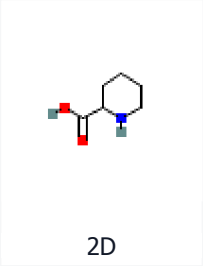
National Library of Medicine
National Center for Biotechnology Information

COMPOUND SUMMARY

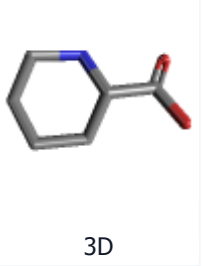
Pipecolic acid

PubChem CID
849

Structure



2D



3D

Chemical Safety

Irritant

Laboratory Chemical Safety Summary (LCSS) Datasheet

Molecular Formula
$C_6H_{11}NO_2$

Synonyms
piperidine-2-carboxylic acid
DL-Pipecolinic acid
535-75-1
Pipecolic acid
Pipecolinic acid
View More...

Molecular Weight
129.16 g/mol
Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

Create:	Modify:
2004-09-16	2024-09-20

Description

Pipecolic acid is a piperidinemonocarboxylic acid in which the carboxy group is located at position C-2. It is a conjugate acid of a pipecolate.

- ChEBI

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

- E. coli Metabolome Database (ECMDB)

Pipecolic acid has been reported in Angelica gigas, Slafractonia leguminicola, and other organisms with data available.

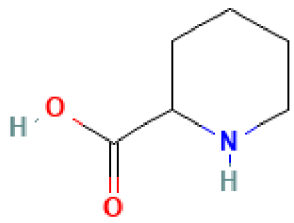
- LOTUS - the natural products occurrence database

Contents

1 Structures

1.1 2D Structure

Chemical Structure Depiction



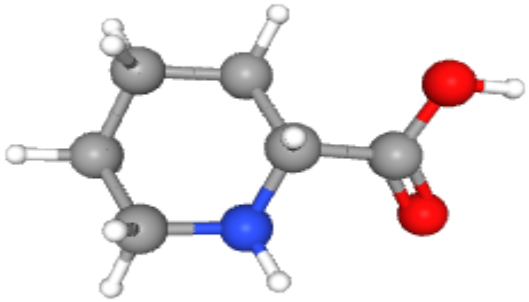
PubChem

1.2 3D Conformer

Interactive Chemical Structure Model

Ball and Stick Sticks Wire-Frame Space-Filling

Show Hydrogens Animate

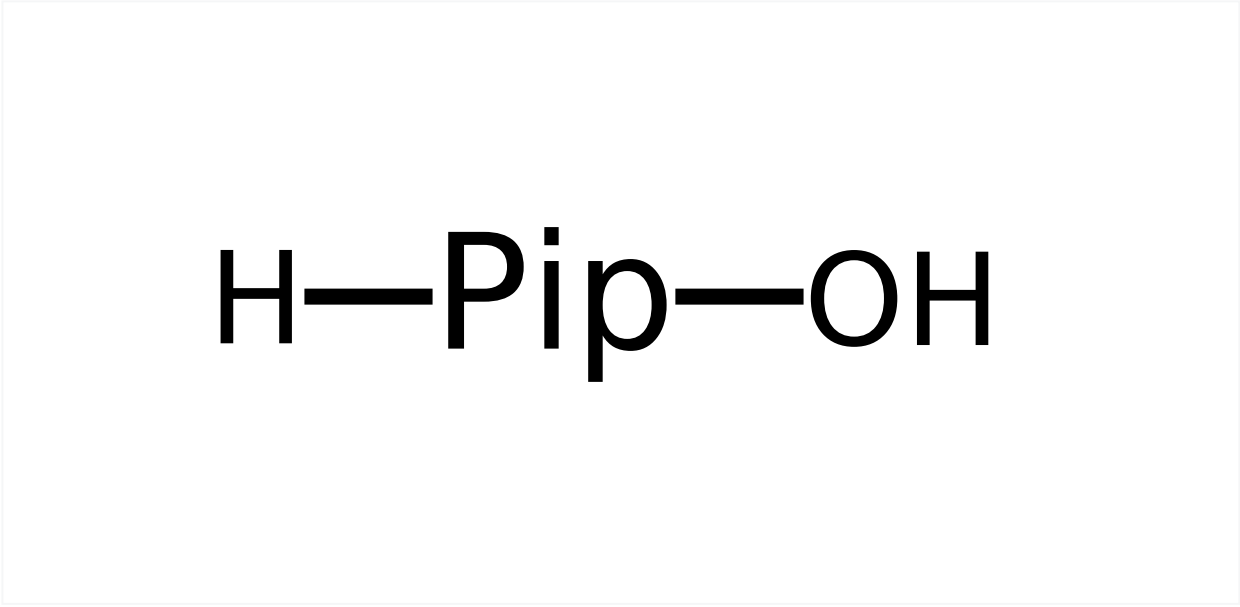


Conformer 1 of 9

PubChem

2 Biologic Description

SVG Image



IUPAC Condensed
H-DL-Pip-OH

Sequence
X

HELM PEPTIDE1{[C1CCNC(C1)C(=O)O]}$$$$
IUPAC DL-homoproline

▸ PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

piperidine-2-carboxylic acid

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

▸ PubChem

3.1.2 InChI

InChI=1S/C6H11NO2/c8-6(9)5-3-1-2-4-7-5/h5,7H,1-4H2,(H,8,9)

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

3.1.3 InChIKey

HXEACLLIILLPRG-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

3.1.4 SMILES

C1CCNC(C1)C(=O)O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

▸ PubChem

3.2 Molecular Formula

$C_6H_{11}NO_2$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

- PubChem

3.3 Other Identifiers

3.3.1 CAS

535-75-1

- CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; ...

3105-95-1

- DTP/NCI

4043-87-2

- European Chemicals Agency (ECHA)

3.3.2 Related CAS

69470-51-5 (mono-potassium salt)
15862-86-9 (hydrochloride salt/solvate)

- ChemIDplus

3.3.3 Deprecated CAS

4043-87-2

- ChemIDplus; EPA Chemicals under the TSCA

3.3.4 European Community (EC) Number

223-737-1

- European Chemicals Agency (ECHA)

208-616-3

- European Chemicals Agency (ECHA)

3.3.5 UNII

H254GW7PVV

- FDA Global Substance Registration System (GSRS)

3.3.6 ChEBI ID

CHEBI:17964

- ChEBI

3.3.7 ChEMBL ID

CHEMBL308408

- ChEMBL

3.3.8 DSSTox Substance ID

DTXSID40862144

- EPA DSSTox

3.3.9 HMDB ID

HMDB0000070

- Human Metabolome Database (HMDB)

3.3.10 Metabolomics Workbench ID

130145

- Metabolomics Workbench

3.3.11 Nikkaji Number

J1.592J

- Japan Chemical Substance Dictionary (Nikkaji)

3.3.12 NSC Number

93089

- DTP/NCI

17125

- DTP/NCI

3.3.13 Wikidata

Q7197255

- Wikidata

3.3.14 Wikipedia

Pipecolic_acid

- Wikipedia

3.4 Synonyms

3.4.1 MeSH Entry Terms

2-piperidinecarboxylic acid
homopipecolic acid
L-pipecolic acid
pipecolic acid
pipecolic acid hydrochloride, (+-)-isomer
pipecolic acid, (+,-)-isomer
pipecolic acid, (-)-
pipecolic acid, (R)-isomer
pipecolic acid, (S)-isomer
pipecolic acid, 14C-labeled cpd, (+,-)-isomer
pipecolic acid, ion (1-)
pipecolic acid, ion(1-), (+,-)-isomer
pipecolic acid, ion(1-), (S)-isomer
pipecolic acid, monopotassium salt

- Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms

piperidine-2-carboxylic acid	Piperolinic acid	83680-83-5
DL-Pipecolinic acid	L-PipecolicAcid	2-Pipecolinic acid
535-75-1	Hexahydropicolinic acid	Pipecolic acid, L-
Pipecolic acid	DL-Homoproline	Acide piperidine-carboxylique-
Pipecolinic acid	Acide pipecolique	.alpha.-Pipecolinic acid
2-PIPERIDINECARBOXYLIC ACID	MFCD00064347	(+/-)-2-Piperidinecarboxylic Ac
4043-87-2	2-Carboxypiperidine	(+/-)-Pipecolinic acid
DL-Pipecolic acid	(R)-(+)-2-Piperidinecarboxylic acid	2-Piperidinecarboxylic acidd
pipecolate	(+/-)-Pipecolic acid	H254GW7PVV
Dihydrobaikiane	Hexahydro-2-picolinic acid	Pipecolic acid, (S)-(-)-

▸ PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name
Molecular Weight

Property Value
129.16 g/mol

Reference
Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name
XLogP3

Property Value
-2.3

Reference
Computed by XLogP3 3.0 (PubChem release 2021.10.14)

Property Name
Hydrogen Bond Donor Count

Property Value
2

Reference
Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Hydrogen Bond Acceptor Count

Property Value

3

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Rotatable Bond Count

Property Value

1

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Exact Mass

Property Value

129.078978594 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Monoisotopic Mass

Property Value

129.078978594 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Topological Polar Surface Area

Property Value

49.3Å²

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

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 2021.10.14)

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

1

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 2021.10.14)

▸ PubChem

4.2 Experimental Properties

4.2.1 Physical Description

Solid

▸ Human Metabolome Database (HMDB)

4.2.2 Melting Point

264 °C

▸ Human Metabolome Database (HMDB)

4.2.3 Solubility

314 mg/mL

▸ Human Metabolome Database (HMDB)

4.2.4 LogP

-2.31

TSAI,RS ET AL. (1991)

▸ Human Metabolome Database (HMDB)

4.2.5 Dissociation Constants

1 item

pKa Type
pKaH2

pKa
10.38

Temperature [°C]

▸ IUPAC Digitized pKa Dataset

4.2.6 Collision Cross Section

138.8 Å² $[M+Na]^+$ [CCS Type: DT; Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

128.9 Å² $[M-H]^-$ [CCS Type: DT; Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

128.3 Å² $[M-H]^-$ [CCS Type: DT; Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

139.4 Å² $[M+Na]^+$ [CCS Type: DT; Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

127.7 Å² $[M+H]^+$ [CCS Type: DT; Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

