Metabolomics Workbench and the National Metabolomics Data Repository
University of California San Diego
and
San Diego Supercomputer Center

RefMet standardized metabolite nomenclature
And Metabolite Structure Database

NIH Common Fund's National Metabolomics Data Repository
(supported by NIH grant, U2C-DK119886)

Metabolomics Workbench: https://www.metabolomicsworkbench.org

Contains the National Metabolomics Data Repository (NMDR)

METABOLOMICS WORKBENCH

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Welcome to the UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health.

National Metabolomics Data Repository

Upload and Manage Studies | Browse and Search Studies | Analyze Studies

As of **02/14/22** a total of **2002 studies** have been processed by the National Metabolomics Data Repository (NMDR). There are **1727 publicly available studies** and the remainder (**275**) will be made available subject to their embargo dates.

Recently released studies on NMDR

ST002058 - **Muscle/Lung/Tumor metabolomics**; *Mus musculus*; University of Colorado Anschutz Medical Campus

ST002059 - **4T1 and SkM cells**; *Homo sapiens*; University of Colorado Anschutz Medical Campus

ST002067 - **Time-Resolved Metabolomics of a Mouse Model of Ovarian High-Grade Serous Carcinoma (LC-MS)**; *Mus musculus*; Georgia Institute of Technology

Metabolite Structure Database

Updates to the Metabolite Structure Database (February 2, 2022)

The updated Metabolite structure database of primary and secondary metabolites at the **Metabolomics Workbench** contains new substructure and text-based searches including by chemical class. Over 164,000 structures have been added including over 10,000 sterols.

Higlights/News archive

Quick Links - Key Resources

Follow @MetabolomicsWB

Tweets by @MetabolomicsWB

Metabolomics Workbench @MetabolomicsWB

The National Metabolomics Data Repository (NMDR) at @MetabolomicsWB has just processed its 2,000th study! MS/NMR data/metadata on studies covering over 130 species. Browse/search/download at

NIH Common Fund Stage 2 Metabolomics Consortium Centers

Metabolomics Consortium Coordinating Center (M3C)
Richard Yost, U. of Florida

Metabolomics Workbench/NMDR
Shankar Subramaniam, UC San Diego (this website)

Compound Identification Cores (CIDCs)
Arthur Edison, U. of Georgia
Alexey Nesvizhskii, U. of Michigan
Oliver Fiehn, UC Davis
Dean Paul Jones, Emory University
Thomas Metz, Pacific Northwest Nat. Lab.

Data and Tools Cores (DTCs)
John Weinstein, MD Anderson Cancer C.
Jamey Young, Vanderbilt University
Xiuxia Du, U. of North Carolina Charlotte
Shuzhao Li, Emory University
Alla Karnovsky, U. of Michigan
Katerina Kechris, U. of Colorado, Denver
Gary Patti, Washington U. at St. Louis

Please cite: **Metabolomics Workbench** You will get more info on how to cite **here**

RefMet standardized metabolite nomenclature

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Overview | Metabolite Database | ...ternal Metabolo...

- Overview
- Metabolite Database
- Human Metabolome Gene/Protein Database (MGP)
- RefMet: Reference List of Metabolite Names
- External Metabolomics Databases (Links)

RefMet: A Refere...

The main objective of RefMet ... h discrete meta... spectroscopic techniques in metabolomics experiments. **This is an essential prerequisite for the abilit... experiments and studies**. The use of identifiers such as PubChem compound id's and InChiKeys offers... depending on parameters such as the salt form and degree of stereochemical detail. In addition, many m... methods as discrete structures but rather as isobaric mixtures (such as PC 34:1 and TG 54:2). To this en... NMR studies on the Metabolomics Workbench has been used as a starting point to generate a highly cur... metabolite structures and isobaric species. Additionally, the vast majority of these names have been linke... of **LIPID MAPS** and **ClassyFire** classification methods. A name-conversion user interface is provi... map them to the corresponding Refmet names. This is a... currently map to RefMet identifiers. Nevertheless, RefMe... "meta-analysis" and systems biology objectives for the m...

