.Gov. Available from, as of June 1, 2018: <https://clinicaltrials.gov/>

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

Niacin and niacinamide are used to prevent **niacin** deficiency and to treat pellagra. Some clinicians prefer niacinamide for the treatment of pellagra because it lacks vasodilating effects. Pellagra may result from dietary deficiency, **isoniazid** therapy, or from decreased conversion of **tryptophan** to **niacin** in Hartnup disease or carcinoid tumors. /Included in US product label/

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

Although **niacin** and niacinamide have not been shown by well-controlled trials to have therapeutic value, the drugs have been used for the management of schizophrenic disorder, drug-induced hallucinations, chronic brain syndrome, hyperkinesia, unipolar depression, motion sickness, alcohol dependence, livedoid vasculitis, acne, and leprosy. /NOT included in US product label/

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

For more Therapeutic Uses (Complete) data for Nicotinamide (14 total), please visit the [HSDB record page](#).

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

7.8 Drug Warnings



Blood **glucose** concentration should be monitored periodically in patients receiving **niacin** or niacinamide, especially early in the course of therapy. Dosage requirements for antidiabetic agents (e.g., insulin, oral sulfonylureas) may change in diabetic patients.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

Potential adverse effects on fetus: Higher levels in fetus than mother, but no fetal anomalies reported. Potential side effects on breast-fed infant: No adverse effects known. FDA Category: C (C = Studies in laboratory animals have revealed adverse effects on the fetus (teratogenic, embryocidal, etc.), but there are no controlled studies in pregnant women. The benefits from use of the drug in pregnant women may be acceptable despite its potential risks, or there are no laboratory animal studies or adequate studies in pregnant women.) /from table II/

Stockton, D.L. and A.S. Paller. J Am Acad Dermatol 23 (1):87-103 (1990)

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

Niacinamide /was administered/ daily as a liquid formulation to head and neck cancer patients receiving a 5- to 7-week course of radiotherapy. Niacinamide was administered orally 1.5 hr before irradiation. The daily dose was 80 mg/kg bw to a maximum of 6 g. A dose reduction to 60 mg/kg was introduced for patients with severe side-effects. ... Side-effects of niacinamide were monitored. In all patients, peak concentrations greater than 700 nM/mL could be obtained 0.25-3 hr after drug intake. During the first week of treatment, plasma concentrations at the time of irradiation were adequate in 82% of the samples. Nausea, with or without vomiting, occurred in 65% of patients. Tolerance improved after a 25% reduction of the dose in six of seven patients but plasma concentrations at the time of irradiation decreased below 700 nM/mL in four out of six patients. Other niacinamide side effects included gastrointestinal symptoms, flushing, dizziness, sweating, fatigue, and headache. The most powerful single predictor for severe niacinamide toxicity was the mean of the plasma concentration measured at the time of irradiation during the first week.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.6; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

Abnormal liver function test results (including increased serum concentrations of [bilirubin](#), AST [SGOT], ALT [SGPT], and LDH), jaundice, and chronic liver damage have occurred during [niacin](#) and niacinamide therapy. Abnormal prothrombin time and hypoalbuminemia have also been reported.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

For more Drug Warnings (Complete) data for Nicotinamide (6 total), please visit the [HSDB record page](#).

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

8 Food Additives and Ingredients



8.1 FDA Substances Added to Food



Substance
NIACINAMIDE
Used for (Technical Effect)

NUTRIENT SUPPLEMENT

Document Number (21 CFR)

[184.1535](#)

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

8.2 Food Additive Status



FDA Food Additive Status

Niacinamide - NUTR/DS, GRAS/FS -182.5535, 184.1535; Part 137 (137.165, 137.185, 137.235, 137.260, 137.305, 137.350), Cereal Flours; Part 139 (139.115, 139.117, 139.122, 139.155, 139.165), Macaroni & Noodle Pds; 136.115, Enriched Bread

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

FDA Food Additive Status

Vitamin B - NUTR/DS, GRAS

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

9 Pharmacology and Biochemistry



9.1 MeSH Pharmacological Classification



Vitamin B Complex

A group of water-soluble vitamins, some of which are COENZYMES. (See [all compounds classified as Vitamin B Complex](#).)

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

9.2 FDA Pharmacological Classification



Non-Proprietary Name

NIACINAMIDE

Pharmacological Classes

[Adenosine](#) Receptor Agonist [EPC]; [Adenosine](#) Receptor Agonists [MoA]

► [National Drug Code \(NDC\) Directory](#)

9.3 ATC Code



A11HA01

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](#)

A - Alimentary tract and metabolism

A11 - Vitamins

A11H - Other plain vitamin preparations

A11HA - Other plain vitamin preparations

A11HA01 - Nicotinamide

► [WHO Anatomical Therapeutic Chemical \(ATC\) Classification](#)

9.4 Bionecessity



At high doses (up to 3.5 g/day), nicotinamide is protective against cell death and inhibits the production of inflammatory mediators in animal and in in vitro models of oxidant-induced cell injury.

Coates, P.M., Blackman, M.R., Cragg, G.M., Levine, M., Moss, J., White, J.D. (Ed), *Encyclopedia of Dietary Supplements*. Marcel Dekker, New York, NY, p. 488 (2005)

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

Nicotinamide, via its major metabolite **NAD+** (**nicotinamide adenine dinucleotide**), is involved in a wide range of biological processes, including the product of energy, the synthesis of fatty acids, **cholesterol** and steroids, signal transduction and the maintenance of the integrity of the genome.

PDR for Nutritional Supplements 2nd ed. Thomson Reuters, Montvale, NJ 2008, p. 450

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

In humans, niacinamide is required for lipid metabolism, tissue respiration, and glycogenolysis. In vivo, niacinamide is formed from conversion of **niacin**. In addition, some dietary **tryptophan** is oxidized to **niacin** and then to niacinamide in vivo. Niacinamide is incorporated into 2 coenzymes: **nicotinamide adenine dinucleotide (NAD)** and **nicotinamide adenine dinucleotide phosphate (NADP)**. **NAD** and **NADP** act as **hydrogen**-carrier molecules in glycogenolysis, tissue respiration, and lipid metabolism.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

9.5 Absorption, Distribution and Excretion



¹⁴(C)Niacinamide was incorporated into an oil-in-**water** (o/w) skin cream and into a 30% (w/w) soap base and applied to the skin of female Colworth Wistar rats. The final concentration of niacinamide in the soap solution was approximately 0.3% (w/v) and was 1% (w/w) in the skin cream. Application of the skin cream and soap paste was made to rat skin at approximately 20 mg/sq cm. The cream was carefully massaged over 10 sq cm of skin for up to 5 min before covering with polythene-lined occlusive protective patches. The rats were placed in metabolism cages for 48 hr during which time all excreta was collected. At 48 hr, the animals were killed and the patch, carcass, and treated area of skin were assayed for ¹⁴(C). Up to 32% ¹⁴(C) was recovered in excreta and in the carcasses from rats treated with skin cream containing ¹⁴(C)Niacinamide and up to 30% from those treated with soap paste.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.5; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

Nicotinamide is efficiently absorbed from the gastrointestinal tract. At low doses, absorption is mediated via **sodium**-dependent facilitated diffusion. Passive diffusion is the principal mechanism of absorption at higher doses. Doses of up to three to four grams of nicotinamide are almost completely absorbed. Nicotinamide is transported via the portal circulation to the liver and via the systemic circulation to the various tissues of the body. Nicotinamide enters most cells by passive diffusion and enters erythrocytes by facilitated transport.

PDR for Nutritional Supplements 2nd ed. Thomson Reuters, Montvale, NJ 2008, p. 452

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

Niacinamide is widely distributed /throughout/ body tissues.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

Niacin and niacinamide are readily absorbed from the GI tract following oral administration, and niacinamide (no longer commercially available in the US) is readily absorbed from subcutaneous and IM injection sites.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

For more Absorption, Distribution and Excretion (Complete) data for Nicotinamide (16 total), please visit the [HSDB record page](#).

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

9.6 Metabolism / Metabolites



In amounts needed for physiologic function as a coenzyme (12-18 mg daily), **niacin** is converted to niacinamide; larger doses of **niacin** are converted to niacinamide to only a minor degree. Niacinamide is metabolized in the liver to N-methylniacinamide, other N-methylated derivatives, and **nicotinuric acid** (the **glycine** conjugate of **niacin**). These metabolites are excreted in urine. Following administration of physiologic doses of **niacin** or niacinamide, only a small amount of niacinamide is excreted unchanged in urine; however, following administration of larger doses, a greater proportion of **niacin** and niacinamide is excreted unchanged.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

N1-Methyl-4-pyridone-3-carboxamide was detected on chromatograms of plasma extracts after oral administration of niacinamide to two human subjects.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.6; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

6-Hydroxynicotinamide and **6-hydroxynicotinic acid** /were detected/ as urinary metabolites by comparison of ultraviolet, infrared, and mass spectra following intraperitoneal injections of ¹⁴(C)**Niacin** or ¹⁴(C)Niacinamide into rats.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.8; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

N1-methyl-4- pyridone-3-carboxamide is a major metabolite of **niacin** and niacinamide which has been found to be synthesized from **N1- methylnicotinamide**.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.8; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

For more Metabolism/Metabolites (Complete) data for Nicotinamide (7 total), please visit the [HSDB record page](#).

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

Uremic toxins tend to accumulate in the blood either through dietary excess or through poor filtration by the kidneys. Most uremic toxins are metabolic waste products and are normally excreted in the urine or feces.

► [Toxin and Toxin Target Database \(T3DB\)](#)

9.7 Biological Half-Life



The mean half life values were 2.7 hr, 5.9 hr, and 8.1 hr after taking 1, 3, or 6 g of Niacinamide, respectively.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.6; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

9.8 Human Metabolite Information



9.8.1 Tissue Locations



Bladder
Epidermis
Fibroblasts
Neuron
Pancreas
Placenta

Prostate
Spleen

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

9.8.2 Cellular Locations



Extracellular

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

9.8.3 Metabolite Pathways



Nicotinate and nicotinamide metabolism

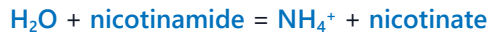
► [Human Metabolome Database \(HMDB\)](#)

9.9 Biochemical Reactions



57 items		↓
Search		
SORT BY		Rhea Accession - Increasing ▼
Rhea Accession		
RHEA:11820		
Reaction		
diphthamide-[translation elongation factor 2] + NAD⁺ = H⁺ + N-(ADP-D-ribosyl)diphthamide-[translation elongation factor 2] + nicotinamide		
PubChem Enzyme		
EC 2.4.2.36		
Evidence PMID		
3927821		
18276581		
6326138		
Rhea Accession		
RHEA:14545		

Reaction



PubChem Enzyme

EC 3.5.1.19

Evidence PMID

4399474

17382284

17335512

8726014

18201201

<< < Page 1 of 12 > >>

► Rhea - Annotated Reactions Database

1,645 items



SORT BY Taxonomy - A to Z



Reaction



PubChem Pathway

Organelle biogenesis and maintenance

Source

Reactome

Taxonomy

Arabidopsis thaliana (thale cress)

Reaction



PubChem Pathway

Mitochondrial biogenesis

Source

Reactome

Taxonomy

Arabidopsis thaliana (thale cress)

Reaction

NAD + Homologues of GLUD1 → NAM

<< < Page 1 of 329 > >>

► PubChem

9.10 Transformations



2 items



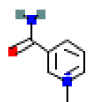
Predecessor ⓘ



Predecessor Name

NIACINAMIDE

Successor ⓘ



► ChEMBL

7 items

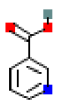


Search

SORT BY Predecessor Name - A to Z



Predecessor



Predecessor Name

Nicotinic acid

Successor



Successor Name

[Nicotinamide](#)

Transformation

Metabolism

Evidence DOI

[10.5281/zenodo.3827487](https://doi.org/10.5281/zenodo.3827487)

Predecessor



Predecessor Name

Page 1 of 2

[▶ NORMAN Suspect List Exchange](#)

10 Use and Manufacturing



10.1 Uses



EPA CPDat Chemical and Product Categories

37 items



SORT BY Category - A to Z



Personal care

Category Description: General personal care products which do not fit into a more refined category**Categorization Type:** Product Use Category (PUC)

Personal care -> acne treatment -> face wash

Category Description: Facial cleansing products (excluding scrubs), for acne treatment

Categorization Type: Product Use Category (PUC)
Personal care -> body hygiene -> bar soap Category Description: Bar and other solid soaps Categorization Type: Product Use Category (PUC)
cosmetic ingredient Categorization Type: Reported Functional Use
hair conditioning agent Categorization Type: Reported Functional Use
<< < Page 1 > >> of 8

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

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

Sources/Uses

Nicotinamide is usually used to treat deficiency, because nicotinamide, unlike [nicotinic acid](#) (the most common form of [niacin](#)), does not cause flushing, itching, burning, or tingling sensations. [Merck Manual, p. 41] Nicotinamide, (...) also known as niacinamide and nicotinic amide, is the amide of [nicotinic acid](#) ([vitamin B3](#) / [niacin](#)). Nicotinamide is a [water](#)-soluble vitamin and is part of the vitamin B group. [Nicotinic acid](#), also known as [niacin](#), is converted to nicotinamide in vivo, and, though the two are identical in their vitamin functions, nicotinamide does not have the same pharmacological and toxic effects of [niacin](#), which occur incidental to [niacin](#)'s conversion. [Wikipedia]

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

Vitamin B Complex

National Library of Medicine's Medical Subject Headings. Niacinamide. Online file (MeSH, 2018). Available from, as of June 1, 2018: https://www.nlm.nih.gov/mesh/2017/mesh_browser/MBrowser.html

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

Nicotinamide is ... used in cosmetics as hair and skin conditioning agent.

