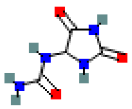
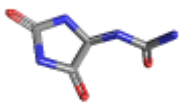
COMPOUND SUMMARY

Allantoin

PubChem CID	204
Structure	 2D  3D
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_4H_6N_4O_3$
Synonyms	allantoin 97-59-6 5-Ureidohydantoin Glyoxyldiureide 1-(2,5-dioxoimidazolidin-4-yl)urea View More...
Molecular Weight	158.12 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2004-09-16 Modify: 2024-02-17
Description	Allantoin is an imidazolidine-2,4-dione that is 5-aminohydantoin in which a carbamoyl group is attached to the exocyclic nitrogen. It has a role as a vulnerary, a human metabolite, a Saccharomyces cerevisiae metabolite and an Escherichia coli metabolite. It is a member of ureas and an imidazolidine-2,4-dione. It is

functionally related to a **hydantoin**. It is a tautomer of a **1-(5-hydroxy-2-oxo-2,3-dihydroimidazol-4-yl)urea**.

▸ ChEBI

Allantoin is a substance that is endogenous to the human body and also found as a normal component of human diets. In healthy human volunteers, the mean plasma concentration of allantoin is about 2-3 mg/l. During exercise, the plasma allantoin concentration rapidly increases about two fold and remains elevated. In human muscle, **urate** is oxidized to allantoin during such exercise. The concentration of allantoin in muscles increases from a resting value of about 5000 ug/kg to about 16000 ug/kg immediately after short-term exhaustive cycling exercise. More specifically, allantoin is a diureide of **glyoxylic acid** that is produced from **uric acid**. It is a major metabolic intermediate in most organisms. Allantoin is found in OTC cosmetic products and other commercial products such as oral hygiene products, in shampoos, lipsticks, anti-acne products, sun care products, and clarifying lotions. Allantoin has also demonstrated to ameliorate the wound healing process in some studies.

▸ DrugBank

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

▸ E. coli Metabolome Database (ECMDB)

View More...

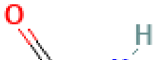
See also: **Alcloxa** (active moiety of); **Comfrey Leaf** (part of); **Comfrey Root** (part of) ... **View More** ...

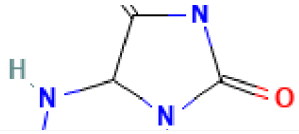
Contents

1 Structures

1.1 2D Structure

Chemical Structure Depiction





PubChem

1.2 3D Conformer

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

(2,5-dioxoimidazolidin-4-yl)urea

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/C4H6N4O3/c5-3(10)6-1-2(9)8-4(11)7-1/h1H,(H3,5,6,10)(H2,7,8,9,11)

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.3 InChIKey

POJWUDADGALRAB-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.4 Canonical SMILES

C1(C(=O)NC(=O)N1)NC(=O)N

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

PubChem

2.2 Molecular Formula

$C_4H_6N_4O_3$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

PubChem

2.3 Other Identifiers

2.3.1 CAS

97-59-6

CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals under the TSCA; E...

2.3.2 Deprecated CAS

37305-69-4, 5377-33-3, 58308-55-7

ChemIDplus

5377-33-3, 58308-55-7, 37305-69-4

EPA DSSTox

2.3.3 European Community (EC) Number

202-592-8

- European Chemicals Agency (ECHA)

2.3.4 UNII

344S277G0Z

- FDA Global Substance Registration System (GSRS)

2.3.5 DrugBank ID

DB11100

- DrugBank

2.3.6 ChEMBL ID

CHEMBL593429

- ChEMBL

2.3.7 DSSTox Substance ID

DTXSID3020043

- EPA DSSTox

2.3.8 KEGG ID

C01551

- KEGG

D00121

- KEGG

2.3.9 Metabolomics Workbench ID

143220

- Metabolomics Workbench

2.3.10 NCI Thesaurus Code

C74277

- NCI Thesaurus (NCIt)

2.3.11 Nikkaji Number

J3.978K

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.12 NSC Number

757792

- DTP/NCI

7606

- DTP/NCI

2.3.13 RXCUI

508

- NLM RxNorm Terminology

2.3.14 Wikidata

Q409804

- Wikidata

2.3.15 Wikipedia

Allantoin

- Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

Allantoin
Herpecin L
Herpecin-L
HerpecinL
Sebical
Woun'dres

▸ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

allantoin
97-59-6
5-Ureidohydantoin
Glyoxyldiureide
1-(2,5-dioxoimidazolidin-4-yl)urea
Cordianine
Glyoxyldiureid
Allantol
Alantan
Sebical
AVC/Dienestrolcream
Urea, (2,5-dioxo-4-imidazolidinyl)-
Psoralon
Septalan
Hydantoin, 5-ureido-
Cutemol emollient
(2,5-Dioxo-4-imidazolidinyl)urea
Uniderm A
(2,5-dioxoimidazolidin-4-yl)urea
Glyoxylic(acid) diureide
DL-Allantoin
Glyoxylic diureide
NSC 7606
5-Ureido-2,4-imidazolidinc
Alwextin
Caswell No. 024
CCRIS 1958
2,5-Dioxo-4-imidazolidinyl
N-(2,5-Dioxo-4-imidazolid
EPA Pesticide Chemical Coc

▸ PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	158.12 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	-2.2	Computed by XLogP3 3.0 (PubChem release 2021.10.14)

Hydrogen Bond Donor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	158.04399007 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	158.04399007 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	113Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	11	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	225	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	1	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

▸ PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Colorless to white odorless solid; [Hawley] White powder; [MSDSonline]

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

Solid

- Human Metabolome Database (HMDB)

3.2.2 Color / Form

Crystals from aqueous methanol

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 49

- Hazardous Substances Data Bank (HSDB)

White to colorless powder or crystals

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

- Hazardous Substances Data Bank (HSDB)

Monoclinic plates

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-10

- Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Odorless

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

- Hazardous Substances Data Bank (HSDB)

Pleasant smelling

Physicians Desk Reference 61st ed, Thomson PDR, Montvale, NJ 2007., p. 2126

- Hazardous Substances Data Bank (HSDB)

3.2.4 Taste

Tasteless

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

▸ Hazardous Substances Data Bank (HSDB)

3.2.5 Melting Point

239 °C /Racemic form/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 49

▸ Hazardous Substances Data Bank (HSDB)

MP: 230 °C (decomposes)

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

▸ Hazardous Substances Data Bank (HSDB)

239 °C

▸ Human Metabolome Database (HMDB)

3.2.6 Solubility

Soluble in alcohol, methanol, pyridine

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 49

▸ Hazardous Substances Data Bank (HSDB)

Soluble in ethanol, sodium hydroxide; insoluble in ethyl ether, methanol

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-10

▸ Hazardous Substances Data Bank (HSDB)

Water: 0.57% (25 °C); ethanol (96%): 0.04% (25 °C); eth/water (1/1): 0.35% (25 °C); propylene glycol/water (1/1): 0.40% (25 °C); glycerol/water (1/1): 0.60% (25 °C)

*Merck; Cosmetics. Active Ingredients. Special Active Ingredients. Anti-Inflammatory. RonaCare Allantoin. Darmstadt, Germany: Merck. Available from, as of Feb 8, 2007: **https://www.merck.de/servlet/PB/menu/1284800/index.html***

▸ Hazardous Substances Data Bank (HSDB)

In water, 5.26X10+3 mg/L at 25 °C

Yalkowsky, S.H., He, Yan., Handbook of Aqueous Solubility Data: An Extensive Compilation of Aqueous Solubility Data for Organic Compounds Extracted from the AQUASOL dATAbASE. CRC Press LLC, Boca

Raton, FL. 2003., p. 93

▸ Hazardous Substances Data Bank (HSDB)

5.26 mg/mL

▸ Human Metabolome Database (HMDB)

3.2.7 pH

pH = 4.5 - 6 (5% in water, 20 °C)

Merck; Cosmetics. Active Ingredients. Special Active Ingredients. Anti-Inflammatory. RonaCare Allantoin. Darmstadt, Germany: Merck. Available from, as of Feb 8, 2007: ***https://www.merck.de/servlet/PB/menu/1284800/index.html***

▸ Hazardous Substances Data Bank (HSDB)

3.2.8 Collision Cross Section

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

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

▸ CCSbase

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

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

▸ CCSbase

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

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

▸ CCSbase

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

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

▸ CCSbase

143.3 Å^2 [M+Na]$^+$

126.7 Å^2 [M-H]$^-$

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

- NORMAN Suspect List Exchange

3.2.9 Other Experimental Properties

Stable at pH 4-9. Hydrolytic decomposition with strong acids and bases

Merck; Cosmetics. Active Ingredients. Special Active Ingredients. Anti-Inflammatory. RonaCare Allantoin. Darmstadt, Germany: Merck. Available from, as of Feb 8, 2007:
https://www.merck.de/servlet/PB/menu/1284800/index.html

- Hazardous Substances Data Bank (HSDB)

3.2.10 Chemical Classes

Biological Agents -> Plant Oils and Extracts

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

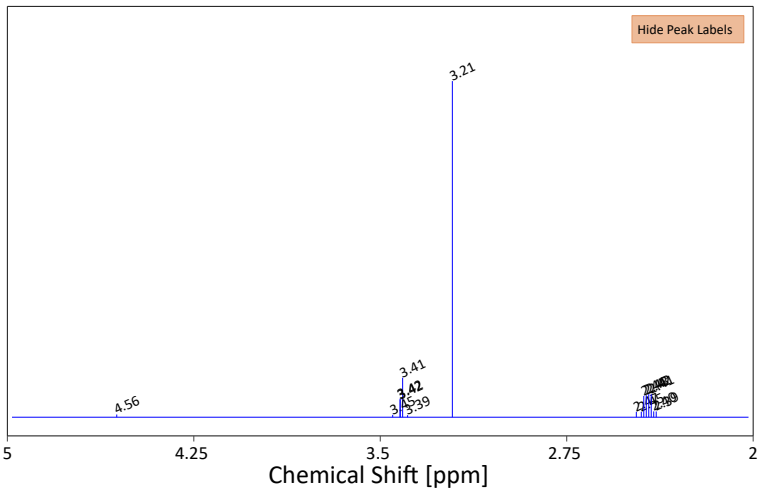
4 Spectral Information

4.1 1D NMR Spectra

4.1.1 1H NMR Spectra

1 of 4	View All
Spectra ID	1380
Instrument Type	Varian
Frequency	500 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	4.56:0.81, 2.40:1.74, 2.45:1.58, 3.41:11.76, 2.47:1.59, 2.41:6.87, 2.42:6.88, 2.39:1.71, 3.21:100.00, 3.42:5.53, 2.43:6.56, 2.44:6.33, 3.45:0.70, 3.42:5.26, 3.39:0.61

Thumbnail

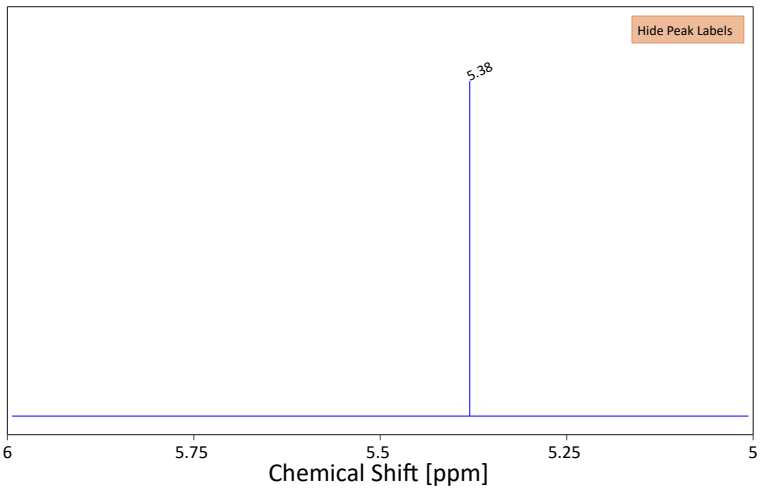


Human Metabolome Database (HMDB)