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- **Convert(map) a list of metabolite names to Re...**
- **Help on RefMet**
- **Lipid Notation in RefMet and lipid m/z calculat...**
- **Mobile phone apps** (App. links are active on pho...
  - **NMDR metabolite summary app.** Search... summary table sorted by frequency of dete...
  - **RefMet search app.** Search RefMet by (p...
  - **RefMet name conversion app.** Convert a...
  - **RefMet MS search app.** Search RefMet w...
  - **Lipid mass/formula app.** Calculate lipid r...
  - View **Screenshot**
- **Run as Shiny app on local R installation**
  - **RefMet name search Shiny App**
  - **RefMet MS search Shiny App**
- **Reference: RefMet: a reference nomenclature...**

RefMet: A Reference set of Metabolite names

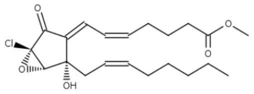
(A total of 154667 compounds or isobaric mixtures as of 04/23/21)

Show all | Structure search | Download RefMet | Convert metabolite names to RefMet | Help on RefMet

InChIKey: Mol. Formula: Exact mass: : 0.1 +/- Daltons Search

Name: Contains Super class(?): Main class(?): Sub class(?): Reset

Metabolite name | *MONA MS spectra*	PubChem CID	Super class	Main class	Sub class	Formula	Exact mass
10,11-DiHDPE	16061145	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{34}O_4$	362.2457
10,11-Dihydro-12-oxo-Resolvin E1	53477458	Fatty Acyls	Eicosanoids	HETE	$C_{20}H_{30}O_5$	350.2093
10,11-Dihydro-Re...			Eicosanoids	HETE	$C_{20}H_{32}O_5$	352.2250
10,11-Dimethoxyt...			Harmala alkaloids	Harmala alkaloids	$C_{29}H_{37}N_3O_2$	459.2886
10(11)-EpDPE			Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10,11-Epoxy-chlo...			Eicosanoids	Clavulones	$C_{21}H_{29}ClO_5$	396.1704
10,12,15-Octadec...			Fatty acids	Unsaturated FA	$C_{18}H_{30}O_2$	278.2246
10,22-Dimethyldo...			Hydrocarbons	Hydrocarbons	$C_{34}H_{70}$	478.5478
10-Deacetyl-2-debenzoylbaccatin III	443489	Prenol Lipids	Isoprenoids	Taxanes	$C_{22}H_{32}O_9$	440.2046
10-Deoxymethymycin	5282032	Polyketides	Macrolides and analogues	Macrolides	$C_{25}H_{43}NO_6$	453.3090
10-Deoxymethynolide	5282031	Polyketides	Macrolides and analogues	Macrolides	$C_{17}H_{28}O_4$	296.1988
10-HDoHE | *MS spectra*	11537494	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10-Hendecenoic acid	5634	Fatty Acyls	Fatty acids	Unsaturated FA	$C_{11}H_{20}O_2$	184.1463
10-HpODE	5282857	Fatty Acyls	Octadecanoids	HpODEs	$C_{18}H_{32}O_4$	312.2301
10-HpOME	13801082	Fatty Acyls	Octadecanoids	HpOMEs	$C_{18}H_{34}O_4$	314.2457



10,11-Epoxy-chlorovulone I

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Check for updates | **correspondence**

RefMet: a reference nomenclature for metabolomics

To the Editor — The past decade has seen an explosive growth in metabolomics, with advances in mass spectrometry (MS) and nuclear magnetic resonance (NMR) enabling the detection of hundreds or even thousands of metabolite species in a single experiment. The wide range of available analytical methods coupled with the even wider range of metabolite databases (vendor-supplied proprietary databases, public-domain databases and private in-house databases) has unfortunately led to a pervasive problem wherein the same metabolite species may be reported by many different names. This nomenclature issue represents a significant barrier for comparative analysis of metabolomics data across studies generated by different institutions and/or platforms[1]. To this end, a repository of over 280,000 named analytes from over 1,400 MS and NMR studies in the National Metabolomics Data Repository (NMDR) on the Metabolomics Workbench[2] has been leveraged to generate a highly curated analytical-chemistry-centric database of common names for metabolite structures and isobaric species. This Reference Set of Metabolite Names (RefMet) has been linked to a metabolite classification system, with numerous positive outcomes including data-sharing potential, facilitation of meta-analysis across studies, and integrated statistical analysis.