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0) p.6 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

.../Has/ been used in the enrichment of bread, flour, and other grain-derived products. Animal feed is routinely supplemented with ... nicotinamide. Nicotinamide is also used in multivitamin preparations.

Van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology (1999-2018). John Wiley & Sons, Inc. Online Posting Date: December 4, 2000

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

MEDICATION

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

MEDICATION (VET)

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

Naturally produced by the body (endogenous).

► [Toxin and Toxin Target Database \(T3DB\)](#)

10.1.1 Use Classification



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

► [FDA Orange Book](#)

Cosmetics -> Smoothing

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

► [NORMAN Suspect List Exchange](#)

10.1.2 Industry Uses



Intermediates

Other (specify)

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

► [EPA Chemicals under the TSCA](#)

10.1.3 Consumer Uses



Other (specify)

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

► [EPA Chemicals under the TSCA](#)

10.1.4 Household Products



Household & Commercial/Institutional Products

Information on 174 consumer products that contain Niacinamide (Vitamin B) in the following categories is provided:

- Personal Care

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

10.2 Methods of Manufacturing



2-Methylglutaronitrile, a byproduct of **adiponitrile** production, is converted to **2-methyl-1,5-diaminopentane**. Cyclic hydrogenation gives **3-methylpiperidine**. Dehydrogenation yields **3-methylpyridine**, which is then ammoxidated and partly hydrolyzed to nicotinamide.

Blum R; Vitamins, 11. Niacin (Nicotinic Acid and Nicotinamide). Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2018). NY, NY: John Wiley & Sons. Online Posting Date: April 14, 2015

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

In a multitubular reactor **3-methylpyridine**, air, **ammonia**, and **hydrogen** react at ca. 350 °C and moderate pressure to give **3-cyanopyridine**. Heterogeneous catalysts containing oxides of **antimony**, **vanadium**, and **titanium**, **antimony**, **vanadium**, and **uranium** or antimony-vanadium-titanium catalyst are highly effective. For instance, with a **vanadium**, **titanium**, **zirconium**, **molybdenum** catalyst, a reactor temperature of 340 °C, and a molar feed ratio of **3-methylpyridine:ammonia: oxygen** of 1:1.3:40 yields 95% of **3-cyanopyridine**. **3-Cyanopyridine** is converted to nicotinamide by alkaline hydrolysis. This reaction has the advantage that saponification to the amide is fast compared to total hydrolysis to **nicotinic acid**. The hydrolysis to the amide is normally carried out with catalytic amounts of bases, mainly **sodium hydroxide**, at 130-150 °C.

Blum R; Vitamins, 11. Niacin (Nicotinic Acid and Nicotinamide). Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2018). NY, NY: John Wiley & Sons. Online Posting Date: April 14, 2015

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

In the Lonza process, [3-cyanopyridine](#) is converted to nicotinamide by means of an immobilized microorganism of the genus *Rhodococcus*. Heterogeneous catalysts are also mentioned. A [copper-chromium oxide](#) catalyst, [manganese dioxide](#), or [manganese dioxide](#) with chromium-nickel oxide, [chromium-cobalt oxide](#), or [manganese dioxide](#) with titanium-silicon dioxide give good yields of nicotinamide.

Blum R; Vitamins, 11. Niacin (Nicotinic Acid and Nicotinamide). Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2018). NY, NY: John Wiley & Sons. Online Posting Date: April 14, 2015

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

[Nicotinic acid](#) is melted and reacted with [ammonia](#) gas to yield nicotinamide. The reaction is catalyzed by the presence of ammonium salts. After distillation, nicotinamide is dissolved in [water](#), purified by the addition of activated [carbon](#), filtered, recrystallized and centrifuged. The nicotinamide contained in the mother liquor is reclaimed by a special recovery operation. The wet pure nicotinamide filter cake is dried under vacuum in a rotary vacuum drier.

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0) p.7 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

For more Methods of Manufacturing (Complete) data for Nicotinamide (6 total), please visit the [HSDB record page](#).

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

10.3 Formulations / Preparations



Table: Niacinamide Preparations

Route of Administration Oral
Dosage Form Powder
Brand or Generic Name (Manufacturer) (Available from one or more manufacturer, distributor, and/or repackager by generic (nonproprietary) name)
Route of Administration Oral

Dosage Form Tablets
Strength 50 mg
Brand or Generic Name (Manufacturer) (Available from one or more manufacturer, distributor, and/or repackager by generic (nonproprietary) name)
Route of Administration Oral
Dosage Form Tablets
Strength 100 mg
Brand or Generic Name (Manufacturer) (Available from one or more manufacturer, distributor, and/or repackager by generic (nonproprietary) name)
Route of Administration Oral
Dosage Form Tablets
Strength 500 mg
Brand or Generic Name (Manufacturer) (Available from one or more manufacturer, distributor, and/or repackager by generic (nonproprietary) name)

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

Grades: United States Pharmacopeia; Food Chemical Codex; also available as the hydrochloride.

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 966

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

10.4 Consumption Patterns



APPROX 80% BY ITSELF AS AN ESSENTIAL B VITAMIN; APPROX 20% AS AN ESSENTIAL B VITAMIN IN OTHER APPLICATIONS SUCH AS FLOUR, BAKED GOODS & CEREAL PRODUCTS, & PHARMACEUTICALS (1973)

SRI

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

10.5 U.S. Production



Aggregated Product Volume

2019: 1,000,000 lb - <20,000,000 lb

2018: 1,000,000 lb - <20,000,000 lb

2017: 1,000,000 lb - <20,000,000 lb

2016: 1,000,000 lb - <20,000,000 lb

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

► [EPA Chemicals under the TSCA](#)

(1972) 2.49X10+9 GRAMS ([NIACIN](#) & NICOTINAMIDE)

SRI

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

(1975) 2.5X10+9 GRAMS ([NIACIN](#) & NICOTINAMIDE)

SRI

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

Non-confidential 2016 Chemical Data Reporting (CDR) information on the production and use of chemicals manufactured or imported into the United States. Chemical: Nicotinamide:

Table: National Aggregate Production Volume (pounds)

2011
789,032
2012
Withheld
2013
Withheld
2014
Withheld

2015

Withheld

USEPA; 2016 Chemical Data Reporting Database. Nicotinamide (98-92-0). Available from, as of June 11, 2018: <https://www.epa.gov/chemical-data-reporting>

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

10.6 U.S. Imports



(1972) 1.45X10+9 GRAMS

SRI

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

(1975) 7.5X10+7 GRAMS (NICOTINAMIDE ONLY)

SRI

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

In 1980, 297.1 tons of nicotinamide were imported.

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V24 59 (1980)

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

10.7 General Manufacturing Information



Industry Processing Sectors

All Other Basic Organic Chemical Manufacturing
Food, beverage, and tobacco product manufacturing
Other (requires additional information)

► [EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

3-Pyridinecarboxamide: ACTIVE

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

► [EPA Chemicals under the TSCA](#)

Niacin is a naturally occurring substance. **Nicotinic acid** is the form present in food of plant origin, whereas nicotinamide occurs in animal products.

Blum R; Vitamins, 11. Niacin (Nicotinic Acid and Nicotinamide). Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2018). NY, NY: John Wiley & Sons. Online Posting Date: April 14, 2015

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

The terms **niacin**, **Vitamin B3**, and Vitamin PP have been used to refer to both nicotinamide and **nicotinic acid**.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1213

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

As feed additive esp for pigs, humans, and rats on diet rich in cereal grain or their by-products since vitamin appears to be trapped within indigestible **cellulose** and **lignin** components of foods.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 643

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

11 Identification



11.1 Analytic Laboratory Methods



AOAC Method 975.41. **Niacin** and Niacinamide in cereal products. Automated method.

Association of Official Analytical Chemists. Official Methods of Analysis. 15th ed. and Supplements. Washington, DC: Association of Analytical Chemists, 1990, p. V2 1055

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

AOAC Method 961.14. **Niacin** and Niacinamide in drugs, foods, and feeds. Colorimetric method.

Association of Official Analytical Chemists. Official Methods of Analysis. 15th ed. and Supplements. Washington, DC: Association of Analytical Chemists, 1990, p. V2 1054

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

AOAC Method 985.34. **Niacin** and niacinamide (**nicotinic acid** and nicotinamide) in ready-to-feed milk-based infant formula. Microbiological-turbidimetric method.

Association of Official Analytical Chemists. Official Methods of Analysis. 15th ed. and Supplements. Washington, DC: Association of Analytical Chemists, 1990, p. V2 1109

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

AOAC Method 968.32. Niacinamide in multivitamin preparations by spectrophotometric method.

Association of Official Analytical Chemists. Official Methods of Analysis. 15th ed. and Supplements. Washington, DC: Association of Analytical Chemists, 1990, p. V2 1057

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

For more Analytic Laboratory Methods (Complete) data for Nicotinamide (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



1 of 2	View All
Pictogram(s)  Irritant	
Signal <u>Warning</u>	
GHS Hazard Statements H315 (27.78%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (99.81%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H335 (49.81%): 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 1083 companies from 22 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.

Reported as not meeting GHS hazard criteria by 3 of 1083 companies. For more detailed information, please visit [ECHA C&L website](#).

Of the 20 notification(s) provided by 1080 of 1083 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 (27.78%)

Eye Irrit. 2A (99.81%)

STOT SE 3 (49.81%)

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

12.1.3 Fire Hazards



Combustible. Gives off irritating or toxic fumes (or gases) in a fire. Finely dispersed particles form explosive mixtures in air.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

12.1.4 Hazards Summary



See Nicotinic acid.

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

12.1.5 Fire Potential



This chemical is a noncombustible solid.

Pohanish, R.P. (ed). *Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z*. William Andrew, Waltham, MA 2012, p. 1917

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

12.2 Safety and Hazard Properties



12.2.1 Physical Dangers



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

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

12.3 First Aid Measures



12.3.1 First Aid



EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with [water](#) or [normal saline](#) solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

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

INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of [water](#) to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

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

► CAMEO Chemicals

12.3.2 Inhalation First Aid



Fresh air, rest.

► ILO-WHO International Chemical Safety Cards (ICSCs)

12.3.3 Skin First Aid



Rinse skin with plenty of **water** or shower.

► ILO-WHO International Chemical Safety Cards (ICSCs)

12.3.4 Eye First Aid



Rinse with plenty of **water** (remove contact lenses if easily possible).

► ILO-WHO International Chemical Safety Cards (ICSCs)

12.3.5 Ingestion First Aid



Rinse mouth. Give one or two glasses of **water** to drink.

► ILO-WHO International Chemical Safety Cards (ICSCs)

12.4 Fire Fighting



Use **water** spray, foam, powder, **carbon dioxide**.

► ILO-WHO International Chemical Safety Cards (ICSCs)

12.4.1 Fire Fighting Procedures



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

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

Advice for firefighters: Wear self contained breathing apparatus for fire fighting if necessary.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

... Use dry chemical, [carbon dioxide](#), [water](#) spray, or alcohol foam extinguishers. ... If material of contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Notify local health and fire officials and pollution control agencies. From a secure, explosion-proof location, use [water](#) spray to cool exposed containers. If cooling streams are ineffective (venting sound increase in volume and pitch, tank discolors, or shows any signs of deforming), withdraw immediately to a secure position. If employees are expected to fight fires, they must be trained and equipped in OSHA 1910.156. The only respirators recommended for firefighting are self-contained breathing apparatuses that have full face-pieces and are operated in a pressure-demand or other positive-pressure mode.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 1917

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

12.5 Accidental Release Measures



12.5.1 Spillage Disposal



Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of [water](#).

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

12.5.2 Cleanup Methods



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

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

Evacuate persons not wearing protective equipment from area of spill or leak until clean up is complete. Remove all ignition sources. Use HEPA vacuum or wet method to reduce dust during cleanup. Do not dry sweep. Collect powdered material in the most convenient and safe manner and deposit in sealed containers. Ventilate after clean up is complete. It may be necessary to contain and dispose of this chemical as a hazardous waste. If material of contaminated runoff enters waterways, notify downstream users of potentially contaminated waters.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 1917

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

12.5.3 Disposal Methods



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

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

SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a permitted wastewater treatment facility is acceptable only after review by the governing authority and assurance that "pass through" violations will not occur. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must be evaluated in accordance with EPA 40 CFR Part 261, specifically Subpart B, in order to determine the appropriate local, state and federal requirements for disposal.

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

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Contaminated packaging: Dispose of as unused product.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

12.5.4 Preventive Measures



... Employees should wash immediately with soap when skin is wet or contaminated. ...

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 1916

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

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Do not let product enter drains.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

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

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

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

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

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

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

12.6 Handling and Storage



12.6.1 Nonfire Spill Response



SMALL SPILLS AND LEAKAGE: If you spill this chemical, you should dampen the solid spill material with [water](#), then transfer the dampened material to a suitable container. Use absorbent paper dampened with [water](#) to pick up any remaining material. Seal your contaminated clothing and the absorbent paper in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with a soap and [water](#) solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should store this material in a refrigerator. (NTP, 1992)

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

► [CAMEO Chemicals](#)

12.6.2 Safe Storage



Separated from oxidants.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

12.6.3 Storage Conditions



Keep container tightly closed in a dry and well-ventilated place. Keep in a dry place.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

12.7 Exposure Control and Personal Protection



12.7.1 Inhalation Risk



A nuisance-causing concentration of airborne particles can be reached quickly when dispersed, especially if powdered.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

12.7.2 Effects of Short Term Exposure



The substance is irritating to the eyes.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

12.7.3 Allowable Tolerances



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

40 CFR 180.920; U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of March 14, 2007: <https://www.ecfr.gov>

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

12.7.4 Personal Protective Equipment (PPE)



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

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

► [CAMEO Chemicals](#)

Eye/face protection: Safety glasses with side-shields conforming to EN166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

Skin protection: Handle with gloves.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

Body Protection: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

Respiratory protection: For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

Wear protective gloves and clothing to prevent any reasonable probability of skin contact. ... All protective clothing (suits, gloves, footwear, headgear) should be clean, available each day, and put on before work. ... Wear dust proof chemical goggles and face shield unless full face piece respiratory protection is worn. ... Provide emergency showers and eyewash.