128 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

129.3 Å² $[M-H]^-$

127.4 Å² $[M+H]^+$

139 Å² $[M+Na]^+$

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

▸ NORMAN Suspect List Exchange

5 Spectral Information

5.1 1D NMR Spectra

1D NMR Spectra
NMRShiftDB Link

▸ NMRShiftDB

5.1.1 1H NMR Spectra

1 of 3 View All

Spectra ID
1067

Instrument Type
Varian

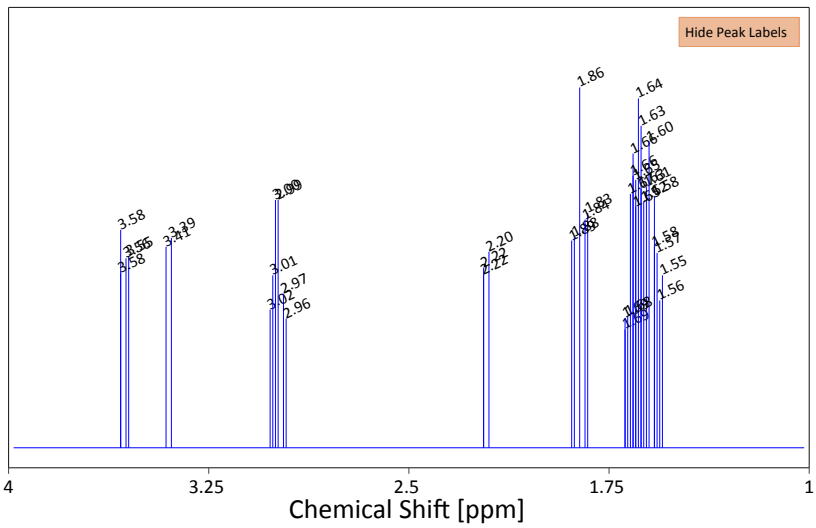
Frequency
500 MHz

Solvent
Water

pH
7.00

Shifts [ppm]:Intensity
2.20:54.37, 1.69:32.84, 1.55:47.86, 3.41:55.76, 1.58:69.83, 3.55:53.11, 3.56:52.57, 1.64:96.95, 1.56:40.89, 1.61:72.36, 1.63:71.98, 1.66:81.65, 1.83:65.11, 3.02:38.34, 1.62:68.33, 1.86:100.00, 2.22:48.04, 1.66:75.51, 1.58:55.78, 1.60:84.96, 3.58:60.48, 3.00:68.76, 1.63:89.36, 3.01:47.86, 1.68:36.50, 1.69:35.93, 1.57:54.06, 2.97:42.72, 1.67:70.47, 2.22:50.00, 2.99:68.82, 2.96:35.87, 1.89:57.51, 1.65:74.35, 1.65:66.91, 3.58:48.42, 1.88:58.45, 1.84:63.34, 3.39:58.26

Thumbnail



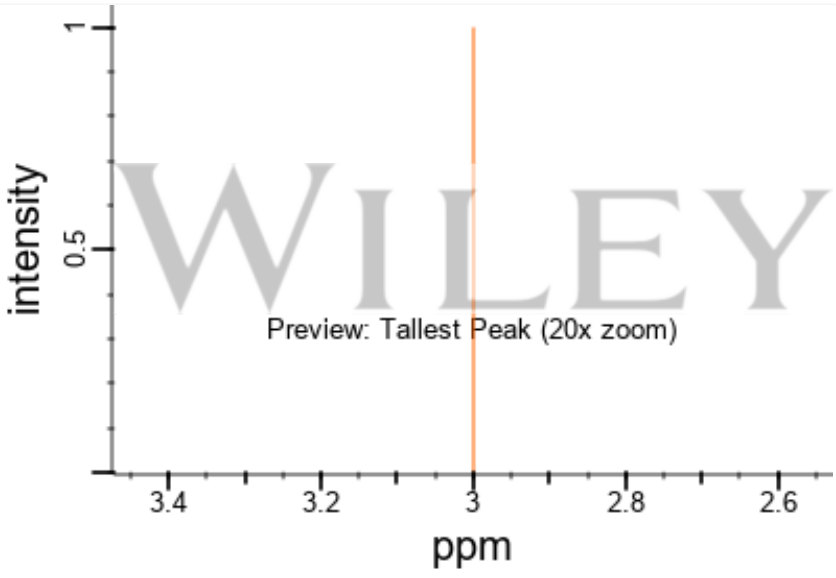
▸ Human Metabolome Database (HMDB)

2 of 3 View All

Instrument Name
Varian CFT-20

Copyright

Thumbnail



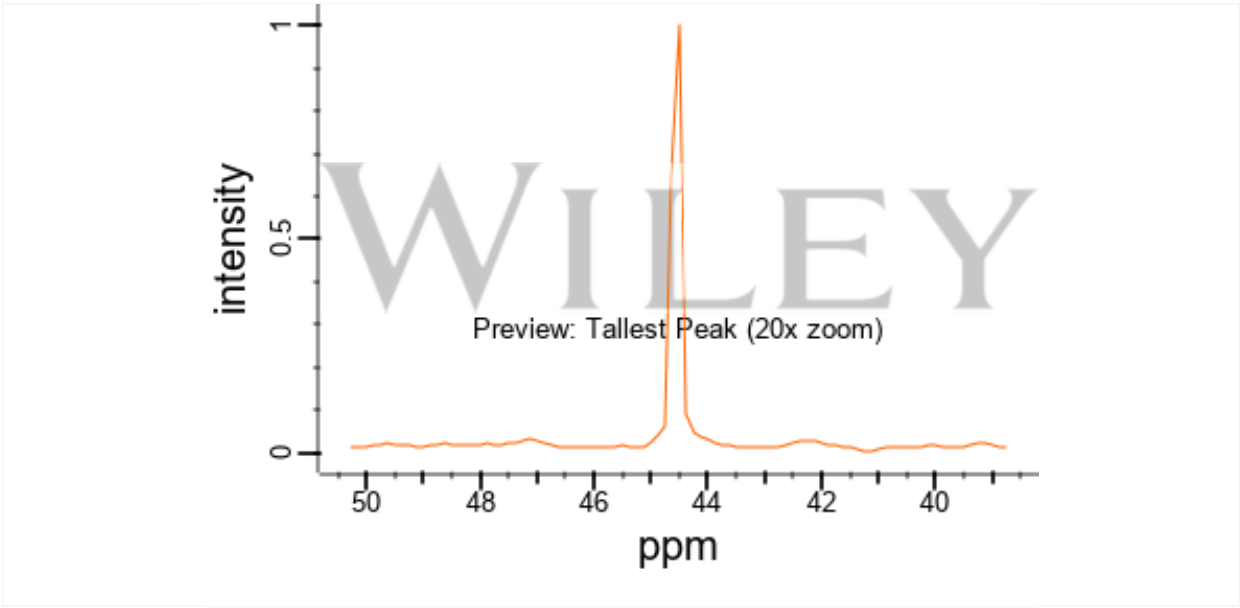
▸ SpectraBase

5.1.2 13C NMR Spectra

1 of 2

Source of Sample
Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan

Thumbnail

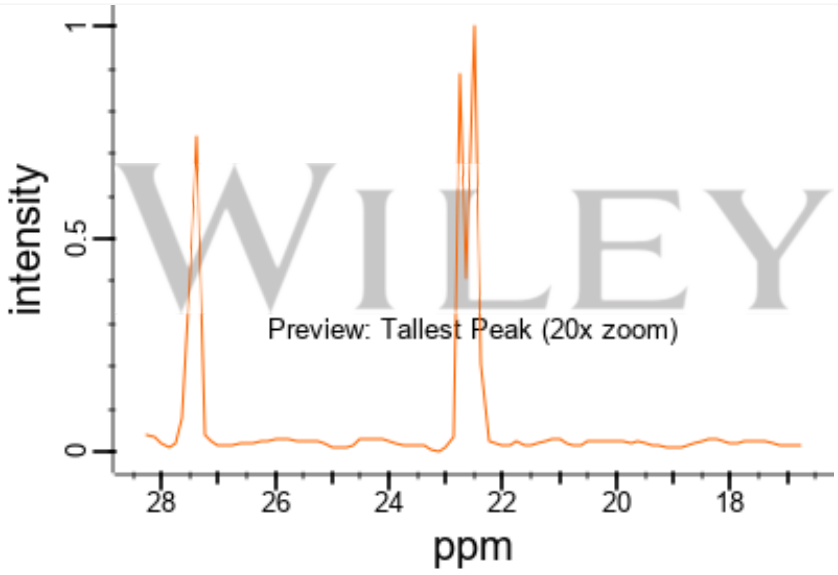


▸ SpectraBase

2 of 2

Source of Sample
Fluka AG, Buchs, Switzerland

Thumbnail



SpectraBase

5.2 2D NMR Spectra

5.2.1 1H-1H NMR Spectra

2D NMR Spectra Type
1H-1H TOCSY

Spectra ID
949

Shifts [ppm] (F2:F1)
3.69:3.92, 3.59:1.59, 2.21:3.42, 3.42:3.39, 1.87:2.19, 3.59:3.03, 1.63:1.87, 3.41:2.23, 1.87:1.68, 3.59:3.00, 3.42:1.71, 3.01:3.00, 3.42:3.42, 3.01:3.39, 3.41:2.20, 1.63:1.64, 1.87:3.56, 2.21:3.59, 1.63:3.03, 2.21:1.87, 2.21:1.68, 1.63:1.61, 3.59:2.20, 3.59:1.84, 2.21:3.00, 3.01:1.64, 3.41:3.59, 2.21:3.56, 1.63:2.97, 3.59:1.65, 3.42:1.68, 3.42:1.59, 1.87:1.84, 2.21:1.71, 3.41:1.56, 3.59:3.59, 3.01:3.57, 1.63:1.59, 1.87:3.00, 1.87:1.61, 3.41:2.97, 1.64:2.23, 1.87:1.59, 3.01:1.61, 1.63:1.56, 1.63:1.84, 3.01:3.42, 3.01:3.59, 3.59:1.68, 3.59:1.87, 3.59:3.40, 1.64:2.19, 2.21:2.23, 1.87:3.59, 1.87:1.71, 3.59:3.43, 3.01:2.20, 1.63:3.56, 1.87:1.64, 2.21:2.19, 3.42:1.64, 3.01:1.68, 3.59:2.23, 3.01:1.59, 1.63:3.42, 2.21:1.59, 3.01:3.03, 3.42:1.61, 1.63:3.00, 1.63:3.39, 1.64:1.71, 2.21:1.56, 3.41:1.84, 1.63:3.59, 3.59:1.62, 3.01:2.23, 3.42:3.00, 2.21:3.39, 2.21:1.61, 2.21:3.03, 3.59:3.57, 1.87:2.97, 1.87:3.03, 3.42:3.03, 3.01:1.87, 1.87:1.56, 2.21:1.84, 1.87:3.39, 1.87:1.87, 3.01:1.84, 3.01:1.56, 3.01:1.71, 2.21:2.97, 1.64:1.68, 2.21:1.64, 3.41:3.56, 1.87:2.23, 1.87:3.42, 3.42:1.87, 3.01:2.97

