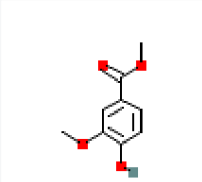
National Library of Medicine
National Center for Biotechnology Information

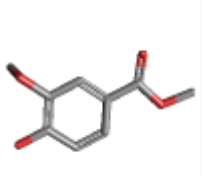
COMPOUND SUMMARY

Methyl vanillate

PubChem CID
19844

Structure


2D


3D

Chemical Safety

Irritant

Laboratory Chemical Safety Summary (LCSS) Datasheet

Molecular Formula
$C_9H_{10}O_4$

Synonyms
Methyl vanillate
3943-74-6
Methyl 4-hydroxy-3-methoxybenzoate
Methyl 3-methoxy-4-hydroxybenzoate
Vanillic acid, methyl ester
View More...

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

Dates

Create:	Modify:
2005-03-26	2024-09-20

Description

Methyl vanillate is a benzoate ester that is the methyl ester of vanillic acid. It has a role as an antioxidant and a plant metabolite. It is a benzoate ester, a member of phenols and an aromatic ether. It is functionally related to a vanillic acid.

- ChEBI

Methyl vanillate has been reported in Rhinacanthus nasutus, Aristolochia kankauensis, and other organisms with data available.

- LOTUS - the natural products occurrence database

Methyl vanillate is a metabolite found in or produced by Saccharomyces cerevisiae.

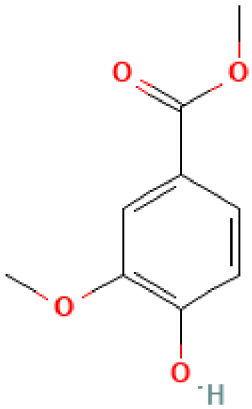
- Yeast Metabolome Database (YMDB)

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

methyl 4-hydroxy-3-methoxybenzoate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

▸ PubChem

2.1.2 InChI

InChI=1S/C9H10O4/c1-12-8-5-6(9(11)13-2)3-4-7(8)10/h3-5,10H,1-2H3

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

2.1.3 InChIKey

BVWTXUYLKBHMOX-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

2.1.4 SMILES

COC1=C(C=CC(=C1)C(=O)OC)O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

▸ PubChem

2.2 Molecular Formula

$C_9H_{10}O_4$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

- Australian Industrial Chemicals Introduction Scheme (AICIS); PubChem

2.3 Other Identifiers

2.3.1 CAS

3943-74-6

- Australian Industrial Chemicals Introduction Scheme (AICIS); CAS Common Chemistry; ChemID…

2.3.2 Deprecated CAS

1220026-96-9

- ChemIDplus; EPA Chemicals under the TSCA

2.3.3 European Community (EC) Number

223-525-9

- European Chemicals Agency (ECHA)

2.3.4 UNII

2HXG8QSO3D

- FDA Global Substance Registration System (GSRS)

2.3.5 ChEBI ID

CHEBI:46477

- ChEBI

2.3.6 ChEMBL ID

CHEMBL486214

- ChEMBL

2.3.7 DrugBank ID

DB08711

- DrugBank

2.3.8 DSSTox Substance ID

DTXSID5074345

- EPA DSSTox

2.3.9 HMDB ID

HMDB0240266

- Human Metabolome Database (HMDB)

2.3.10 Metabolomics Workbench ID

56659

- Metabolomics Workbench

2.3.11 Nikkaji Number

J45.025A

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.12 NSC Number

74385

- DTP/NCI

2.3.13 Wikidata

Q27097897

▸ Wikidata

2.4 Synonyms

2.4.1 MeSH Entry Terms

methyl vanillate

▸ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Methyl vanillate	2HXG8QSO3D
3943-74-6	CHEBI:46477
Methyl 4-hydroxy-3-methoxybenzoate	4-hydroxy-3-methoxy methyl benzoate
Methyl 3-methoxy-4-hydroxybenzoate	NSC-74385
Vanillic acid, methyl ester	VXX
4-Hydroxy-3-methoxybenzoic acid methyl ester	EINECS 223-525-9
BENZOIC ACID, 4-HYDROXY-3-METHOXY-, METHYL ESTER	UNII-2HXG8QSO3D
Methylvanillate	NSC 74385
Vanillic acid methyl ester	BRN 1369113
MFCD00008438	AI3-20212

▸ PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name
Molecular Weight

Property Value
182.17 g/mol

Reference
Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name
XLogP3

Property Value

1.8

Reference

Computed by XLogP3 3.0 (PubChem release 2021.10.14)

Property Name

Hydrogen Bond Donor Count

Property Value

1

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Hydrogen Bond Acceptor Count

Property Value

4

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Rotatable Bond Count

Property Value

3

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Exact Mass

Property Value

182.05790880 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Monoisotopic Mass

Property Value

182.05790880 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Topological Polar Surface Area

Property Value

55.8Å²

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name
Heavy Atom Count

Property Value
13

Reference
Computed by PubChem

Property Name
Formal Charge

Property Value
0

Reference
Computed by PubChem

Property Name
Complexity

Property Value
181

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
0

Reference
Computed by PubChem

Property Name
Defined Bond Stereocenter Count

Property Value
0

Reference
Computed by PubChem

Property Name
Undefined Bond Stereocenter Count

Property Value
0

Reference
Computed by PubChem

Property Name
Covalently-Bonded Unit Count

Property Value
1

Reference
Computed by PubChem

Property Name
Compound Is Canonicalized

Property Value
Yes

Reference
Computed by PubChem (release 2021.10.14)

▸ PubChem

3.2 Experimental Properties

3.2.1 Dissociation Constants

▸ IUPAC Digitized pKa Dataset

3.2.2 Kovats Retention Index

Standard non-polar
1481

Semi-standard non-polar
1516.9, 1525, 1525, 1496, 1526, 1527, 1526, 1518, 1509.7, 1516

Standard polar
2600, 2585, 2600, 2586, 2580, 2586, 2600, 2567, 2578, 2629, 2565, 2629, 2613, 2629, 2607, 2635, 2603, 2604, 2598, 2603

▸ NIST Mass Spectrometry Data Center

3.3 SpringerMaterials Properties

13C nuclear magnetic resonance spectrum
Chemical shift
Spin-spin coupling constant

▸ SpringerMaterials

3.4 Chemical Classes

3.4.1 Cosmetics

Cosmetics related ingredient -> CompTox list(s): [COSMOSDB], [EUCOSMETICS]

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

▸ EPA DSSTox

3.4.2 Endocrine Disruptors

Potential endocrine disrupting compound

S109 | PARCEDC | List of 7074 potential endocrine disrupting compounds (EDCs) by PARC T4.2 | DOI:10.5281/zenodo.10944198

- NORMAN Suspect List Exchange

3.4.3 Fragrances

Fragrance Ingredient (Methyl vanillate) -> IFRA transparency List

- International Fragrance Association (IFRA)

4 Spectral Information

4.1 1D NMR Spectra

1D NMR Spectra
NMRShiftDB Link

- NMRShiftDB

4.1.1 1H NMR Spectra

1 of 3 View All

Spectra ID
4475

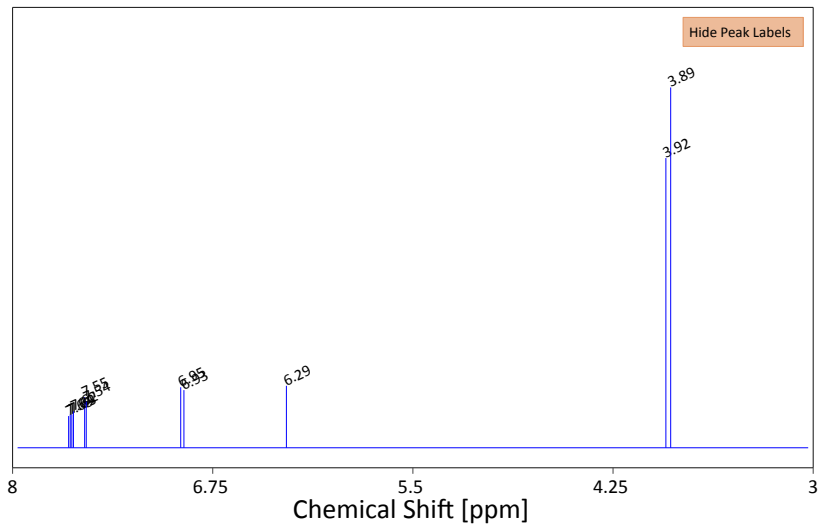
Instrument Type
JEOL

Frequency
400 MHz

Solvent
CDCl3

Shifts [ppm]:Intensity
7.63:93.00, 6.29:172.00, 3.92:804.00, 7.55:140.00, 7.64:92.00, 7.62:101.00, 6.95:168.00, 7.65:88.00, 7.54:128.00, 6.93:160.00, 3.89:1000.00

Thumbnail



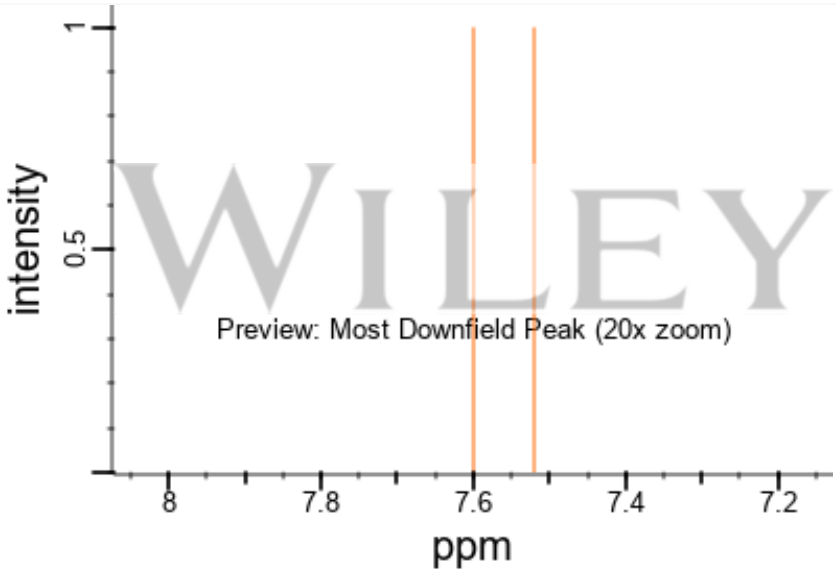
▸ Human Metabolome Database (HMDB)