Pohanish, R.P. (ed). Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z. William Andrew, Waltham, MA 2012, p. 1916

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

12.7.5 Fire Prevention



Prevent deposition of dust. Closed system, dust explosion-proof electrical equipment and lighting.

► **ILO-WHO International Chemical Safety Cards (ICSCs)**

12.7.6 Exposure Prevention



PREVENT DISPERSION OF DUST!

- ▶ ILO-WHO International Chemical Safety Cards (ICSCs)

12.7.7 Inhalation Prevention



Avoid inhalation of dust.

- ▶ ILO-WHO International Chemical Safety Cards (ICSCs)

12.7.8 Skin Prevention



Protective gloves.

- ▶ ILO-WHO International Chemical Safety Cards (ICSCs)

12.7.9 Eye Prevention



Wear safety goggles.

- ▶ ILO-WHO International Chemical Safety Cards (ICSCs)

12.7.10 Ingestion Prevention



Do not eat, drink, or smoke during work.

- ▶ ILO-WHO International Chemical Safety Cards (ICSCs)

12.8 Stability and Reactivity



12.8.1 Air and Water Reactions



Water soluble.

- ▶ CAMEO Chemicals

12.8.2 Reactive Group



Amides and Imides

Amines, Phosphines, and Pyridines

► [CAMEO Chemicals](#)

12.8.3 Reactivity Profile



An amine and amide. Acts as a weak base in solution. Amines are chemical bases. They neutralize acids to form salts plus [water](#). These acid-base reactions are exothermic. The amount of heat that is evolved per mole of amine in a neutralization is largely independent of the strength of the amine as a base. Amines may be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous [hydrogen](#) is generated by amines in combination with strong reducing agents, such as hydrides. Organic amides/imides react with azo and diazo compounds to generate toxic gases. Flammable gases are formed by the reaction of organic amides/imides with strong reducing agents. Amides are very weak bases (weaker than [water](#)). Imides are less basic yet and in fact react with strong bases to form salts. That is, they can react as acids. Mixing amides with dehydrating agents such as P2O5 or SOCl2 generates the corresponding nitrile. The combustion of these compounds generates mixed oxides of nitrogen (NOx).

► [CAMEO Chemicals](#)

12.9 Regulatory Information



12.9.1 FIFRA Requirements



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

40 CFR 180.920 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 1, 2018: <https://www.ecfr.gov>

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

12.9.2 FDA Requirements



Nicotinamide-**ascorbic acid** complex may be safely used in accordance with the following prescribed conditions: (a) The additive is the product of the controlled reaction between **ascorbic acid** and nicotinamide, melting in the range 141 °C to 145 °C. (b) It is used as a source of **ascorbic acid** and nicotinamide in multivitamin preparations. /Nicotinamide-**Ascorbic Acid** Complex/

21 CFR 172.315 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 1, 2018: <https://www.ecfr.gov>

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

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

21 CFR 184.1535 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 1, 2018: <https://www.ecfr.gov>

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

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

21 CFR 310.545 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 1, 2018: <https://www.ecfr.gov>

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

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

21 CFR 582.5535 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 1, 2018: <https://www.ecfr.gov>

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

12.10 Other Safety Information



12.10.1 Toxic Combustion Products



... Poisonous gases are produced in a fire. ...

Pohanish, R.P. (ed). *Sittig's Handbook of Toxic and Hazardous Chemical Carcinogens 6th Edition Volume 1: A-K, Volume 2: L-Z*. William Andrew, Waltham, MA 2012, p. 1917

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

Special hazards arising from the substance or mixture: Carbon oxides, nitrogen oxides (NO_x).

Sigma-Aldrich; Safety Data Sheet for Nicotinamide. Product Number: N3376, Version 4.4 (Revision Date 01/16/2015). Available from, as of June 18, 2018: <https://www.sigmaaldrich.com/safety-center.html>

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

12.10.2 Special Reports



Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and [Niacin](#); Intl J of Toxicology 24 (Suppl 5): 1-31 (2005)

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

13 Toxicity



13.1 Toxicological Information



13.1.1 Toxicity Summary



IDENTIFICATION AND USE: Nicotinamide is a white, crystalline powder. Nicotinamide is used to prevent [niacin](#) deficiency and to treat pellagra. Nicotinamide is also used in cosmetics as a hair and skin conditioning agent. It has been used in the enrichment of bread, flour, and other grain-derived products. Animal feed is routinely supplemented with nicotinamide. It is also used in multi-vitamin preparations. Nicotinamide and [niacin](#) are similarly effective as a vitamin because they can be converted into each other within the organism. The blanket term vitamin B(3) is used for both. Niacinamide is a component of important coenzymes involved in [hydrogen](#) transfer. HUMAN STUDIES: In humans, nicotinamide is required for lipid metabolism, tissue respiration, and glycogenolysis. In vivo, nicotinamide is formed from conversion of [niacin](#). In addition, some dietary [tryptophan](#) is oxidized to [niacin](#) and then to nicotinamide in vivo. Nicotinamide is incorporated into 2 coenzymes: [nicotinamide adenine dinucleotide \(NAD\)](#) and [nicotinamide adenine dinucleotide phosphate \(NADP\)](#). [NAD](#) and [NADP](#) act as [hydrogen](#)-carrier molecules in glycogenolysis, tissue respiration, and lipid metabolism. In a study with 6 volunteers (single dose between 3 and 9 g/day) toxic symptoms associated with nicotinamide were mild and consisted mainly of nausea. The effect of 2 mM nicotinamide on unscheduled DNA synthesis on resting human lymphocytes was studied. In

cells treated with UV irradiation or with **N-methyl-N-nitro- N-nitrosoguanidine**, nicotinamide caused a two-fold stimulation of unscheduled DNA synthesis. ANIMAL STUDIES: Application of 0.1 g nicotinamide to the eyes of rabbits induced reversible irritation. It did not produced sensitization in guinea pig test. Single ip injection of nicotinamide (100 mg/kg) to male rats was shown to significantly induce all components of the hepatic microsomal mixed function oxidase system as well as activities of drug-metabolizing enzymes. Groups of 12 male rats were fed nicotinamide in their diet for a period of 8 to 12 weeks. At 0.1% of the diet (100 mg/kg bw per day), nicotinamide caused no significant change in the growth rate, at 0.2%, growth rate was enhanced, but at 0.4%, a marked inhibition of growth rate resulted. Almost complete growth inhibition occurred in rats fed 1% nicotinamide. Lifelong treatment with 1% nicotinamide had no carcinogenic effect in mice. However, nicotinamide promoted **diethylnitrosamine**-induced renal tubular cell tumorigenesis in rats. In mice nicotinamide in doses of 500-2000 mg/kg depresses orientation reflexes and exploring behavior, and has antiaggressive and anticonvulsant properties. Nicotinamide supplementation in pregnant rats led to a decrease in placental and fetal hepatic genomic DNA methylation and genomic **uracil** contents (a factor modifying DNA for diversity) in the placenta and fetal liver and brain, which could be completely or partially prevented by **betaine**. Moreover, nicotinamide supplementation induced tissue-specific alterations in the mRNA expression of the genes encoding nicotinamide N-methyltransferase, DNA methyltransferase 1, catalase and tumor protein p53 in the placenta and fetal liver. High-dose nicotinamide supplementation increased fetal hepatic α -fetoprotein mRNA level, which was prevented by **betaine** supplementation. It is concluded that maternal nicotinamide supplementation can induce changes in fetal epigenetic modification and DNA base composition. Nicotinamide was negative in an Ames test performed with Salmonella strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538 both with and without metabolic activation. Nicotinamide was not mutagenic in Saccharomyces stain D4. It was reported that nicotinamide at concentrations of 3 mg/mL (25 mM) induced large structural chromosome aberrations in vitro in Chinese hamster ovary cells.

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

Uremic toxins such as nicotinamide are actively transported into the kidneys via organic ion transporters (especially OAT3). Increased levels of uremic toxins can stimulate the production of reactive oxygen species. This seems to be mediated by the direct binding or inhibition by uremic toxins of the enzyme **NADPH** oxidase (especially NOX4 which is abundant in the kidneys and heart) (A7868). Reactive oxygen species can induce several different DNA methyltransferases (DNMTs) which are involved in the silencing of a protein known as KLOTHO. KLOTHO has been identified as having important roles in anti-aging, mineral metabolism, and vitamin D metabolism. A number of studies have indicated that KLOTHO mRNA and protein levels are reduced during acute or chronic kidney diseases in response to high local levels of reactive oxygen species (A7869).

► [Toxin and Toxin Target Database \(T3DB\)](#)

13.1.2 Carcinogen Classification



Carcinogen Classification

No indication of carcinogenicity to humans (not listed by IARC).

► [Toxin and Toxin Target Database \(T3DB\)](#)

13.1.3 Health Effects



Chronic exposure to uremic toxins can lead to a number of conditions including renal damage, chronic kidney disease and cardiovascular disease.

► [Toxin and Toxin Target Database \(T3DB\)](#)

13.1.4 Exposure Routes



Endogenous, Ingestion, Dermal (contact)

► [Toxin and Toxin Target Database \(T3DB\)](#)

13.1.5 Symptoms



As a uremic toxin, this compound can cause uremic syndrome. Uremic syndrome may affect any part of the body and can cause nausea, vomiting, loss of appetite, and weight loss. It can also cause changes in mental status, such as confusion, reduced awareness, agitation, psychosis, seizures, and coma. Abnormal bleeding, such as bleeding spontaneously or profusely from a very minor injury can also occur. Heart problems, such as an irregular heartbeat, inflammation in the sac that surrounds the heart (pericarditis), and increased pressure on the heart can be seen in patients with uremic syndrome. Shortness of breath from fluid buildup in the space between the lungs and the chest wall (pleural effusion) can also be present.

► [Toxin and Toxin Target Database \(T3DB\)](#)

13.1.6 Inhalation Symptoms



Cough.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

13.1.7 Eye Symptoms



Redness. Pain.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

13.1.8 Acute Effects



6 items 	
Search	
Compound CID	936
Organism	rat
Test Type	LD50
Route	oral
Dose	3500 mg/kg
Effect	
Reference	Prehled Prumyslove Toxikologie; Organicke Latky, Marhold, J., Prague, Czechoslovakia, Avicenum, 1986, -(1390), 1986
Compound CID	936

► [ChemIDplus](#)

13.1.9 Treatment



Kidney dialysis is usually needed to relieve the symptoms of uremic syndrome until normal kidney function can be restored.

► [Toxin and Toxin Target Database \(T3DB\)](#)

13.1.10 Interactions



Addition of 0.5 mg of nicotinamide reduced the action of [dicrotophos](#) on cultured chick embryo tibiae.

Autissier-Navarro C et al; Cr Seances Soc Biol Ses Fil 171 (6): 1235 (1977)

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

Nicotinamide will prevent depletion of [NAD](#) coenzymes by alkylating agents.

Schoental R; Cancer (Phila) 40 (4): 1833 (1977)

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

Renal oncogenic activity of [Streptozotocin](#) in male rats was significantly decreased by nicotinamide.

[PMID:175379](#)

Rakieten N et al; Proc Soc Exp Biol Med 151 (2): 356 (1976)

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

Oral or iv administered nicotinamide prevented [Streptozotocin](#)-induced diabetes in Rhesus monkeys and dogs.

[PMID:4267772](#)

Schein PS et al; Proc Soc Exp Biol Med 143 (2): 514 (1973)

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

For more Interactions (Complete) data for Nicotinamide (25 total), please visit the [HSDB record page](#).

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

13.1.11 Antidote and Emergency Treatment



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

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160

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

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

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160

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

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema Consider administering a beta agonist such as **albuterol** for severe bronchospasm Monitor cardiac rhythm and treat arrhythmias as necessary Start IV administration of D5W TKO /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload Treat seizures with **diazepam (Valium)** or **lorazepam (Ativan)** Use **proparacaine hydrochloride** to assist eye irrigation /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160-1

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

13.1.12 Human Toxicity Excerpts



/HUMAN EXPOSURE STUDIES/ In studies with diabetic and at-risk-of-diabetes patients who were treated for several years with 1.5 to 3 g nicotinamide daily (25 and 42 mg/kg/day, respectively) no effect on a range of biochemical parameters including liver and kidney function was observed.

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0) p.15 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

/HUMAN EXPOSURE STUDIES/ In a study with 6 volunteers (single dose between 3 and 9 g/day) toxic symptoms associated with nicotinamide were mild and consisted mainly of nausea.