2 of 4 View All

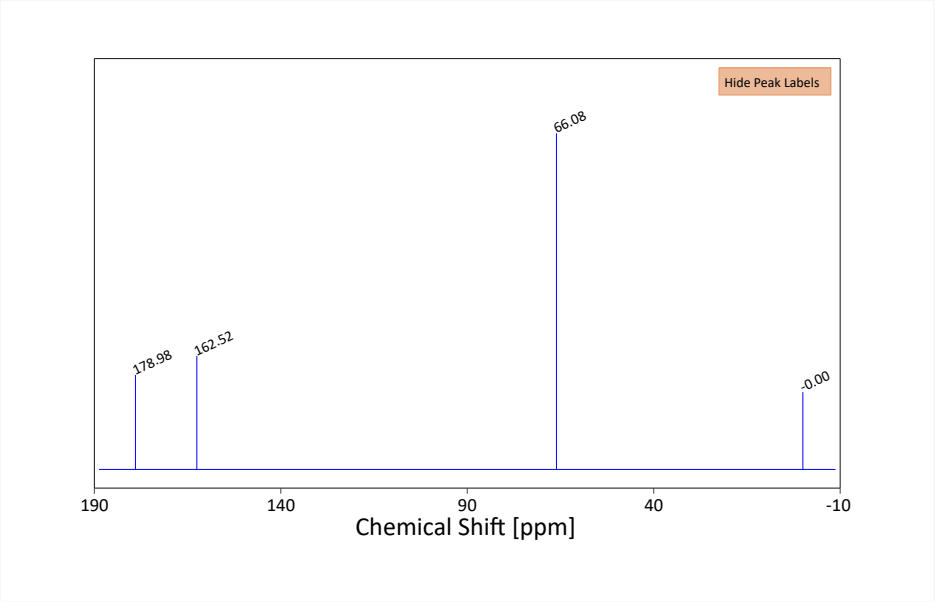
Spectra ID	4792
Instrument Type	Bruker
Solvent	D2O
pH	7.4
Shifts [ppm]:Intensity	5.38:7.74

Thumbnail



Human Metabolome Database (HMDB)

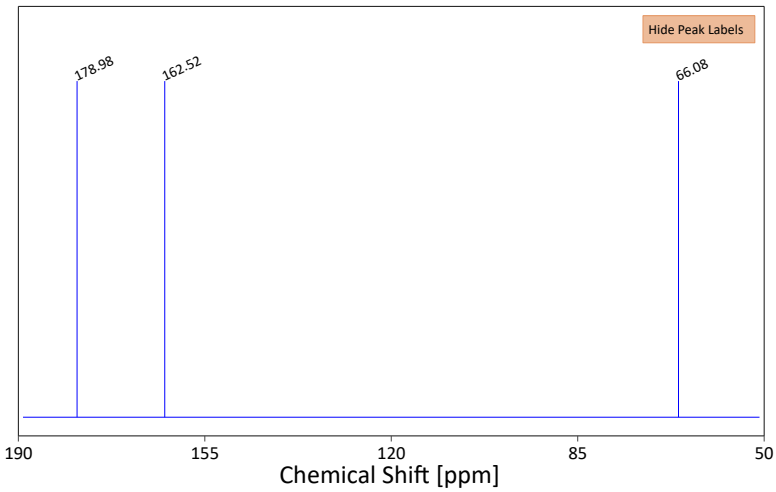
4.1.2 13C NMR Spectra

1 of 5	View All
Spectra ID	1233
Instrument Type	Bruker
Frequency	125 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	162.52:6.41, 178.98:5.34, 66.08:19.00, -0.00:4.37
Thumbnail	

▸ Human Metabolome Database (HMDB)

2 of 5	View All
Spectra ID	166437
Frequency	400 MHz
Solvent	H2O
Shifts [ppm]	162.52, 66.08, 178.98

Thumbnail



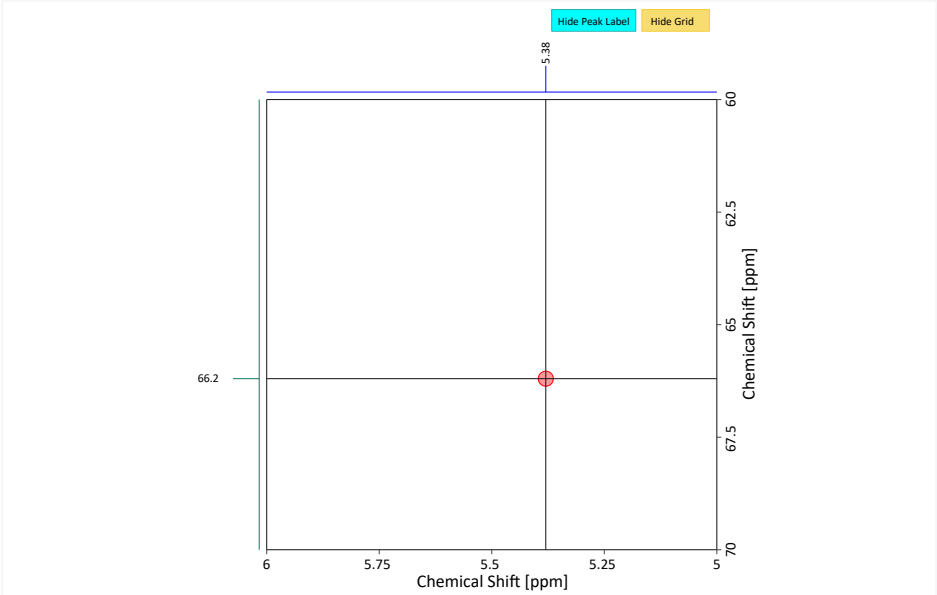
▸ Human Metabolome Database (HMDB)

4.2 2D NMR Spectra

4.2.1 1H-13C NMR Spectra

2D NMR Spectra Type	1H-13C HSQC
Spectra ID	1324
Instrument Type	Bruker
Frequency	400 MHz
Solvent	Water
pH	7.00
Shifts [ppm] (F2:F1):Intensity	5.38:66.20:1.00

Thumbnail



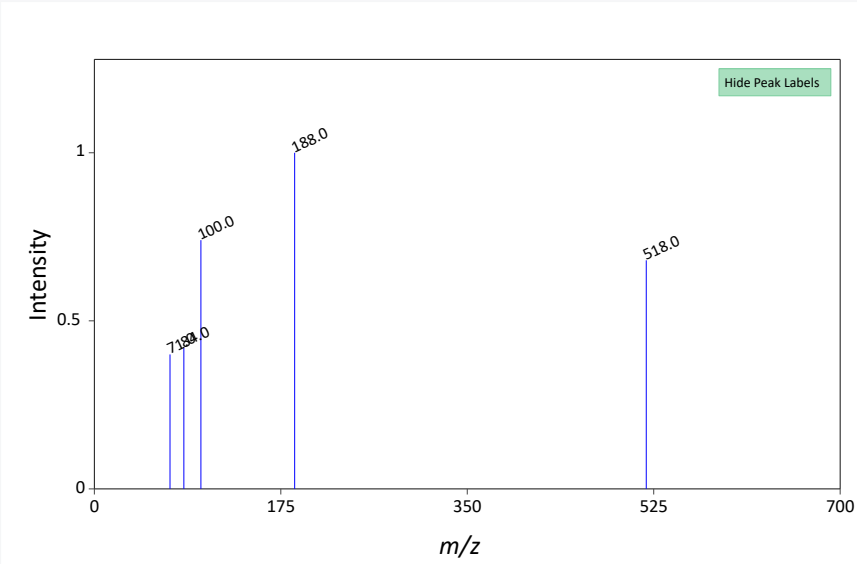
▸ Human Metabolome Database (HMDB)

4.3 Mass Spectrometry

4.3.1 GC-MS

1 of 16	View All
Spectra ID	1583
Instrument Type	GC-MS
SPLASH	splash10-00kr-4911230000-f2112ac79e45fb821ab6
Top 5 Peaks	188.0 1 100.0 0.74 518.0 0.68 84.0 0.42 71.0 0.40

Thumbnail

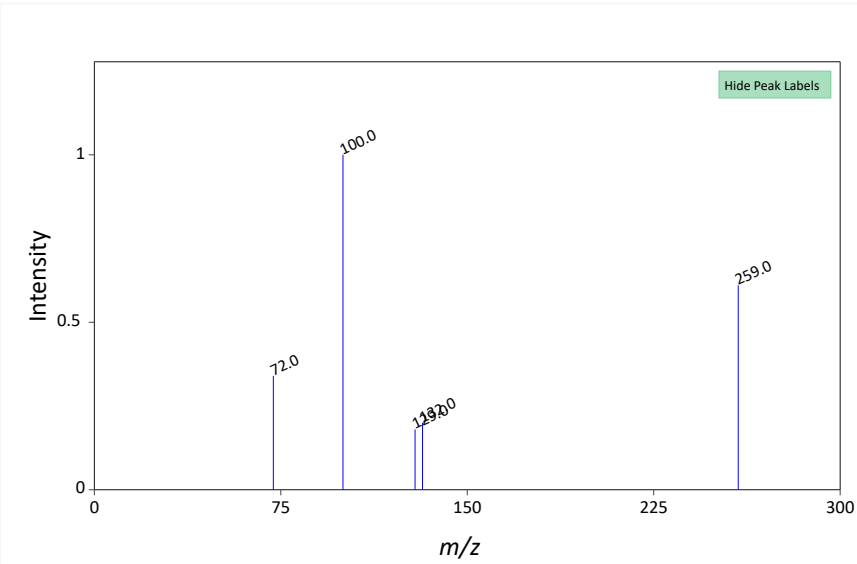


▸ Human Metabolome Database (HMDB)

2 of 16 View All

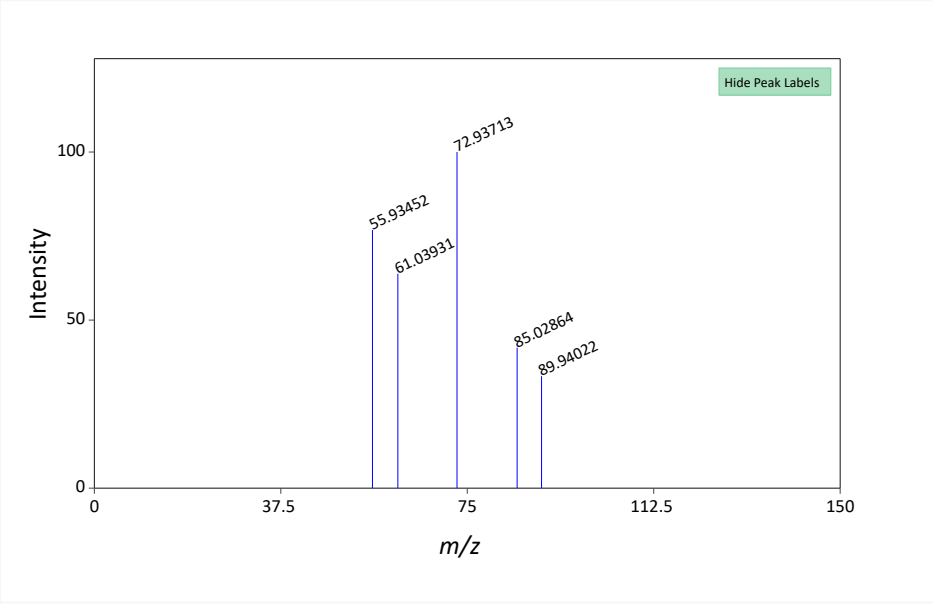
Spectra ID	1778
Instrument Type	GC-MS
SPLASH	splash10-0zfr-4951100000-88808e71aea4d5ad7885
Top 5 Peaks	100.0 1 259.0 0.61 72.0 0.34 132.0 0.20 129.0 0.18

Thumbnail



▸ Human Metabolome Database (HMDB)