RefMet is composed of four groups of annotations (Supplementary Table 1):

1. Annotations with complete structural characterization of regiochemistry, stereochemistry and double bond

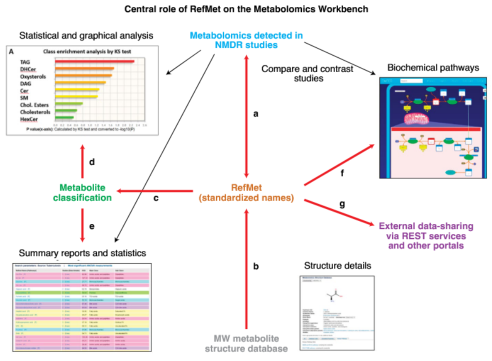


Fig. 1 | Overview of the central role of RefMet in the Metabolomics Workbench infrastructure. **a**, Metabolite annotations reported in studies submitted to the NMDR are used as a key data source for development of the RefMet database. Metabolite names in each study in turn are harmonized and converted to their RefMet equivalents. **b**,**c**, RefMet names are linked to a database (**b**) of molecular structures (in the case of entries with defined structures) and to a metabolite classification system (**c**). **d**,**e**, The set of classified RefMet annotations may be used for multiple modes of statistical analysis (**d**) and summary reports (**e**). **f**, Biochemical pathways from the Kyoto Encyclopedia of Genes and Genomes (KEGG) and Human Metabolome Database (HMDB) that have been supplemented with RefMet annotations are used on the Metabolomics Workbench (MW) to map NMDR study data using pathway enrichment tools. **g**, A REST service for RefMet enables data-sharing efforts with external metabolomics-related portals.

Fahy, E., Subramaniam, S. RefMet: a reference nomenclature for metabolomics. *Nature Methods* **17**, 1173–1174 (2020).

RefMet (A Reference list of Metabolite names): what is it?

A standardized reference nomenclature for metabolite species identified in metabolomics experiments.

Why do we need it?

There's a huge amount of diversity in reporting names of metabolite species detected by MS and NMR analyses. Having a standardized nomenclature is an essential prerequisite for the ability to compare and contrast metabolite data across different experiments and studies, and also to link to other key resources such as data integration, biochemical pathways, chemical classification and systems biology objectives.

How is it implemented?

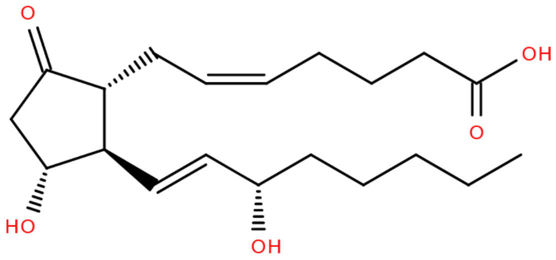
A set of over 2,000 studies with over 350,000 named metabolites deposited on the Metabolomics Workbench has been leveraged to generate a highly curated **analytical chemistry-centric database** of common names for metabolite structures and isobaric species. All entries are linked to a metabolite classification system. RefMet is searchable and may be freely downloaded. A name-conversion user interface is provided where users can submit a list of metabolite names and map them to the corresponding RefMet names.

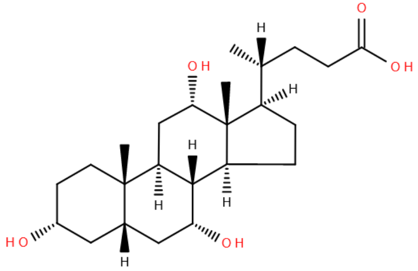
RefMet annotation levels

Level 1: Complete structure level

Comments Exact structure (including stereochemistry and bond geometry)