2 of 3 View All

Instrument Name
Varian A-60

Copyright

Thumbnail



▸ SpectraBase

4.1.2 13C NMR Spectra

1 of 3 View All

Spectra ID
4603

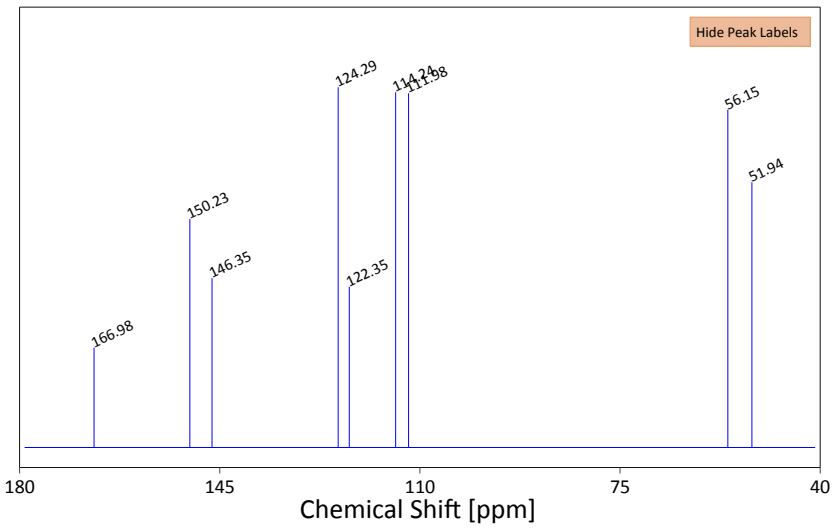
Instrument Type
JEOL

Frequency
22.53 MHz

Solvent
CDCl3

Shifts [ppm]:Intensity
51.94:736.00, 124.29:1000.00, 146.35:470.00, 150.23:634.00, 111.98:983.00, 122.35:446.00, 56.15:937.00, 166.98:277.00, 114.24:986.00

Thumbnail



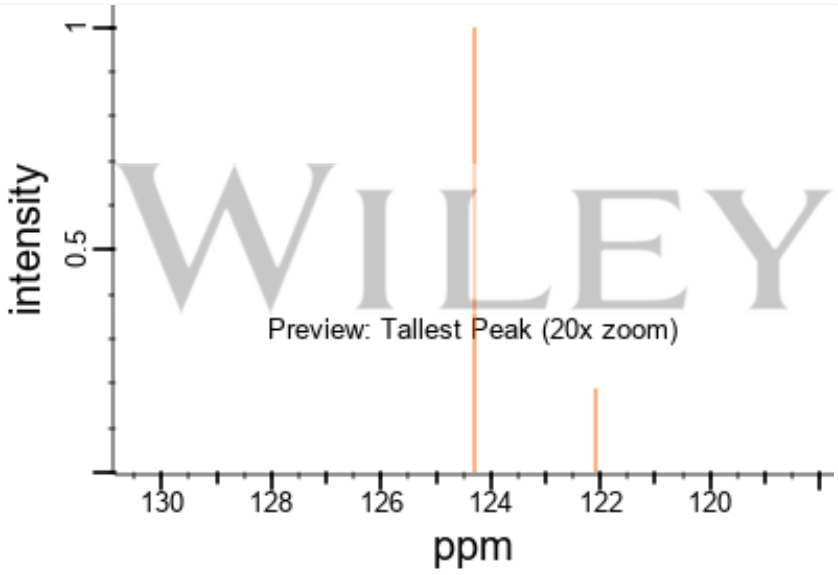
▸ Human Metabolome Database (HMDB)

2 of 3 View All

Source of Sample
Fluka AG, Buchs, Switzerland

Copyright

Thumbnail



SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

1 of 12 View All

Spectra ID
27760

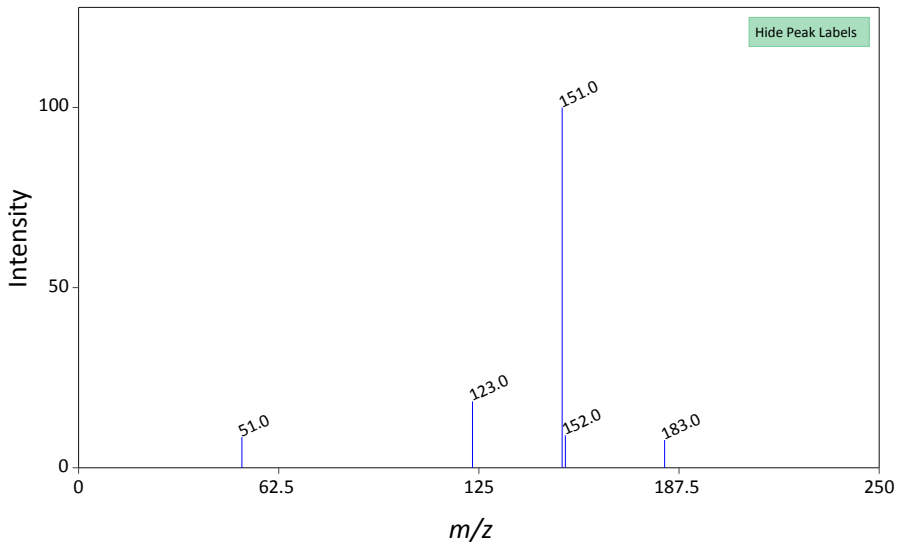
Instrument Type
EI-B

Ionization Mode
positive

SPLASH
splash10-0udi-3900000000-baea5cfe4e199a5ff3bc

Top 5 Peaks
151.0 99.99
123.0 18.40
152.0 9
51.0 8.50
183.0 7.70

Thumbnail



Notes
instrument=SHIMADZU LKB-9000B

▸ Human Metabolome Database (HMDB)

2 of 12 View All

Spectra ID
29870

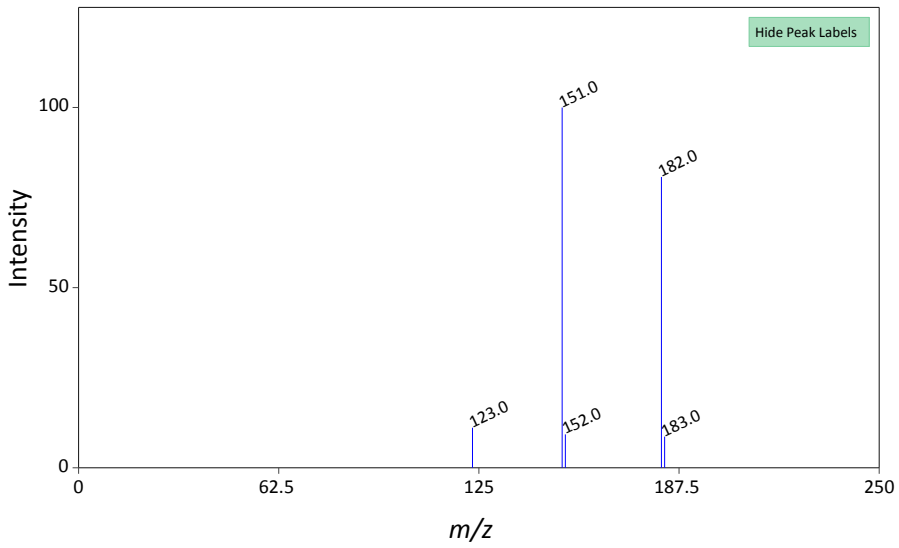
Instrument Type
EI-B

Ionization Mode
positive

SPLASH
splash10-0ue9-0900000000-c2808da990a74bab5038

Top 5 Peaks
151.0 99.99
182.0 80.71
123.0 11.12
152.0 9.27
183.0 8.65

Thumbnail



Notes
instrument=HITACHI M-80

▸ Human Metabolome Database (HMDB)

4.2.2 MS-MS

1 of 8 View All

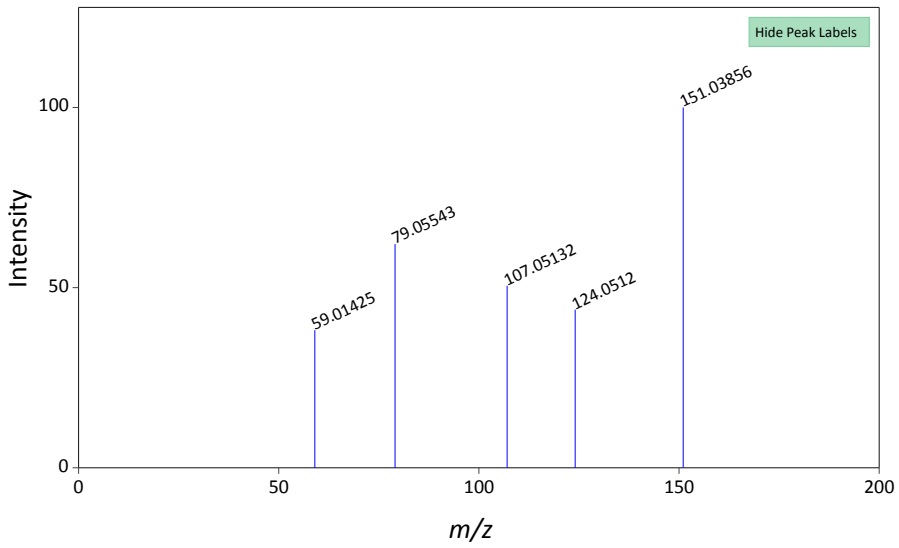
Spectra ID
2252678

Ionization Mode
Positive

SPLASH
splash10-0zor-5900000000-a4ed8f03061acdf96ef7

Top 5 Peaks
151.03856 100
79.05543 62.10
107.05132 50.50
124.0512 43.90
59.01425 38.20

Thumbnail



▸ Human Metabolome Database (HMDB)

2 of 8 View All

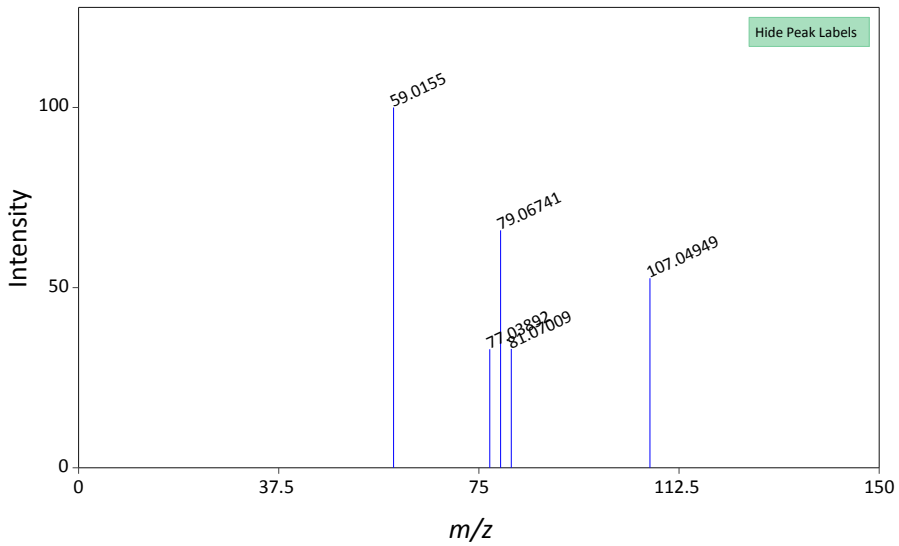
Spectra ID
2253812

Ionization Mode
Positive

SPLASH
splash10-0a6r-9400000000-bc72ccdad3422a05a984

Top 5 Peaks
59.0155 100
79.06741 65.90
107.04949 52.60
81.07009 33
77.03892 32.90

Thumbnail



▸ Human Metabolome Database (HMDB)