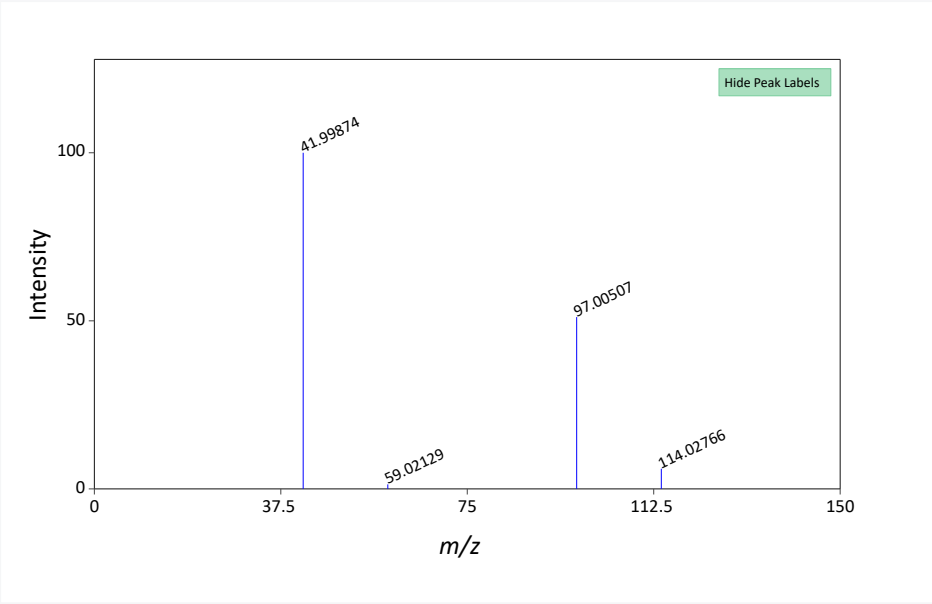
4.3.2 MS-MS

1 of 6	View All
Spectra ID	2226522
Ionization Mode	Positive
SPLASH	splash10-074r-9000000000-63e528ecadeb18126065
Top 5 Peaks	72.93713 100 55.93452 76.80 61.03931 63.80 85.02864 41.80 89.94022 33.30
Thumbnail	

▸ Human Metabolome Database (HMDB)

2 of 6	View All
Spectra ID	2228171
Ionization Mode	Negative
SPLASH	splash10-0007-9000000000-0300b52fe70e77739514
Top 5 Peaks	41.99874 100 97.00507 51.11 114.02766 6 59.02129 1.34

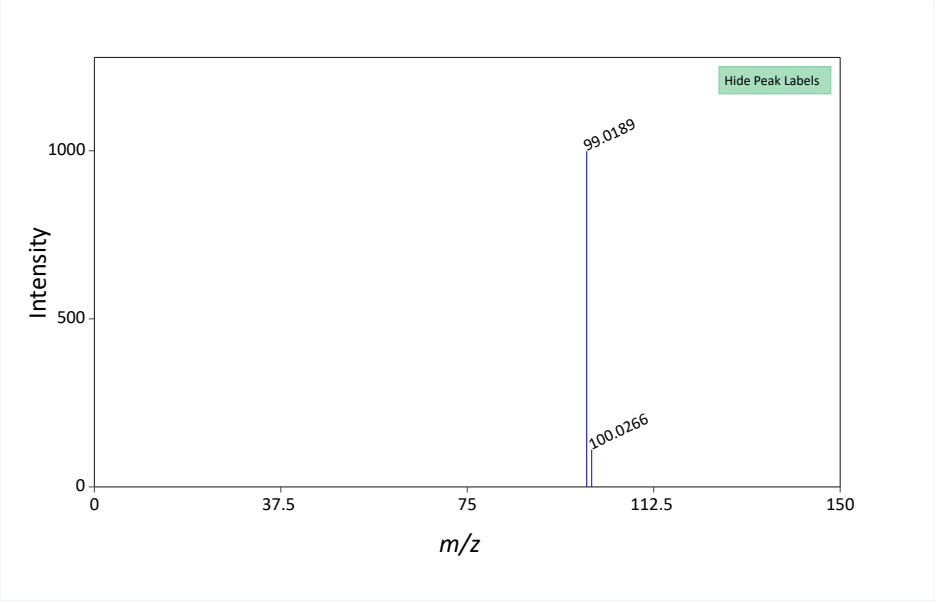
Thumbnail



▸ Human Metabolome Database (HMDB)

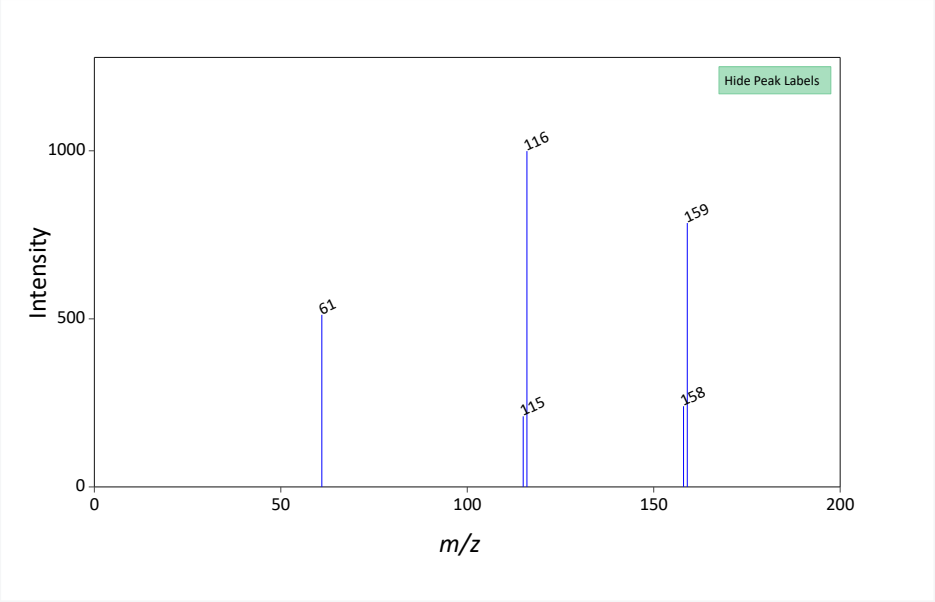
4.3.3 LC-MS

1 of 8	View All
Accession ID	MSBNK-MetaboLights-ML002501
Authors	Mark Earll, Stephan Beisken, EMBL-EBI
Instrument	LTQ Orbitrap Velos Thermo Scientific
Instrument Type	LC-ESI-ITFT
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	50 % (nominal)
Fragmentation Mode	HCD
Column Name	HSS T3 1.7 um, 2x150 mm, Waters
Retention Time	1.6 min
Precursor m/z	159.0513
Precursor Adduct	[M+H]+
Top 5 Peaks	99.0189 999 100.0266 111

SPLASH	splash10-0002-9100000000-8c779bd6b0021171c0c2
Thumbnail	
License	CC BY-SA
Reference	Beisken S et al (2014) Scientific Data, 1:140029, DOI:10.1038/sdata.2014.29. http://www.ebi.ac.uk/metabolights/MTBLS38

MassBank Europe

2 of 8	View All
Accession ID	MSBNK-RIKEN_ReSpect-PS016901
Authors	Sawada Y, Matsuda F, and Hirai MY. Plant Science Center, RIKEN
Instrument	TQD, Waters
Instrument Type	LC-ESI-QQ
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	10
Precursor m/z	159.11
Top 5 Peaks	116 999 159 785 61 512 158 240 115 210

SPLASH	splash10-066r-2900000000-7156a3134550c1a0599f
Thumbnail	
License	CC BY-NC
Reference	Sawada, Y.; Akiyama, K.; Sakata, A.; Kuwahara, A.; Otsuki, H.; Sakurai, T.; Saito, K.; Hirai, M. Y. Widely Targeted Metabolomics Based on Large-Scale MS/MS Data for Elucidating Metabolite Accumulation Patterns in Plants. Plant and Cell Physiology 2008, 50 (1), 37–47. DOI:10.1093/pcp/pcn183

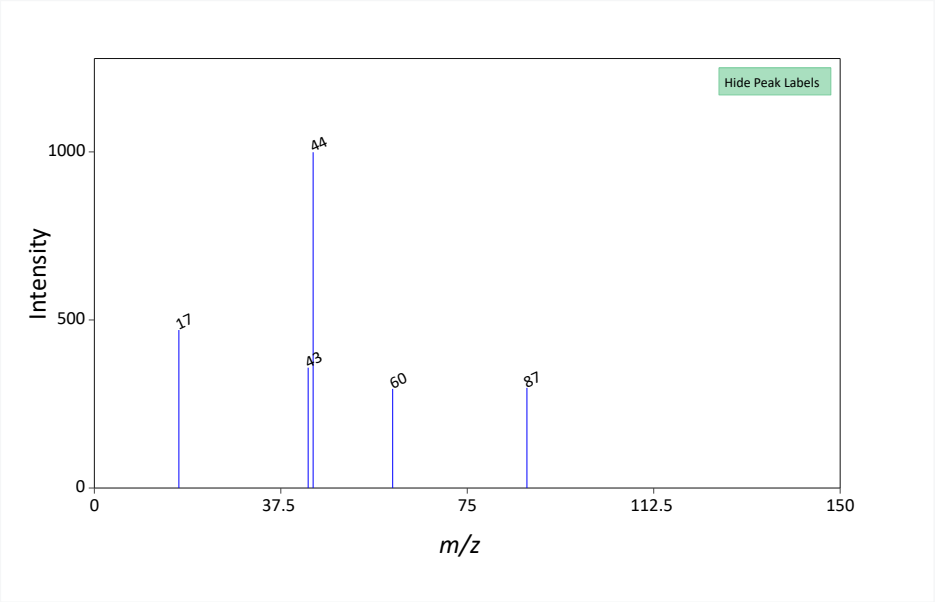
▸ MassBank Europe

4.3.4 Other MS

1 of 6	View All
Other MS	MASS: 76364 (NIST/EPA/MSDC Mass Spectral database, 1990 version); 173 (Aldermaston, Eight Peak Index of Mass Spectra, U.K.)

▸ Hazardous Substances Data Bank (HSDB)

2 of 6	View All
Accession ID	MSBNK-Fac_Eng_Univ_Tokyo-JP002868
Authors	MASS SPECTROSCOPY SOC. OF JAPAN (MSSJ)
Instrument	Unknown
Instrument Type	EI-B
MS Level	MS
Ionization Mode	POSITIVE

Top 5 Peaks	44 999 17 470 43 358 87 298 60 295
SPLASH	splash10-0006-9100000000-5f4cd23ea44234e5a455
Thumbnail	
License	CC BY-NC-SA

▸ MassBank Europe

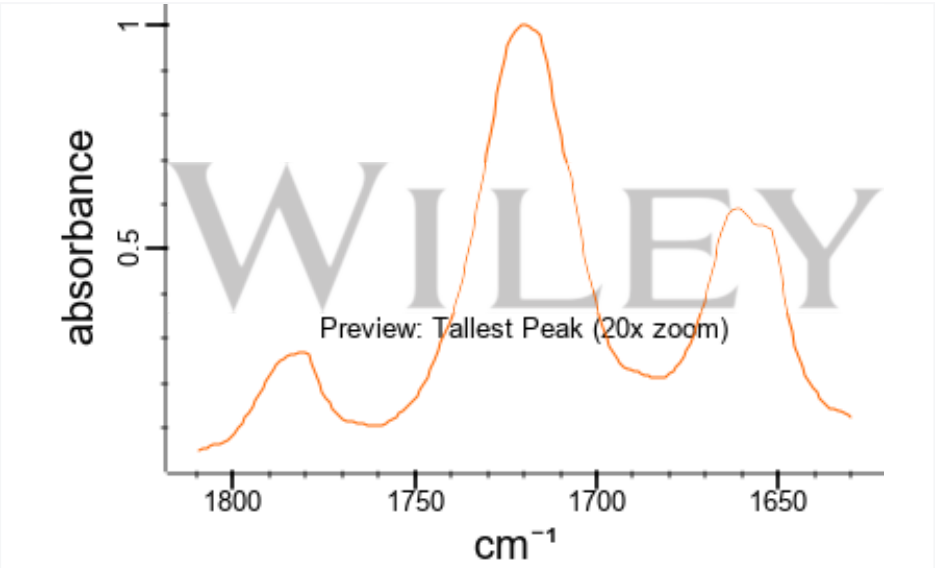
4.4 IR Spectra

IR Spectra	IR: 1808 (Coblentz Society spectral collection)