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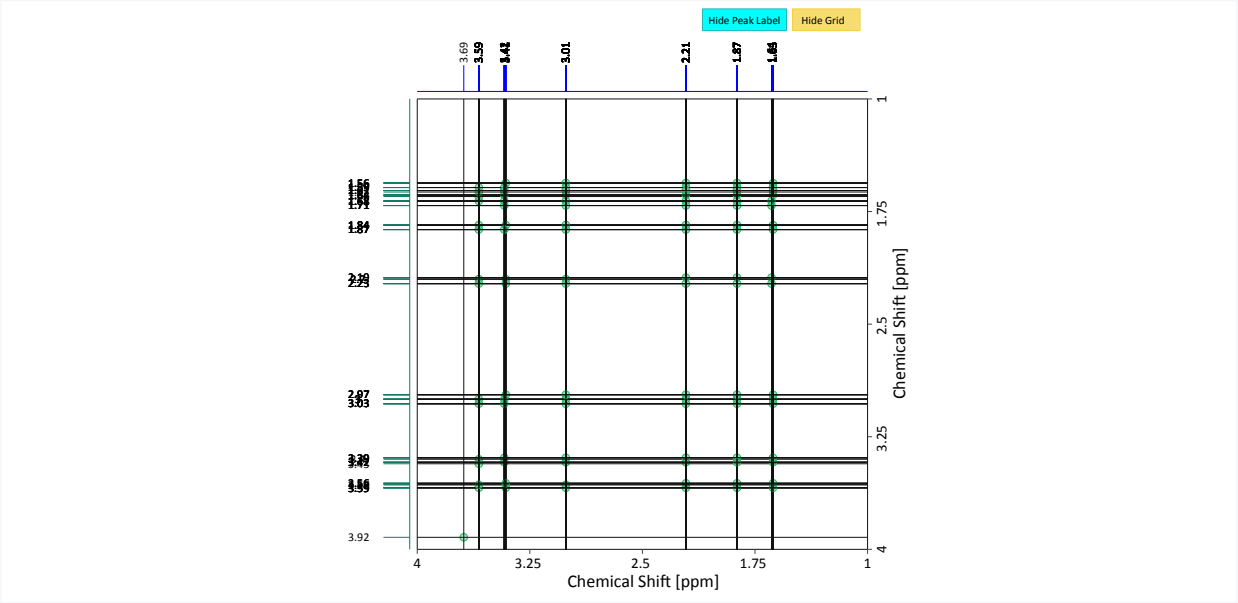


▸ Human Metabolome Database (HMDB)

5.2.2 1H-13C NMR Spectra

2D NMR Spectra Type
1H-13C HSQC

Spectra ID
1125

Instrument Type
Bruker

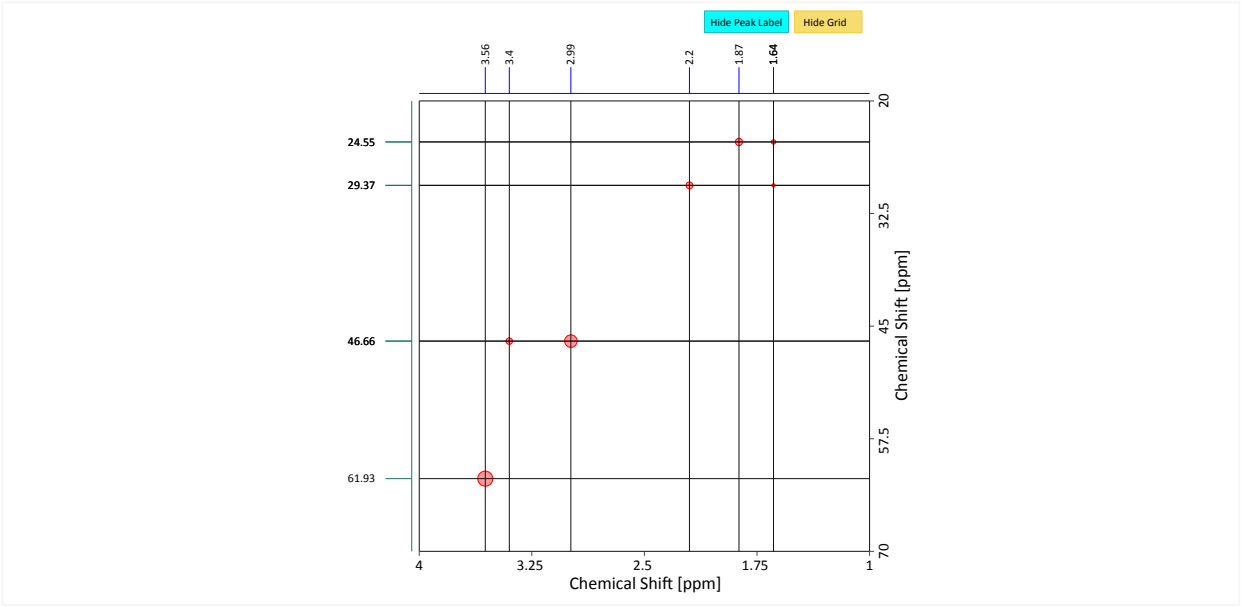
Frequency
600 MHz

Solvent
Water

pH
7.00

Shifts [ppm] (F2:F1):Intensity
3.56:61.93:1.00, 2.20:29.37:0.45, 1.64:29.37:0.21, 3.40:46.66:0.43, 1.64:24.55:0.29, 2.99:46.66:0.83, 1.87:24.55:0.48

Thumbnail



▸ Human Metabolome Database (HMDB)

5.3 Mass Spectrometry

5.3.1 GC-MS

1 of 13 View All

Spectra ID
32094

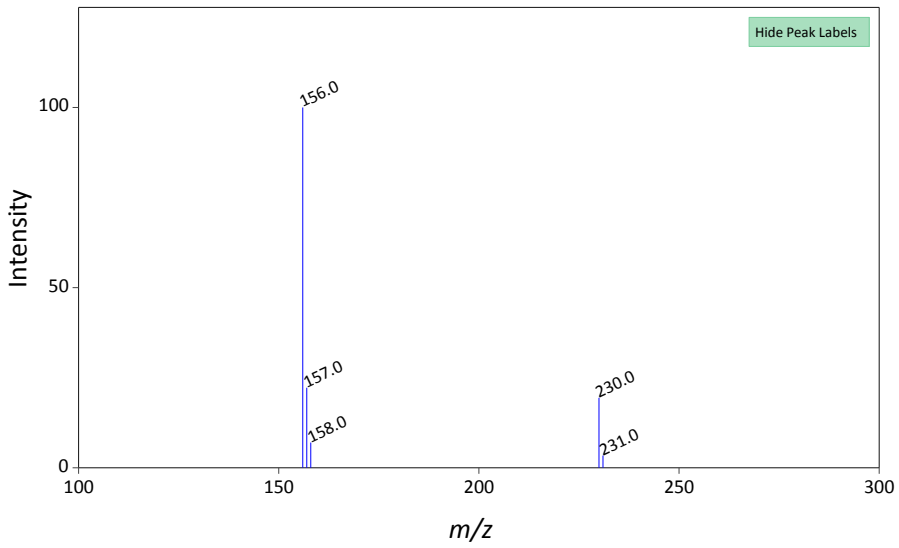
Instrument Type
GC-EI-TOF

Ionization Mode
positive

SPLASH
splash10-0a4i-0910000000-d9cfd443adb5187a3f21

Top 5 Peaks
156.0 100
157.0 22.22
230.0 19.42
158.0 7.01
231.0 3.40

Thumbnail



Notes
instrument=Leco Pegasus IV

▸ Human Metabolome Database (HMDB)

2 of 13 View All

Spectra ID
102574

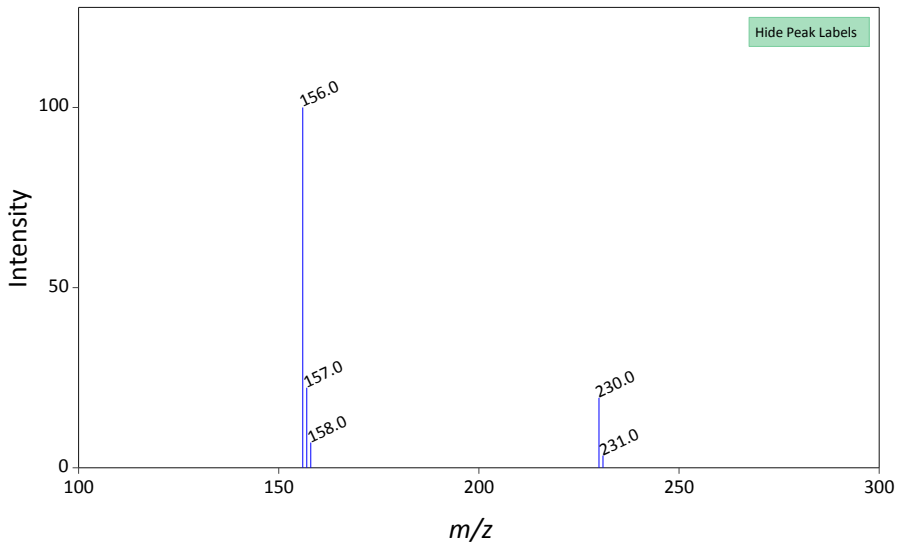
Instrument Type
GC-EI-TOF

Ionization Mode
positive

SPLASH
splash10-0a4i-0910000000-d9cfd443adb5187a3f21

Top 5 Peaks
156.0 100
157.0 22.22
230.0 19.42
158.0 7.01
231.0 3.40

Thumbnail



Notes
instrument=Leco Pegasus IV

▸ Human Metabolome Database (HMDB)