Examples: PGE2, 12S-HETE, Cholic acid

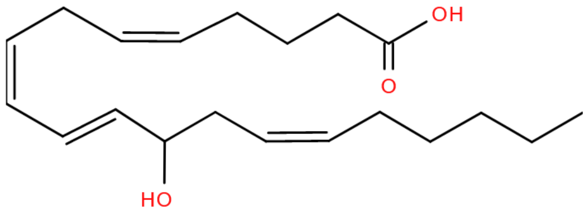


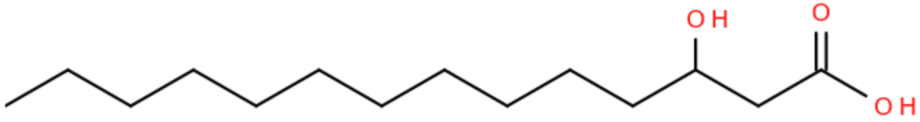


Level 2: Regiochemistry level

Comments Known regiochemistry (excluding stereochemistry and bond geometry)

Examples: 12-HETE, 3-Hydroxytetradecanoic acid, Hexose





Level 3: Molecular Species level

Comments Information on structural features, but complete regiochemistry unknown

Examples: PC 16:0_18:1 , Hydroxytetradecanoic acid, Citric acid/Isocitric acid, Leucine/Isoleucine

Level 4: Species level

Comments Metabolite class, number of chain carbons and unsaturations known

Examples: PC 34:1 , TG 54:3 , Cer d42:2 or Cer 42;2;O2

Metabolite identifications From NMDR

Harmonization,
Annotation,
Classification

Standardized metabolite nomenclature

Grp 1: Exact structures (chirality, DB geometry)
e.g. Alanine, PGE2, 12S-HETE, Cholic acid
Grp 2: Known regiochemistry
e.g. 12-HETE, 3-Hydroxytetradecanoic acid
Grp 3: Partial structures
e.g. PC(16:0_18:1), Hydroxytetradecanoic acid
Grp 4: Sum-composition
e.g. Cer(d42:2), PC(34:1), TG(54:3)