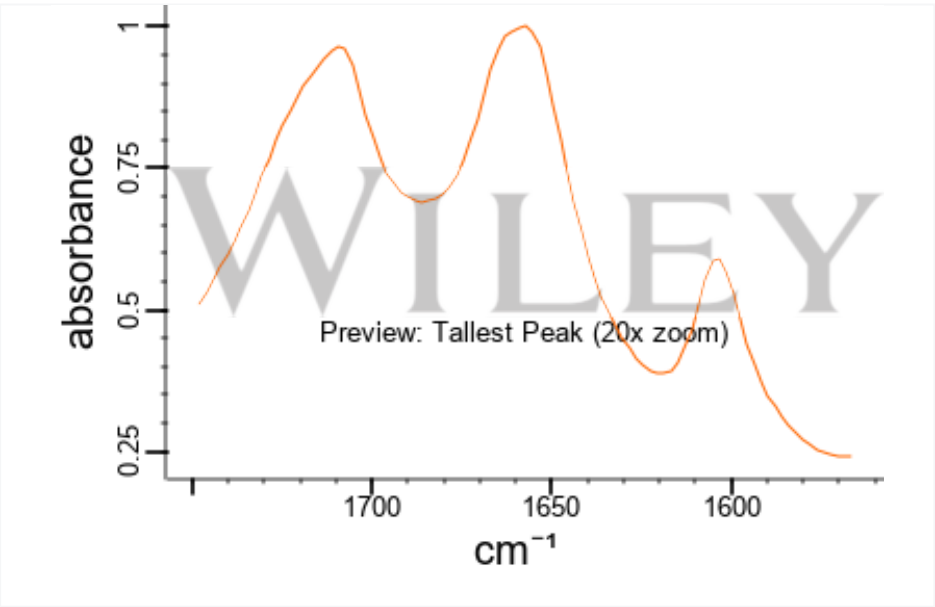
▸ Hazardous Substances Data Bank (HSDB)

4.4.1 FTIR Spectra

1 of 2	
Technique	KBr WAFER
Source of Sample	Fine Organics, Inc., Lodi, New Jersey
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

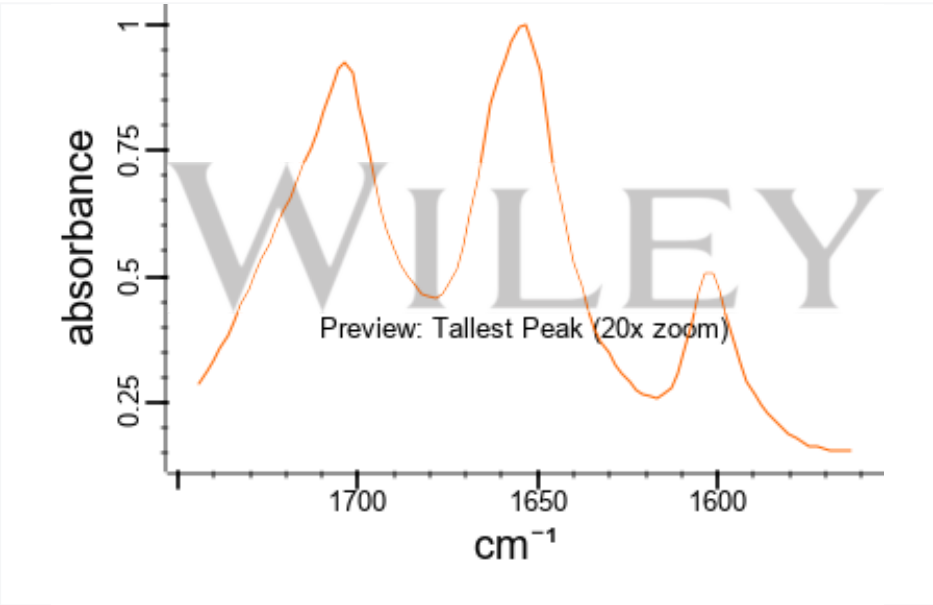
Thumbnail	

▸ SpectraBase

2 of 2	
Instrument Name	Bruker IFS 85
Technique	KBr-Pellet
Source of Sample	Riedel de Haen AG, Seelze
Copyright	Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

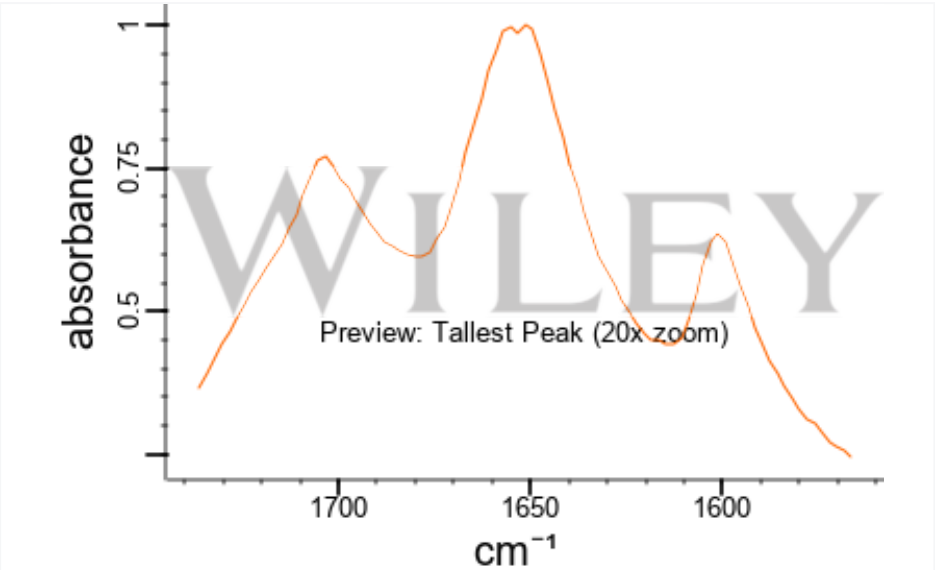
▸ SpectraBase

4.4.2 ATR-IR Spectra

1 of 2	
Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Spectrum Chemical Manufacturing Corp.
Catalog Number	A1196
Lot Number	48133A0
Copyright	Copyright © 2012-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

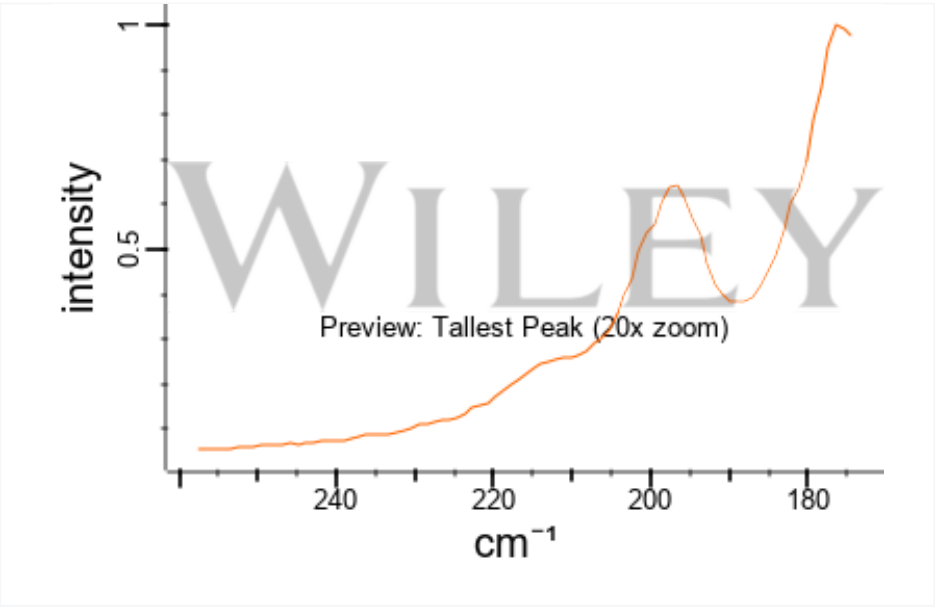
▸ SpectraBase

2 of 2	
Source of Sample	Aldrich
Catalog Number	A28392
Copyright	Copyright © 2018-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail	

▸ SpectraBase

4.5 Raman Spectra

Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Spectrum Chemical Manufacturing Corp.
Catalog Number	A1196
Lot Number	48133A0
Copyright	Copyright © 2012-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

- SpectraBase

4.6 Other Spectra

Optically active forms are known

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

- Hazardous Substances Data Bank (HSDB)

5 Related Records

5.1 Related Compounds with Annotation

- PubChem

5.2 Related Compounds

Same Connectivity Count	5
Same Stereo Count	3
Same Isotope Count	3
Same Parent, Connectivity Count	50

Same Parent, Stereo Count	48
Same Parent, Isotope Count	48
Same Parent, Exact Count	46
Mixtures, Components, and Neutralized Forms Count	154
Similar Compounds Count	83
Similar Conformers Count	482

PubChem

5.3 Substances

5.3.1 PubChem Reference Collection SID

481106862

PubChem

5.3.2 Related Substances

All Count	798
Same Count	296
Mixture Count	502

PubChem

5.3.3 Substances by Category

PubChem

5.4 Other Relationships

Alcloxa (active moiety of)	Allantoin; oatmeal (component of)	Allanto
Comfrey Leaf (part of)	Allantoin; Lidocaine Hydrochloride (component of)	Allanto
Comfrey Root (part of)	Adenosine; allantoin (component of)	Allanto
Allantoin; Lidocaine (component of)	Allantoin; Benzalkonium Chloride (component of)	Allanto
Allantoin; Glycerin (component of)	Allantoin; Sodium Fluoride (component of)	Allanto
Allantoin; panthenol (component of)	Allantoin; shea butter (component of)	Allanto
Allantoin; Dimethicone (component of)	Allantoin; Benzethonium Chloride (component of)	Allanto
Allantoin; zinc oxide (component of)	Allantoin; witch hazel (component of)	Adeno
Allantoin; MENTHOL (component of)	Allantoin; salicylic acid (component of)	Allanto
Allantoin; petrolatum (component of)	Allantoin; SILICON DIOXIDE (component of)	Allanto

PubChem

5.5 Entrez Crosslinks

PubMed Count	13
Taxonomy Count	5
Gene Count	17

PubChem

6 Chemical Vendors

- PubChem

7 Drug and Medication Information

7.1 Drug Indication

Allantoin is commonly applied in a variety of topical vehicles or applications such as cosmetic creams, toothpastes, mouthwashes, shampoos, lipsticks, anti-acne products, and lotions for the purpose of moisturizing skin, enhancing the smoothness of skin, stimulating the healing of wounds, and soothing irritated skin.

- DrugBank

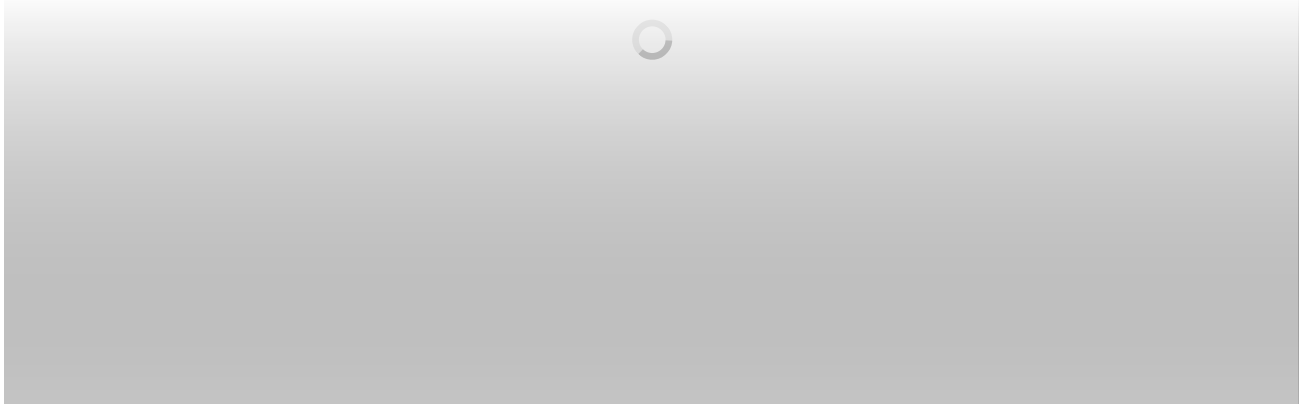
FDA Label

- DrugBank

Treatment of epidermolysis bullosa

- European Medicines Agency (EMA)

7.2 FDA National Drug Code Directory



National Drug Code (NDC) Directory

7.3 Drug Labels

Drug and label

DailyMed

Active ingredient and drug

DailyMed

7.4 Clinical Trials

7.4.1 ClinicalTrials.gov

ClinicalTrials.gov

7.4.2 EU Clinical Trials Register

EU Clinical Trials Register

7.5 EMA Drug Information

Type	Paediatric investigation
Active Substance	Allantoin
Therapeutic Area	Dermatology
Drug Form	Cream
Administration Route	Topical use
Decision Type	PM: decision on the application for modification of an agreed PIP
Decision Date	2017-08-11

▸ European Medicines Agency (EMA)

7.6 Therapeutic Uses

A urea hydantoin that is found in URINE and PLANTS and is used in dermatological preparations.