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0) p.16 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

/GENOTOXICITY/ The effect of 2 mM Niacinamide on unscheduled DNA synthesis on resting human lymphocytes /was studied/. In cells treated with UV irradiation or with **N-methyl-N-nitro- N-nitrosoguanidine**, niacinamide caused a two-fold stimulation of unscheduled DNA synthesis and retarded the rate of **NAD+** lowering caused by these treatments. Niacinamide also reduced the burst of poly(ADP-ribose) synthesis caused by **N-methyl-N-nitro- N-nitrosoguanidine** treatment. The effect of niacinamide on unscheduled DNA synthesis was shown to be independent of protein or polyamine synthesis.

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.15; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

13.1.13 Non-Human Toxicity Excerpts



/LABORATORY ANIMALS: Acute Exposure/ Application of 0.1 g nicotinamide to the eyes of 3 rabbits induced irritation in two of the animals, which was reversible within 7 days. The third animal showed irritation after 2 hours and was killed for humane reasons. In a second study with a similar design irritant effects were reversible within one week except for hyperemia of the conjunctivae in one animal.

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0) p.14 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

/LABORATORY ANIMALS: Acute Exposure/ Single ip injection of nicotinamide (100 mg/kg) to male rats was shown to significantly induce all components of the hepatic microsomal mixed function oxidase system as well as activities of drug-metabolizing enzymes.

[PMID:6444527](#)

Kamat JP et al; *Biochim Biophys Acta* 628 (1): 26 (1980)

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

/LABORATORY ANIMALS: Acute Exposure/ Seven New Zealand White rabbits were intradermally injected with a series of low concentrations of niacinamide, [sodium lauryl sulfate](#), and saline control. Niacinamide at 0.1, 0.25, 1, and 2.5% dissolved in saline, [sodium lauryl sulfate](#) at 0.02, 0.005, 0.1, and 0.5%, and saline were given in aliquots of 0.1 mL at different sites on the clipped dorsum of each rabbit. The size and nature of the reactions were assessed under a uniform white light at 24 and 48 hr after injection. ... Niacinamide produced a slight irritation in three out of seven animals at 2.5%, with a mean reaction size of 2.43 mm at 24 hr, and no visible response at 1, 0.25, and 0.1%. The level of response to all concentrations of niacinamide was less than to 0.5 and 0.1% [sodium lauryl sulfate](#). At 0.5% [sodium lauryl sulfate](#), distinct to fairly well developed irritation and slight necrosis was seen in all seven animals with a mean reaction size of 20.29 mm at 24 hr. Under the conditions of this study, 2.5% niacinamide was only marginally irritating to rabbit skin. The overall level of irritation was significantly less than that produced by [sodium lauryl sulfate](#).

Cosmetic Ingredient Review (CIR) Expert Panel; Final Report of the Safety Assessment of Niacinamide and Niacin p.14; Intl J of Toxicology 24 (Suppl 5): 1-31 (2005). Available from, as of June 4, 2018: <https://www.cir-safety.org/ingredients>

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

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ ... Male rats (10/treatment) were fed diets with high or low fat content with or without added nicotinamide (100 mg/kg bw per day) during 3 or 6 weeks. Increased concentrations of fat in the liver were found only when the high fat diet was combined with an excessive intake of nicotinamide. A further study suggested that the fatty livers resulted from an induced [choline](#) deficiency brought about by the methylation of nicotinamide to the excretory product [N1-methylnicotinamide](#).

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0) p.15 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

For more Non-Human Toxicity Excerpts (Complete) data for Nicotinamide (21 total), please visit the [HSDB record page](#).

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

13.1.14 Non-Human Toxicity Values



LD50 Rat oral 3500 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2623

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

LD50 Rat sc 1680 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2623

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

LD50 Mouse oral 2500 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2623

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

LD50 Mouse ip 2050 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2623

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

For more Non-Human Toxicity Values (Complete) data for Nicotinamide (9 total), please visit the [HSDB record page](#).

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

13.1.15 Ecotoxicity Values



LC50; Species: *Poecilia reticulata* (Guppy) age 1.5-2.5 weeks; Conditions: freshwater, static, 22-23 °C, pH 7.8-8.2, dissolved [oxygen](#) >5 mg/L; Concentration: >1000 mg/L for 96 hr />99%

purity/

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, Nicotinamide (98-92-0) p.37 (October 2002). Available from, as of August 12, 2018:

<https://www.inchem.org/pages/sids.html>

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

EC50; Species: *Daphnia magna* (Water flea) age <24 hr; Conditions: freshwater, static, 18.5-20 °C, pH 8.1-8.2; Concentration: >1000 mg/L for 24 hr; Effect: immobilization />99% purity/

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, Nicotinamide (98-92-0) p.37 (October 2002). Available from, as of August 12, 2018:

<https://www.inchem.org/pages/sids.html>

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

EC50; Species: *Scenedesmus subspicatus* (algae) strain CCAP 276/20; Conditions: freshwater, static, 21.5-25.5 °C, pH 8.1-9.9; Concentration: >1000 mg/L for 72 hr; Effect: growth inhibition />99% purity/

OECD; Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, Nicotinamide (98-92-0) p.38 (October 2002). Available from, as of August 12, 2018:

<https://www.inchem.org/pages/sids.html>

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

EC50; Species: *Xenopus laevis* (African clawed frog) embryos; Conditions: freshwater, renewal, 23 °C; Concentration: 340 ug/L for 96 hr (95% confidence interval: 310-360 ug/L); Effect: abnormal growth

Dawson DA, Wilke TS; *Environ Toxicol Chem* 10: 941-948 (1991) Available from, as of February 12, 2007

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

13.1.16 Ongoing Test Status



EPA has released the Interactive Chemical Safety for Sustainability (iCSS) Dashboard. The iCSS Dashboard provides an interactive tool to explore rapid, automated (or in vitro high-throughput) chemical screening data generated by the Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration. /The title compound was tested by ToxCast and/or Tox21 assays/[USEPA; iCSS Dashboard Application; Available from, as of August 9, 2018: <http://actor.epa.gov/dashboard/>]

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

The following link will take the user to the National Toxicology Program (NTP) Test Status of Agents Search page, which tabulates the results and current status of tests such as "Short-Term Toxicity Studies", "Long-term Carcinogenicity Studies", "Developmental Studies", "Genetic Toxicology Studies", etc., performed with this chemical. Testing status for nicotinamide is available.[Available from, as of August 8, 2018: <https://ntpsearch.niehs.nih.gov/?e=True&ContentType=Testing+Status>]

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

13.1.17 Populations at Special Risk



Large doses of **niacin** or niacinamide should be administered with caution to patients with gallbladder disease or a history of jaundice or liver disease, diabetes mellitus, gout, peptic ulcer, or allergy. **Niacin** and niacinamide are contraindicated in patients with liver disease, active peptic ulcer, or hypersensitivity to the drugs.

American Society of Health-System Pharmacists 2017; Drug Information 2017. Bethesda, MD. 2017

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

13.2 Ecological Information



13.2.1 Environmental Fate / Exposure Summary



Nicotinamide's production and use as a dietary supplement and administration as a medicine and in cosmetics as a hair and skin conditioning agent may result in its release to the environment through various waste streams. Nicotinamide (**vitamin B3**) is a precursor of the coenzymes **NAD** and **NADP**. If released to air, an estimated vapor pressure of 4.2X10⁻⁴ mm Hg at 25 °C indicates nicotinamide will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase nicotinamide 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 6 days. Particulate-phase nicotinamide will be removed from the atmosphere by wet or dry deposition. Nicotinamide absorbs UV light at wavelengths >300 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, nicotinamide is expected to have very high mobility based upon an estimated K_{oc} of 15. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 2.9X10⁻¹² atm-cu m/mole. Nicotinamide was determined to be readily biodegradable in an aerobic screening test, suggesting that biodegradation may be an important environmental fate process in soil and **water**. If released into **water**, nicotinamide is not expected to adsorb to suspended solids and sediment based upon the estimated K_{oc}.

Volatilization from **water** surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. Hydrolysis is not expected to be an important environmental fate process since amides hydrolyze slowly under environmental conditions. Occupational exposure to nicotinamide may occur through inhalation of dust and dermal contact with this compound at workplaces where nicotinamide is produced or used. Monitoring data indicate that the general population may be exposed to nicotinamide via ingestion of food, smoking cigarettes and dermal contact with consumer products containing this compound. Exposure to nicotinamide will also occur by direct medical treatment. (SRC)

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

13.2.2 Natural Pollution Sources



Nicotinamide is a precursor of the coenzymes **NAD** and **NADP**(1). Nicotinamide and **nicotinic acid** occur in nature almost exclusively in the bound form. In plants, **nicotinic acid** is prevalent whereas in animals nicotinamide is the predominant form. This nicotinamide is exclusively in the form of **NAD** and **NADP**(2).

(1) O'Neil MJ, ed; *The Merck Index*. 15th ed., Cambridge, UK: Royal Society of Chemistry, p. 1213 (2013) (2) van Arnum SD; *Niacin, Nicotinamide, and Nicotinic Acid*. *Kirk-Othmer Encyclopedia of Chemical Technology*. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

13.2.3 Artificial Pollution Sources



Nicotinamide's production and use as a dietary supplement and administration as a medicine(1) and in cosmetics as a hair and skin conditioning agent(2) may result in its release to the environment through various waste streams(SRC).

(1) Larranaga MD et al; *Hawley's Condensed Chemical Dictionary* 16th ed., Hoboken, NJ: John Wiley & Sons, Inc. p. 966 (2016) (2) OECD; *Screening Information Data Set (SIDS) Initial Assessment Report for SIDS Initial Assessment Meeting (SIAM) 15, 3-Pyridinecarboxamide (Nicotinamide) (98-92-0)* p.6 (October 2002). Available from, as of June 4, 2018: <https://www.inchem.org/pages/sids.html>

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

13.2.4 Environmental Fate



TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 8(SRC), determined from a structure estimation method(2), indicates that nicotinamide is expected to have very high /mobility in soil(SRC). Volatilization of nicotinamide from moist soil surfaces is

not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 2.9×10^{-12} atm-cu m/mole(SRC), developed using a fragment constant estimation method(2). Nicotinamide is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 4.2×10^{-4} mm Hg at 25 °C(SRC), determined from a fragment constant method(2). Nicotinamide was determined to be readily biodegradable in an aerobic screening test(3) suggesting that biodegradation may be an important environmental fate process in soil(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (3) Richardson ML, Bowron JM; J Pharm Pharmacol 37: 1-12 (1985)

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

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 8(SRC), determined from a structure estimation method(2), indicates that nicotinamide is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from **water** surfaces is not expected(3) based upon an estimated Henry's Law constant of 2.9×10^{-12} atm-cu m/mole(SRC), developed using a fragment constant estimation method(2). According to a classification scheme(4), an estimated BCF of 3(SRC), from its log Kow of -0.37(5) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Nicotinamide was determined to be readily biodegradable in an aerobic screening test(6) suggesting that biodegradation may be an important environmental fate process in **water**(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (4) Franke C et al; Chemosphere 29: 1501-14 (1994) (5) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 19 (1995) (6) Richardson ML, Bowron JM; J Pharm Pharmacol 37: 1-12 (1985)

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

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), nicotinamide, which has an estimated vapor pressure of 4.2×10^{-4} 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 nicotinamide 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 6 days(SRC), calculated from its rate constant of 2.5×10^{-12} cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(2). Particulate-phase nicotinamide may be removed from the air by wet and dry deposition(SRC). Nicotinamide absorbs UV light at wavelengths >300 nm(3) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

(1) Bidleman TF; *Environ Sci Technol* 22: 361-367 (1988) (2) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (3) NIST; *NIST Chemistry WebBook*. Nicotinamide (98-92-0). NIST Standard Reference Database No. 69, Feb 2015 Release. Washington, DC: US Sec Commerce. Available from, as of June 19, 2018: <https://webbook.nist.gov>

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

13.2.5 Environmental Biodegradation



AEROBIC: Nicotinamide was determined to be readily biodegradable in an aerobic screening test recommended by the Department of Environment, Standing Committee of Analysts, UK(1).

[PMID:2858520](#)

(1) Richardson ML, Bowron JM; *J Pharm Pharmacol* 37: 1-12 (1985)

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

ANAEROBIC: Nicotinamide was not degraded using an anaerobic spore-forming rod (*Clostridia* sp.) bacteria isolated from Potamac River mud(1).

(1) Shukla OP; *J Sci Ind Res* 43: 98-116 (1984)

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

13.2.6 Environmental Abiotic Degradation



The rate constant for the vapor-phase reaction of nicotinamide with photochemically-produced hydroxyl radicals has been estimated as 2.5×10^{-12} cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 6 days at an atmospheric concentration of 5×10^5 hydroxyl radicals per cu cm(1). Some hydrolysis of nicotinamide may occur; however, amides are only slowly hydrolyzed under environmental conditions(2). The rate constant for the reaction of hydroxyl radicals in aqueous solutions at pH 5.9 and 9.0 is 1.4×10^9 and 1.5×10^9 L/mol-sec, respectively(3); this corresponds to aquatic half-lives of 1.6 and 1.5 yrs, respectively, at an aquatic concentration of 1×10^{-17} hydroxyl radicals per liter(4). Nicotinamide absorbs UV light at wavelengths >300 nm(5) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

(1) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (2) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*. Washington, DC: Amer Chem Soc pp. 7-4, 7-5 (1990) (3) Buxton GV et al; *J Phys Chem Ref Data* 17: 513-882 (1988) (4) Mill T et al; *Science* 207: 886-887 (1980) (5) NIST; *NIST Chemistry WebBook*. Nicotinamide (98-92-0). NIST Standard Reference Database No. 69, Feb 2015 Release. Washington, DC: US Sec Commerce. Available from, as of June 19, 2018: <https://webbook.nist.gov>

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

13.2.7 Environmental Bioconcentration



An estimated BCF of 3 was calculated in fish for nicotinamide(SRC), using a log Kow of -0.37(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Hansch C et al; *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants*. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 19 (1995) (2) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (3) Franke C et al; *Chemosphere* 29: 1501-14 (1994)

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

13.2.8 Soil Adsorption / Mobility



Using a structure estimation method based on molecular connectivity indices(1), the Koc of nicotinamide can be estimated to be 8(SRC). According to a classification scheme(2), this estimated Koc value suggests that nicotinamide is expected to have very high mobility in soil(SRC).