4.2.3 LC-MS

1 of 3 View All

MoNA ID
MoNA038793

MS Category
Experimental

MS Type
LC-MS

MS Level
MS2

Precursor Type
[M+H]+

Precursor m/z
183.0651848

Instrument
Thermo Q Exactive HF

Instrument Type
LC-ESI-QFT

Ionization Mode

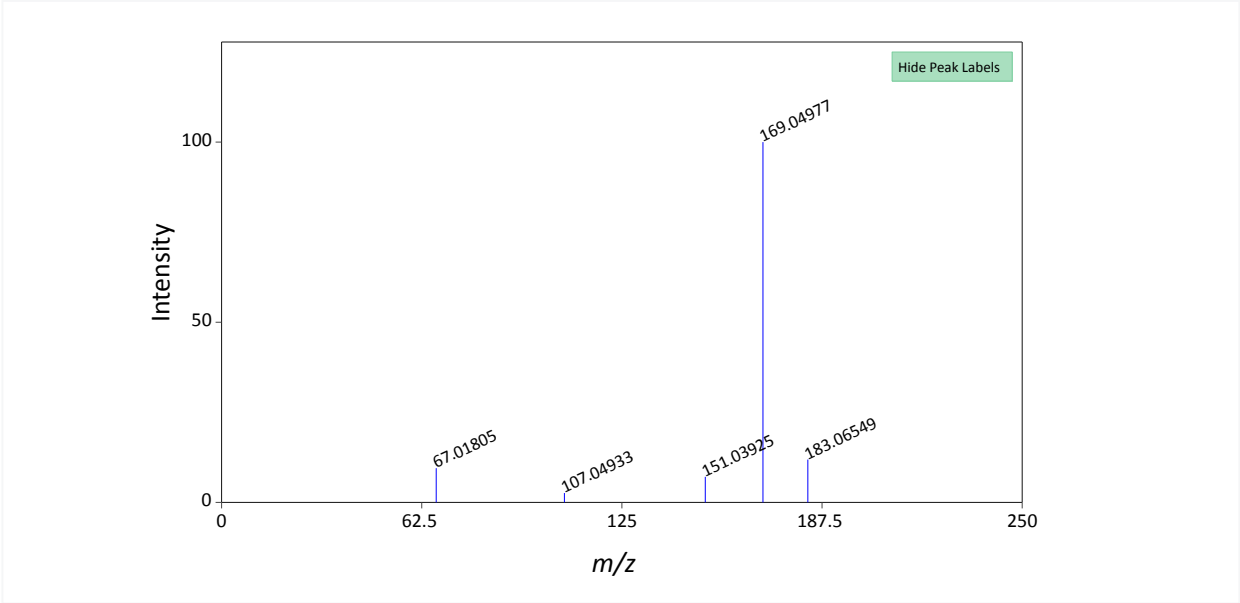
positive

Collision Energy
HCD (NCE 20-30-40%)

Top 5 Peaks
169.04977 100
183.06549 11.90
67.01805 9.50
151.03925 7.10
107.04933 2.60

SPLASH
splash10-014i-0900000000-ad170a04351cb8c76364

Thumbnail



▸ MassBank of North America (MoNA)

2 of 3 View All

MoNA ID
MoNA038644

MS Category
Experimental

MS Type
LC-MS

MS Level
MS2

Precursor Type
[M+H]+

Precursor m/z
183.0651848

Instrument
Thermo Q Exactive HF

Instrument Type
LC-ESI-QFT

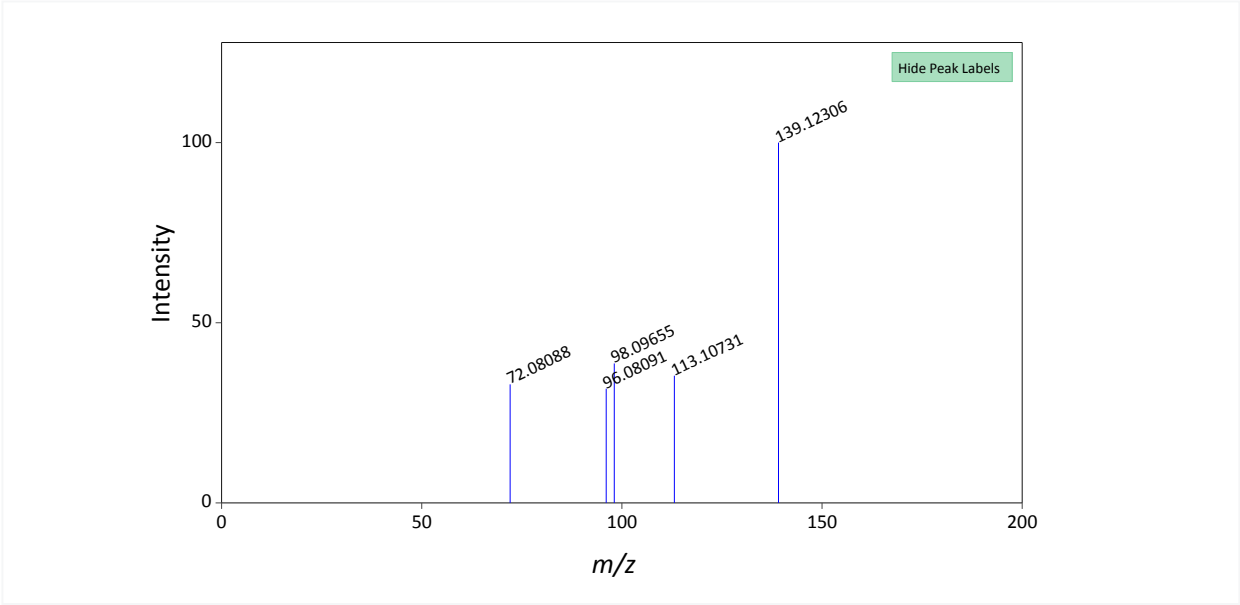
Ionization Mode
positive

Collision Energy
HCD (NCE 20-30-40%)

Top 5 Peaks
139.12306 100
98.09655 38.70
113.10731 35.30
72.08088 32.90
96.08091 31.70

SPLASH
splash10-01w1-4900000000-dd1126586adcaf4250a1

Thumbnail



▸ MassBank of North America (MoNA)

4.2.4 Other MS

1 of 2

Accession ID
MSBNK-Fac_Eng_Univ_Tokyo-JP004564

Authors
HAYASHI A, DEPT. OF CHEMISTRY, FAC. OF SCI. AND TECHNOLOGY, KINKI UNIV.