5.3.2 MS-MS

1 of 6 View All

Spectra ID
111

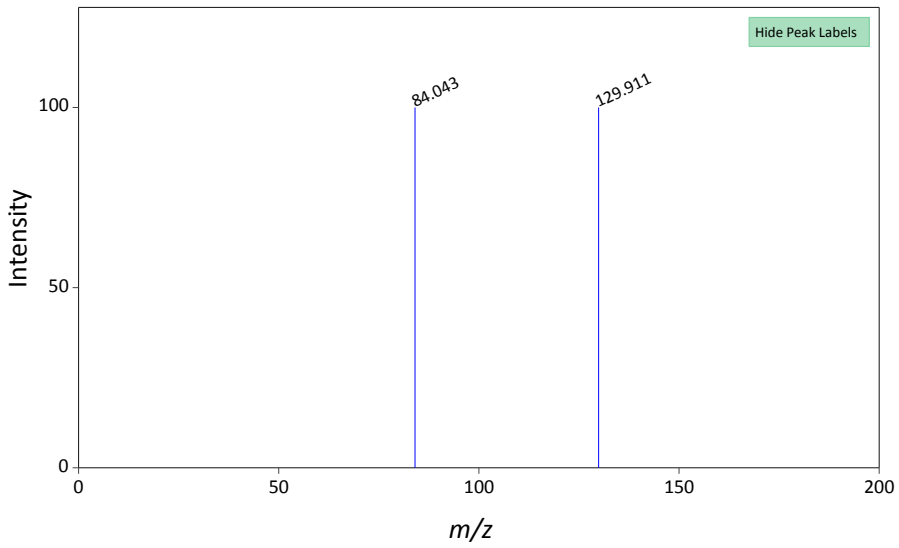
Instrument Type
Quattro_QQQ

Ionization Mode
Positive

SPLASH
splash10-0060-9900000000-c5b5bf28424d5d5d1bda

Top 5 Peaks
129.911 100
84.043 100

Thumbnail



Notes
delivery=Flow_Injectionanalyzer=Triple_Quad

▸ Human Metabolome Database (HMDB)

2 of 6 View All

Spectra ID
113

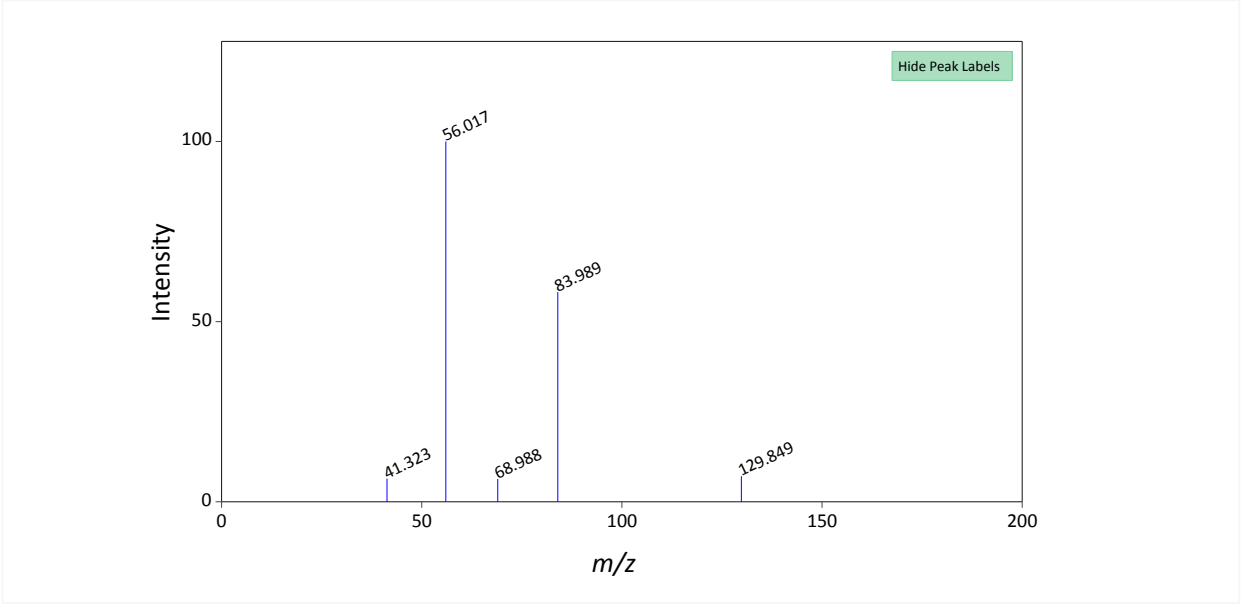
Instrument Type
Quattro_QQQ

Ionization Mode
Positive

SPLASH
splash10-0a59-9000000000-b779372fa816467754c1

Top 5 Peaks
56.017 100
83.989 58.21
129.849 7.09
41.323 6.44
68.988 6.34

Thumbnail



Notes
delivery=Flow_Injectionanalyzer=Triple_Quad

▸ Human Metabolome Database (HMDB)

5.3.3 LC-MS

1 of 26 View All

Accession ID
MSBNK-Keio_Univ-KO001631

Authors
Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio Univ.

Instrument
API3000, Applied Biosystems

Instrument Type
LC-ESI-QQ

MS Level
MS2

Ionization Mode
NEGATIVE

Collision Energy
10 V

Precursor m/z

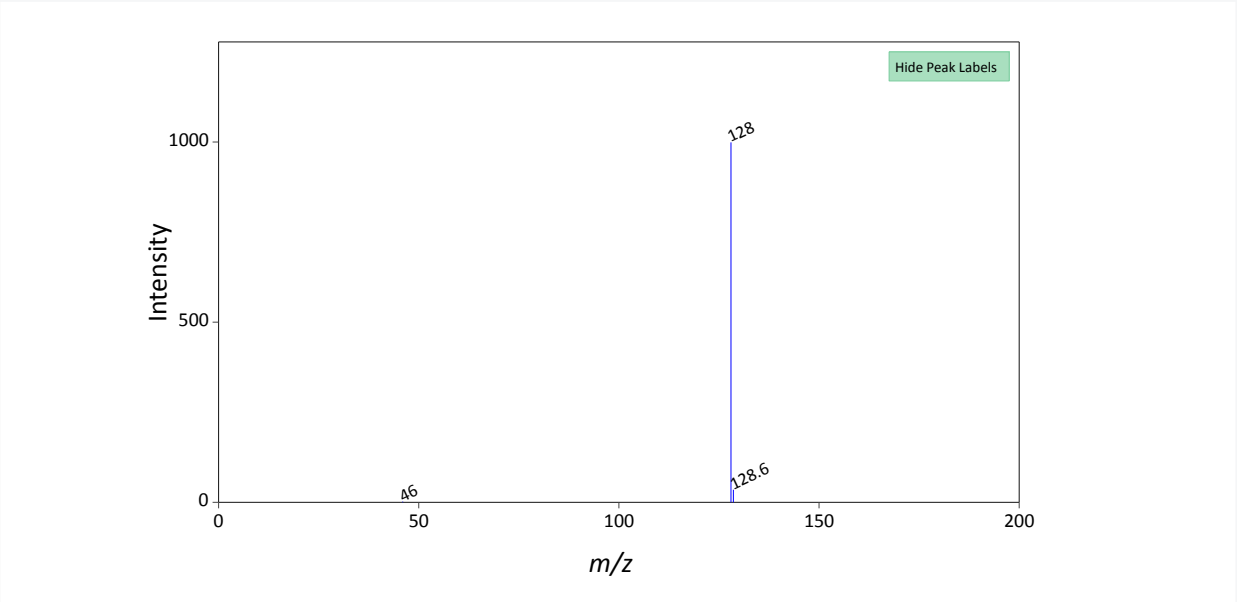
128

Precursor Adduct
[M-H]-

Top 5 Peaks
128 999
128.6 35
46 2

SPLASH
splash10-004i-0900000000-6d82525e15d98dd794db

Thumbnail



License
CC BY-NC-SA

MassBank Europe

2 of 26 View All

Accession ID
MSBNK-Keio_Univ-KO001632

Authors
Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio Univ.