(1) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (2) Swann RL et al; *Res Rev* 85: 17-28 (1983)

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

13.2.9 Volatilization from Water / Soil



The Henry's Law constant for nicotinamide is estimated as 2.9×10^{-12} atm-cu m/mole(SRC) developed using a fragment constant estimation method(1). This Henry's Law constant indicates that nicotinamide is expected to be essentially nonvolatile from [water](#) and moist soil surfaces(2). Nicotinamide is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 4.2×10^{-4} mm Hg(SRC), determined from a fragment constant method(1).

(1) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.11. Nov, 2012. Available from, as of June 19, 2018: <https://www2.epa.gov/tsca-screening-tools> (2) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)

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

13.2.10 Food Survey Values



Nicotinamide is prevalent in many common foodstuffs and is especially concentrated in brewer's yeast, wheat germ and liver(1).

(1) van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

Nicotinic Acid and Nicotinamide (Vitamin B3) Foodstuff Content(1).

Table: [Vitamin B3](#) content as compared to [niacin](#) potential from [tryptophan](#)

Food
Cow milk, whole fresh summer
Potential, mg/kg
0.8
Food
Cheese, cream cheese
Potential, mg/kg
0.8
Food
Eggs, whole, raw
Potential, mg/kg
0.7
Food
Butter, salted
Potential, mg/kg
trace
Food
Beef, lean, avg, raw
Potential, mg/kg
52
Food
Beef liver, fresh
Potential, mg/kg
178

Food Pork, lean, avg, raw Potential, mg/kg 62
Food Pork liver, fresh Potential, mg/kg 118
Food Corn, whole Potential, mg/kg 12
Food Corn, flour Potential, mg/kg trace
Food Breakfast cereals, all-bran Potential, mg/kg 490
Food Cornflakes, fortified Potential, mg/kg 210
Food Cornflakes, unfortified Potential, mg/kg 6
Food Wheat flour whole meal Potential, mg/kg 56
Food White, 72% for bread fortified; unfortified

Potential, mg/kg 20; 7
Food Brown, 85% fortified; unfortified
Potential, mg/kg 42; 12
Food Bread, white
Potential, mg/kg 14
Food Macaroni, boiled
Potential, mg/kg 3
Food Rice, polished, boiled
Potential, mg/kg 3
Food Rice, bran
Potential, mg/kg 366-437
Food Soybean flour, full fat
Potential, mg/kg 20
Food Spaghetti, boiled
Potential, mg/kg 3
Food Potatoes, raw
Potential, mg/kg 12

Food

Yeast, Baker's dry

Potential, mg/kg

257

(1) van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

Nicotinic Acid and Nicotinamide (**Vitamin B3**) in Coffee(1).

Table: **Vitamin B3** content as compared to **niacin** potential from **tryptophan**

Food item

Green

Potential, mg/kg

20

Food item

Medium roasted

Potential, mg/kg

80-150

Food item

Dark Roasted

Potential, mg/kg

<500

(1) van Arnum SD; Niacin, Nicotinamide, and Nicotinic Acid. Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2018). New York, NY: John Wiley & Sons. Online Posting Date: 4 Dec 2000

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

13.2.11 Plant Concentrations



Nicotinamide occurrence in plants(1).

Genus species

Agrimonia eupatoria

Family

Rosaceae

Common name(s)

Arimony, Sticklewort

Part Leaf
Concn (ppm) 100-300
Genus species Linum usitatissimum
Family Linaceae
Common name(s) Linseed, Flax
Part Seed
Concn (ppm) 38
Genus species Theobroma cacao
Family Sterculiaceae
Common name(s) Cacao
Part Seed
Concn (ppm) 21
Genus species Pisum sativum
Family Fabaceae
Common name(s) Pea
Part Sprout seedling
Concn (ppm) 0.7
Genus species

Panax ginsend
Family Araliaceae
Common name(s) Oriental Ginseng; Korean Ginseng; Chinese Ginseng; Ginseng
Part Root
Concn (ppm) not reported
Genus species Petroselinum crispum
Family Apiaceae
Common name(s) Parsley
Part Plant
Concn (ppm) not reported
Genus species Anemarrhena asphodeloides
Family Liliaceae
Common name(s) Zhi-Mu; Chih-Mu
Part Rhizome
Concn (ppm) not reported
Genus species Angelica sinensis
Family Apiaceae
Common name(s) Dang Gui; Dong Quai; Dang Qui; Dong Gui; Chinese Angelica; Dang Quai
Part

Root
Concn (ppm) not reported
Genus species Trigonella foenum-graecum
Family Fabaceae
Common name(s) Alholva (Sp.); Greek Hay; Fenugreek; Greek Clover; Bockshornklee (Ger.)
Part Seed
Concn (ppm) not reported

(1) Dr. Duke's Phytochemical and Ethnobotanical Databases. Nicotinic Acid. Available from, as of June 19, 2018: <https://phytochem.nal.usda.gov/phytochem/search>

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

13.2.12 Other Environmental Concentrations



Nicotinamide is a component of tobacco, tobacco smoke and tobacco substitute smoke(1).

(1) Rodgman A, Perfetti TA; *The Chemical Components of Tobacco and Tobacco Smoke*. Boca Raton, FL: CRC Press p. 674 (2009)

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

13.2.13 Probable Routes of Human Exposure



According to the 2016 [TSCA](#) Inventory Update Reporting data, 2 reporting facilities estimate the number of persons reasonably likely to be exposed during the manufacturing, processing, or use of nicotinamide in the United States may be as low as 25 workers and as high as 50 workers per plant; the data may be greatly underestimated due to confidential business information (CBI) or unknown values(1).

(1) US EPA; *Chemical Data Reporting (CDR). Non-confidential 2016 Chemical Data Reporting information on chemical production and use in the United States*. Available from, as of Jun 19, 2018:

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

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

NIOSH (NOES Survey 1981-1983) has statistically estimated that 64,950 workers (44,524 of these are female) are potentially exposed to nicotinamide in the US(1). Occupational exposure to nicotinamide may occur through inhalation of dust and dermal contact with this compound at workplaces where nicotinamide is produced or used(SRC). Monitoring data indicate that the general population may be exposed to nicotinamide via ingestion of food and smoking cigarettes. Exposure to nicotinamide will also occur by direct medical treatment(SRC).

(1) CDC; *International Chemical Safety Cards (ICSC) 2012*. Atlanta, GA: Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health (NIOSH). Ed Info Div. Available from, as of June 19, 2018: <https://www.cdc.gov/niosh/ipcs/default.html>

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

14 Associated Disorders and Diseases



44 items



Disease

Diabetes Mellitus, Type 1

Evidence Type

therapeutic

Evidence PMID

17430113

Disease

Hyperinsulinism

Evidence Type

therapeutic

Evidence PMID

32298659

Disease

Child Behavior Disorders

Evidence Type

Page 1 of 9



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

1 item	
Indication Inflammatory skin condition	
ICD-11 Code ⓘ FE20.Y	

► **Therapeutic Target Database (TTD)**

Disease Uremia
References PubMed: 11865086 , 10509899 , 9607216 , 7482520 , 6520173 , 22626821 , 21359215 , 2026685 , 9573551 , 24023812 , 15353324 , 19309105 , 8087979 , 17132244 , 12675874 Merck Manual of Diagnosis and Therapy. David F. Putnam Composition and Concentrative Properties of Human Urine. NASA Contractor Report. July 1971 Geigy Scientific Tables, 8th Rev edition, pp. 130. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp. Basel, Switzerland c1981-1992. Geigy Scientific Tables, 8th Rev edition, pp. 165-177. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp., Basel, Switzerland c1981-1992. National Health and Nutrition Examination Survey (NHANES Survey) 2013 Geigy Scientific Tables, 8th Rev edition, pp. 80-82. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp., Basel, Switzerland c1981-1992.
Disease Crohn's disease
References PubMed: 16440420 , 11418788 , 8723414 , 19491857 , 17269711 , 23516449 , 23867873 , 24811995 , 25598765 , 26806034 , 26848182 , 27609529 , 28842642
Disease Ulcerative colitis
References PubMed: 21059682 , 1740537 , 17269711 , 17314143 , 21761941 , 23516449 , 23867873 , 24811995 , 25598765 , 26806034 , 26848182 , 27609529 , 28842642
Disease Diverticular disease
References PubMed: 8723414 , 27622378

Disease

Colorectal cancer

References

PubMed: [7482520](#), [19006102](#), [23940645](#), [24424155](#), [20156336](#), [19678709](#), [22148915](#), [25105552](#), [21773981](#), [25037050](#), [27015276](#), [27107423](#), [27275383](#), [28587349](#)

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

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

15 Literature



15.1 Consolidated References



29,386 items



SORT BY Publication Date - Most Recent

**Enzymatic cofactor regeneration systems: A new perspective on efficiency assessment****Publication Name:** The Science of the total environment**Publication Date:** 2023-04-10**PMID:** [36657682](#)**DOI:** [10.1016/j.scitotenv.2023.161630](#)**Cancer immunity and immunotherapy beyond COVID-19****Publication Name:** Cancer immunology, immunotherapy : CII**Publication Date:** 2023-03-30**PMID:** [36995489](#)**DOI:** [10.1007/s00262-023-03411-9](#)**Pathological mechanisms of cigarette smoking, dietary, and sedentary lifestyle risks in vascular dysfunction: mitochondria as a common target of risk factors****Publication Name:** Pflugers Archiv : European journal of physiology**Publication Date:** 2023-03-30**PMID:** [36995495](#)**DOI:** [10.1007/s00424-023-02806-y](#)**Preparation of niacinamide imprinted starch-based biomaterials for treating of hyperpigmentation****Publication Name:** International Journal of Biological Macromolecules

Publication Date: 2023-03-30

PMID: [36693604](#)

DOI: [10.1016/j.ijbiomac.2023.123382](#)

[An integrated multi-omic approach demonstrates distinct molecular signatures between human obesity with and without metabolic complications: a case-control study](#)

Page 1 of 5,878

► PubChem

15.2 NLM Curated PubMed Citations



All NLM Curated PubMed Citations



administration and dosage	deficiency	statistics and numerical data
adverse effects	economics	supply and distribution
agonists	genetics	therapeutic use
analogs and derivatives	immunology	therapy
analysis	isolation and purification	toxicity
antagonists and inhibitors	metabolism	urine
biosynthesis	pharmacokinetics	
blood	pharmacology	
cerebrospinal fluid	physiology	
chemical synthesis	poisoning	
chemistry	radiation effects	
classification	standards	

► PubChem

15.3 Springer Nature References



13,653 items



Search

SORT BY Publication Date - Oldest

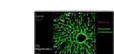


[Nicotinamide promotes cardiomyocyte derivation and survival through kinase inhibition in human pluripotent stem cells](#)

PMID: [34845199](#)

Publication Date: 2021

Publication Name: Cell Death & Disease

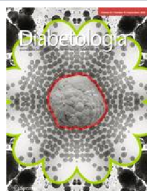


Nicotinamide is an inhibitor of SIRT1 in vitro, but can be a stimulator in cells

PMID: 28417163

Publication Date: 2017

Publication Name: Cellular and Molecular Life Sciences



Nicotinamide — biological actions and therapeutic potential in diabetes prevention

Publication Date: 1993

Publication Name: Diabetologia



Page 1 of 2,731

Springer Nature

15.4 Thieme References



47 items



Search

SORT BY Publication Date - Most Recent



Synthesis from 2-Bromoaryl Methyl Ketones

Publication Date: 2022

Publication Name: Science of Synthesis

Mesoporous Carbon-Catalyzed Oxidative Amination of C-Methyl Groups in N-Heterocycles

DOI: 10.1055/s-0041-1737263

Publication Date: 2021

Publication Name: Synfacts

[Synthesis of Primary Amides by Site-Selective Hydrolysis](#)DOI: [10.1055/s-0040-1706182](#)

Publication Date: 2021

Publication Name: Synfacts

[Synthesis of Alogliptin](#)DOI: [10.1055/s-0040-1719789](#)

Publication Date: 2021

Publication Name: Synfacts

[Aerobic Oxidation Using Nitroxides and Metal Ions](#)

Publication Date: 2021

Publication Name: Science of Synthesis

<< < Page 1 of 10 > >>

[► Thieme Chemistry](#)

15.5 Wiley References



11 items



SORT BY Publication Date - Most Recent

[Development of a Second Generation Palladium Catalyst System for the Aminocarbonylation of Aryl Halides with CO and Ammonia](#)DOI: [10.1002/asia.201000418](#)

Publication Name: Chem. Asian J.

[New Heterocyclic Compounds Derived from 4,6-Diamino-3-cyano-2-methylthiopyridine and their Biological Activity](#)DOI: [10.1002/jhet.2649](#)

Publication Date: 2017

Publication Name: J. Heterocyclic Chem.

[Design, Synthesis, and Biological Evaluation of Some Cyclohepta\[b\]Thiophene and Substituted Pentahydrocycloheptathieno\[2,3-d\]Pyrimidine Derivatives](#)DOI: [10.1002/jhet.2678](#)

Publication Date: 2017

Publication Name: J. Heterocyclic Chem.