Instrument
SHIMADZU LKB-9000B

Instrument Type
EI-B

MS Level
MS

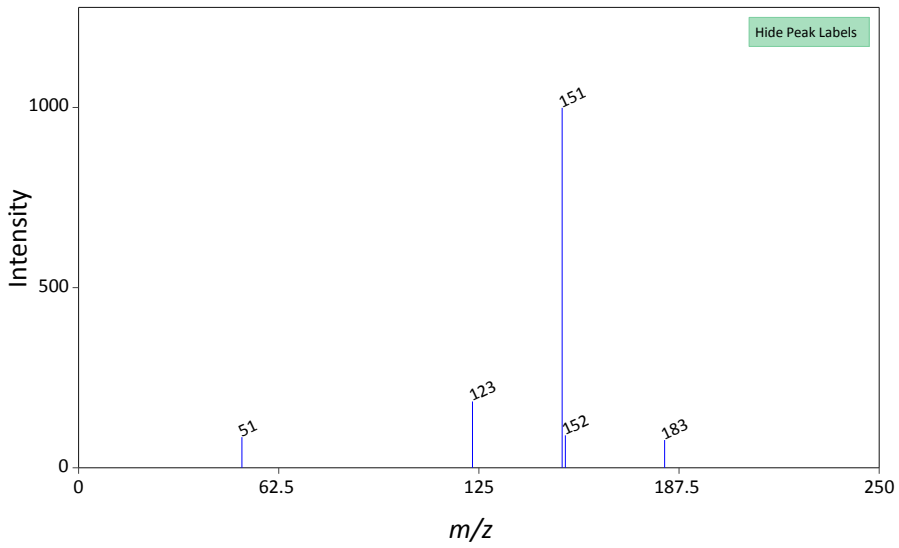
Ionization Mode
POSITIVE

Ionization
ENERGY 70 eV

Top 5 Peaks
151 999
123 184
152 90
51 85
183 77

SPLASH
splash10-0udi-3900000000-baea5cfe4e199a5ff3bc

Thumbnail



License
CC BY-NC-SA

MassBank Europe

2 of 2

Accession ID
MSBNK-Fac_Eng_Univ_Tokyo-JP011441

Authors
SUMITA Y, KYOTO COLLEGE OF PHARMACY

Instrument
HITACHI M-80

Instrument Type
EI-B

MS Level
MS

Ionization Mode
POSITIVE

Ionization
ENERGY 20 eV

Top 5 Peaks
151 999
182 807
123 111

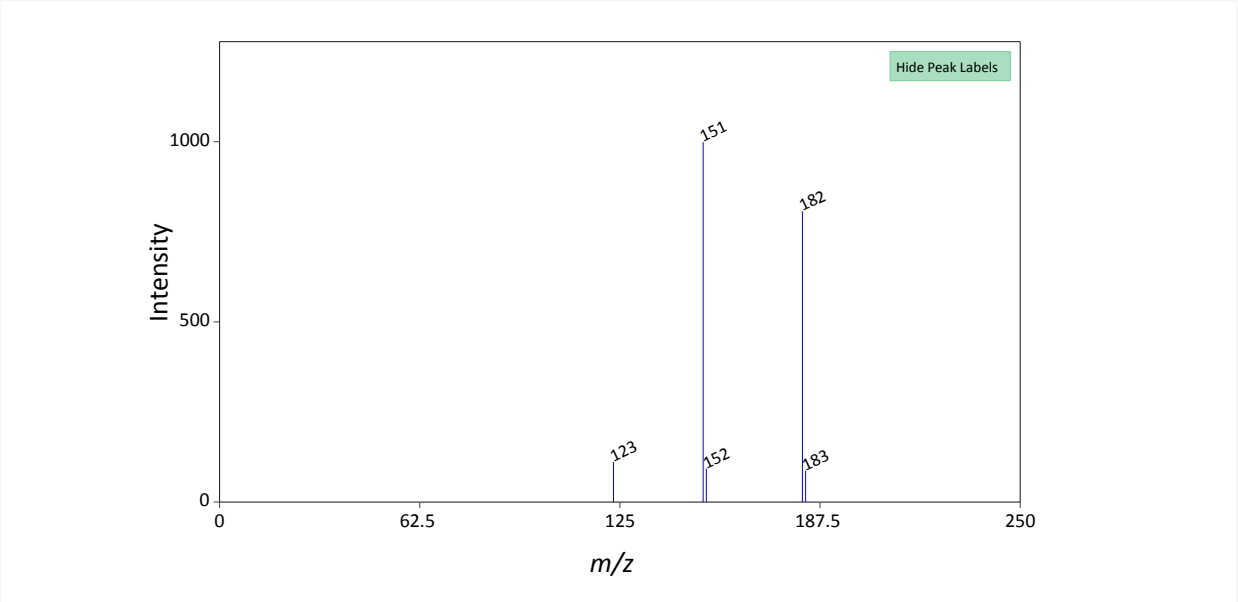
152 93

183 87

SPLASH

splash10-0ue9-0900000000-c2808da990a74bab5038

Thumbnail



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▸ MassBank Europe

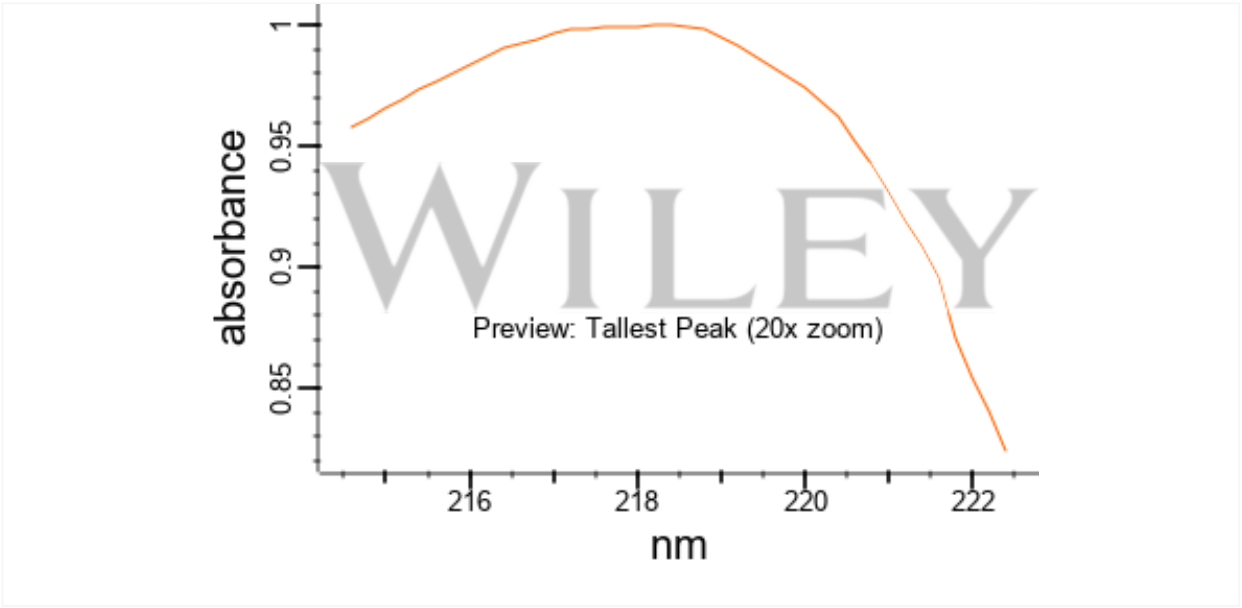
4.3 UV Spectra

4.3.1 UV-VIS Spectra

1 of 2

Copyright

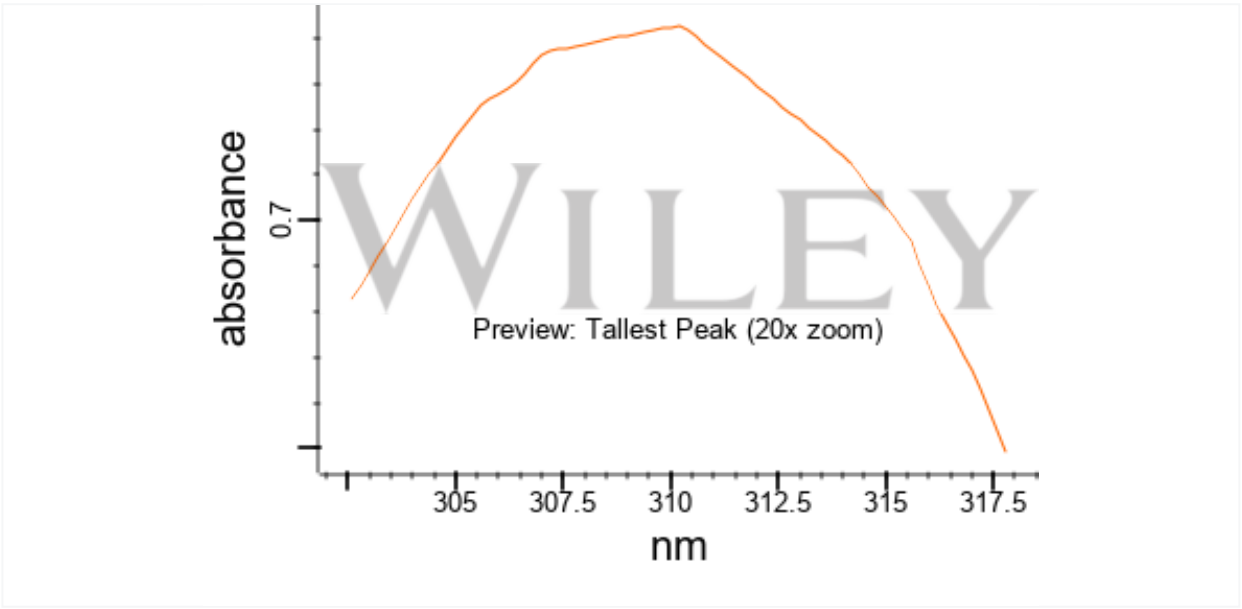
Thumbnail



SpectraBase

2 of 2

Thumbnail



SpectraBase

4.4 IR Spectra

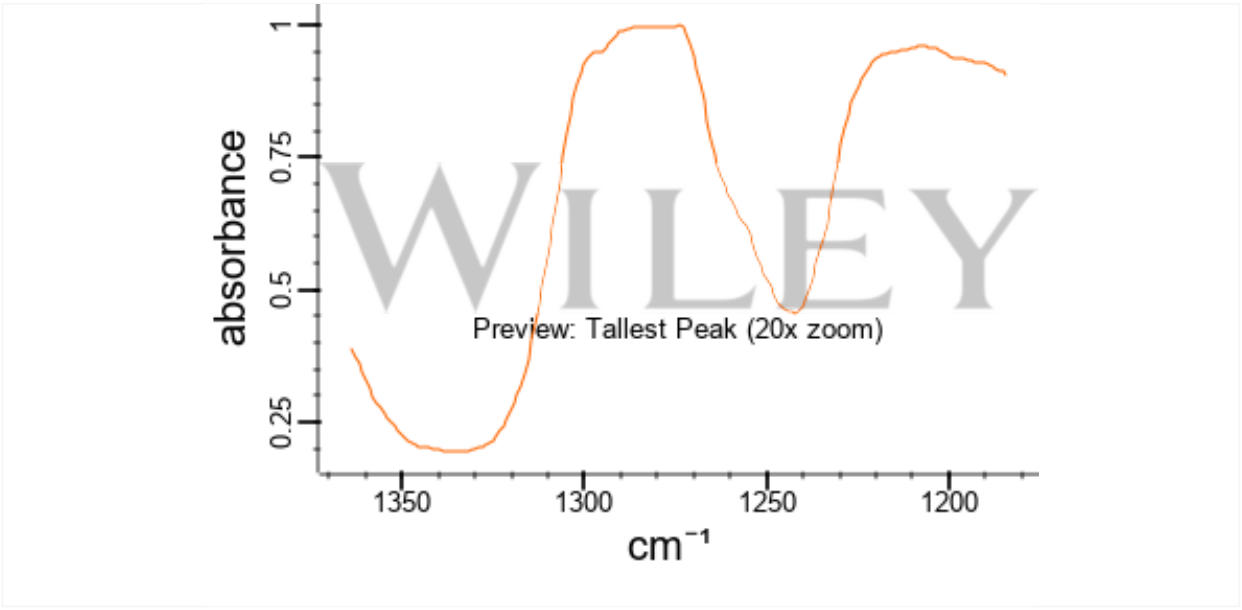
4.4.1 FTIR Spectra

1 of 2

Technique
CAPILLARY CELL: MELT

Source of Sample
Fluka Chemie AG, Buchs, Switzerland

Thumbnail



▸ SpectraBase

2 of 2

Instrument Name
Bruker Tensor 27 FT-IR

Technique
Film (Acetone)

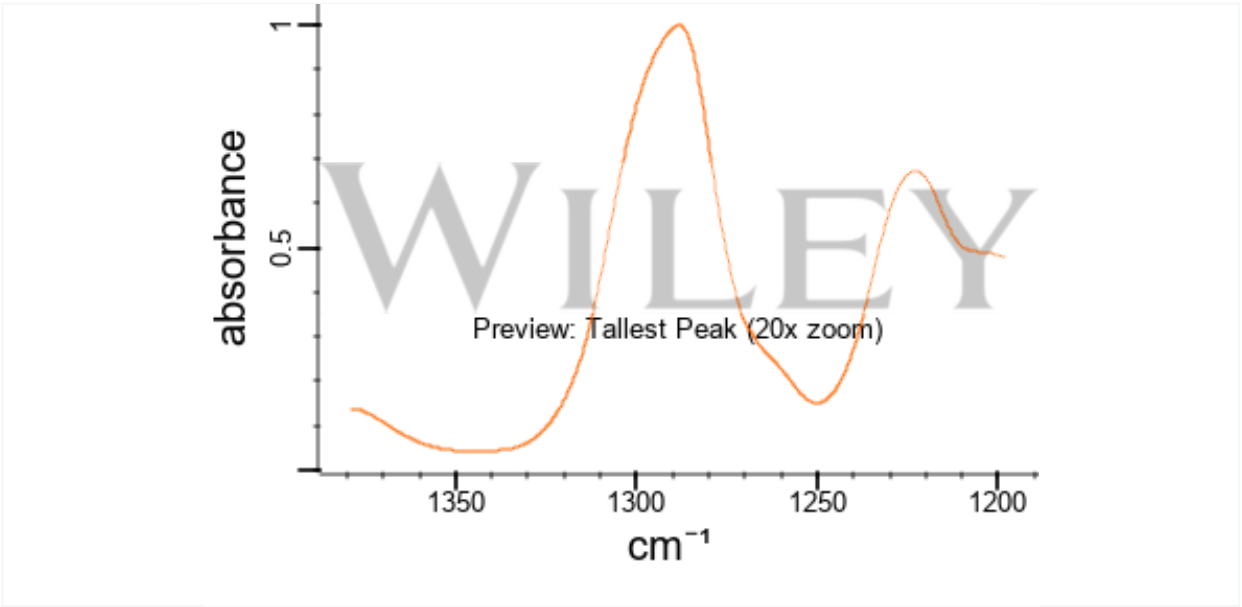
Source of Spectrum
Bio-Rad Laboratories, Inc.

Source of Sample
Alfa Aesar, Thermo Fisher Scientific

Catalog Number
B24209

Lot Number
FA016602

Thumbnail



▸ SpectraBase

4.4.2 ATR-IR Spectra

1 of 2

Instrument Name
Bio-Rad FTS

Technique
ATR-Neat (DuraSamplIR II)

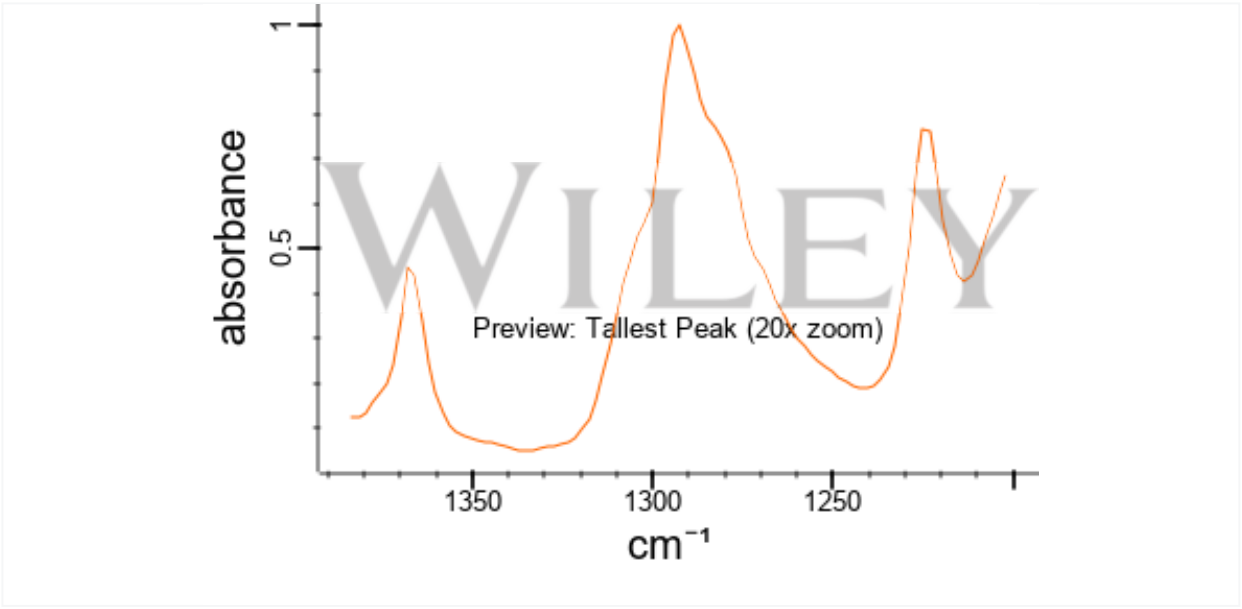
Source of Spectrum
Forensic Spectral Research

Source of Sample
Indofine Chemical Company, Inc.