Instrument
API3000, Applied Biosystems

Instrument Type
LC-ESI-QQ

MS Level
MS2

Ionization Mode
NEGATIVE

Collision Energy
20 V

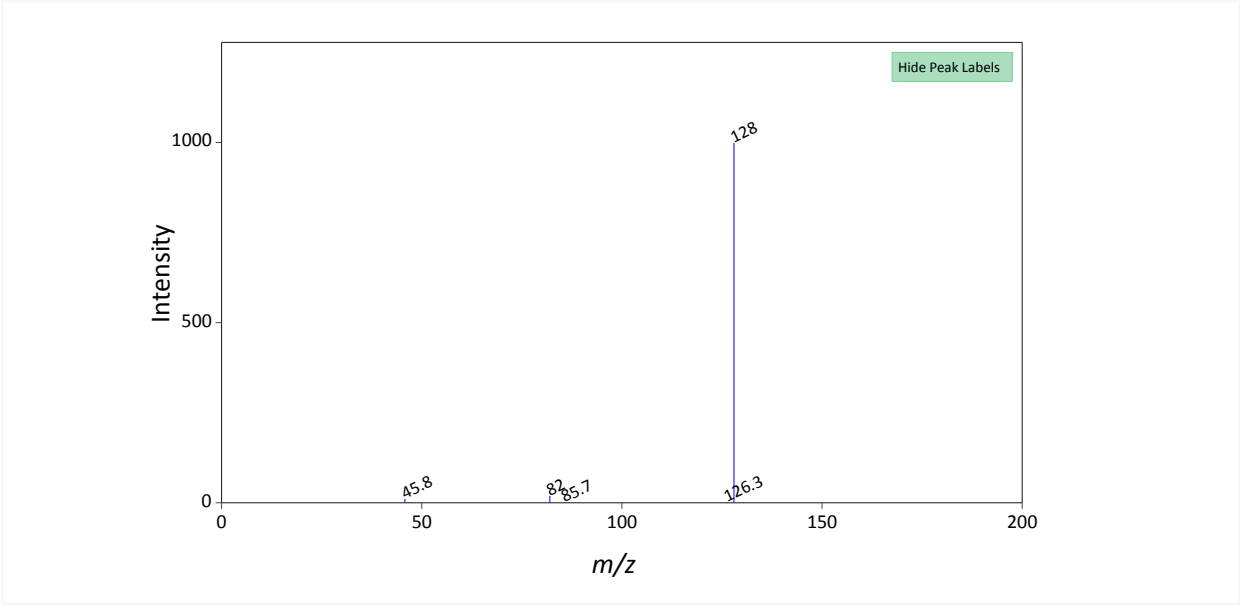
Precursor m/z
128

Precursor Adduct
[M-H]-

Top 5 Peaks
128 999
82 19
45.8 11
126.3 2
85.7 1

SPLASH
splash10-004i-0900000000-abb8b4f2daaa91bfa758

Thumbnail



License
CC BY-NC-SA

▸ MassBank Europe

5.3.4 Other MS

1 of 3 View All

MoNA ID
MoNA011274

MS Category
Experimental

MS Type
Other

MS Level
MS2

Precursor Type
[M+H]+

Precursor m/z
130.08625793457

Instrument
Agilent 6550 iFunnel

Instrument Type
Q-TOF

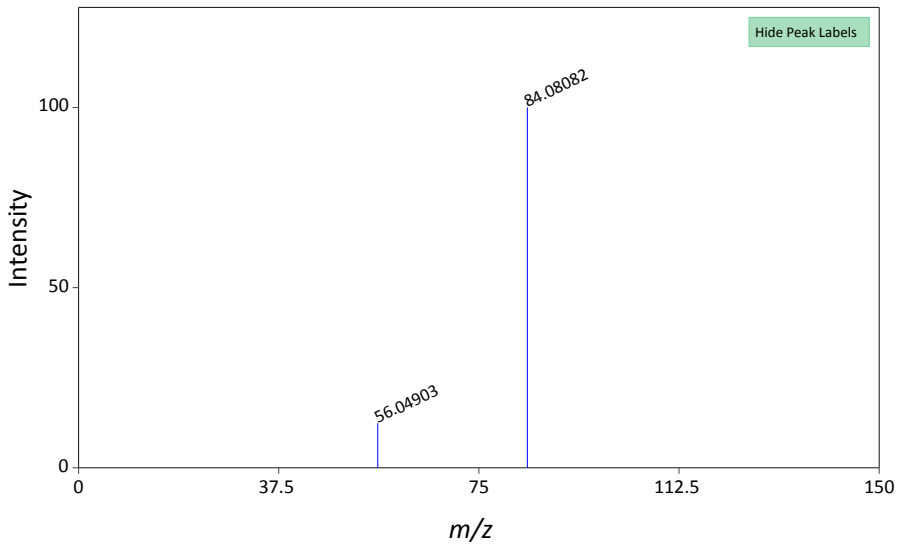
Ionization Mode
ESI

Collision Energy
20

Top 5 Peaks
84.08082 100
56.04903 12.38

SPLASH
splash10-001i-9000000000-b8661d66f50b0d73aad9

Thumbnail



License
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▸ MassBank of North America (MoNA)

2 of 3 View All

MoNA ID
MoNA011275

MS Category
Experimental

MS Type
Other

MS Level
MS2

Precursor Type
[M+H]+

Precursor m/z
130.08625793457

Instrument
Agilent 6550 iFunnel

Instrument Type
Q-TOF

Ionization Mode

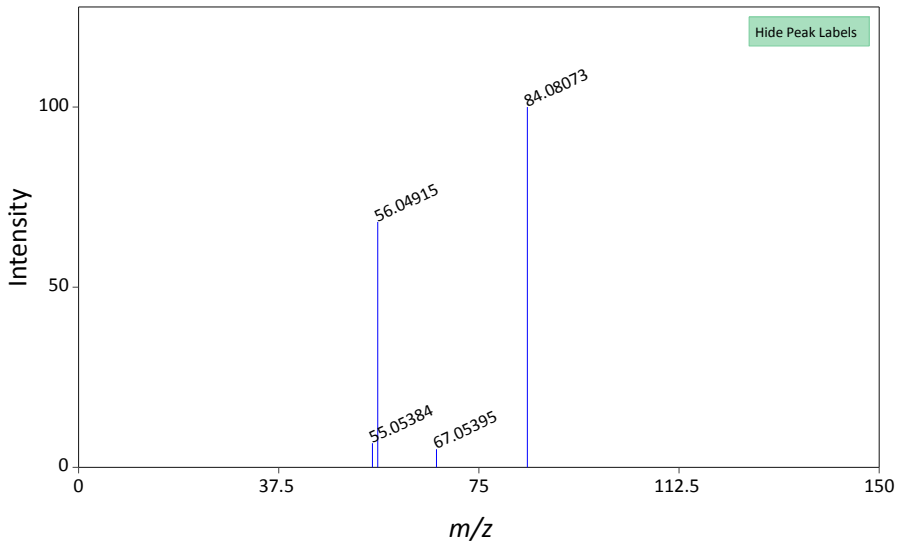
ESI

Collision Energy
30

Top 5 Peaks
84.08073 100
56.04915 68.12
55.05384 6.70
67.05395 5.03

SPLASH
splash10-053r-9000000000-431801cb76e1ab122d35

Thumbnail



License
CC-BY

▸ MassBank of North America (MoNA)

5.4 IR Spectra

5.4.1 FTIR Spectra

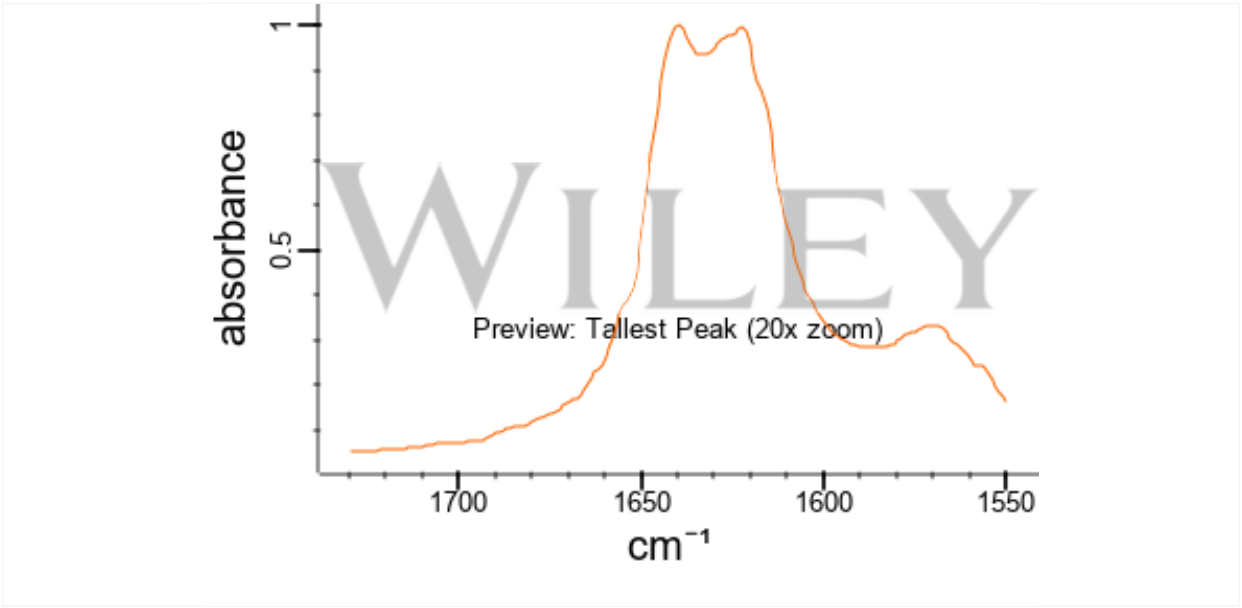
1 of 2

Technique
KBr WAFER

Source of Sample

Aldrich Chemical Company, Inc., Milwaukee, Wisconsin

Thumbnail



▸ SpectraBase

2 of 2

Instrument Name
Bruker Tensor 27 FT-IR

Technique
KBr1

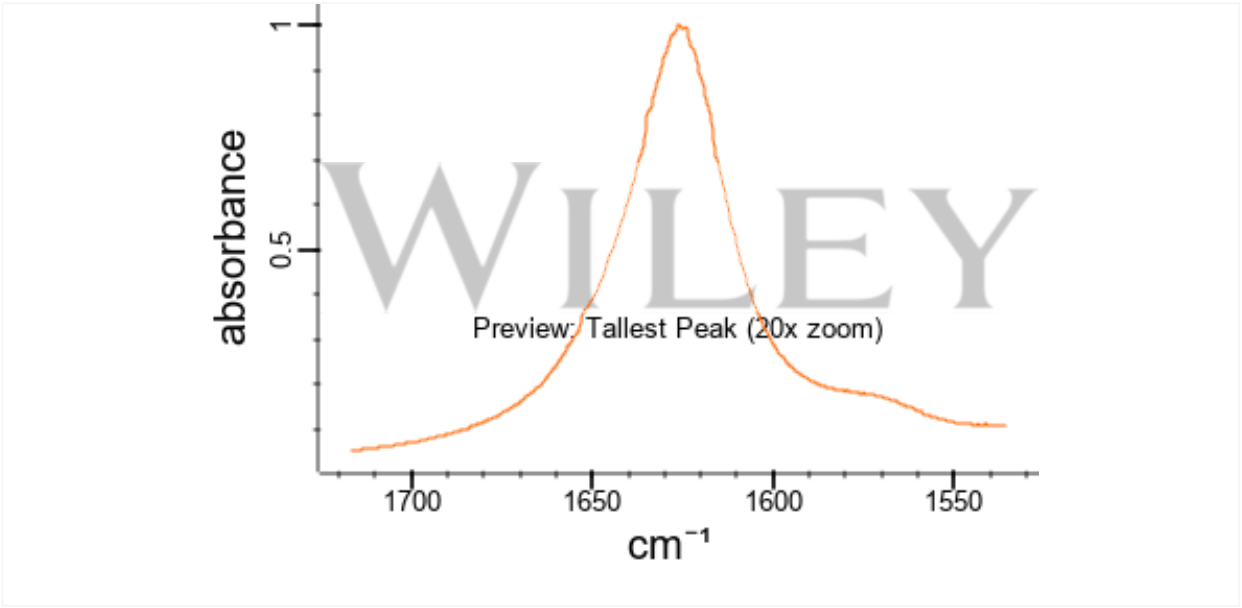
Source of Spectrum
Bio-Rad Laboratories, Inc.