RefMet DB

Metabolite structures from public sources

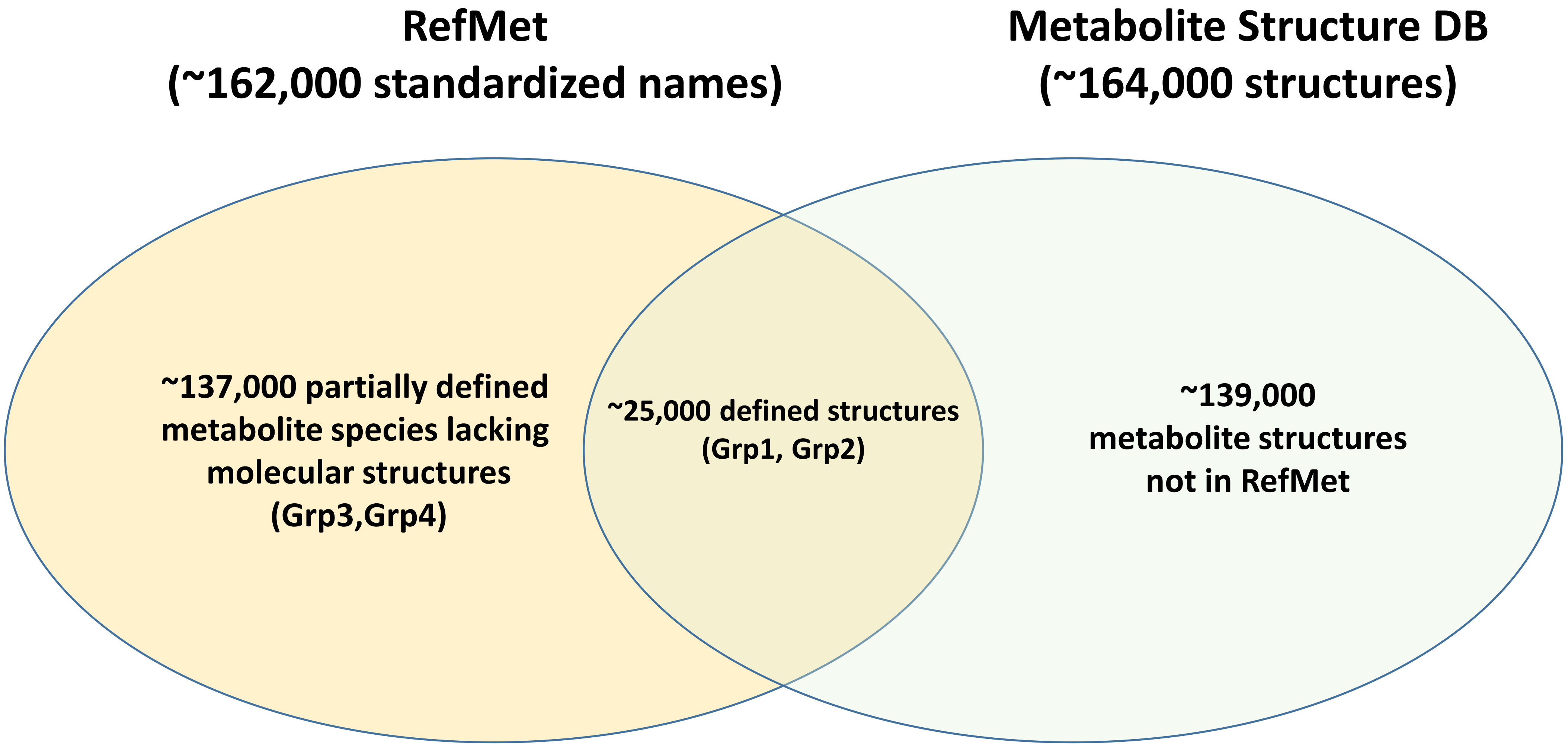
Database of molecular structures

RefMet Structures
Group 1 and 2

Other metabolite structures

Metabolite structure DB

Relationship between RefMet and Metabolite Structure DB



Metabolite nomenclature harmonization is an important consideration

NMDR: DIFFERENT SUBMITTED NAMES for the same metabolite

lysoPhosphatidylcholine acyl C16:0
lysoPC 16:0; [M+H]+@1.47
LysoPC (16:0)_R1
lysoPC 16:0; [M+H]+@1.55
LPC 16:0
lysoPC 16:0; [M+H]+@1.80
lysoPC 16:0; [M+Na]+@1.95
Lyso-PC(16:0)
Hexadecanoyl-sn-glycero-3-phosphocholine-
palmitoylglycerophosphocholine
palmitoylglycerophosphocholine (16:0)
Palmitoyl-Gpc (16:0)
LPC C16:0
LPC(16:0)
LPC(16:0) [sn1]
LPC(a-16:0)
LPC(a-16:0)-1
LPC(a-16:0)-2
LysoPC (16:0)
LysoPC (16:0)_R2
LysoPC(16:0)
PALMITOYLGLYCEROPHOSPHOCHOLINE
PALMITOYLGLYCEROPHOSPHOCHOLINE (*)
PC(16:0_0:0)
… etc

LPC 16:0

(RefMet name)

Examples of metabolite names which were mapped to RefMet names in order to enable comparative analysis across studies

9Z-palmitoleic acid
Cis-9-palmitoleic acid
cis-9-Palmitoleic acid
cis-9-Palmitoleic acid TOTAL
FFA(16:1n-7)
palmitoleic acid
PALMITOLEIC ACID
palmitoleic acid

Palmitoleic acid

AC(8:0)
Acylcarnitine C8:0
Acylcarnitine(C8:0)
C8, Octanoylcarnitine
C8:0 acylcarnitine
Octanoylcarnitine
OCTANOYLCARNITINE
Octanoyl-L-carnitine

CAR 8:0

alpha-glucose
beta-glucose
D-Glucose
glucose

Glucose

PC(p-38:2) or PC(o-38:3)
PC(p-38:3) or PC(o-38:4) A
PC(p-38:3)/PC(o-38:4)

PC P-38:3 or PC O-38:4

C24 Ceramide
C24-Cer
Cer(d18:1/24:0)

Cer 18:1;O2/24:0

GPEtn 16:0_18:2
PE(16:0_18:2)