Catalog Number
19-354

Lot Number
806036

Thumbnail



▸ SpectraBase

2 of 2

Instrument Name
Bruker Tensor 27 FT-IR

Technique
ATR-Neat (DuraSamplIR II)

Source of Spectrum
Bio-Rad Laboratories, Inc.

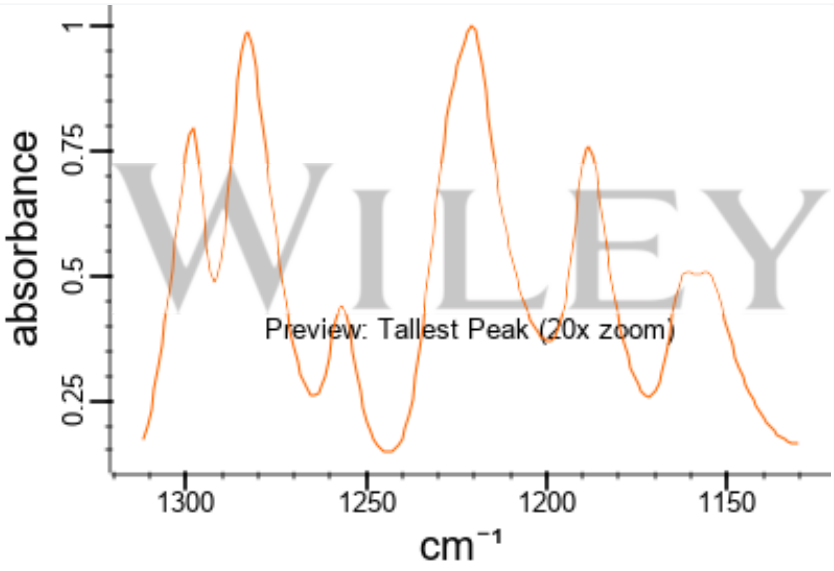
Source of Sample
TCI Chemicals India Pvt. Ltd.

Catalog Number
B24209

Lot Number
FA016602

Copyright

Thumbnail



▸ SpectraBase

4.4.3 Vapor Phase IR Spectra

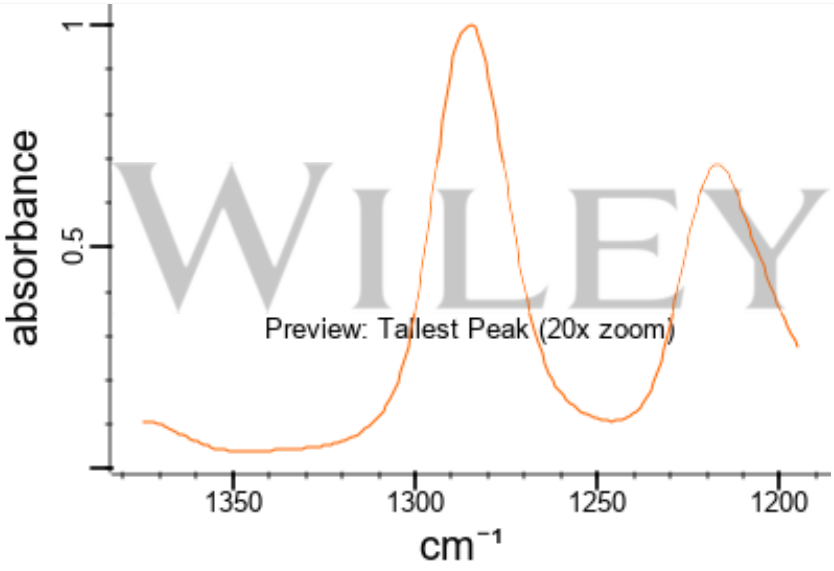
1 of 2

Instrument Name
DIGILAB FTS-14

Technique
Vapor Phase

Copyright

Thumbnail



SpectraBase

2 of 2

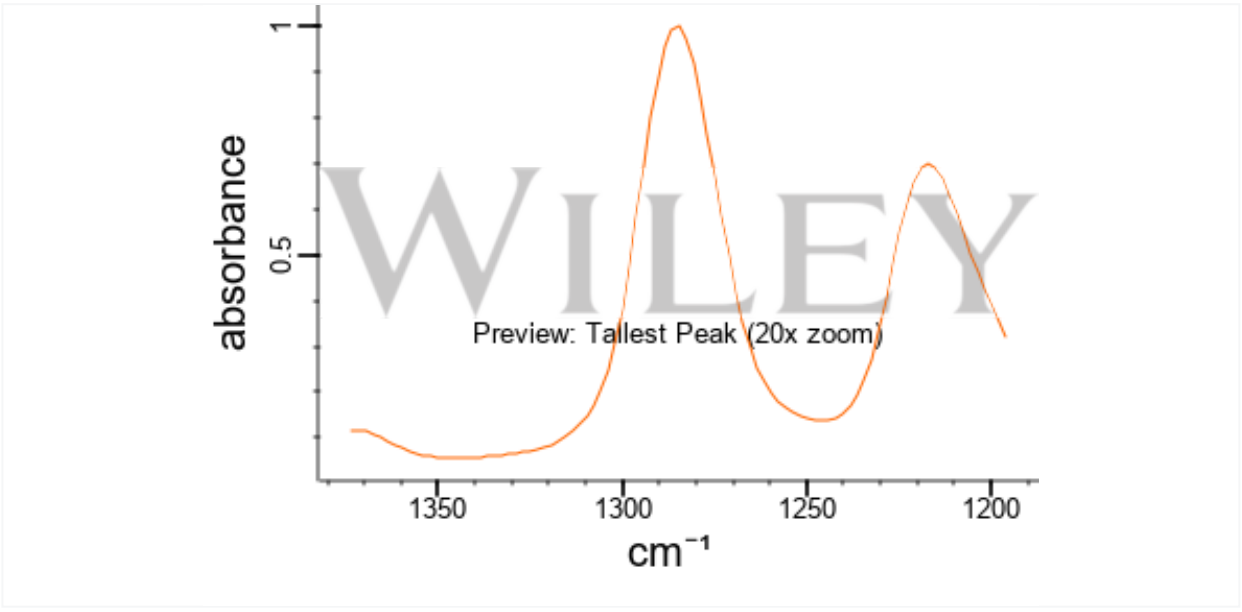
Technique
Vapor Phase

Source of Spectrum
Sigma-Aldrich Co. LLC.

Source of Sample
Aldrich

Catalog Number
138126

Thumbnail



SpectraBase

4.5 Raman Spectra

1 of 2

Instrument Name
Bruker MultiRAM Stand Alone FT-Raman Spectrometer

Technique

FT-Raman

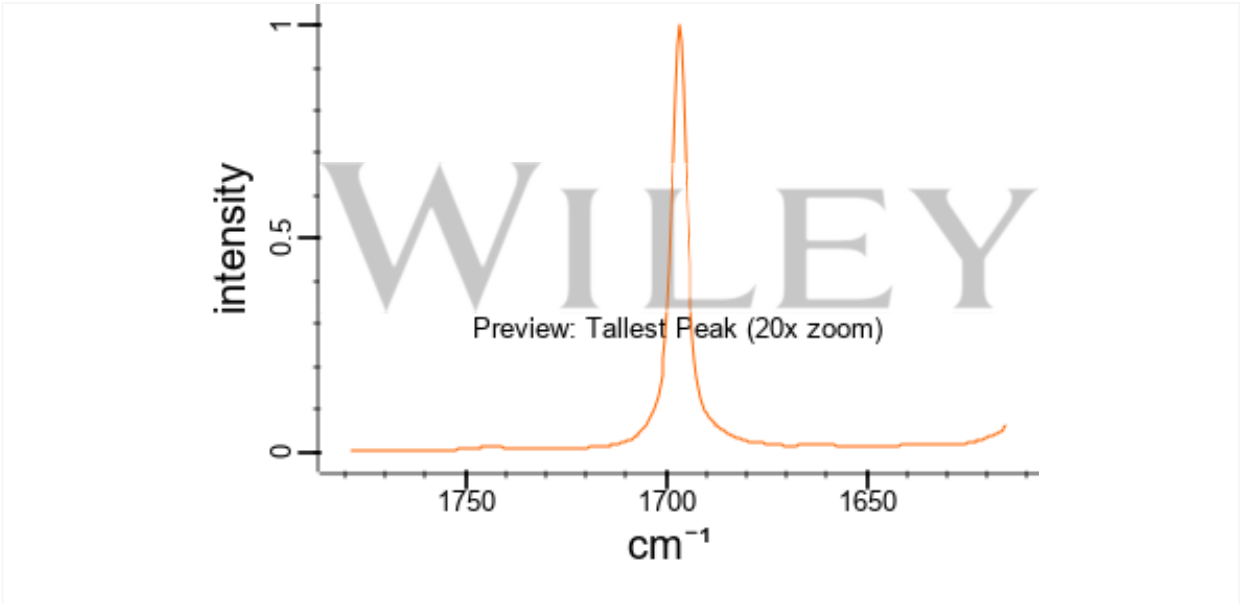
Source of Spectrum
Bio-Rad Laboratories, Inc.

Source of Sample
Alfa Aesar, Thermo Fisher Scientific

Catalog Number
B24209

Lot Number
FA016602

Thumbnail



▸ SpectraBase

2 of 2

Technique
FT-Raman

Source of Spectrum
Forensic Spectral Research

Source of Sample
Indofine Chemical Company, Inc.