Source of Sample
Alfa Aesar, Thermo Fisher Scientific

Catalog Number
B23541

Lot Number
10190660

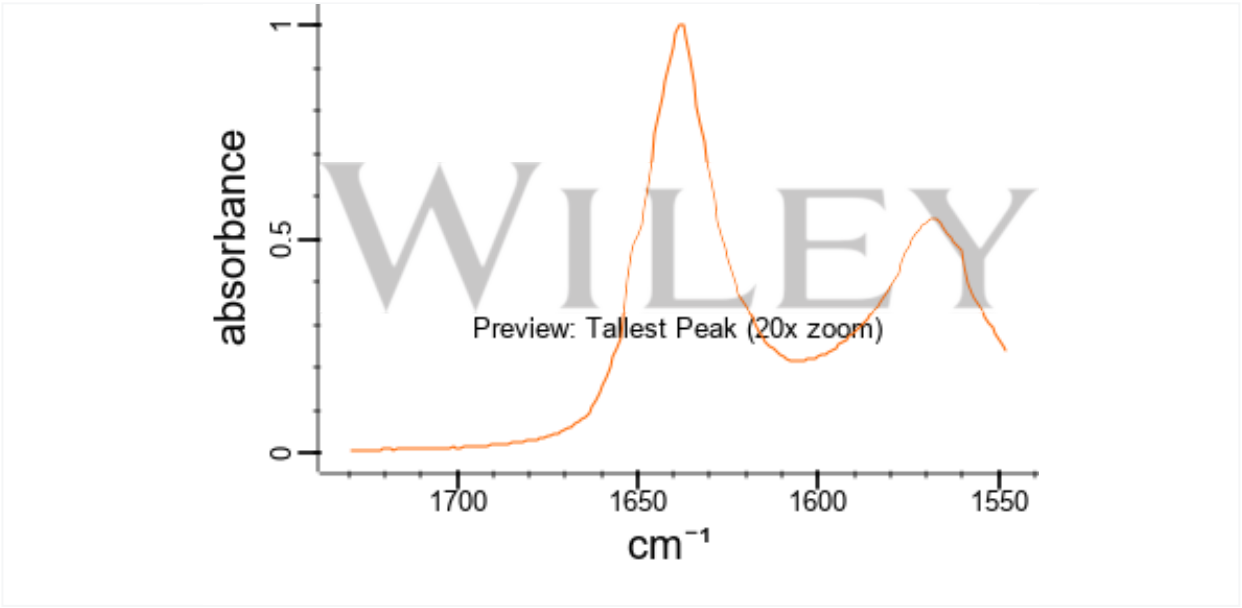
Thumbnail



▸ SpectraBase

5.4.2 ATR-IR Spectra

1 of 2
Instrument Name Bruker Tensor 27 FT-IR
Technique ATR-Neat (DuraSamplIR II)
Source of Spectrum Bio-Rad Laboratories, Inc.
Source of Sample Alfa Aesar, Thermo Fisher Scientific
Catalog Number B23541
Lot Number 10190660
Copyright Copyright © 2016-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail



SpectraBase

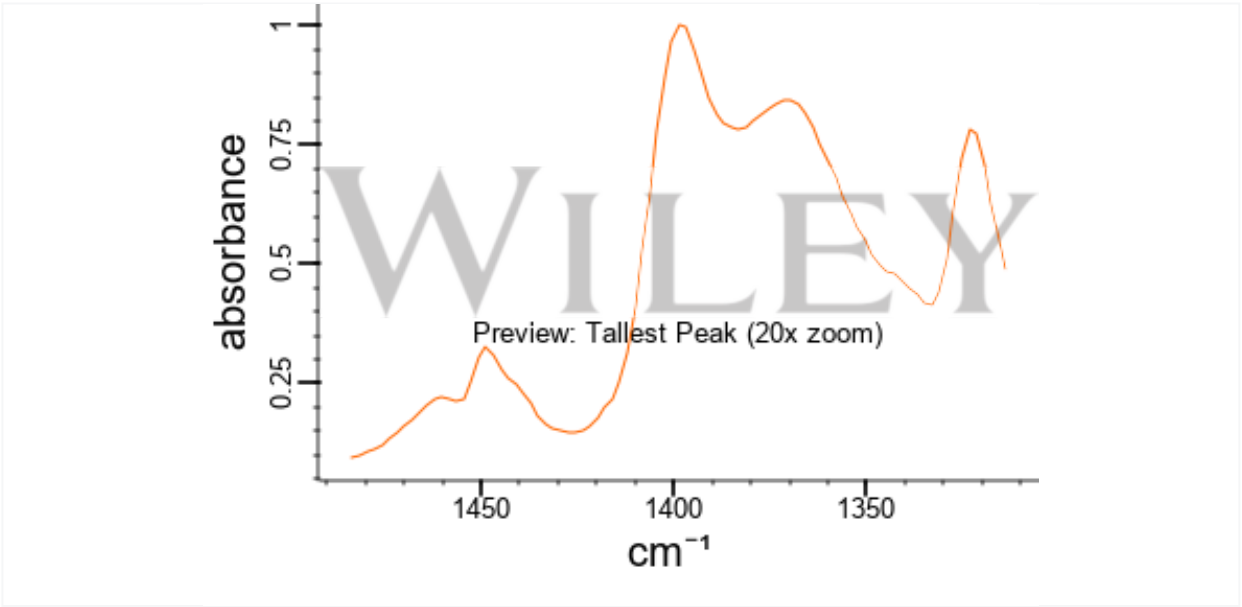
2 of 2

Source of Sample
Aldrich

Catalog Number
P45850

Copyright

Thumbnail



SpectraBase

5.5 Raman Spectra

Instrument Name
Bruker MultiRAM Stand Alone FT-Raman Spectrometer

Technique
FT-Raman

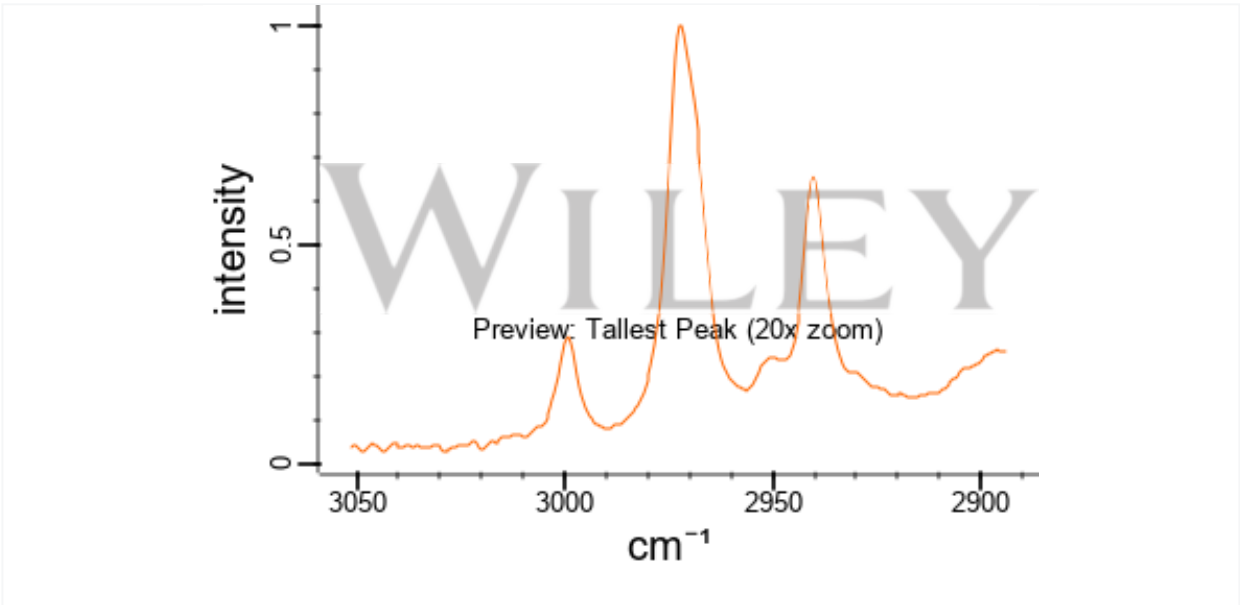
Source of Spectrum
Bio-Rad Laboratories, Inc.

Source of Sample
Alfa Aesar, Thermo Fisher Scientific

Catalog Number
B23541

Lot Number
10190660

Thumbnail



SpectraBase

6 Related Records

6.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

▸ PubChem

6.2 Related Compounds

Same Connectivity Count	12
Same Stereo Count	5
Same Isotope Count	3
Same Parent, Connectivity Count	70
Same Parent, Stereo Count	45
Same Parent, Isotope Count	61
Same Parent, Exact Count	41
Mixtures, Components, and Neutralized Forms Count	199
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

▸ PubChem

6.3 Substances

6.3.1 Related Substances

All Count
806

Same Count
360

Mixture Count
446

PubChem

6.3.2 Substances by Category

PubChem

6.4 Entrez Crosslinks

PubMed Count
197

Taxonomy Count
3

Gene Count
2

PubChem

7 Chemical Vendors

▸ PubChem

8 Drug and Medication Information

8.1 Biomarker Information

▸ MarkerDB

9 Pharmacology and Biochemistry

9.1 Human Metabolite Information

9.1.1 Tissue Locations

Intestine
Liver
Placenta
Prostate

▸ Human Metabolome Database (HMDB)

9.1.2 Cellular Locations

Cytoplasm
Extracellular

▸ Human Metabolome Database (HMDB)

10 Use and Manufacturing

10.1 General Manufacturing Information

EPA TSCA Commercial Activity Status

2-Piperidinecarboxylic acid: INACTIVE

▸ EPA Chemicals under the TSCA

11 Safety and Hazards

11.1 Hazards Identification

11.1.1 GHS Classification

1 of 2 View All

Pictogram(s)

Irritant

Signal
Warning

GHS Hazard Statements
H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation]
H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]
H335 (100%): 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 per 47 reports by companies from 6 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.
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)

11.1.2 Hazard Classes and Categories

Skin Irrit. 2 (100%)
Eye Irrit. 2 (100%)
STOT SE 3 (100%)

▸ European Chemicals Agency (ECHA)

Skin Irrit. 2 (100%)
Eye Irrit. 2 (100%)
STOT SE 3 (50%)

▸ European Chemicals Agency (ECHA)

12 Toxicity

12.1 Toxicological Information

12.1.1 Acute Effects

- ChemIDplus

13 Associated Disorders and Diseases

- Comparative Toxicogenomics Database (CTD)