PE 16:0_18:2

https://www.metabolomicsworkbench.org/databases/refmet/

RefMet: A Reference list of Metabolite names

The main objective of RefMet is to provide a standardized reference nomenclature for both discrete metabolite structures and metabolite species identified by spectroscopic techniques in metabolomics experiments. **This is an essential prerequisite for the ability to compare and contrast metabolite data across different experiments and studies**. The use of identifiers such as PubChem compound id's and InChiKeys offers only a partial solution because these identifiers will vary depending on parameters such as the salt form and degree of stereochemical detail. In addition, many metabolite species, especially lipids, are not reported by MS methods as discrete structures but rather as isobaric mixtures (such as PC 34:1 and TG 54:2). To this end, a list of over 380,000 names from a set of over 2,000 MS and NMR studies on the Metabolomics Workbench has been used as a starting point to generate a highly curated **analytical chemistry-centric** list of common names for metabolite structures and isobaric species. Additionally, the vast majority of these names have been linked to a **metabolite classification system** using a combination of **LIPID MAPS** and **ClassyFire** classification methods. A name-conversion user interface is provided where users can submit a list of metabolite names and map them to the corresponding Refmet names. This is a work-in-progress with the caveat that many metabolite names generated by metabolomics experiments will not currently map to RefMet identifiers. Nevertheless, RefMet has the ability to greatly increase the **data-sharing potential of metabolomics experiments** and facilitate "meta-analysis" and systems biology objectives for the majority of commonly encountered metabolite species.

- **Browse/Search/Download Refmet**
- **Convert(map) a list of metabolite names to RefMet nomenclature**
- **Help on RefMet**
- **Lipid Notation in RefMet and lipid m/z calculation tools**
- **Mobile phone apps** (App. links are active on phones only. Save the URLs below as icons on your home screen):
  - **NMDR metabolite summary app.** Search over 1,500 studies in NMDR by anlytical technique, sample source, species and metabolite class. Retrieve a summary table sorted by frequency of detection of metabolite species, linked to structures and individual NMDR study information.
  - **RefMet search app.** Search RefMet by (partial) name and/or neutral mass.
  - **RefMet name conversion app.** Convert a metabolite name to RefMet nomenclature. Display structure. Calculate m/z.
  - **RefMet MS search app.** Search RefMet with m/z value.
  - **Lipid mass/formula app.** Calculate lipid neutral mass and m/z for over 160 lipid species.
  - View **Screenshot**
- **Run as Shiny app on local R installation**
  - **RefMet name search Shiny App**
  - **RefMet MS search Shiny App**
- **Reference: RefMet: a reference nomenclature for metabolomics (Nature Methods, 2020)**

Currently, there are over 160,000 metabolite species in RefMet

Convert a list of metabolite names to RefMet nomenclature

- Browse/Search/Download Refmet
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Enter a list of metabolite names (one per line) for conversion to RefMet nomenclature

```
PC 35:2; [M-Ac-H]-@6.77
Phosphatidylcholine acyl-alkyl C36:0
SM 34:2; [M]+@5.65
Ceramide d18:0/26:2
TAG(54:3)-13C4+15N0[M+Na]
Trilauroyl-glycerol
PE(aa-40:4)
C32:0 PC
Octenoyl-L-carnitine
TG(16:1_17:0_18:1)
lysoPC 16:0; [M+Na]+@0.49
TAG(50:8)-13C30[M+Na]
PE(39:4) [M-H]-_R2
PC(36:3)-13C3+15N0[M+Na]
PE-pmg(40:6)-13C0[+NH4]+
PA(34:1)-13C0
SQDG 43:1
CE(23:0)-13C5[+K]+
DAG(44:7)-13C0[M+H]
FFA(C20:1;2)
PE 38:5 [M-H]-
```

Submit | Reset

Metabolite name-to-RefMet conversion results

Return to RefMet conversion form

Download standardized names and annotations as tab-delimited text (including classification)