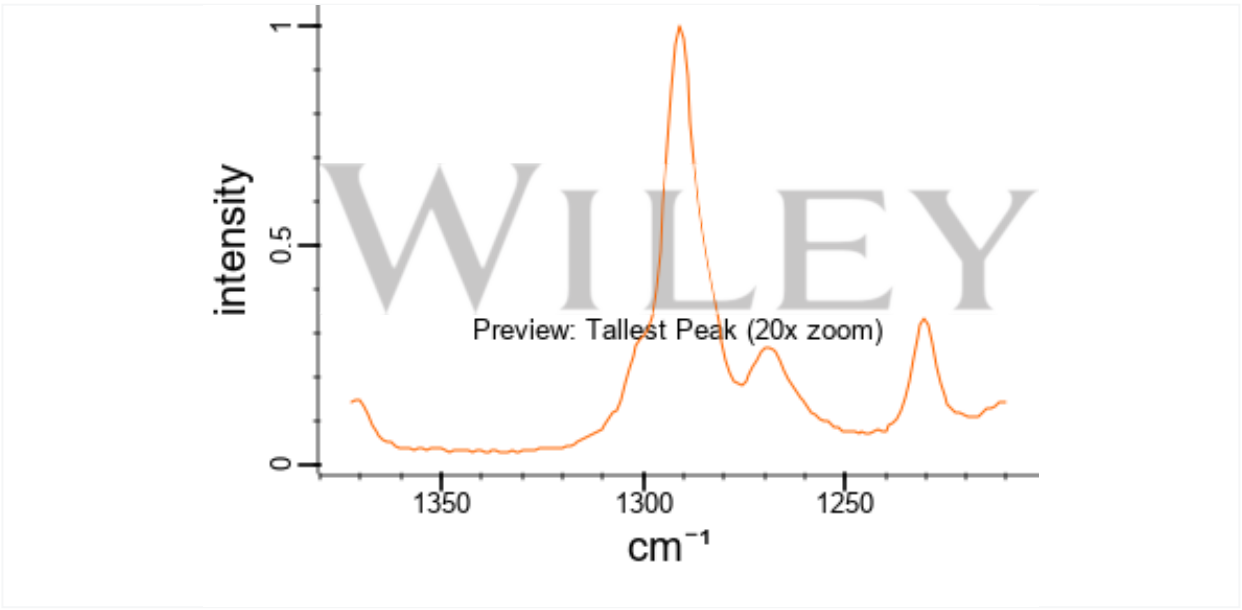
Catalog Number

19-354

Lot Number
0806036

Copyright

Thumbnail



▸ SpectraBase

5 Related Records

5.1 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

5.2 Related Compounds

Same Connectivity Count
2

Same Parent, Connectivity Count
8

Same Parent, Exact Count
7

Mixtures, Components, and Neutralized Forms Count
118

Similar Compounds (2D)
View in PubChem Search

Similar Conformers (3D)
View in PubChem Search

PubChem

5.3 Substances

5.3.1 Related Substances

All Count
315

Same Count
197

Mixture Count
118

PubChem

5.3.2 Substances by Category

PubChem

5.4 Entrez Crosslinks

PubMed Count	19
Protein Structures Count	3
Taxonomy Count	1
Gene Count	3

PubChem

6 Chemical Vendors

PubChem

7 Food Additives and Ingredients

7.1 Food Additive Classes

Flavoring Agents

- EU Food Improvement Agents

8 Use and Manufacturing

8.1 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)

8.1.1 Use Classification

Food additives -> Flavoring Agents

- EU Food Improvement Agents

Fragrance Ingredients

- International Fragrance Association (IFRA)

8.2 General Manufacturing Information

EPA TSCA Commercial Activity Status

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester: ACTIVE

- EPA Chemicals under the TSCA

EPA TSCA Regulatory Flag

PMN - indicates a commenced PMN (Pre-Manufacture Notices) substance.

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

- EPA Chemicals under the TSCA

9 Safety and Hazards

9.1 Hazards Identification

9.1.1 GHS Classification

Note

This chemical does not meet GHS hazard criteria for 83% (235 of 283) of all reports. Pictograms displayed are for 17% (48 of 283) of reports that indicate hazard statements.

Pictogram(s)

Irritant

Signal

Warning

GHS Hazard Statements

H315 (16.6%): Causes skin irritation [Warning Skin corrosion/irritation]

H319 (17%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

H335 (16.3%): 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 283 reports by companies from 7 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.

Reported as not meeting GHS hazard criteria per 235 of 283 reports by companies. For more detailed information, please visit ECHA C&L website.

There are 6 notifications provided by 48 of 283 reports by 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)

9.1.2 Hazard Classes and Categories

Skin Irrit. 2 (16.6%)

Eye Irrit. 2A (17%)

STOT SE 3 (16.3%)

- European Chemicals Agency (ECHA)

9.2 Regulatory Information

The Australian Inventory of Industrial Chemicals

Chemical: Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

- Australian Industrial Chemicals Introduction Scheme (AICIS)

New Zealand EPA Inventory of Chemical Status

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester: Does not have an individual approval but may be used under an appropriate group standard

- New Zealand Environmental Protection Authority (EPA)

9.3 Other Safety Information

Chemical Assessment

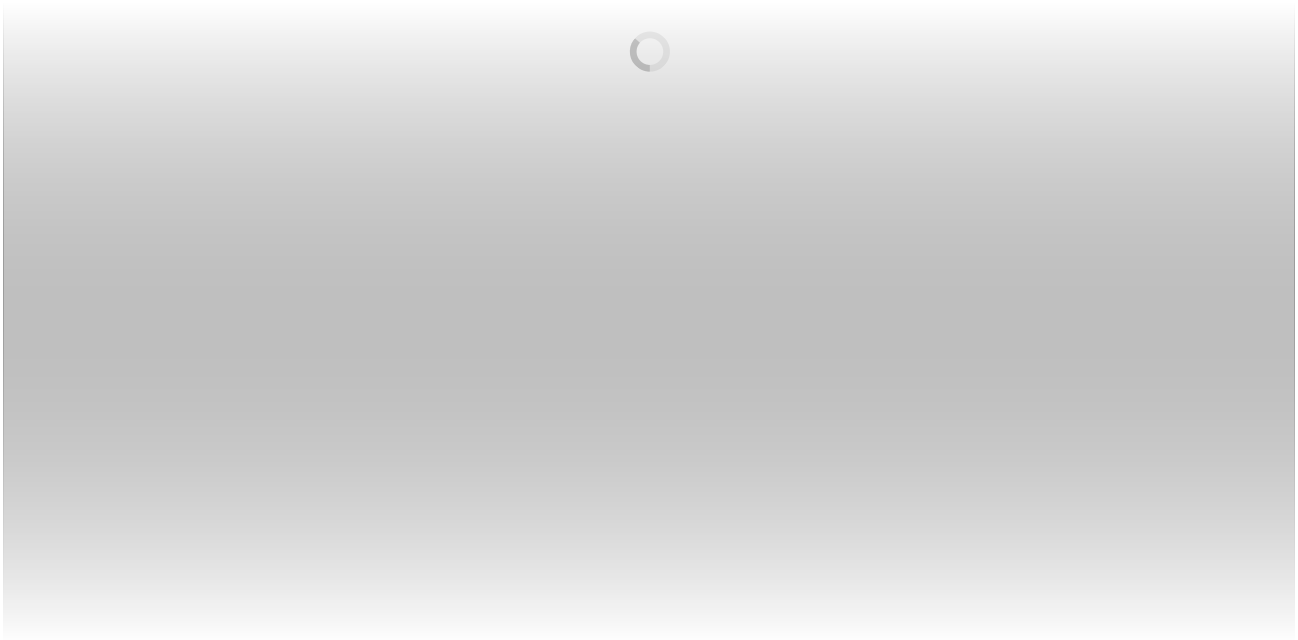
IMAP assessments - Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester: Environment tier I assessment

- Australian Industrial Chemicals Introduction Scheme (AICIS)

10 Toxicity

10.1 Toxicological Information

10.1.1 Acute Effects



- ChemIDplus

11 Literature

11.1 Consolidated References

- PubChem

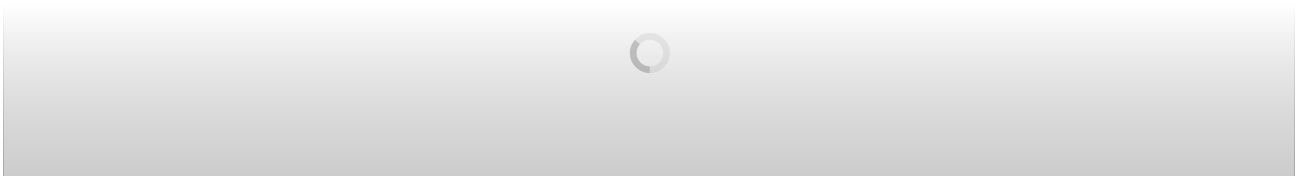
11.2 NLM Curated PubMed Citations

PubChem

11.3 Springer Nature References

Springer Nature

11.4 Thieme References



- Thieme Chemistry

11.5 Nature Journal References

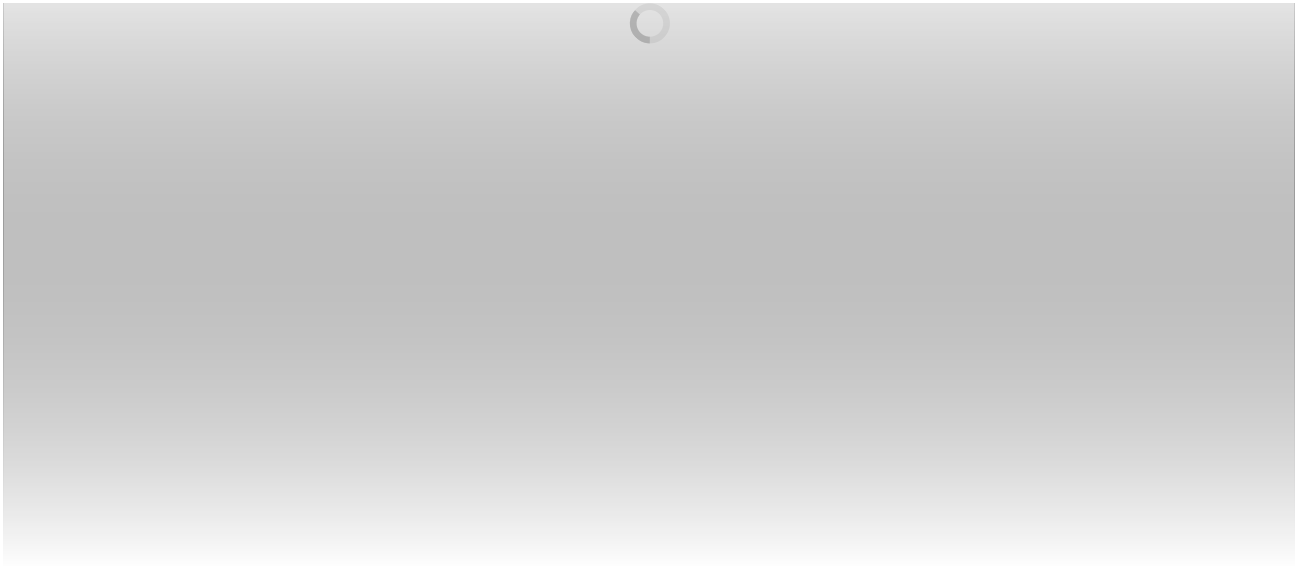
Vedadi et al. A chemical probe selectively inhibits G9a and GLP methyltransferase activity in cells. Nature Chemical Biology, doi: 10.1038/nchembio.599, published online 10 July 2011 http://www.nature.com/naturechemicalbiology