[Utility of Acetylenedicarboxylate in Organic Synthesis](#)

DOI: [10.1002/jhet.2697](https://doi.org/10.1002/jhet.2697)

Publication Date: 2017

Publication Name: J. Heterocyclic Chem.

[Design and Synthesis of New 9-Substituted Norharmene Derivatives as Potential Sirt5 Inhibitors](#)DOI: [10.1002/jhet.2732](https://doi.org/10.1002/jhet.2732)

Publication Date: 2017

Publication Name: J. Heterocyclic Chem.

<< < Page 1 of 3 > >>

► Wiley

15.6 Depositor Provided PubMed Citations



6,274 items



Search

SORT BY Publication Date - Most Recent



Therapeutic targeting of hepatocellular carcinoma cells with antrocinol, a novel, dual-specificity, small-molecule inhibitor of the KRAS and ERK oncogenic signaling pathways

PMID: [36565974](#)

Publication Date: 2023-01-25

Journal: Chemico-biological interactions

A phase 3, open-label, randomized study of asciminib, a STAMP inhibitor, vs bosutinib in CML after 2 or more prior TKIs

PMID: [34407542](#)

Publication Date: 2021-11-25

Journal: Blood

Resveratrol-induced Sirt1 phosphorylation by LKB1 mediates mitochondrial metabolism

PMID: [34216621](#)

Publication Date: 2021-08-01

Journal: The Journal of biological chemistry

Modulation of antioxidant enzymes, SIRT1 and NF-κB by resveratrol and nicotinamide in alcohol-aflatoxin B1-induced hepatocellular carcinoma

PMID: [32894639](#)

Publication Date: 2021-01-01

Journal: Journal of biochemical and molecular toxicology

Reduction of fatty liver in rats by nicotinamide via the regeneration of the methionine cycle and the inhibition of aldehyde oxidase

PMID: [33408299](#)

Publication Date: 2021-01-01

Journal: The Journal of toxicological sciences

Page 1 of 1,255

► [PubChem](#)

15.7 Synthesis References



Helmut Beschke, Heinz Friedrich, Klaus-Peter Muller, Gerd Schreyer, "Process for the production of nicotinamide." U.S. Patent US4314064, issued May, 1949.

► [DrugBank](#)

Galat, Alexander. Nicotinamide from [nicotinonitrile](#) by catalytic hydration. Journal of the American Chemical Society (1948), 70 3945.

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

15.8 Metabolite References



86 items



Search

SORT BY [PMID - Increasing](#)



PMID

Reference

Galat, Alexander. Nicotinamide from nicotinonitrile by catalytic hydration. Journal of the American Chemical Society (1948), 70 3945.

PMID

[11865086](#)

Reference

Canepa A, Filho JC, Gutierrez A, Carrea A, Forsberg AM, Nilsson E, Verrina E, Perfumo F, Bergstrom J: Free amino acids in plasma, red blood cells, polymorphonuclear leukocytes, and muscle in normal and uraemic children. Nephrol Dial Transplant. 2002 Mar;17(3):413-21.

PMID

[10509899](#)

Reference

Fujita T, Amuro Y, Hada T, Higashino K: Plasma levels of pipercolic acid, both L- and D-enantiomers, in patients with chronic liver diseases. especially hepatic encephalopathy. Clin Chim Acta. 1999

Page 1 of 18

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

15.9 General References



Neumann et al. Genetically encoding N^ε-acetyllysine in recombinant proteins Nature Chemical Biology, doi: 10.1038/nchembio.73, published online 17 February 2008. <http://www.nature.com/naturechemicalbiology>

► [Nature Chemical Biology](#)

Chen et al. A small molecule that directs differentiation of human ESCs into the pancreatic lineage Nature Chemical Biology, doi: 10.1038/nchembio.154, published online 15 March 2009 <http://www.nature.com/naturechemicalbiology>

► [Nature Chemical Biology](#)

Kim et al. Permissive epigenomes endow reprogramming competence to transcriptional regulators. Nature Chemical Biology, doi: 10.1038/s41589-020-0618-6, published online 17 August 2020

► [Nature Chemical Biology](#)

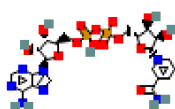
15.10 Chemical Co-Occurrences in Literature



Showing 3 of 25 [View More](#)



Chemical



Nadide

CID 5892

Selected evidence

2,230 articles

[View All](#)**The use of Nicotinamide and Nicotinamide riboside as an adjunct therapy in the treatment of glaucoma**

PMID 36916064; DOI 10.1177/11206721231161101; European journal of ophthalmology 2023 Mar; ?(?):11206721231161101 (Review Article)

Name matches: **nicotinamide adenine dinucleotide** *nicotinamide*

Recent advances of targeting nicotinamide phosphoribosyltransferase (NAMPT) for cancer drug discovery

PMID 37413882; DOI 10.1016/j.ejmech.2023.115607; European journal of medicinal chemistry 2023 Jul; 258(?):115607 (Review Article)

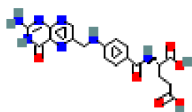
Name matches: **NAD+** *nicotinamide*

Effect of Exercise and Oral Niacinamide Mononucleotide on Improving Mitochondrial Autophagy in Alzheimer's Disease

PMID 37447179; DOI 10.3390/nu15132851; Nutrients 2023 Jun; 15(13): (Review Article)

Name matches: **NAD+** *niacinamide*

Chemical



Folic Acid

CID 135398658

Selected evidence

1,573 articles

[View All](#)**Physiological Associations between Vitamin B Deficiency and Diabetic Kidney Disease**

PMID 37189771; DOI 10.3390/biomedicines11041153; Biomedicines 2023 Apr; 11(4): (Review Article)

Name matches: **folate** *nicotinamide; vitamin b*

Association of Vitamin B Status with Risk of Dementia in Cohort Studies: A Systematic Review and Meta-Analysis

PMID 35779574; DOI 10.1016/j.jamda.2022.05.022; Journal of the American Medical Directors Association 2022 Nov; 23(11):1826.e21-1826.e35 (Review Article)

Name matches: **folate** *vitamin b*

Dietary Vitamin B Complex: Orchestration in Human Nutrition throughout Life with Sex Differences

PMID 36235591; DOI 10.3390/nu14193940; Nutrients 2022 Sep; 14(19): (Review Article)

Name matches: folic acid *vitamin b*

Chemical



Nicotinic acid

CID 938

Selected evidence

1,190 articles

[View All](#)

[The use of Nicotinamide and Nicotinamide riboside as an adjunct therapy in the treatment of glaucoma](#)

PMID 36916064; DOI 10.1177/11206721231161101; European journal of ophthalmology 2023 Mar; ?
(?):11206721231161101 (Review Article)

Name matches: **vitamin b3** *nicotinamide*

[Physiological Associations between Vitamin B Deficiency and Diabetic Kidney Disease](#)

PMID 37189771; DOI 10.3390/biomedicines11041153; Biomedicines 2023 Apr; 11(4): (Review Article)

Name matches: **niacin** *nicotinamide*; *vitamin b*

[Dietary Vitamin B Complex: Orchestration in Human Nutrition throughout Life with Sex Differences](#)

PMID 36235591; DOI 10.3390/nu14193940; Nutrients 2022 Sep; 14(19): (Review Article)

Name matches: **niacin** *vitamin b*

► [PubChem](#)

15.11 Chemical-Gene Co-Occurrences in Literature



Showing 3 of 100 [View More](#)



Gene/Protein/Enzyme

[ins](#)

Selected evidence

933 articles

[View All](#)

[Model of Streptozotocin-nicotinamide Induced Type 2 Diabetes: a Comparative Review](#)

PMID 34789130; DOI 10.2174/1573399818666211117123358; Current diabetes reviews 2022; 18(8):e171121198001 (Review Article)

Name matches: **insulin** *nicotinamide*

Metabolic alterations in streptozotocin-nicotinamide-induced diabetic rats treated with *Muntingia calabura* L. extract via ¹H-NMR-based metabolomics

PMID 36914160; DOI 10.1055/a-2053-0950; Planta medica 2023 Mar; ?(?):

Name matches: **insulin** *nicotinamide*

Antidiabetic and Liver Histological and Ultrastructural Effects of *Cynara scolymus* Leaf and Flower Head Hydroethanolic Extracts in Nicotinamide/Streptozotocin-Induced Diabetic Rats

PMID 37163198; DOI 10.1155/2023/4223026; Evidence-based complementary and alternative medicine : eCAM 2023; 2023(?):4223026

Name matches: **insulin** *nicotinamide*

Gene/Protein/Enzyme

sirt1

Selected evidence

397 articles

[View All](#) 

The Role of Nicotinamide in Cancer Chemoprevention and Therapy

PMID 32245130; DOI 10.3390/biom10030477; Biomolecules 2020 03; 10(3): (Review Article)

Name matches: **sirtuin 1** *nicotinamide*

Immunotherapy of COVID-19 with poly (ADP-ribose) polymerase inhibitors: starting with **nicotinamide**

PMID 33063092; DOI 10.1042/bsr20202856; Bioscience reports 2020 10; 40(10): (Review Article)

Name matches: **sirtuin 1** *nicotinamide*

Nicotinamide: Oversight of Metabolic Dysfunction Through SIRT1, mTOR, and Clock Genes

PMID 33183203; DOI 10.2174/1567202617999201111195232; Current neurovascular research 2020; 17(5):765-783 (Review Article)

Name matches: **sirt1** *nicotinamide*

Gene/Protein/Enzyme

EC:2.4.2.30

Selected evidence

306 articles

[View All](#) 

Immunotherapy of COVID-19 with poly (ADP-ribose) polymerase inhibitors: starting with **nicotinamide**

PMID 33063092; DOI 10.1042/bsr20202856; Bioscience reports 2020 10; 40(10): (Review Article)

Name matches: **poly(adp-ribose)polymerase** *nicotinamide*

Cellular toxicity of nicotinamide metabolites

PMID 22200423; DOI 10.1053/j.jrn.2011.10.033; Journal of renal nutrition : the official journal of the Council on Renal Nutrition of the National Kidney Foundation 2012 Jan; 22(1):95-7 (Review Article)

Name matches: **poly(adp-ribose)polymerase** *nicotinamide*

Streptozotocin-nicotinamide-induced diabetes in the rat. Characteristics of the experimental model

PMID 22619373; DOI 10.1258/ebm.2012.011372; Experimental biology and medicine (Maywood, N.J.) 2012 May; 237(5):481-90 (Review Article)

Name matches: **poly(adp-ribose)polymerase** *nicotinamide*

► [PubChem](#)

15.12 Chemical-Disease Co-Occurrences in Literature



Showing 3 of 25 [View More](#)



Disease

Diabetes Mellitus

Selected evidence

1,276 articles
[View All](#)

Physiological Associations between Vitamin B Deficiency and Diabetic Kidney Disease

PMID 37189771; DOI 10.3390/biomedicines11041153; Biomedicines 2023 Apr; 11(4): (Review Article)

Name matches: **diabetes** *nicotinamide*; *vitamin b*

The Nicotinamide/Streptozotocin Rodent Model of Type 2 Diabetes: Renal Pathophysiology and Redox Imbalance Features

PMID 36139064; DOI 10.3390/biom12091225; Biomolecules 2022 09; 12(9): (Review Article)

Name matches: **diabetes** *nicotinamide*

Model of Streptozotocin-nicotinamide Induced Type 2 Diabetes: a Comparative Review

PMID 34789130; DOI 10.2174/1573399818666211117123358; Current diabetes reviews 2022; 18(8):e1711121198001 (Review Article)

Name matches: **diabetes**; **diabetogenic** *nicotinamide*

Disease

Hyperhomocysteinemia

Selected evidence

354 articles
[View All](#)

Vitamin B-related Gene Polymorphisms and Cardiovascular Disease

PMID 35346016; DOI 10.2174/1381612828666220328115605; Endocrine, metabolic & immune disorders drug targets 2022; 22(10):979-984 (Review Article)

Name matches: **hyperhomocysteinemia** *vitamin b*

The Effects of Bariatric Surgery on Vitamin B Status and Mental Health

PMID 33923999; DOI 10.3390/nu13041383; Nutrients 2021 Apr; 13(4): (Review Article)

Name matches: **hyperhomocysteinemia** *vitamin b*

Efficacy of Vitamin B Supplementation on Cognition in Elderly Patients With Cognitive-Related Diseases

PMID 28248558; DOI 10.1177/0891988716673466; Journal of geriatric psychiatry and neurology 2017 Jan; 30(1):50-59 (Review Article)

Name matches: **hyperhomocysteinemia** *vitamin b*

Disease**Diabetes Mellitus, Type 2****Selected evidence**

535 articles

[View All](#) 

The Nicotinamide/Streptozotocin Rodent Model of Type 2 Diabetes: Renal Pathophysiology and Redox Imbalance Features

PMID 36139064; DOI 10.3390/biom12091225; Biomolecules 2022 09; 12(9): (Review Article)

Name matches: **type 2 diabetes**; **type-2 diabetic** *nicotinamide*

Model of Streptozotocin-nicotinamide Induced Type 2 Diabetes: a Comparative Review

PMID 34789130; DOI 10.2174/157339981866621117123358; Current diabetes reviews 2022; 18(8):e171121198001 (Review Article)

Name matches: **type 2 diabetes**; **type-2 diabetes** *nicotinamide*

In vitro and in vivo antidiabetic activity of bitter honey in streptozotocin-nicotinamide-induced diabetic Wistar rats