Disease
Infantile Refsum's disease

References

PubMed: 2427795, 2408988

MetaGene: Metabolic & Genetic Information Center (MIC: http://www.metagene.de)

Disease
Rhizomelic chondrodysplasia punctata

References
PubMed: 9818927

Disease
Refsum's disease

References
PubMed: 12700346, 6186413, 2408988, 2427795, 2433405

Disease
Peroxisomal disorders, new type, liver

References
PubMed: 7931872

MetaGene: Metabolic & Genetic Information Center (MIC: http://www.metagene.de)

Disease
Pyridoxine-dependent epilepsy

References
PubMed: 1454145, 17068770

Disease
D-Bifunctional protein deficiency

References
PubMed: 2921319, 12646728

Disease
Pseudoneonatal adrenoleukodystrophy

References
PubMed: 2894756

Disease
Traumatic brain injury

References
PubMed: 15206793, 11978879, 15756940, 17684518

Disease
Malaria

References
PubMed: 10877011, 11865422, 12964115, 12185554, 9231201

Disease
Anemia

References

PubMed: 12964115

Disease

Tuberculous meningitis

References

PubMed: 12581805, 9542731, 15627241, 2885596, 12964115

Disease

Convulsion

References

PubMed: 12964115, 1794121

Disease

Hyperlysinemia I, familial

References

PubMed: 23890588

Disease

Hyperpipecolatemia

References

PubMed: 5700850

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

Disease

Perillyl alcohol administration for cancer treatment

References

PubMed: 17668437, 15607313, 14569192, 10379660, 17403619, 22284503, 20300169, 22061338, 19783829, 19010317

Disease

Pancreatic cancer

References

PubMed: 2315288, 20300169, 22613268, 21505807, 25429707

Disease

Periodontal disease

References

PubMed: 20300169

Disease
Periodontal Probing Depth

References
PubMed: 31026179

Disease
Peroxisomal biogenesis defect

References
PubMed: 3769211, 2921319, 12705501, 10509903, 9818927, 2418187, 7931872, 8825400
MetaGene: Metabolic & Genetic Information Center (MIC: http://www.metagene.de)

Disease
Adrenoleukodystrophy

References
PubMed: 2921319, 2408988, 7807943, 7609459
MetaGene: Metabolic & Genetic Information Center (MIC: http://www.metagene.de)

Disease
Schizophrenia

References
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

▸ Human Metabolome Database (HMDB)

14 Literature

14.1 Consolidated References

PubChem

14.2 NLM Curated PubMed Citations

PubChem

14.3 Springer Nature References

Springer Nature

14.4 Thieme References

Thieme Chemistry

14.5 Wiley References

Wiley

14.6 Nature Journal References

Kohler et al. Synthetic cascades are enabled by combining biocatalysts with artficial metalloenzymes. Nature Chemistry, doi: 10.1038/nchem.1498, published online 25 November 2012 http://www.nature.com/nchem

- Nature Chemistry

Over et al. Natural-product-derived fragments for fragment-based ligand discovery. Nature Chemistry, doi: 10.1038/nchem.1506, published online 2 December 2012 http://www.nature.com/nchem

- Nature Chemistry

14.7 Chemical Co-Occurrences in Literature

- PubChem

14.8 Chemical-Gene Co-Occurrences in Literature

PubChem

14.9 Chemical-Disease Co-Occurrences in Literature

PubChem

15 Patents

15.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

- PubChem

15.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

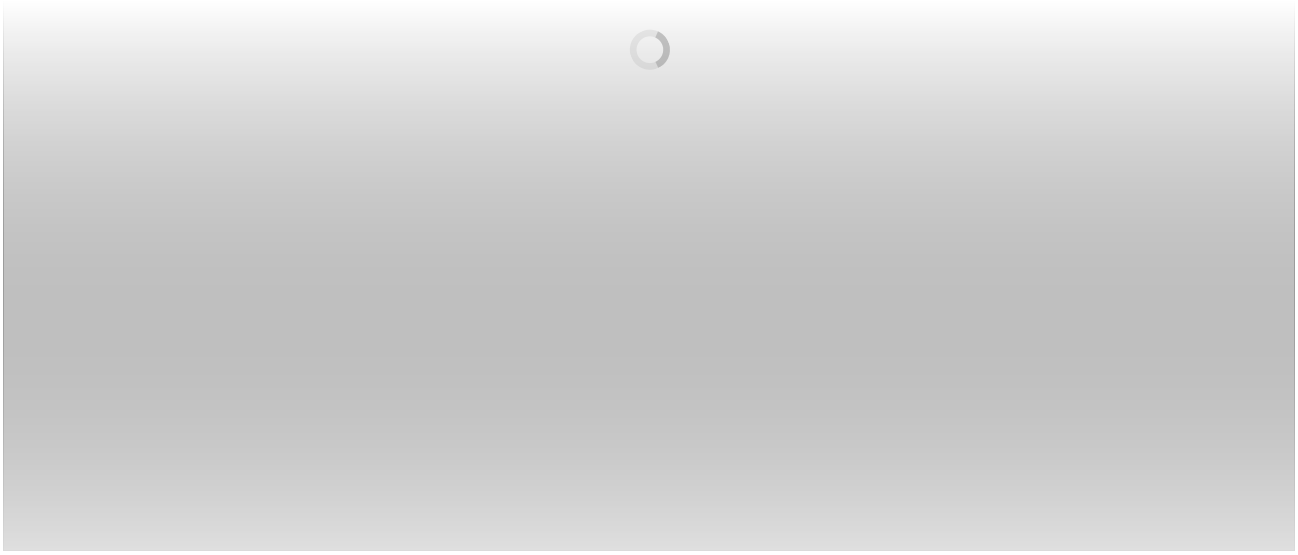
https://patentscope.wipo.int/search/en/result.jsf?inchikey=HXEACLLIILLPRG-UHFFFAOYSA-N

- PATENTSCOPE (WIPO)

15.3 Chemical Co-Occurrences in Patents

- PubChem

15.4 Chemical-Disease Co-Occurrences in Patents



PubChem

15.5 Chemical-Gene Co-Occurrences in Patents

PubChem

16 Interactions and Pathways

16.1 Chemical-Target Interactions

- Comparative Toxicogenomics Database (CTD)

17 Biological Test Results

17.1 BioAssay Results

- PubChem

18 Taxonomy

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

- E. coli Metabolome Database (ECMDB); LOTUS - the natural products occurrence database; Nat…

19 Classification

19.1 MeSH Tree

- Medical Subject Headings (MeSH)