Input name	Standardized name	Formula	Exact mass	Sub class
1-oleoyl-GPI (18:1)	LPI 18:1	C27H51O12P	598.3118	LPI
2'-Deoxyuridine	Deoxyuridine	C9H12N2O5	228.0746	Pyrimidine deoxyribonucleosides
2-eicosapentaenoylglycerophosphoethanolamine*	LPE 20:5	C25H42NO7P	499.2699	LPE
4-hydroxyphenylpyruvate	4-Hydroxyphenylpyruvic acid	C9H8O4	180.0423	Phenylpyruvic acid derivatives
acetylcarnitine	CAR 2:0	C9H17NO4	203.1158	Acyl carnitines
Acylcarnitine (C10:0) [M+H]+	CAR 10:0	C17H33NO4	315.2410	Acyl carnitines
Adenosine triphosphate	ATP	C10H16N5O13P3	506.9958	Purine rNTP
Asn	Asparagine	C4H8N2O3	132.0535	Amino acids
Butyrylcarnitine	CAR 4:0	C11H21NO4	231.1471	Acyl carnitines
C16:1 SM	SM 18:1;O2/16:1	C39H77N2O6P	700.5519	SM
C32:0 PC	PC 32:0	C40H80NO8P	733.5622	PC
PC(56:8)	PC 56:8*	C64H112NO8P	1053.8126	PC
PC C36:4	PC 36:4	C44H80NO8P	781.5622	PC
CE(18:2); [M+NH4]+	CE 18:2	C45H76O2	648.5845	Chol. esters
CE(23:0) [M+NH4]+	CE 23:0	C50H90O2	722.6941	Chol. esters
Cer(15:0)	-			
Ceramide d18:0/26:2	Cer 18:0;O2/26:2	C44H85NO3	675.6529	DHCer
DAG C36:3	DG 36:3	C39H70O5	618.5223	DAG
DAG(44:7) [M+H]	DG 44:7	C47H78O5	722.5849	DAG
Decanoic acid	Capric acid	C10H20O2	172.1463	Saturated FA
D-Mannonate	Mannonic acid	C6H12O7	196.0583	Medium-chain hydroxy acids
Eicosanoic acid	Arachidic acid	C20H40O2	312.3028	Saturated FA
Erucamide	13-Docosenamide	C22H43NO	337.3345	Fatty amides
FA(16:0)	Palmitic acid	C16H32O2	256.2402	Saturated FA
FFA(C20:1;2)	-			
indolepropionate	3-Indolepropionic acid	C11H11NO2	189.0790	Indolyl carboxylic acids
Isovalerylcarnitine	CAR 4:0;3Me	C12H23NO4	245.1627	Acyl carnitines
Leucyl-Glycine	Leu-Gly	C8H16N2O3	188.1161	Dipeptides
L-Histidine	Histidine	C6H9N3O2	155.0695	Amino acids
lysoPC 16:0; [M+Na]+	LPC 16:0	C24H50NO7P	495.3325	LPC
malate	Malic acid	C4H6O5	134.0215	TCA acids
myristate (14:0)	Myristic acid	C14H28O2	228.2089	Saturated FA
N,N,N-Trimethyllysine_R2	N-6-Trimethyllysine	C9H20N2O2	188.1525	Amino acids
Octenoyl-L-carnitine	CAR 8:1	C15H27NO4	285.1940	Acyl carnitines

RefMet Search Page

Search by: Exact mass, Formula, Name, chemical class, InChI Key, structure

- Browse/Search/Download Refmet
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RefMet: A Reference set of Metabolite names

(A total of 154667 compounds or isobaric mixtures as of 04/23/21)

Show all   Structure search   Download RefMet   Convert metabolite names to RefMet   Help on RefMet

InChIKey: ____ Mol. Formula: ____ Exact mass: ____ : 0.1 +/- Daltons [Search]

Name: Contains ____ Super class(?): ____ Main class(?): ____ Sub class(?): ____ [Reset]