*National Library of Medicine, SIS; ChemIDplus Record for Allantoin (97-59-6), MESH Heading. Available from, as of February 1, 2006: **https://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp***

▸ Hazardous Substances Data Bank (HSDB)

Allantoin, a component in Comfrey, stimulates tissue repair and wound healing through cell proliferation. Allantoin has also had significant effect on cellular multiplication in degenerating and regenerating peripheral nerves.

PDR for Herbal Medicines; Medical Economics Co., Montvale, NJ. p. 212 (2000)

▸ Hazardous Substances Data Bank (HSDB)

In humans, the allantoin to uric acid ratio in plasma increases during oxidative stress, thus this ratio has been suggested to be an in vivo marker for oxidative stress in humans.

PMID:16705445

Tsahar E et al; J Comp Physiol (B) 176 (7): 653-61 (2006)

▸ Hazardous Substances Data Bank (HSDB)

Diagnostic marker for oxidative stress during antituberculous (anti-TB) therapy.

PMID:7546339

Walubo A et al; Biomed Environ Sci 8 (2): 106-13 (1995)

- Hazardous Substances Data Bank (HSDB)

For more Therapeutic Uses (Complete) data for ALLANTOIN (8 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

7.7 Drug Warnings

Skin: For external use only. Ocular: Avoid contact with eyes. Sensitization: Mederma is contraindicated in individuals who have shown hypersensitivity to any of its components /Mederma/

Merz Pharmaceuticals, LLC; Material Safety Data Sheet, Mederma. December 12, 2002

- Hazardous Substances Data Bank (HSDB)

7.8 Biomarker Information

- MarkerDB

8 Minerals

1 of 2	
Name	ALLANTOIN
Formula	C4H6N4O3

Athena Minerals

2 of 2	
Name	Allantoin
IMA Number	IMA2020-004a
Formula	$C_4H_6N_4O_3$
IMA Symbol	Aan
Crystal Structure Data Link	American Mineralogist Crystal Structure Database

RRUFF Project

9 Pharmacology and Biochemistry

9.1 Pharmacodynamics

There is no well controlled and appropriate data that can formally substantiate the pharmacodynamic properties of allantoin. Nevertheless, ongoing studies suggest that allantoin possesses moisturizing and keratolytic effects, as well as abilities to increase the water content of the extracellular matrix and enhance the desquamation of upper layers of dead skin cells, all of which are activities that can promote cell proliferation and facilitate wound healing.

DrugBank

9.2 MeSH Pharmacological Classification

Dermatologic Agents

Drugs used to treat or prevent skin disorders or for the routine care of skin. (See all compounds classified as Dermatologic Agents.)

Medical Subject Headings (MeSH)

9.3 Absorption, Distribution and Excretion

Absorption

In studies on human subjects, a recovery of 19% and 34% of allantoin in the urine was observed but only in two individuals and only after the administration of massive doses of

allantoin. After intravenous administration, recovery in the urine was practically quantitative with doses of 75 to 600 mgm in the human model. After 240 mgm, excretion continued for 72 hours in human subjects and the results were similar in regards to subcutaneous injection.

- DrugBank

Route of Elimination

Urinary clearance is the predominant excretion route.

- DrugBank

Clearance

Some studies suggest that the average renal clearance of allantoin in normal, healthy human subjects is approximately 123 cc per minute. It is generally agreed upon that exogenously administered allantoin is rapidly excreted.

- DrugBank

Allantoin administered to dogs orally as solid or solution was excreted in the urine to an extent of between 35 and 92 per cent within 24 hours. No allantoin was recovered either in urine or feces when given to rabbits orally. In man the recovery was 19 and 34 per cent in two individuals after massive doses. After intravenous administration recovery in the urine was practically quantitative with doses of 75 to 600 mgm. in the dog and in man. After 240 mgm. in man excretion continued for 72 hours. The results were similar after subcutaneous injection. **Uric acid** injected intravenously into a dog was converted into allantoin within two hours.

Young EG et al; J Pharmacol Exptl Ther 81 (1): 1-9 (1944)

- Hazardous Substances Data Bank (HSDB)

9.4 Metabolism / Metabolites

Uricase is the enzyme that possesses the functionality to convert **uric acid** to allantoin. Considering humans do not possess any endogenous uricase, **uric acid** is the only final breakdown product in the **purine** degradation of unwanted waste product purine nucleotides. The presence of allantoin in human urine is subsequently the result of non-enzymatic processes on **uric acid** with reactive oxygen species. Such non-enzymatic processes are consequently potentially suitable biomarkers for measuring oxidative stress in chronic illnesses and aging. Furthermore, as allantoin is found endogenously and is part of basic, natural metabolic pathways, no accumulation is expected of it. Additionally, allantoin is not believed to be metabolized to a measurable extent in humans and animals.

- DrugBank

In humans, uric acid is the final breakdown product of unwanted purine nucleotides. Uric acid is the last stage in purine degradation, because humans lack the enzyme uricase which converts uric acid into allantoin.

PMID:15493112

Hediger MA; Ther Umsch 61 (9): 541-5 (2004)

▸ Hazardous Substances Data Bank (HSDB)

Allantoin in the presence of calcium ions has been implicated as a potential toxic agent in Reye's syndrome. An investigation of possible alternative sources of allantoin in humans, which lack the enzyme uricase, has been initiated. Urate is a strong reducing agent which can reduce cytochrome c nonenzymatically, with the concomitant production of CO2 and H+. The stoichiometries measured for the various reactants and products were 1 urate:2 cytochrome c:1 H+:1 CO2. The initial reaction rate depended on the concentrations of both urate and cytochrome c, with reaction kinetics that were first order with respect to urate and second order with respect to cytochrome c. The participation of molecular oxygen in this reaction could not be detected. The pH and ionic strength optima for this reaction were determined to be 9.5-10.5 and 10(-5) M, respectively. Based on the results reported here, the following balanced equation can be written: urate-2 + 2 cytochrome c+3 + 2 H2O---- allantoin + 2 cytochrome c+2 + H+ + HCO3-. /The authors/ propose that allantoin can be generated from the oxidation of urate by cytochrome c+3, and that this is a potential source of allantoin in human tissues.

PMID:3028263

Martens ME et al; Arch Biochem Biophys 252 (1):91-6 (1987)

▸ Hazardous Substances Data Bank (HSDB)

Uric acid is the main nitrogenous waste product in birds but it is also known to be a potent antioxidant. Hominoid primates and birds lack the enzyme urate oxidase, which oxidizes uric acid to allantoin. Consequently, the presence of allantoin in their plasma results from non-enzymatic oxidation.

PMID:16705445

Tsahar E et al; J Comp Physiol (B) 176 (7): 653-61 (2006)

▸ Hazardous Substances Data Bank (HSDB)

In most mammals purine degradation ultimately leads to the formation of allantoin. Humans lack the enzyme uricase, which catalyzes the conversion of uric acid to allantoin.

PMID:16375732

Masseoud D et al; Curr Pharm Des 11 (32): 4117-24 (2005)

▸ Hazardous Substances Data Bank (HSDB)

For more Metabolism/Metabolites (Complete) data for ALLANTOIN (11 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

9.5 Biological Half-Life

When studied in cattle, sheep, and horses, the half-life of allantoin is in the range of 1 to 2.5 hours.

- DrugBank

9.6 Mechanism of Action

There is no well controlled data that can formally substantiate the method of action. However, ongoing studies suggest that there may exist a histological wound healing profile induced by allantoin in rats that leads to the amelioration and fastening of the reestablishment of normal skin. This facilitation of wound healing is supported by observations that wounds inflicted to rat subjects to which topical allantoin preparations were applied histologically demonstrated increased vasodilation, presence of inflammatory exudates, number of inflammatory cells, angiogenesis, fibroblast proliferation, and increased collagen deposition when compared to rat subjects with wounds that did not receive any allantoin administration.

- DrugBank

9.7 Human Metabolite Information

9.7.1 Tissue Locations

Placenta

- Human Metabolome Database (HMDB)

9.7.2 Cellular Locations

Cytoplasm

- Human Metabolome Database (HMDB)

9.8 Biochemical Reactions

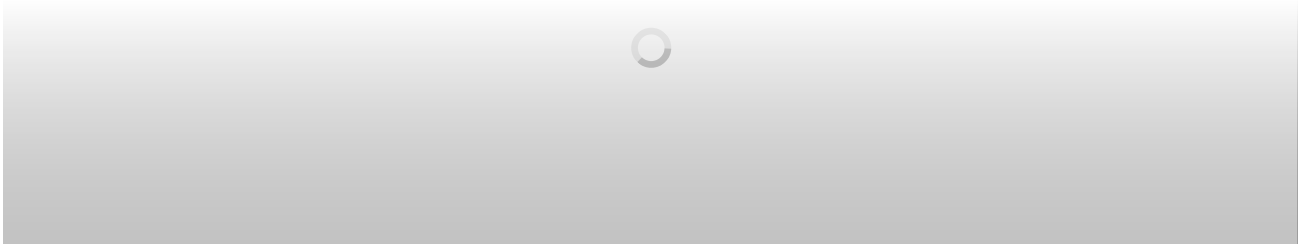
Rhea - Annotated Reactions Database

PubChem

10 Use and Manufacturing

10.1 Uses

EPA CPDat Chemical and Product Categories



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

- **EPA Chemical and Products Database (CPDat)**

Sources/Uses

Occurs naturally in tobacco seeds, sugar beets, and wheat sprouts; [Hawley] Used as a medicine for wound healing, in biochemical research, and in the preparation of estrogenic compounds; Also used as a dermatological preparation to treat dandruff, seborrheic dermatitis, psoriasis, hair loss, corns, and calluses; It is an ingredient in sunscreens; [HSDB]

Hawley - Lewis RJ. _Hawley's Condensed Chemical Dictionary, _15th Ed. New York: John Wiley & Sons, 2007.

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

For allantoin (USEPA/OPP Pesticide Code: 085701) there are 0 labels match. /SRP: Not registered for current use in the U.S., but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently approved uses./

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Allantoin (97-59-6). Available from, as of February 9, 2007: ***https://npirspublic.ceris.purdue.edu/ppis/***

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

Subpart B: Section 310.545: Drug products containing certain active ingredients offered over-thecounter (OTC) for certain uses. Ingredients-Approved as of May 7, 1991: Allantoin (wound healing claims only).

FDA; Federal Register / Vol. 68, No. 107 / Wednesday, June 4, 2003

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

Subpart B: Section 347.10 Skin protectant active ingredients. The active ingredients of the product consist of any of the following, within the concentration specified for each ingredient: (a) Allantoin, 0.5 to 2 percent.

FDA; Federal Register / Vol. 68, No. 107 / Wednesday, June 4, 2003

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

Allantoin is listed on the FDA OTC Ingredient List as used for or having reviews pending for use as a wound healing agent, skin protectant and external analgesic, a dandruff/seborrheic dermatitis/psoriasis product, a grower for hair loss, a corn/callus remover, and a sunscreen ingredient.

FDA; Allantoin. OTC Ingredient List. Updated August 2006. Available from, as of January 31, 2007: ***https://www.fda.gov/cder/Offices/OTC/Ingredient_List_A-C.pdf***

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

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

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

10.1.1 Use Classification

Human Drugs -> EU pediatric investigation plans

- **European Medicines Agency (EMA)**

Cosmetics -> Soothing

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

- **NORMAN Suspect List Exchange**

10.1.2 Consumer Uses

Preservative

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

- **EPA Chemicals under the TSCA**

10.1.3 Household Products

Household & Commercial/Institutional Products

Information on 158 consumer products that contain Allantoin in the following categories is provided:

• Personal Care

• Pet Care

- **Consumer Product Information Database (CPID)**

10.2 Methods of Manufacturing

Produced by oxidation of **uric acid**. Also present in tobacco seeds, sugar beets, wheat sprouts.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

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

Various heterocyclic compounds can be obtained by coupling polynucleophiles with **glyoxylic acid**: ... with **urea** and an acid catalyst, allantoin is obtained in 60% yield.