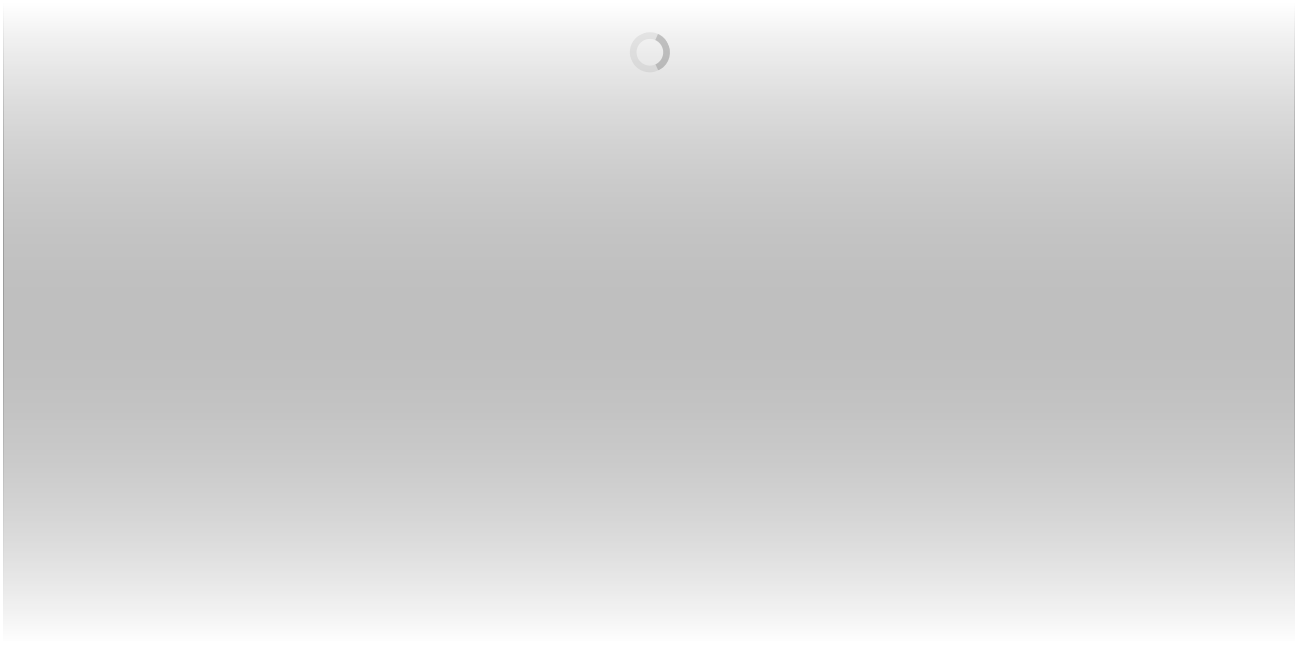
19.2 ChEBI Ontology

- ChEBI

19.3 ChemIDplus

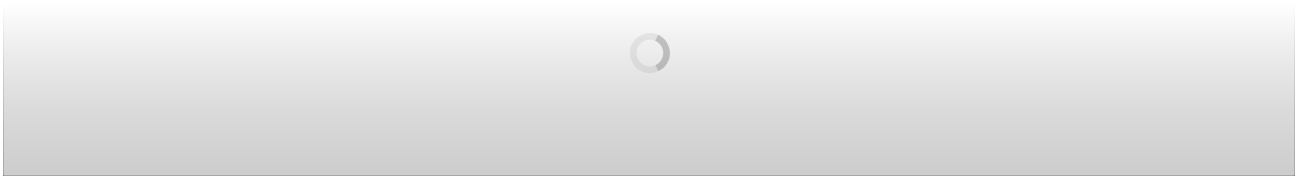
▸ ChemIDplus

19.4 ChEMBL Target Tree



▸ ChEMBL

19.5 UN GHS Classification

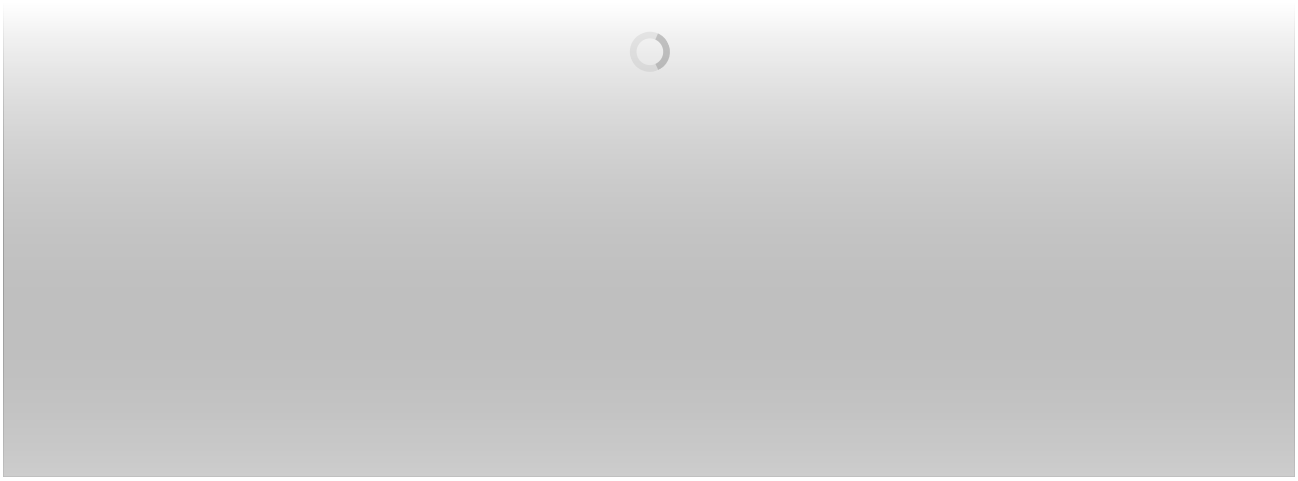


▸ GHS Classification (UNECE)

19.6 NORMAN Suspect List Exchange Classification

▸ NORMAN Suspect List Exchange

19.7 CCSBase Classification



- CCSbase

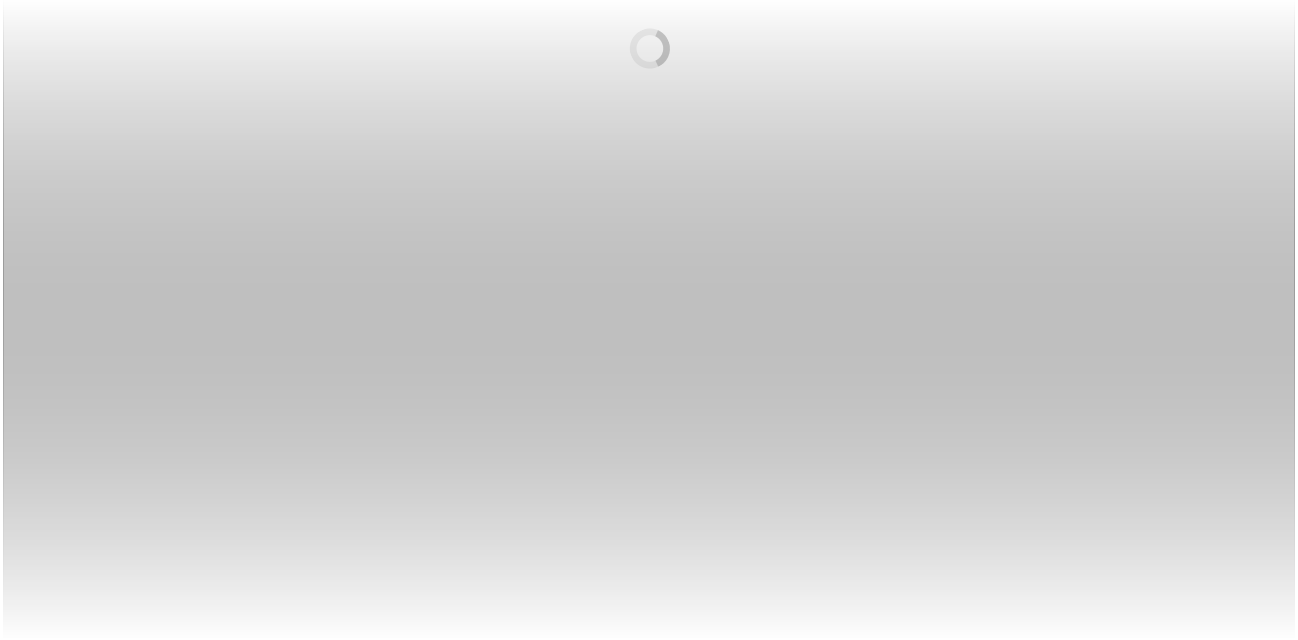
19.8 EPA DSSTox Classification

- EPA DSSTox

19.9 EPA TSCA and CDR Classification

- EPA Chemicals under the TSCA

19.10 LOTUS Tree



LOTUS - the natural products occurrence database

19.11 EPA Substance Registry Services Tree

EPA Substance Registry Services

20 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. ## CAS Common Chemistry

Pipecolic acid

https://commonchemistry.cas.org/detail?cas_rn=535-75-1

2. ## ChemIDplus

Pipecolic acid

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000535751

ChemIDplus Chemical Information Classification

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

3. ## DTP/NCI

Pipecolic acid

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=93089

Pipecolic acid

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=17125

4. ## EPA Chemicals under the TSCA

2-Piperidinecarboxylic acid

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

EPA TSCA Classification

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

5. ## EPA DSSTox

2-Piperidinecarboxylic acid

https://comptox.epa.gov/dashboard/DTXSID40862144

CompTox Chemicals Dashboard Chemical Lists

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

6. ## European Chemicals Agency (ECHA)

DL-piperidine-2-carboxylic acid

https://echa.europa.eu/substance-information/-/substanceinfo/100.021.580

Piperidine-2-carboxylic acid

https://chem.echa.europa.eu/100.007.835

Piperidine-2-carboxylic acid (EC: 208-616-3)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/52035

DL-piperidine-2-carboxylic acid (EC: 223-737-1)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/75738

7. FDA Global Substance Registration System (GSRS)

PIPECOLIC ACID

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/H254GW7PVV

8. Human Metabolome Database (HMDB)

Pipecolic acid

http://www.hmdb.ca/metabolites/HMDB0000070

HMDB0000070_cms_32094

https://hmdb.ca/metabolites/HMDB0000070#spectra

9. CCSbase

CCSbase Classification

https://ccsbase.net/

10. NORMAN Suspect List Exchange

DL-Pipecolate

NORMAN Suspect List Exchange Classification

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

11. ChEBI

Pipecolic acid

https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:17964

ChEBI Ontology

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

12. E. coli Metabolome Database (ECMDB)

LICENSE
ECMDB is offered to the public as a freely available resource.
https://ecmdb.ca/citations

https://ecmdb.ca/compounds/M2MDB001780

13. LOTUS - the natural products occurrence database

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

Pipecolic acid

https://www.wikidata.org/wiki/Q7197255

LOTUS Tree

https://lotus.naturalproducts.net/

14. ChEMBL

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

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL308408/

ChEMBL Protein Target Tree

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

15. Comparative Toxicogenomics Database (CTD)

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

pipecolic acid

https://ctdbase.org/detail.go?type=chem&acc=C031345

16. Natural Product Activity and Species Source (NPASS)

Pipecolic Acid

https://bidd.group/NPASS/compound.php?compoundID=NPC64250

17. MassBank Europe

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

DL-Pipecolic acid

https://massbank.eu/MassBank/Result.jsp?inchikey=HXEACLLIILLPRG-YFKPBYRVSA-N

DL-Pipecolinic acid

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

18. MassBank of North America (MoNA)

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

D-pipecolate

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

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

LLPRG-UHFFFAOYSA-N%27)

19. NIST Mass Spectrometry Data Center

LICENSE
Data covered by the Standard Reference Data Act of 1968 as amended.
https://www.nist.gov/srd/public-law

L-Pipecolinic acid

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

20. SpectraBase

Piperidine-2-carboxylic acid

https://spectrabase.com/spectrum/FZXRtMiji3A

Piperidine-2-carboxylic acid

https://spectrabase.com/spectrum/Fs0mC5deFJW

DL-pipecolic acid

https://spectrabase.com/spectrum/HWQ3aOlvFXs

2-piperidinecarboxylic acid

https://spectrabase.com/spectrum/2RqzhyPINvq

PIPECOLINIC ACID

https://spectrabase.com/spectrum/9WfObTp8C9q

L-PIPECOLIC ACID

https://spectrabase.com/spectrum/Iq25GVxf1A1

PIPECOLINIC ACID

https://spectrabase.com/spectrum/988l0JEYPSG

D,L-Pipecolinic acid

https://spectrabase.com/spectrum/6v0aG56Nzil

D,L-Pipecolinic acid

https://spectrabase.com/spectrum/EpjQRHB6frn

D,L-Pipecolinic acid

https://spectrabase.com/spectrum/JiLDZHcmS5w

Pipecolinic acid

https://spectrabase.com/spectrum/Ey9Tee1LO68

21. IUPAC Digitized pKa Dataset

Piperidine-2-carboxylic acid

https://github.com/IUPAC/Dissociation-Constants

22. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J1.592J

23. MarkerDB

Pipecolic acid

https://markerdb.ca/chemicals/48

24. Metabolomics Workbench

Pipecolic Acid

https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=130145

25. Nature Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/152186697

https://pubchem.ncbi.nlm.nih.gov/substance/152199283

26. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/87689735

27. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=9042471-256751779

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=9042471-256761956

28. Thieme Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=9042471-256751779

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=9042471-256761956

29. Wikidata

Pipecolic_acid

https://www.wikidata.org/wiki/Q7197255

30. Wikipedia

Pipecolic acid

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

31. Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=118693

32. PubChem

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

33. Medical Subject Headings (MeSH)

pipecolic acid

https://www.ncbi.nlm.nih.gov/mesh/67031345

MeSH Tree

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

34. GHS Classification (UNECE)

GHS Classification Tree

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

35. EPA Substance Registry Services

EPA SRS List Classification

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

36. PATENTSCOPE (WIPO)

SID 403389637

https://pubchem.ncbi.nlm.nih.gov/substance/403389637