- Nature Chemical Biology

11.6 Chemical Co-Occurrences in Literature

- PubChem

11.7 Chemical-Gene Co-Occurrences in Literature



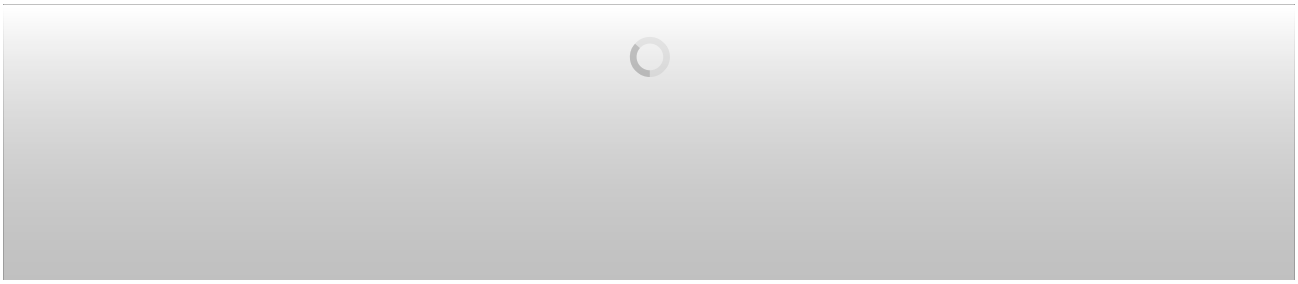
- PubChem

11.8 Chemical-Disease Co-Occurrences in Literature

- PubChem

12 Patents

12.1 Depositor-Supplied Patent Identifiers



- PubChem

Link to all deposited patent identifiers

- PubChem

12.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

- PATENTSCOPE (WIPO)

Patents are available for this chemical structure:

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

- PATENTSCOPE (WIPO)

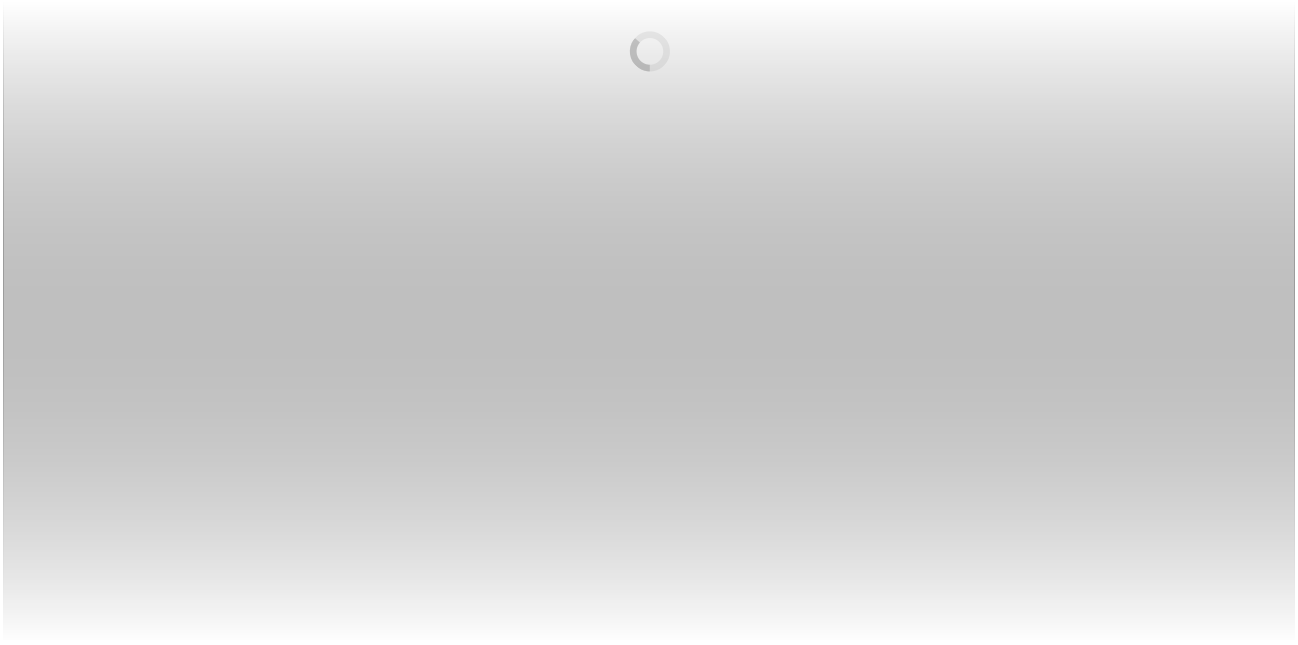
12.3 Chemical Co-Occurrences in Patents

PubChem

12.4 Chemical-Disease Co-Occurrences in Patents

PubChem

12.5 Chemical-Gene Co-Occurrences in Patents



PubChem

13 Interactions and Pathways

13.1 Protein Bound 3D Structures

- RCSB Protein Data Bank (RCSB PDB)

View 3 proteins in NCBI Structure

- PubChem

13.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code
VXX

PDBe Structure Code
1WB6

PDBe Conformer

- Protein Data Bank in Europe (PDBe)

13.2 Chemical-Target Interactions

- Comparative Toxicogenomics Database (CTD)

- DrugBank

14 Biological Test Results

14.1 BioAssay Results

- PubChem

15 Taxonomy

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

- KNApSAcK Species-Metabolite Database; LOTUS - the natural products occurrence database; N...

16 Classification

16.1 MeSH Tree

- Medical Subject Headings (MeSH)