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V15 697 (2003)

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

10.3 Formulations / Preparations

Mederma, a topical skin gel produced by Merz Pharmaceuticals, LLC, 4215 Tudor Lane Greensboro, NC 27410, contains **water** (purified), **PEG-4**, allium cepa (onion) bulb extraxt, xanthan gum, allantoin, fragrance, **methylparaben** and **sorbic acid**.

Physicians' Desk Reference entry for Mederma Topical Gel (Merz). Micromedex Healthcare Series. Thomson MICROMEDEX (2004)

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

10.4 U.S. Production

Aggregated Product Volume

2018: <1,000,000 lb

2017: <1,000,000 lb

2016: <1,000,000 lb

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

▸ **EPA Chemicals under the TSCA**

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	No Reports
1990	10 thousand - 500 thousand

1994	No Reports
1998	10 thousand - 500 thousand
2002	10 thousand - 500 thousand

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Urea, (2,5-dioxo-4-imidazolidinyl)- (97-59-6). Available from, as of February 16, 2007: ***https://www.epa.gov/oppt/iur/tools/data/2002-vol.html***

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

10.5 General Manufacturing Information

EPA TSCA Commercial Activity Status

Urea, N-(2,5-dioxo-4-imidazolidinyl)-: ACTIVE

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

▸ **EPA Chemicals under the TSCA**

One of several compounds identified in comfrey (Symphytum officinale)

PDR for Herbal Medicines; Medical Economics Co., Montvale, NJ. p. 212 (2000)

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

The main effect of allantoin is the powerful stimulation of cell proliferation and the enhancement of the rebuilding of intact granulation tissue. In pharmaceutical applications, allantoin is used ... in the treatment of ulcers, slow-healing wounds and burns.

Merck; Cosmetics. Active Ingredients. Special Active Ingredients. Anti-Inflammatory. RonaCare Allantoin. Darmstadt, Germany: Merck. Available from, as of Feb 8, 2007: ***https://www.merck.de/servlet/PB/menu/1284800/index.html***

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

Pesticide: Cancelled

USEPA/Office of Pesticide Programs; Status Of Pesticides in Reregistration and Special Review (1994) EPA 738-R-94-008, p. 233

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

The Food and Drug Administration (FDA) final monograph establishing conditions under which over-the-counter (OTC) skin protectant drug products are generally recognized as safe and effective and not misbranded includes allantoin as an active ingredient for symptoms of /skin/ dryness and as a Category III skin protectant for wound-healing based on the lack of effectiveness data (43 FR 34628 at 34644 through 34647).

FDA; Federal Register / Vol. 68, No. 107 / Wednesday, June 4, 2003

▸ Hazardous Substances Data Bank (HSDB)

Allantoin ... /has/ been present in oral mucosal injury drug products for use as oral wound healing agents. Oral wound healing agents have been marketed as aids in the healing of minor oral wounds by means other than cleansing and irrigating, or by serving as a protectant. Allantoin /is/ safe for use as oral wound healing agents, but there are inadequate data to establish general recognition of the effectiveness of these ingredients as oral wound healing agents. ...Clinical investigations designed to obtain evidence that any drug product labeled, represented, or promoted for OTC use as an oral wound healing agent is safe and effective for the purpose intended must comply with the requirements and procedures governing the use of investigational new drugs set forth in part 312 of this chapter. (d) After the effective date of the final regulation, any OTC drug product that is labeled, represented, or promoted for use as an oral wound healing agent may not be initially introduced or initially delivered for introduction into interstate commerce unless it is the subject of an approved new drug application.

FDA; 51 FR 26114, July 18, 1986, as amended at 55 FR 11579, Mar. 29, 1990

▸ Hazardous Substances Data Bank (HSDB)

11 Identification

11.1 Analytic Laboratory Methods

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

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p1320 (2007)

▸ Hazardous Substances Data Bank (HSDB)

Analyte: allantoin; matrix: chemical identification; procedure: thin-layer chromatography with comparison to standards

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p1320 (2007)

▸ Hazardous Substances Data Bank (HSDB)

Analyte: allantoin; matrix: chemical identification; procedure: reaction with **sodium hydroxide** and **water**; addition of **hydrochloric acid**; addition of **potassium bromide** solution, **resorcinol** solution and **sulfuric acid**; heating results in a dark blue color, which turns red after cooling and adding to **water**

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p1320 (2007)

▸ Hazardous Substances Data Bank (HSDB)

Analyte: allantoin; matrix: chemical purity; procedure: dissolution in water; potentiometric titration with sodium hydroxide, using a suitable electrode system

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p1320 (2007)

▸ Hazardous Substances Data Bank (HSDB)

11.2 Clinical Laboratory Methods

A new enzymatic assay using allantoinase and allantoate amidohydrolase for specifically measuring allantoin concentration in serum has been developed. The procedure is simple, rapid, and accurate. The method has been used to measure serum allantoin levels after oral administration of purine nucleotides to experimental animals, including rats that have uricase catalyzing the conversion of urate to allantoin.

PMID:17081493

Muratsubaki H et al; Anal Biochem 359 (2): 161-6 (2006)

▸ Hazardous Substances Data Bank (HSDB)

A micellar electrokinetic chromatographic method is described for the determination and quantitation of allantoin, an end-product of purine metabolism in mammals. This method is applicable to biofluids of different mammal species and man.

Alfazema LN et al; J Chromatog A. 817 (102): 345-52 (1998)

▸ Hazardous Substances Data Bank (HSDB)

An analytical procedure was developed for determining allantoin using high pressure liquid chromatography (HPLC) separation of an ultraviolet labeled allantoin derivative. The method was applied to the quantitative measurement of allantoin in cosmetic preparations. ... The allantoin was derivatized to an ultraviolet labeled product and read by reverse phase chromatography on an octadecylsilyl silica column.

Nakao K et al; J Assoc Off Anal Chem 65 (6): 1362-5 (1982)

▸ Hazardous Substances Data Bank (HSDB)

A stability indicating HPLC method for the determination of allantoin in cream and lotion formulations is presented. An extraction step in methanol-distilled water and separation from interferences by reversed phase chromatography precedes the LC.

PMID:7131287

Zaida ZR et al; J Pharm Sci 71: 997-9 (1982)

▸ Hazardous Substances Data Bank (HSDB)

A high performance liquid chromatography (HPLC) method was developed for determination of allantoin derivatives in cosmetic and pharmaceutical products. Solutions of allantoin or chlorohydroxy aluminium allantoinate (ALCA) or samples of toothpastes, creams, shampoos, soaps, lipsticks, and powders were extracted in hot water and injected on a resin based strong cation exchanger using water as eluent. The allantoin derivatives were determined from post column reactions.

Kawase J et al; J Chromatography 253 (2): 237-42 (1982)

▸ Hazardous Substances Data Bank (HSDB)

12 Safety and Hazards

12.1 Hazards Identification

12.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	**Warning**
GHS Hazard Statements	H302 (100%): Harmful if swallowed [**Warning** Acute toxicity, oral]
Precautionary Statement Codes	P264, P270, P301+P317, P330, 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 294 companies from 4 notifications to the ECHA C&L Inventory.* *Reported as not meeting GHS hazard criteria by 246 of 294 companies. For more detailed information, please visit ECHA C&L website.* *Of the 3 notification(s) provided by 48 of 294 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

Acute Tox. 4 (100%)

- European Chemicals Agency (ECHA)

12.1.3 Hazards Summary

May cause irritation; [MSDSonline] No increased congenital anomalies found in children of 51 women treated with allantoin during the first trimester of pregnancy; [REPROTOX]

REPROTOX - Scialli AR, Lione A, Boyle Padgett GK. Reproductive Effects of Chemical, Physical, and Biological Agents. Baltimore: The Johns Hopkins University Press, 1995.

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

12.2 Accidental Release Measures

12.2.1 Disposal Methods

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

- Hazardous Substances Data Bank (HSDB)

12.3 Regulatory Information

REACH Registered Substance

Status: Active Update: 30-11-2021 https://echa.europa.eu/registration-dossier/-/registered-dossier/13641

- European Chemicals Agency (ECHA)

New Zealand EPA Inventory of Chemical Status

Allantoin: Does not have an individual approval but may be used under an appropriate group standard

- New Zealand Environmental Protection Authority (EPA)

12.3.1 FIFRA Requirements

As the federal pesticide law FIFRA directs, EPA is conducting a comprehensive review of older pesticides to consider their health and environmental effects and make decisions about their future use. Under this pesticide reregistration program, EPA examines health and safety data for pesticide active ingredients initially registered before November 1, 1984, and determines whether they are eligible for reregistration. In addition, all pesticides must meet the new safety standard of the Food Quality Protection Act of 1996. Pesticides for which EPA had not issued Registration Standards prior to the effective date of FIFRA '88 were divided into three lists based upon their potential for human exposure and other factors, with List B containing pesticides of greater concern and List D pesticides of less concern. Allantoin is found on List C. Case No: 3015; Pesticide type: insecticide; Case Status: No products containing the pesticide are actively registered. Therefore, we are characterizing the case as "cancelled." Under FIFRA, pesticide producers may voluntarily cancel their registered products. EPA also may cancel pesticide registrations if registrants fail to pay required fees or make/meet certain reregistration commitments, or if EPA reaches findings of unreasonable adverse effects; Active ingredient (AI): allantoin; AI Status: The active ingredient is no longer contained in any registered products. Thus, we characterize it as "cancelled."

United States Environmental Protection Agency/ Prevention, Pesticides and Toxic Substances; Status of Pesticides in Registration, Reregistration, and Special Review. (1998) EPA 738-R-98-002, p. 233

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

12.3.2 FDA Requirements

Skin protectant active ingredients. The active ingredients of the products consist of any of the following, within the concentration specified for each ingredient. Allantoin, 0.5 to 2 percent.

21 CFR 347.10; U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 5, 2007: ***https://www.ecfr.gov***

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

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

21 CFR 310.545(a)(7); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 5, 2007: ***https://www.ecfr.gov***

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

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

21 CFR 310.545(a)(18); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 5, 2007: ***https://www.ecfr.gov***

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

Drug products containing active ingredients offered over-the-counter (OTC) for human use as oral wound healing agents. Allantoin ... /has/ been present in oral mucosal injury drug products for use as oral wound healing agents. Oral wound healing agents have been marketed as aids in the healing of minor oral wounds by means other than cleansing and irrigating, or by serving as a protectant. Allantoin, **carbamide peroxide** in anhydrous **glycerin**, **water** soluble chlorophyllins, and **hydrogen peroxide** in aqueous solution are safe for use as oral wound healing agents, but there are inadequate data to establish general recognition of the effectiveness of these ingredients as oral wound healing agents.

21 CFR 310.534(a); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 5, 2007: ***https://www.ecfr.gov***

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

13 Toxicity

13.1 Toxicological Information

13.1.1 Carcinogen Classification

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

▸ **Toxin and Toxin Target Database (T3DB)**

13.1.2 Interactions

Feed containing 0.2% allantoin ... with or without 0.2% **sodium nitrite**, was given ad lib. to groups of 20 or 24 male and 20 or 24 female F344 rats for 106 wk. ... Control rats were given untreated feed ... and **nitrite**-treated controls were given **sodium nitrite** at a concentration of 0.2% in feed or drinking-**water**. At the end of the treatment period the rats were given untreated feed ...and observed until death. There was little or no life-shortening

effect in any treatment group. /Allantoin / administered alone /and in combination with **sodium nitrite** did not induce/ an increase in the incidence of any tumor in comparison with the untreated control groups ...