PMID 36873120; DOI 10.25122/jml-2022-0099; Journal of medicine and life 2023 Jan; 16(1):91-100

Name matches: **type-2 diabetic** *nicotinamide*

[► PubChem](#)

16 Patents**16.1 Depositor-Supplied Patent Identifiers**

117,374 items



SORT BY

Priority Date - Most Recent

▼

[Novel mixtures and uses of \(2e\)-3-\(1,3-benzodioxol-5-yl\)-n-phenyl-n-\(tetrahydro-3-furanyl\)-2-propenamide](#)
Publication Number: [WO-2022207944-A9](#)
Priority Date: 2022-07-11

[Active ingredient complexes, compositions and methods for hangover relief and to ameliorate alcohol-induced liver damage](#)
Publication Number: [US-11458155-B1](#)
Priority Date: 2021-11-16
Grant Date: 2022-10-04

[Specific conjugation of an antibody](#)
Publication Number: [WO-2022078524-A2](#)
Priority Date: 2021-11-03

[Specific conjugation of an antibody](#)
Publication Number: [WO-2022078524-A4](#)
Priority Date: 2021-11-03

[Topical formulations containing erythritol and methods of treating skin conditions](#)
Publication Number: [US-11517578-B1](#)

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Page 1

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of 23,475

► [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=DFPAKSUCGFBDDF-UHFFFAOYSA-N>

► [PATENTSCOPE \(WIPO\)](#)

17 Interactions and Pathways



17.1 Protein Bound 3D Structures



66 items

SORT BY Resolution - Increasing

Structure of *P. luminescens* TccC3-F-actin complex
PDB Code: [7Z7H](#)
Resolution: 0 Å

Structure image

Cryo-EM structure of CopC-CaM-caspase-3 with ADPR
PDB Code: [7XN5](#)
Resolution: 0 Å

Structure image

Cryo-EM structure of CopC-CaM-caspase-3 with ADPR-deacylation
PDB Code: [7XN6](#)
Resolution: 0 Å

► [RCSB Protein Data Bank \(RCSB PDB\)](#)

[View 67 proteins in NCBI Structure](#)

[► PubChem](#)

17.1.1 Ligands from Protein Bound 3D Structures



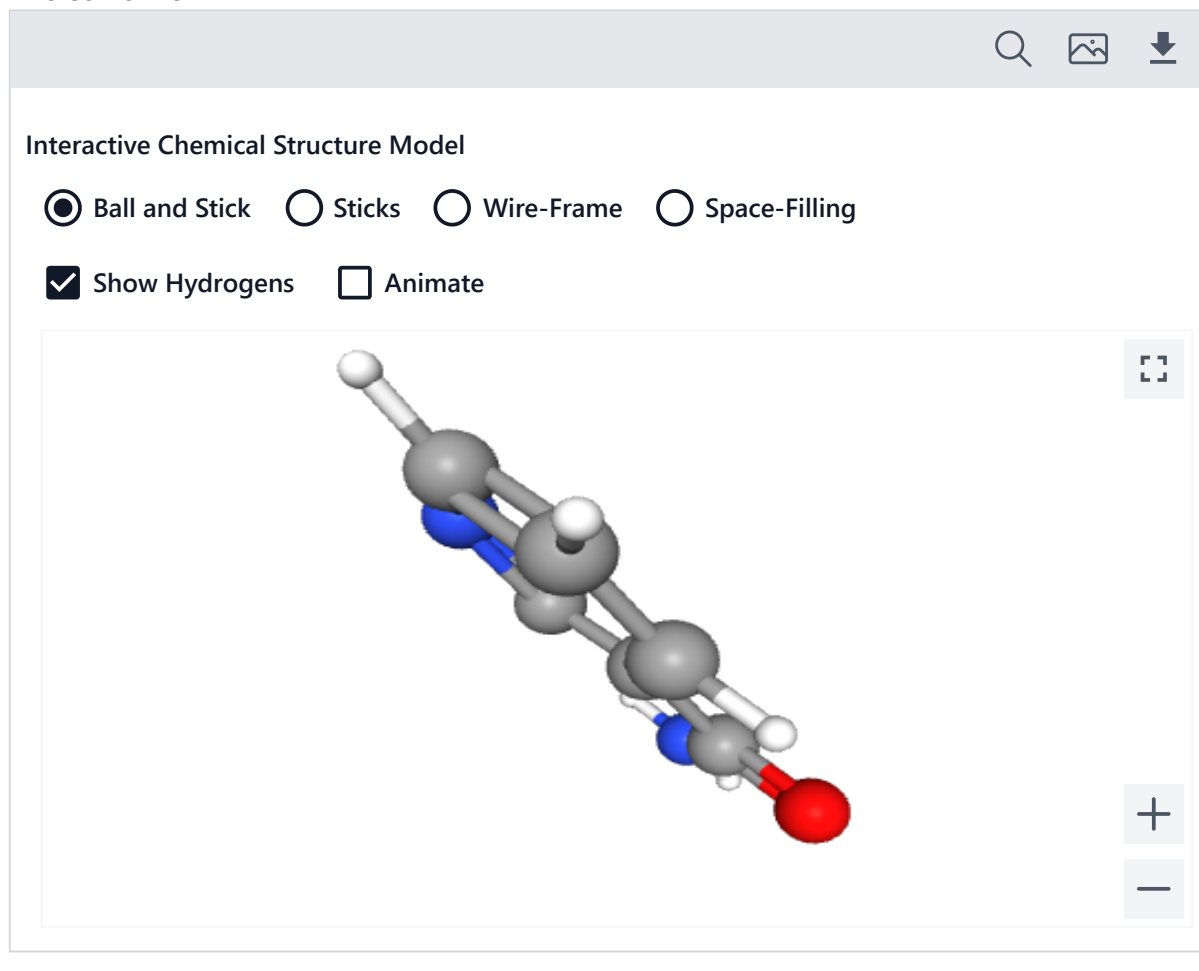
PDBe Ligand Code

[NCA](#)

PDBe Structure Code

[1DMA](#)

PDBe Conformer

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

17.2 Chemical-Target Interactions



283 items



SORT BY

Data Source - A to Z

▼

Structure



Protein

Gene

PARP1

Taxonomy

Homo sapiens (human)

Evidence IDs ⓘ

Data Source

Drug Gene Interaction database (DGIdb)

Structure



Protein

NAD-dependent protein deacetylase sirtuin-2

Gene

SIRT2

Taxonomy

Homo sapiens (human)

Evidence IDs ⓘ

PMID:25041433

PMID:22419041

PMID:17145705

PMID:19700324

PMID:17149860

...

► BindingDB; Comparative Toxicogenomics Database (CTD); Drug Gene Interaction database (DGIdl...

17.3 Pathways



110 items

SORT BY Taxonomy - A to Z

thiazole component of thiamine diphosphate biosynthesis III
Source: [PlantCyc](#)
External ID: [PWY-6909](#)
Taxonomy: [Arabidopsis halleri](#)

Differentiation pathway
Source: [WikiPathways](#)
External ID: [WP3223](#)
Taxonomy: [Bos taurus \(cattle\)](#)

NAD salvage pathway I
Source: [WikiPathways](#)
External ID: [WP2486](#)
Taxonomy: [Escherichia coli](#)

NAD Salvage
Source: [PathBank](#)
External ID: [SMP0000850](#)
Taxonomy: [Escherichia coli](#)

<< < Page 1 of 22 > >>

► PubChem

18 Biological Test Results



18.1 BioAssay Results



3,162 items 

 Search

SORT BY **Activity Value - Increasing** 



BK Channel Variant Modulator Selectivity Assay
Activity: [Inactive](#)
Activity Value: -0.0296531 μ M
BioAssay AID: [1259406](#)
Substance SID: [363920149](#)
Compound CID: [936](#)



BK Channel Variant Modulator Selectivity Assay
Activity: [Inactive](#)
Activity Value: -0.0169048 μ M
BioAssay AID: [1259406](#)
Substance SID: [363920149](#)
Compound CID: [936](#)



<< < Page 1 of 633 > >>

[► PubChem](#)

19 Taxonomy



120 items 

 Search

SORT BY Data Source - A to Z
Structure 
Taxonomy Homo sapiens (human)
Data Source Human Metabolome Database (HMDB)
Structure 
Taxonomy Virola multinervia
Data Source Natural Product Activity and Species Source (NPASS)
Structure 
Taxonomy

<< < Page 1 of 24 > >>

WormJam Metabolites Local CSV for MetFrag | [DOI:10.5281/zenodo.3403364](https://doi.org/10.5281/zenodo.3403364)

WormJam: A consensus *C. elegans* Metabolic Reconstruction and Metabolomics Community and Workshop Series, Worm, 6:2, e1373939, [DOI:10.1080/21624054.2017.1373939](https://doi.org/10.1080/21624054.2017.1373939)

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

► [E. coli Metabolome Database \(ECMDB\); ECI Group, LCSB, University of Luxembourg; KNApSack S...](#)

20 Classification



20.1 MeSH Tree



1 item

[View in Classification Browser](#)

MeSH Tree > Technology and Food and Beverages Category > Food and Beverages > Food > Nutrients > Micronutrients > Vitamins

Niacinamide

An important compound functioning as a component of the coenzyme NAD. Its primary significance is in the prevention and/or cure of blacktongue and PELLAGRA. Most animals cannot manufacture this compound in amounts sufficient to prevent nutritional deficiency and it therefore must be supplemented through dietary intake.

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

20.2 NCI Thesaurus Tree



1 item

[View in Classification Browser](#)

NCI Thesaurus Tree > Drug, Food, Chemical or Biomedical Material > Dietary Supplement

Niacinamide

The active form of vitamin B3 and a component of the coenzyme nicotinamide adenine dinucleotide (NAD). Niacinamide acts as a chemo- and radio-sensitizing agent by enhancing tumor blood flow, thereby reducing tumor hypoxia. This agent also inhibits poly(ADP-ribose) polymerases, enzymes involved in the rejoining of DNA strand breaks induced by radiation or chemotherapy.

► [NCI Thesaurus \(NCIt\)](#)

20.3 ChEBI Ontology



1 item

[View in Classification Browser](#)

ChEBI Ontology > chemical entity > molecular entity > main group molecular entity > p-block molecular entity > carbon group molecular entity > organic molecular entity > heteroorganic entity > organic heterocyclic compound > organic heteromonocyclic compound > pyridines

nicotinamide

A pyridinecarboxamide that is pyridine in which the hydrogen at position 3 is replaced by a carboxamide group.

► [ChEBI](#)

20.4 KEGG: Metabolite



1 item

[View in Classification Browser](#)

Compounds with biological roles > Vitamins and cofactors > Vitamins

[Nicotinamide \(Vitamin B3\)](#)

► [KEGG](#)

20.5 KEGG: Phytochemical Compounds



1 item

[View in Classification Browser](#)

Phytochemical compounds > Alkaloids > Alkaloids derived from nicotinic acid

[Nicotinamide](#)

► [KEGG](#)

20.6 KEGG: Drug



1 item

[View in Classification Browser](#)

Therapeutic category of drugs in Japan > 3 Agents affecting metabolism > 31 Vitamins > 313 Vitamin B preparations

[Niacinamide \(USP\); Nicotinamide \(JP18/INN\)](#)

► [KEGG](#)

20.7 KEGG: ATC



1 item

[View in Classification Browser](#)

Anatomical Therapeutic Chemical (ATC) classification > A ALIMENTARY TRACT AND METABOLISM > A11 VITAMINS > A11H OTHER PLAIN VITAMIN PREPARATIONS > A11HA Other plain vitamin preparations

[Niacinamide \(USP\)](#)

► [KEGG](#)

20.8 KEGG: JP15



1 item

[View in Classification Browser](#)

Drugs listed in the Japanese Pharmacopoeia

Nicotinamide

► KEGG

20.9 KEGG: Risk Category of Japanese OTC Drugs



1 item

View in Classification Browser

Risk category of Japanese OTC drugs > Third-class OTC drugs > Inorganic and organic chemicals

[Nicotinamide \(USP\)](#)

► KEGG

20.10 KEGG: OTC drugs



1 item

View in Classification Browser

Classification of Japanese OTC drugs > Agents for otolaryngologic use

[Nicotinamide \(USP\)](#)

► KEGG

20.11 WHO ATC Classification System



1 item

View in Classification Browser

ATC Code > A - Alimentary tract and metabolism > A11 - Vitamins > A11H - Other plain vitamin preparations

[A11HA01 - Nicotinamide](#)

► WHO Anatomical Therapeutic Chemical (ATC) Classification

20.12 ChemIDplus



57 items

View in Classification Browser

ChemIDplus Chemical Information Classification

CAMEO

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

stored in the United States

ChemIDplus Chemical Information Classification

CCRIS

Chemical Carcinogenesis Research Information System - Carcinogenicity, mutagenicity, tumor promotion and tumor inhibition data from the National Cancer Institute (NCI). CCRIS provides historical information from the years 1985 - 2011. It is no longer updated.

ChemIDplus Chemical Information Classification

CTD

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

ChemIDplus Chemical Information Classification

ChEBI

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

ChemIDplus Chemical Information Classification

ClinicalTrials.gov

ClinicalTrials.gov - ClinicalTrials.gov offers a public database of information for clinical research, including clinical trials.