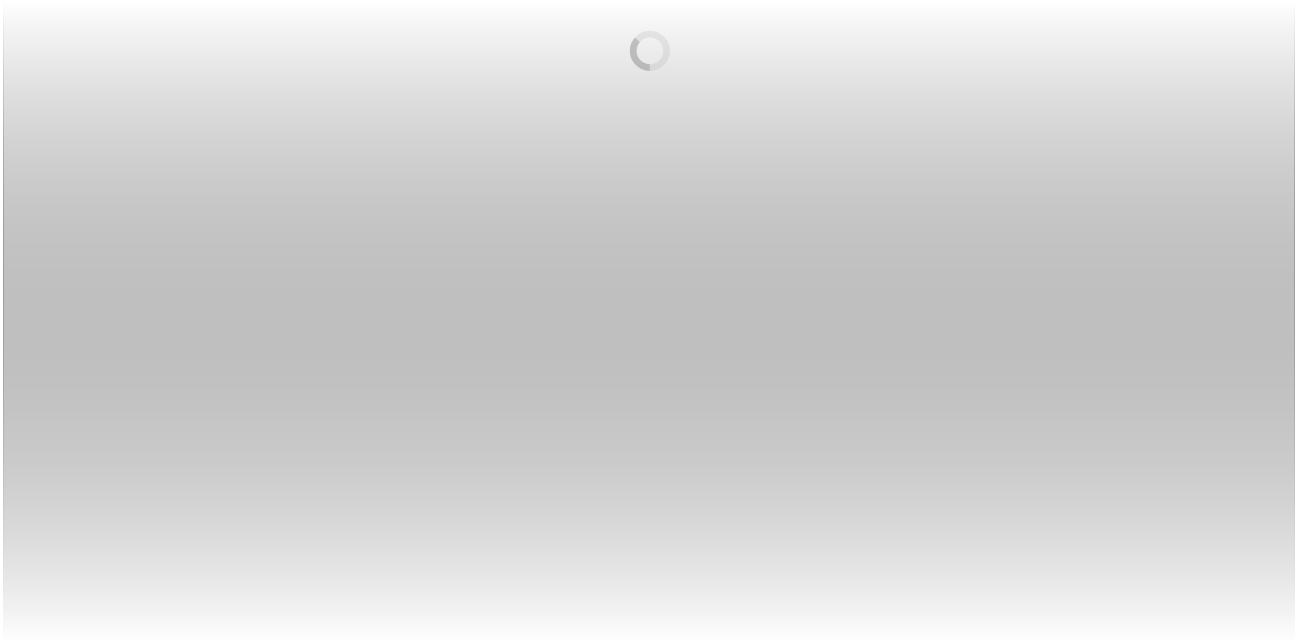
16.2 ChEBI Ontology

- ChEBI

16.3 ChemIDplus

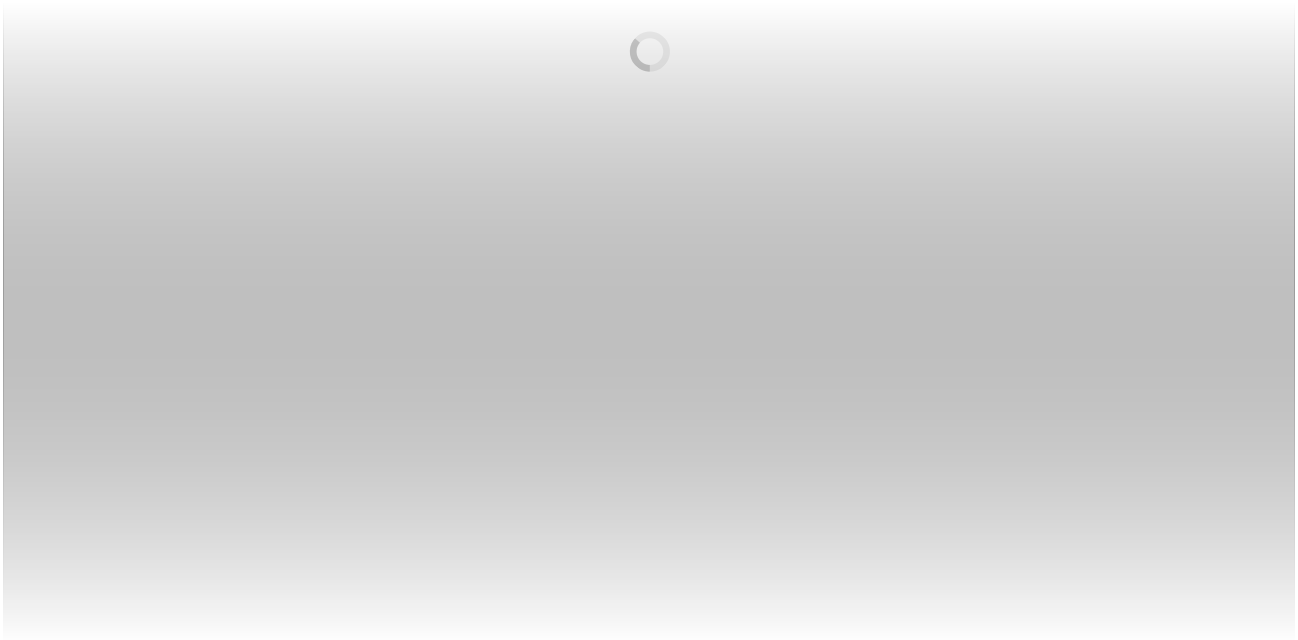
ChemIDplus

16.4 ChEMBL Target Tree



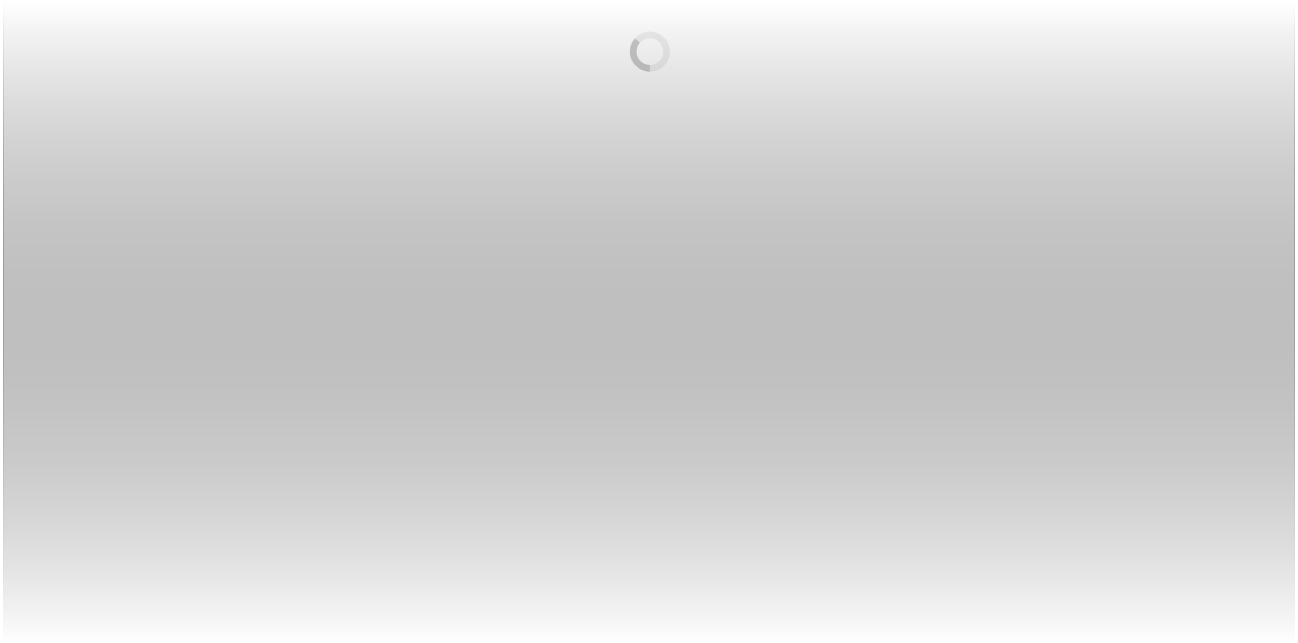
ChEMBL

16.5 UN GHS Classification



- GHS Classification (UNECE)

16.6 EPA CPDat Classification



- EPA Chemical and Products Database (CPDat)

16.7 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

16.8 EPA DSSTox Classification

- EPA DSSTox

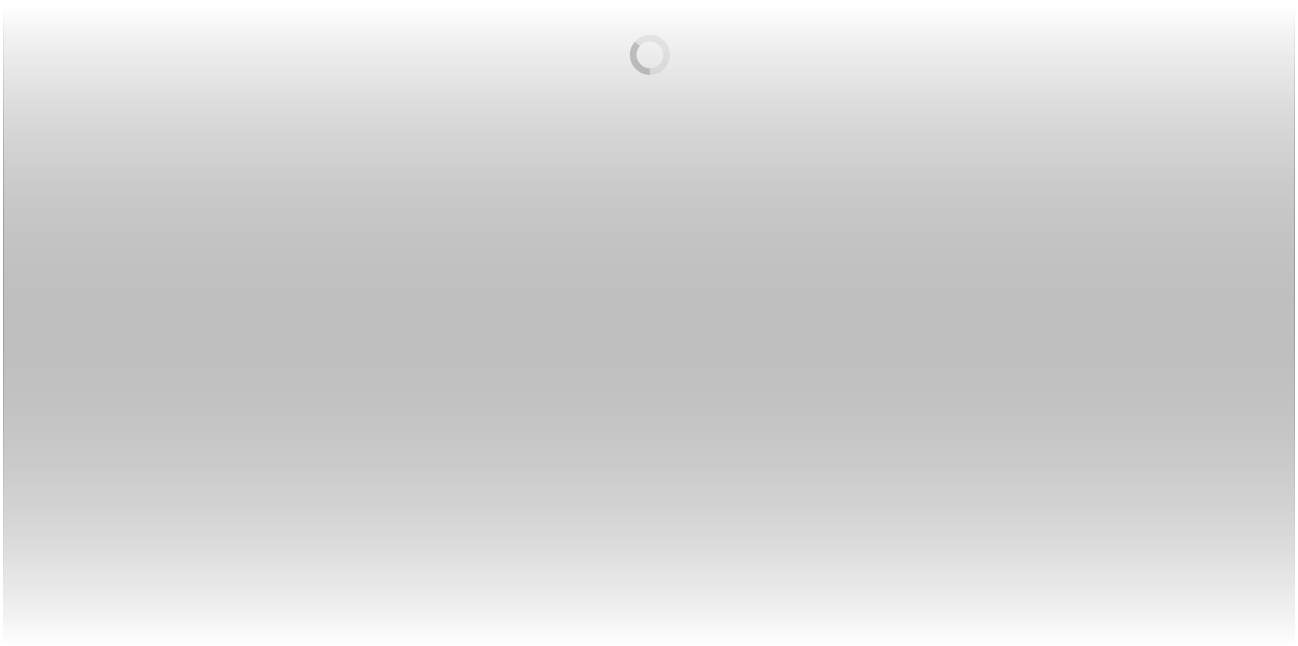
16.9 EPA TSCA and CDR Classification

- EPA Chemicals under the TSCA

16.10 LOTUS Tree

LOTUS - the natural products occurrence database

16.11 EPA Substance Registry Services Tree



EPA Substance Registry Services

17 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. Australian Industrial Chemicals Introduction Scheme (AICIS)

LICENSE
https://www.industrialchemicals.gov.au/copyright

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester
https://services.industrialchemicals.gov.au/search-assessments/

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester
https://services.industrialchemicals.gov.au/search-inventory/

2. CAS Common Chemistry

LICENSE
The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.

Methyl vanillate

https://commonchemistry.cas.org/detail?cas_rn=3943-74-6

3. ChemIDplus

Methyl vanillate

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0003943746

ChemIDplus Chemical Information Classification

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

4. DrugBank

Methyl vanillate

https://www.drugbank.ca/drugs/DB08711

5. DTP/NCI

Methyl vanillate

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=74385

6. EPA Chemicals under the TSCA

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

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

EPA TSCA Classification

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

7. EPA DSSTox

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

https://comptox.epa.gov/dashboard/DTXSID5074345

CompTox Chemicals Dashboard Chemical Lists

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

8. European Chemicals Agency (ECHA)

Methyl vanillate

https://echa.europa.eu/substance-information/-/substanceinfo/100.021.388

Methyl vanillate (EC: 223-525-9)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/35174

9. FDA Global Substance Registration System (GSRS)

METHYL VANILLATE

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/2HXG8QSO3D

10. Human Metabolome Database (HMDB)

Methyl vanillate

http://www.hmdb.ca/metabolites/HMDB0240266

HMDB0240266_cms_27760

https://hmdb.ca/metabolites/HMDB0240266#spectra

11. International Fragrance Association (IFRA)

Methyl vanillate

https://ifrafragrance.org/priorities/ingredients/ifra-transparency-list

12. New Zealand Environmental Protection Authority (EPA)

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

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

13. ChEBI

Methyl vanillate

https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:46477

ChEBI Ontology

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

14. 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/

Methyl vanillate

https://www.wikidata.org/wiki/Q27097897

LOTUS Tree

https://lotus.naturalproducts.net/

15. Yeast Metabolome Database (YMDB)

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

Methyl vanillate

https://www.ymdb.ca/compounds/YMDB01747

16. 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/CHEMBL486214/

ChEMBL Protein Target Tree

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

17. Comparative Toxicogenomics Database (CTD)

LICENSE
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http://ctdbase.org/about/legal.jsp

methyl vanillate

https://ctdbase.org/detail.go?type=chem&acc=C000618837

18. EPA Chemical and Products Database (CPDat)

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

https://comptox.epa.gov/dashboard/DTXSID5074345#exposure

EPA CPDat Classification

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

19. EU Food Improvement Agents

Methyl vanillate

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

20. MassBank of North America (MoNA)

METHYL 4-HYDROXY-3-METHOXYBENZOATE

https://mona.fiehnlab.ucdavis.edu/spectra/browse?query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27BVWTXUYLKBHMOX-UHFFFAOYSA-N%27)

21. NIST Mass Spectrometry Data Center

Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

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

22. SpectraBase

Methylparaben-M (methoxy-)

https://spectrabase.com/spectrum/LrDRyBF0rvB

Vanillic acid ME @

https://spectrabase.com/spectrum/4rTFDdxrOa

vanillic acid, methyl ester

https://spectrabase.com/spectrum/BM8tsCi4z7F

Methyl vanillate

https://spectrabase.com/spectrum/GdMSw76dd3w

VANILLIC ACID, METHYL ESTER

https://spectrabase.com/spectrum/3HfllgaWKka

METHYL-4-HYDROXY-3-METHOXYBENZOATE

https://spectrabase.com/spectrum/xhZAwQ5Cx0

Ethyl vanillate

https://spectrabase.com/spectrum/IJF5SmXLUGa

Methyl vanillate

https://spectrabase.com/spectrum/45IOh9l28X7

VANILLIC ACID, METHYL ESTER

https://spectrabase.com/spectrum/ICu0GkE8f80

Methyl vanillate

https://spectrabase.com/spectrum/CHuJ7W6J3mx

methyl vanillate

https://spectrabase.com/spectrum/JJVP2ypOoZ0

methyl vanillate

https://spectrabase.com/spectrum/GjMFtIwHXn

VANILLIC ACID, METHYL ESTER

https://spectrabase.com/spectrum/H5orM2fCgbQ

Methyl vanillate

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

Methyl vanillate

https://spectrabase.com/spectrum/BWoDO9oIdLW

Ethyl vanillate

https://spectrabase.com/spectrum/BkXnfdYR2rX

23. IUPAC Digitized pKa Dataset

Methyl 4-hydroxy-3-methoxybenzoate

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

24. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J45.025A

25. KNApSAcK Species-Metabolite Database

Methyl vanillate

http://www.knapsackfamily.com/knapsack_core/info.php?sname=C_ID&word=C00030768

26. Natural Product Activity and Species Source (NPASS)

Methyl Vanillate

https://bidd.group/NPASS/compound.php?compoundID=NPC159418

27. MassBank Europe

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

METHYL 4-HYDROXY-3-METHOXYBENZOATE

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

28. Metabolomics Workbench

Methyl vanillate

https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=56659

29. Nature Chemical Biology

https://pubchem.ncbi.nlm.nih.gov/substance/123105094

30. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/8002099

31. NORMAN Suspect List Exchange

NORMAN Suspect List Exchange Classification

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

32. Protein Data Bank in Europe (PDBe)

http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/VXX

33. RCSB Protein Data Bank (RCSB PDB)

https://www.rcsb.org/

34. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=13051054-839486306

35. SpringerMaterials

methyl vanillate

https://materials.springer.com/substanceprofile/docs/smsid_szesakcijwboxagz

36. Thieme Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=13051054-839486306

37. Wikidata

methyl vanillate

https://www.wikidata.org/wiki/Q27097897

38. PubChem

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

39. Medical Subject Headings (MeSH)

methyl vanillate

https://www.ncbi.nlm.nih.gov/mesh/2019657

MeSH Tree

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

40. GHS Classification (UNECE)

GHS Classification Tree

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

41. EPA Substance Registry Services

EPA SRS List Classification

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

42. PATENTSCOPE (WIPO)

SID 403391679

https://pubchem.ncbi.nlm.nih.gov/substance/403391679

SID 427339181

https://pubchem.ncbi.nlm.nih.gov/substance/427339181