PMID:6541624

Lijinsky W; Food Chem Toxicol 22(9): 715-20 (1984)

▸ Hazardous Substances Data Bank (HSDB)

13.1.3 Antidote and Emergency Treatment

/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 edition, Elsevier Mosby, St. Louis, MO 2005, 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 /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload ... . Treat seizures with **diazepam** or **lorazepam** ... . Use **proparacaine hydrochloride** to assist eye irrigation ... . /Poisons A and B/

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

▸ Hazardous Substances Data Bank (HSDB)

13.1.4 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Chronic Exposure or Carcinogenicity/ Feed containing 0.2% allantoin ... with or without 0.2% **sodium nitrite**, was given ad lib. to groups of 20 or 24 male and 20 or 24 female F344 rats for 106 wk. ... Control rats were given untreated feed ... and **nitrite**-treated controls were given **sodium nitrite** at a concentration of 0.2% in feed or drinking-**water**. At the end of the treatment period the rats were given untreated feed ...and observed until death. There was little or no life-shortening effect in any treatment group. /Allantoin / administered alone /and in combination with **sodium nitrite** did not induce/ an increase in the incidence of any tumor in comparison with the untreated control groups ...

PMID:6541624

Lijinsky W; Food Chem Toxicol 22(9): 715-20 (1984)

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

/ALTERNATIVE and IN VITRO TESTS/ Rabbit renal cortical slices were incubated at 25 degrees C, pH 7.4, for 2 hr under 100% O2 in a **phosphate**-buffered medium. (14-C)allantoin was accumulated to a tissue **water**/medium ratio of 1.38 +/- 0.03 (mean +/- S.E., n = 22). Under 100% N2, the tissue **water**/medium ratio fell significantly to 0.90 +/- 0.02 (n = 14, P less than .001). **Probenecid** (an anion) inhibited the uptake of allantoin at doses which had no effect on the **water** content of the slices, i.e., did not appear to have a toxic effect on the tissue. Its effect was specific. In contrast, **salicylate** (another anion) and **quinine** (a cation) inhibited the uptake of allantoin only at concentrations which simultaneously increased the **water** content of the slices. These results suggest a toxic effect on cell metabolism. **Salicylate** (an anion) and **quinine** (a cation), in dosage which inhibited allantoin uptake, also inhibit the uptake of the **para-aminohippuric acid** (an anion) and **tetraethylammonium bromide** (a cation). Net secretion of allantoin was observed in urinary clearance experiments on anesthetized rabbits acutely loaded with allantoin, under **mannitol** diuresis. At flow rates less than 1 ml/kg/min, fractional excretion of (14-C)allantoin was 0.85 +/- 0.03 (n = 27 clearance periods) indicating significant net reabsorption. When urine flow was increased above 1 ml/kg/min, fractional excretion of (14-C)allantoin reached 1.07 +/- 0.03 (n = 18 clearance periods), i.e., net secretion.

PMID:7359365

Schali C and Roch-Ramel F; J Pharmacol Exp Ther 213 (1): 168-72 (1980)

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

13.2 Ecological Information

13.2.1 Environmental Fate / Exposure Summary

Allantoin's production and use as a topical medication may result in its release to the environment through various waste streams. Allantoin is the metabolic end product of **purine** from mammals other than primates. Allantoin is present in tobacco seeds, sugar

beets and white sprouts. If released to air, an estimated vapor pressure of 4.3X10-9 mm Hg at 25 °C indicates allantoin will exist solely in the particulate phase in the atmosphere. Particulate-phase allantoin will be removed from the atmosphere by wet or dry deposition. If released to soil, allantoin is expected to have very high mobility based upon an estimated Koc of 10. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 3.4X10-18 atm-cu m/mole. Allantoin is expected to biodegrade in soil and **water** based on a study giving 6, 10, and 88% degradation in 5, 15, and 30 days, respectively, using a sewage inoculum. If released into **water**, allantoin is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from **water** surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Occupational exposure to allantoin may occur through dermal contact with this compound at workplaces where allantoin is produced or used. Exposure to allantoin among the general population may occur to those administered the drug allantoin, a cell poliferation and enhancement agent. Exposure to allantoin will also occur through contact with natural sources containing allantoin. (SRC)

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

13.2.2 Natural Pollution Sources

The end product of **purine** metabolism in mammals other than humans and other primates; it results from the oxidation of **uric acid**

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

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

... present in tobacco seeds, sugar beets, white sprouts

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 34

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

13.2.3 Artificial Pollution Sources

Allantoin's production and use as a topical medication(1) may result in its release to the environment through various waste streams(SRC).

(1) PDR; Physicians Desk Reference 61st ed, Thomson PDR, Montvale, NJ p. 2126 (2007)

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

13.2.4 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 10(SRC), determined from a structure estimation method(2), indicates that allantoin is expected to have very high mobility in soil(SRC). Volatilization of allantoin from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 3.4X10-18 atm-cu m/mole(SRC), using a fragment constant estimation method(3). Allantoin is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 4.3X10-9 mm Hg(SRC), determined from a fragment constant method(4). Allantoin was biodegraded 6, 10, and 88% in 5, 15, and 30 days, respectively(5).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (3) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (4) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985) (5) Fischer WK et al; Wasser-UND Abwasser-Forxchung 7:99-118 (1974)

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

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 10(SRC), determined from a structure estimation method(2), indicates that allantoin 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 3.4X10-18 atm-cu m/mole(SRC), developed using a fragment constant estimation method(4). According to a classification scheme(5), an estimated BCF of 3(SRC), from an estimated log Kow of -3.14(6) and a regression-derived equation(7), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Allantoin was biodegraded 6, 10, and 88% in 5, 15, and 30 days, respectively(8).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990) (4) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (5) Franke C et al; Chemosphere 29: 1501-14 (1994) (6) Meylan WM, Howard PH; J Pharm Sci 84: 83-92 (1995) (7) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (8) Fischer WK et al; Wasser-UND Abwasser-Forxchung 7:99-118 (1974)

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

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), allantoin, which has an estimated vapor pressure of 4.3X10-9 mm Hg at 25 °C(SRC), determined from a fragment constant method(2), is expected to exist solely in the particulate phase in the ambient atmosphere. Particulate-phase allantoin may be removed from the air by wet or dry deposition(SRC).

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

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

13.2.5 Environmental Biodegradation

AEROBIC: Allantoin was biodegraded 6, 10, and 88% in 5, 15, and 30 days, respectively in closed bottle tests at 20 °C(1).

(1) Fischer WK et al; Wasser-UND Abwasser-Forxchung 7:99-118 (1974)

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

13.2.6 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of allantoin with photochemically-produced **hydroxyl** radicals has been estimated as 2.0X10-11 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 20 hours at an atmospheric concentration of 5X10+5 **hydroxyl** radicals per cu cm(1).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

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

13.2.7 Environmental Bioconcentration

An estimated BCF of 3 was calculated in fish for allantoin(SRC), using an estimated log Kow of -3.14(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Meylan WM, Howard PH; J Pharm Sci 84: 83-92 (1995) (2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

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

13.2.8 Soil Adsorption / Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc of allantoin can be estimated to be 10(SRC). According to a classification scheme(2), this estimated Koc value suggests that allantoin is expected to have very high mobility in soil(SRC).

(1) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (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 allantoin is estimated as 3.4X10-18 atm-cu m/mole(SRC) using a fragment constant estimation method(1). This Henry's Law constant indicates that allantoin is expected to be essentially nonvolatile from **water** surfaces(2). Allantoin is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 4.3X10-9 mm Hg(SRC), determined from a fragment constant method(3).

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

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

13.2.10 Probable Routes of Human Exposure

NIOSH (NOES Survey 1981-1983) has statistically estimated that 33,966 workers (20,108 of these are female) are potentially exposed to allantoin in the US(1). Occupational exposure to allantoin may occur through dermal contact with this compound at workplaces where allantoin is produced or used(SRC). Exposure to allantoin among the general population may occur to those administered the drug allantoin, a cell poliferation and enhancement agent(SRC). Exposure to allantoin will occur through contact with natural sources containing allantoin(SRC).

*(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available at **https://www.cdc.gov/noes/** as of Feb 2007.*

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

14 Associated Disorders and Diseases

Comparative Toxicogenomics Database (CTD)

Therapeutic Target Database (TTD)

Disease	References
Chronic renal failure	PubMed: 2474282, 11380830, 9141788, 7296840, 18636793
Schizophrenia	PubMed: 115032, 7126379, 2480613, 17276036, 11877547, 12796220, 7595563, 20814316, 25004141, 24713860, 23823132, 2415198, 1694425, 7711000, 19390223, 22024767, 22007635, 21483431, 3741918, 11979513, 20206656, 436860, 19401681, 6184954, 26952797, 22800120, 24789758, 22944140, 22892715, 17440431, 25729574, 22257447
Meningitis	PubMed: 12581805, 15627241, 7729054, 9542731, 15061359, 11805243, 6326460, 16150112, 6198481, 2835791, 8899053
Crohn's disease	PubMed: 16440420, 11418788, 8723414, 19491857, 17269711, 23516449, 23867873, 24811995, 25598765, 26806034, 26848182, 27609529, 28842642
Ulcerative colitis	PubMed: 21059682, 1740537, 17269711, 17314143, 21761941, 23516449, 23867873, 24811995, 25598765, 26806034, 26848182, 27609529, 28842642
Colorectal cancer	PubMed: 7482520, 19006102, 23940645, 24424155, 20156336, 19678709, 22148915, 25105552, 21773981, 25037050, 27015276, 27107423, 27275383, 28587349 Silke Matysik, Caroline Ivanne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255: http://www.sciencedirect.com/science/article/pii/S0924224416301984
Eosinophilic esophagitis	Mordechai, Hien, and David S. Wishart

- Human Metabolome Database (HMDB)

15 Literature

15.1 Consolidated References

- PubChem

15.2 NLM Curated PubMed Citations

- PubChem

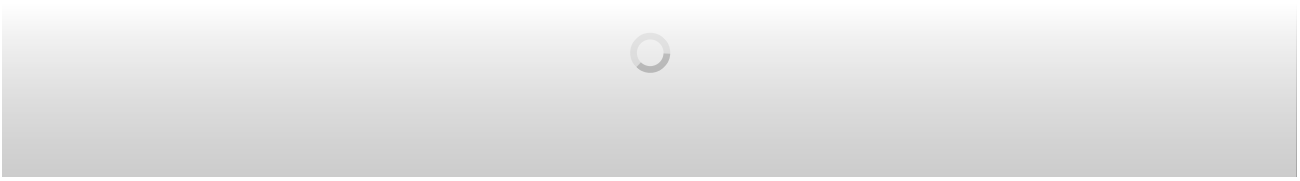
15.3 Springer Nature References

Springer Nature

15.4 Thieme References

Thieme Chemistry

15.5 Wiley References

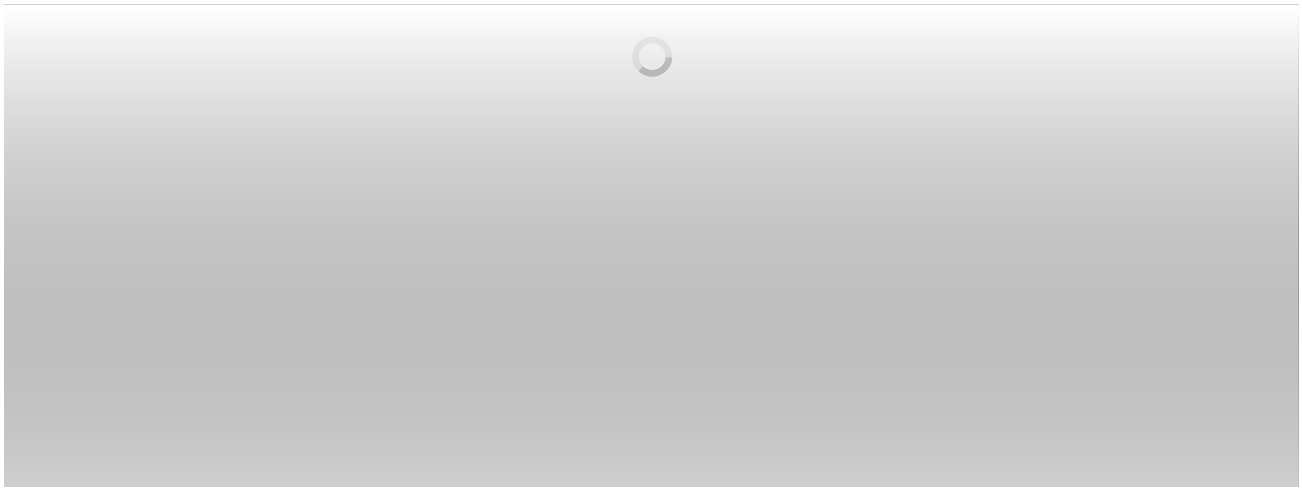


- Wiley

15.6 Chemical Co-Occurrences in Literature

- PubChem

15.7 Chemical-Gene Co-Occurrences in Literature



PubChem

15.8 Chemical-Disease Co-Occurrences in Literature

PubChem

16 Patents

16.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

16.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

- PATENTSCOPE (WIPO)

16.3 Chemical Co-Occurrences in Patents

- PubChem

16.4 Chemical-Disease Co-Occurrences in Patents

PubChem

16.5 Chemical-Gene Co-Occurrences in Patents

PubChem

17 Interactions and Pathways

17.1 Chemical-Target Interactions

- Comparative Toxicogenomics Database (CTD); Drug Gene Interaction database (DGIdb); Toxin...