Page 1 of 12

► [ChemIDplus](#)

20.13 CAMEO Chemicals



2 items

[View in Classification Browser](#)

Amides and Imides

Reactive group: Amides and Imides

Amines, Phosphines, and Pyridines

Reactive group: Amines, Phosphines, and Pyridines

► [CAMEO Chemicals](#)

20.14 ChEMBL Target Tree



61 items

[View in Classification Browser](#)

Enzyme

Biological molecules that possess catalytic activity. They may occur naturally or be synthetically created. Enzymes are usually proteins, however CATALYTIC RNA and CATALYTIC DNA molecules have also been identified. [MESH:D004798]

Surface antigen

Antigens on surfaces of cells, including infectious or foreign cells or viruses. They are usually protein-containing groups on cell membranes or walls and may be isolated. [MESH:D000954]

ChEMBL Protein Target Tree

Oxidoreductase

The class of all enzymes catalyzing oxidoreduction reactions. The substrate that is oxidized is regarded as a hydrogen donor. The systematic name is based on donor:acceptor oxidoreductase. The recommended name will be dehydrogenase, wherever this is possible; as an alternative, reductase can be used. Oxidase is only used in cases where O₂ is the acceptor. (Enzyme Nomenclature, 1992, p9) [MESH:D010088]

Membrane receptor

Cell surface proteins that bind signalling molecules external to the cell with high affinity and convert this extracellular event into one or more intracellular signals that alter the behavior of the target cell (From Alberts, Molecular Biology of the Cell, 2nd ed, pp693-5). Cell surface receptors, unlike enzymes, do not chemically alter their ligands. [MESH:D011956]

ChEMBL Protein Target Tree > Enzyme > Protease > Metallo protease

Metallo protease M2 family

<< < Page 1 of 13 > >>

► [ChEMBL](#)

20.15 EPA CPDat Classification



37 items

[View in Classification Browser](#)

EPA CPDat Classification > Functional Use

softener and conditioner

EPA CPDat Classification > Functional Use

cosmetic ingredient

EPA CPDat Classification > Functional Use

hair conditioning agent

EPA CPDat Classification > Functional Use

skin conditioning agent

EPA CPDat Classification > Functional Use

skin-conditioning agent - miscellaneous

<< < Page 1 of 8 > >>

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

20.16 NORMAN Suspect List Exchange Classification



39 items	View in Classification Browser
NORMAN Suspect List Exchange Classification	
Smoothing	
NORMAN Suspect List Exchange Classification	
Parents (Predecessors)	
These are parent compounds (predecessors) documented in the Parent-Transformation Product Pairs from HSDB (S68).	
NORMAN Suspect List Exchange Classification	
Transformation products (TPs, successors)	
These are transformation products (TPs, successors) documented in the Parent-Transformation Product Pairs from HSDB (S68).	
NORMAN Suspect List Exchange Classification	
[M+Na]⁺	
NORMAN Suspect List Exchange Classification	
[M+H]⁺	
Page 1 of 8	

► NORMAN Suspect List Exchange

20.17 CCSBase Classification



2 items	View in Classification Browser
[M+H]⁺	
[M+Na]⁺	

► CCSbase

20.18 EPA DSSTox Classification



88 items	View in Classification Browser
CompTox Chemicals Dashboard Chemical Lists	
[BLOODEXPOSOME] LIST: BLOODEXPOSOME Chemicals identified as part of the blood exposome	

Short_Description: Chemicals identified as part of the blood exposome

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

CompTox Chemicals Dashboard Chemical Lists

[\[CANADADSL\] Canadian Domestic Substances List 2019](#)

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

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

CompTox Chemicals Dashboard Chemical Lists

[\[CCSCOMPEND\] NORMAN|MASSPECDB: The Unified Collision Cross Section \(CCS\) Compendium](#)

Short_Description: Chemicals associated with >3800 experimental collision cross section (CCS) values

Long_Description: Chemicals associated with >3800 experimental collision cross section (CCS) values (drift tube MS), provided to the NORMAN Suspect List Exchange by Jackie Picache and John McLean, Vanderbilt University. Mapped to DTXSIDs by CAS Registry Number by E. Schymanski (Luxembourg Center for Systems Biomedicine); further curation ongoing. Further details available [here](#)

CompTox Chemicals Dashboard Chemical Lists

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

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

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

CompTox Chemicals Dashboard Chemical Lists

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

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

Long_Description: CHEMINV consists of the full list of unique DSSTox substance records mapped to the historical chemical inventory of physical samples registered by EPA's ToxCast Chemical Contractor (Evotec) in their sample tracking database since the launch of the ToxCast program in 2007. The CHEMINV file includes all chemical samples procured by Evotec for possible inclusion in EPA's ToxCast program since the start of the program in 2007, as well as a relatively small set of donated or EPA-supplied samples that were shipped to Evotec to be included in EPA's physical sample library. The list includes all samples received and registered by Evotec, but all samples were not necessarily solubilized or plated for testing, i.e., the full list includes volatiles, DMSO insolubles, depleted chemicals, and discarded

chemicals deemed too dangerous for storage and handling. All physical samples plated for screening in the ToxCast program (TOXCAST), which includes EPA's full contribution to the Tox21 screening program (TOX21SL), are included as a subset of CHEMINV, as is the full list of samples currently available for ToxCast plating. Hence, the CHEMINV inventory file is a snapshot of all past and present samples. The CHEMINV file provides a complete historical record of chemicals that were prioritized for inclusion in EPA's ToxCast and Tox21 screening programs based on multiple criteria (toxicity data, exposure potential, use, etc.), and that were successfully procured by (or provided to) EPA's ToxCast Chemical Contractor (Evotec) for possible inclusion in those programs. The CHEMINV file is a subset of EPA's ChemTrack database (CHEMTRACK), the latter including all chemicals for which ToxCast or Tox21 screening data have been

Page 1 of 18

► EPA DSSTox

20.19 Consumer Product Information Database Classification



1 item

View in Classification Browser

Personal Care

► Consumer Product Information Database (CPID)

20.20 LOTUS Tree



42 items

View in Classification Browser

LOTUS Tree > Biological Tree > Eukaryota > Archaeplastida > Streptophyta > Magnoliopsida > Celastrales > Celastraceae

Euonymus sanguineus

LOTUS Tree > Biological Tree > Eukaryota > Archaeplastida > Streptophyta > Magnoliopsida > Celastrales > Celastraceae

Euonymus hamiltonianus

LOTUS Tree > Biological Tree > Eukaryota > Archaeplastida > Streptophyta > Magnoliopsida > Celastrales > Celastraceae

Euonymus phellomanus

LOTUS Tree > Biological Tree > Eukaryota > Archaeplastida > Streptophyta > Magnoliopsida > Celastrales > Celastraceae

Euonymus grandiflorus

Page 1 of 9

► [LOTUS - the natural products occurrence database](#)

20.21 EPA Substance Registry Services Tree



29 items
View in Classification Browser

EPA SRS List Classification
Synonyms Provided by Submitters to the TSCA Inventory
TSCA INV SYN :: Synonyms Provided by Submitters to the TSCA Inventory

EPA SRS List Classification
2012 Chemical Data Reporting
2012 CDR :: This list contains chemicals that were reported to EPA's 2012 Chemical Data Reporting (CDR). Companies that manufacture (including import) certain chemicals at certain volumes in the U.S. must report to EPA every four years through its CDR. The vast majority of chemicals on this 2012 CDR list needed to be reported, but some of these chemicals were not required to be reported. EPA uses the CDR data to support many health, safety, and environmental protection activities.

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

EPA SRS List Classification
Ecotoxicology Database
ECOTOX :: Comprehensive database providing adverse effects of single chemical stressors to ecologically relevant aquatic and terrestrial species.

EPA SRS List Classification
Green Chemistry Expert System
GCES :: The Green Chemistry Expert System (GCES) is a tool currently under development by the U.S. EPA, which will allow users to build a green chemical process, design a green chemical, or survey the field of green chemistry. Its primary purpose is to guide users in the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. This new approach to pollution prevention is the central focus of EPA's Green

Page 1 of 6

► [EPA Substance Registry Services](#)

21 Information Sources



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3-Pyridinecarboxamide<https://www.bindingdb.org/rwd/bind/chemsearch/marvin/MolStructure.jsp?monomerid=27507>

2. Comparative Toxicogenomics Database (CTD)

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

Niacinamide<https://ctdbase.org/detail.go?type=chem&acc=D009536>

3. Drug Gene Interaction database (DGIdb)

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The data used in DGIdb is all open access and where possible made available as raw data dumps in the downloads section.
<http://www.dgldb.org/downloads>

NIACINAMIDE<https://www.dgldb.org/drugs/NIACINAMIDE>

4. DrugBank

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

Nicotinamide<https://www.drugbank.ca/drugs/DB02701>

5. Therapeutic Target Database (TTD)

Nicotinamide<https://idrblab.net/ttd/data/drug/details/D06NVJ>

6. Toxin and Toxin Target Database (T3DB)

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<http://www.t3db.ca/downloads>

Niacinamide

<http://www.t3db.ca/toxins/T3D4168>

7. Burnham Center for Chemical Genomics

SID8139965

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

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

NICOTINAMIDE

<https://cameochemicals.noaa.gov/chemical/20736>

CAMEO Chemical Reactivity Classification

<https://cameochemicals.noaa.gov/browse/react>

9. Hazardous Substances Data Bank (HSDB)

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<http://www.hmdb.ca/citing>

Niacinamide

<http://www.hmdb.ca/metabolites/HMDB0001406>

HMDB0001406_nmr_one_1299

<https://hmdb.ca/metabolites/HMDB0001406#spectra>

11. ILO-WHO International Chemical Safety Cards (ICSCs)

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NICOTINAMIDE

https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=1703

12. CAS Common Chemistry

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Nicotinamide

https://commonchemistry.cas.org/detail?cas_rn=98-92-0

13. ChemIDplus

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Niacinamide [USP]

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000098920>

ChemIDplus Chemical Information Classification

<https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus>

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15. EPA Chemicals under the TSCA

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

3-Pyridinecarboxamide

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

16. EPA DSSTox

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

Niacinamide

<https://comptox.epa.gov/dashboard/DTXSID2020929>

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

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19. Wikipedia

nicotinamide<https://en.wikipedia.org/wiki/Nicotinamide>

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

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<https://haz-map.com/About>*Nicotinamide*<https://haz-map.com/Agents/15948>

21. ChEBI

Nicotinamide

<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:17154>

ChEBI Ontology

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

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23. LOTUS - the natural products occurrence database

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<https://lotus.nprod.net/>

Nicotinamide

<https://www.wikidata.org/wiki/Q192423>

LOTUS Tree

<https://lotus.naturalproducts.net/>

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NCI Thesaurus Tree

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

25. Yeast Metabolome Database (YMDB)

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<http://www.ymdb.ca/downloads>

Niacinamide

<http://www.ymdb.ca/compounds/YMDB00274>

26. CCSbase

Nicotinamide

CCSbase Classification

<https://ccsbase.net/>

27. NORMAN Suspect List Exchange

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NORMAN Suspect List Exchange Classification

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

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https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1140/

ChEMBL Protein Target Tree

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

Niacinamide (Vitamin B)

<https://www.whatsinproducts.com/chemicals/view/1/1006/000098-92-0>

Consumer Products Category Classification

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

31. Crystallography Open Database (COD)

<https://www.crystallography.net/cod/4511296.html>

32. The Cambridge Structural Database

<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=131756>

<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=131757>
<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=131758>
<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=794756>
<https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=841466>

33. DailyMed

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Drug: NIACINAMIDE | NICOTINAMIDE

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<https://www.accessdata.fda.gov/scripts/cder/daf/>

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nicotinamide

36. KNApSack Species-Metabolite Database

Nicotinamide

http://www.knapsackfamily.com/knapsack_core/info.php?sname=C_ID&word=C00000209

37. Natural Product Activity and Species Source (NPASS)

Niacinamide

<https://bidd.group/NPASS/compound.php?compoundID=NPC306397>

38. West Coast Metabolomics Center-UC Davis

Nicotinamide

39. EPA Chemical and Products Database (CPDat)

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

<https://comptox.epa.gov/dashboard/DTXSID2020929#exposure>

EPA CPDat Classification<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>40. **EU Clinical Trials Register**<https://www.clinicaltrialsregister.eu/>41. **FDA Center for Food Safety and Applied Nutrition (CFSAN)****LICENSE**

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Nicotinamide

<https://spectrabase.com/spectrum/5V1Fex7g6LG>

Nicotinamide

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

Nicotinamide

<https://spectrabase.com/spectrum/9xJi2BF69tJ>

Nicotinamide

<https://spectrabase.com/spectrum/KjFRvA8CF4h>

3-CARBAMOYL-PYRIDINE

<https://spectrabase.com/spectrum/838BydraZ0b>

NIC-NH₂;NICOTINAMIDE;3-PYRIDINE-CARBOXAMIDE

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

Nicotinamide

<https://spectrabase.com/spectrum/A55KEMfux7s>

Nicotinamide

<https://spectrabase.com/spectrum/5Yyj97DpoR9>

Nicotinamide

<https://spectrabase.com/spectrum/GngFnh835Oz>

3-Pyridinecarboxamide; Nicotinamide

<https://spectrabase.com/spectrum/HROfWAUhGt8>

45. MassBank Europe

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

DFPAKSUCGFBDDF-UHFFFAOYSA-N

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

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

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

48. **Japan Chemical Substance Dictionary (Nikkaji)**

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J3.988H

49. **Kruve Lab, Ionization & Mass Spectrometry, Stockholm University**

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50. **Metabolomics Workbench**

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<https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=37778>

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

52. **Nature Chemical Biology**

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Phytochemical compounds

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Therapeutic category of drugs in Japan

http://www.genome.jp/kegg-bin/get_htext?br08301.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

Risk category of Japanese OTC drugs

http://www.genome.jp/kegg-bin/get_htext?br08312.keg

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