17.2 Pathways

- PubChem

18 Biological Test Results

18.1 BioAssay Results

- PubChem

19 Taxonomy

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

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

- **ECI Group, LCSB, University of Luxembourg; LOTUS - the natural products occurrence databas...**

20 Classification

20.1 MeSH Tree

- **Medical Subject Headings (MeSH)**

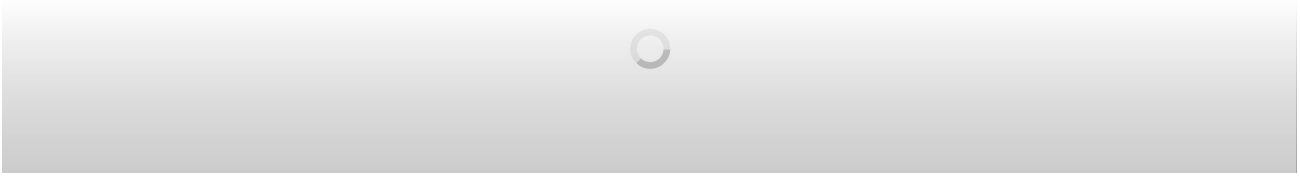
20.2 NCI Thesaurus Tree

NCI Thesaurus (NCIt)

20.3 ChEBI Ontology

ChEBI

20.4 KEGG: Risk Category of Japanese OTC Drugs

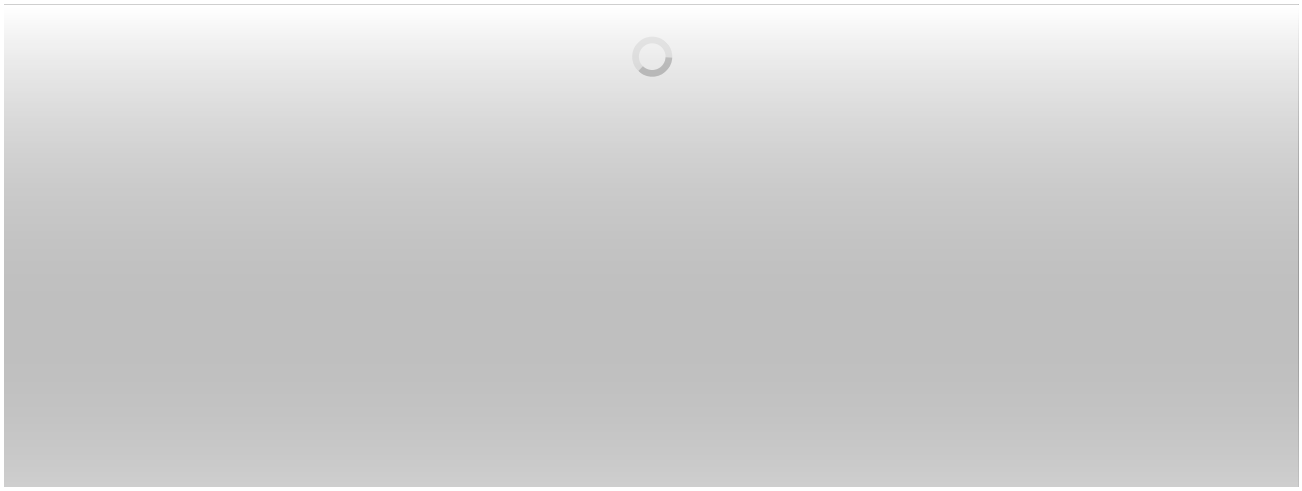


KEGG

20.5 KEGG: OTC drugs

KEGG

20.6 ChemIDplus



ChemIDplus

20.7 ChEMBL Target Tree

ChEMBL

20.8 UN GHS Classification

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

20.9 EPA CPDat Classification

EPA Chemical and Products Database (CPDat)

20.10 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

20.11 CCSBase Classification

CCSbase

20.12 EPA DSSTox Classification

EPA DSSTox

20.13 Consumer Product Information Database Classification

Consumer Product Information Database (CPID)

20.14 LOTUS Tree

LOTUS - the natural products occurrence database

20.15 EPA Substance Registry Services Tree

EPA Substance Registry Services

21 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. ## Athena Minerals

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Allantoin
https://athena.unige.ch/cgi-bin/minfich.cgi?s=ALLANTOIN

2. ## RRUFF Project

Allantoin
https://rruff.info/

3. ## CAS Common Chemistry

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Allantoin
https://commonchemistry.cas.org/detail?cas_rn=97-59-6

4. ## ChemIDplus

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

Allantoin [USAN:USP:BAN:JAN]
https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000097596

ChemIDplus Chemical Information Classification
https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

5. ## DrugBank

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

Allantoin
https://www.drugbank.ca/drugs/DB11100

6. ## DTP/NCI

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allantoin

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=757792

allantoin

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=7606

7. EPA Chemicals under the TSCA

Urea, N-(2,5-dioxo-4-imidazolidinyl)-

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

8. EPA DSSTox

Allantoin

https://comptox.epa.gov/dashboard/DTXSID3020043

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

9. European Chemicals Agency (ECHA)

Allantoin

https://echa.europa.eu/substance-information/-/substanceinfo/100.002.358

Allantoin

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/84256

10. FDA Global Substance Registration System (GSRS)

Allantoin

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/344S277G0Z

11. Hazardous Substances Data Bank (HSDB)

ALLANTOIN

https://pubchem.ncbi.nlm.nih.gov/source/hsdb/7490

12. Human Metabolome Database (HMDB)

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http://www.hmdb.ca/metabolites/HMDB0000462

HMDB0000462_cms_1583

https://hmdb.ca/metabolites/HMDB0000462#spectra

13. New Zealand Environmental Protection Authority (EPA)

Allantoin

https://www.epa.govt.nz/industry-areas/hazardous-substances/guidance-for-importers-and-manufacturers/hazardous-substances-databases/

14. CCSbase

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CCSbase Classification

https://ccsbase.net/

15. NORMAN Suspect List Exchange

Allantoin

NORMAN Suspect List Exchange Classification

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

16. ChEBI

Allantoin

http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:15676

ChEBI Ontology

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

17. E. coli Metabolome Database (ECMDB)

https://ecmdb.ca/compounds/M2MDB000139

18. LOTUS - the natural products occurrence database

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

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https://www.wikidata.org/wiki/Q409804

LOTUS Tree

https://lotus.naturalproducts.net/

19. Toxin and Toxin Target Database (T3DB)

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http://www.t3db.ca/downloads

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http://www.t3db.ca/toxins/T3D4936

20. Yeast Metabolome Database (YMDB)

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

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http://www.ymdb.ca/compounds/YMDB00213

21. ChEMBL

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http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL593429/

ChEMBL Protein Target Tree

https://www.ebi.ac.uk/chembl/g/#browse/targets

22. ClinicalTrials.gov

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https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use

https://clinicaltrials.gov/

23. Comparative Toxicogenomics Database (CTD)

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https://ctdbase.org/detail.go?type=chem&acc=D000481

24. Drug Gene Interaction database (DGIdb)

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

25. Therapeutic Target Database (TTD)

Allantoin

https://idrblab.net/ttd/data/drug/details/D01HNL

26. Consumer Product Information Database (CPID)

Allantoin

https://www.whatsinproducts.com/chemicals/view/1/682/000097-59-6

Consumer Products Category Classification

https://www.whatsinproducts.com/

27. DailyMed

ALLANTOIN

https://dailymed.nlm.nih.gov/dailymed/search.cfm?labeltype=all&query=ALLANTOIN

28. European Medicines Agency (EMA)

Allantoin (P/0225/2017)

https://www.ema.europa.eu/en/medicines/human/paediatric-investigation-plans/emea-001590-pip01-13-m04

29. ECI Group, LCSB, University of Luxembourg

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30. Natural Product Activity and Species Source (NPASS)

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https://bidd.group/NPASS/compound.php?compoundID=NPC153556

31. West Coast Metabolomics Center-UC Davis

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32. EPA Chemical and Products Database (CPDat)

https://comptox.epa.gov/dashboard/DTXSID3020043#exposure

EPA CPDat Classification

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

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

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https://haz-map.com/Agents/3560

34. EU Clinical Trials Register

https://www.clinicaltrialsregister.eu/

35. MassBank Europe

POJWUDADGALRAB-UHFFFAOYSA-N

https://massbank.eu/MassBank/Result.jsp?inchikey=POJWUDADGALRAB-UHFFFAOYSA-N

36. MassBank of North America (MoNA)

Allantoin

https://mona.fiehnlab.ucdavis.edu/spectra/browse?

query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27POJWUDA

DGALRAB-UHFFFAOYSA-N%27)

37. NIST Mass Spectrometry Data Center

Allantoin

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

38. SpectraBase

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https://spectrabase.com/spectrum/6qt1Xmx4lDH

Allantoin

https://spectrabase.com/spectrum/7DSi4y8jkHr

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https://spectrabase.com/spectrum/7j6Zo3CyTuK

Allantoin

https://spectrabase.com/spectrum/8w7sou6qXJs

ALLANTOIN

https://spectrabase.com/spectrum/IePQ4tjP2he

Allantoin

https://spectrabase.com/spectrum/7AQkgl1edDF

5-Ureidohydantoin

https://spectrabase.com/spectrum/KYgg93gLUHW

Allantoin

https://spectrabase.com/spectrum/CqZAD2OFdZm

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https://spectrabase.com/spectrum/5wBHTVrlRvv

Allantoin

https://spectrabase.com/spectrum/GEJXXdJPbcE

5-Ureidohydantoin

https://spectrabase.com/spectrum/LZtCnHig10z

39. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J3.978K

40. KEGG

https://www.kegg.jp/entry/C01551

https://www.kegg.jp/entry/D00121

Risk category of Japanese OTC drugs

http://www.genome.jp/kegg-bin/get_htext?br08312.keg

Classification of Japanese OTC drugs

http://www.genome.jp/kegg-bin/get_htext?br08313.keg

41. MarkerDB

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https://markerdb.ca/

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https://markerdb.ca/chemicals/248

42. Metabolomics Workbench

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https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=143220

43. National Drug Code (NDC) Directory

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

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

44. NCI Thesaurus (NCIt)

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https://ncithesaurus.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=ncit&code=C74277

NCI Thesaurus Tree

https://ncit.nci.nih.gov

45. NLM RxNorm Terminology

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

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https://rxnav.nlm.nih.gov/id/rxnorm/508

46. Rhea - Annotated Reactions Database

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https://www.rhea-db.org/rhea?query=CHEBI:15676

47. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=11043822-85905023

48. Thieme Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=11043822-85905023

49. Wikidata

Allantoin

https://www.wikidata.org/wiki/Q409804

50. Wikipedia

Allantoin

https://en.wikipedia.org/wiki/Allantoin

51. Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=25975

52. Medical Subject Headings (MeSH)

Allantoin

https://www.ncbi.nlm.nih.gov/mesh/68000481

MeSH Tree

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

Dermatologic Agents

https://www.ncbi.nlm.nih.gov/mesh/68003879

53. PubChem

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

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

GHS Classification Tree

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

55. EPA Substance Registry Services

EPA SRS List Classification

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

56. PATENTSCOPE (WIPO)

SID 403033391

https://pubchem.ncbi.nlm.nih.gov/substance/403033391