Metabolite name | *MONA MS spectra*	PubChem CID	Super class	Main class	Sub class	Formula	Exact mass
10,11-DiHDPE	16061145	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{34}O_4$	362.2457
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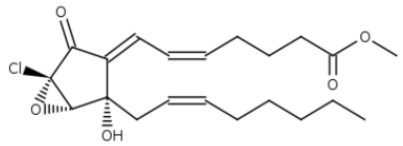
10,12,15-Octadec			Fatty acids	Unsaturated FA	$C_{18}H_{30}O_2$	278.2246
10,22-Dimethyldo			Hydrocarbons	Hydrocarbons	$C_{34}H_{70}$	478.5478
10-Deacetyl-2-debenzoylbaccatin III	[illegible]	Prenol Lipids	Isoprenoids	Taxanes	$C_{22}H_{32}O_9$	440.2046
10-Deoxymethymycin	5282032	Polyketides	Macrolides and analogues	Macrolides	$C_{25}H_{43}NO_6$	453.3090
10-Deoxymethynolide	5282031	Polyketides	Macrolides and analogues	Macrolides	$C_{17}H_{28}O_4$	296.1988
10-HDoHE | *MS spectra*	11537494	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10-Hendecenoic acid	5634	Fatty Acyls	Fatty acids	Unsaturated FA	$C_{11}H_{20}O_2$	184.1463
10-HpODE	5282857	Fatty Acyls	Octadecanoids	HpODEs	$C_{18}H_{32}O_4$	312.2301
10-HpOME	13801082	Fatty Acyls	Octadecanoids	HpOMEs	$C_{18}H_{34}O_4$	314.2457

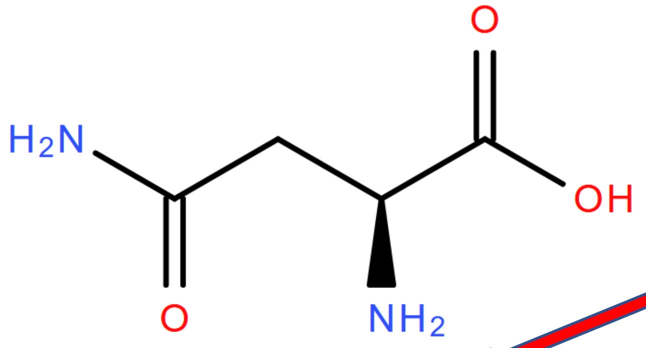


10,11-Epoxy-chlorovulone I

First   Previous   1   2   3   4   5   6   7   Next   Last   Go to page   Page 1 of 10312

RefMet detail page for Asparagine

RefMet Compound Details



MW structure	37114 (View MW Metabolite Database details)
RefMet name	Asparagine
Systematic name	(2S)-2-amino-3-carbamoylpropanoic acid
SMILES	NC(=O)C[C@@H](N)C(O)=O
Exact mass	132.053493 (neutral) Calculate m/z: (Choose adduct) View other RefMet entries with this exact (neutral) mass: +/- 0.05 amu +/- 0.1 amu +/- 0.2 amu +/- 0.5 amu
Formula	C4H8N2O3 View other entries in RefMet with this formula
InChI	InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
InChIKey	DCXYFEDJOCDNAF-REOHCLBHSA-N View other enantiomers/diastereomers of this metabolite in RefMet
Super Class	Organic acids
Main Class	Amino acids and peptides
Sub Class	Amino acids
Pubchem CID	6267
Annotation level	1 (1:Known structure; 2:Known regiochemistry; 3:Partial structure; 4:Sum-composition)
Human quantitation	View measurements in targeted assays on human samples

View entry in the Metabolite Structure database (more detailed structural information)

Calculate m/z for a MS adduct of asparagine

View other metabolites with this formula

View enantiomers/diastereomers (if any)

View biochemical reactions involving asparagine

Table of KEGG reactions in human pathways involving Asparagine

Rxn ID	KEGG Reaction	Enzyme
R00485	L-Asparagine + H2O <=> L-Aspartate + Ammonia	L-asparagine amidohydrolase
R00578	ATP + L-Aspartate + L-Glutamine + H2O <=> AMP + Diphosphate + L-Asparagine + L-Glutamate	L-aspartate:L-glutamine amido-ligase (AMP-forming)
R00483	ATP + L-Aspartate + Ammonia <=> AMP + Diphosphate + L-Asparagine	L-aspartate:ammonia ligase (AMP-forming)

Table of KEGG human pathways containing Asparagine

Pathway ID	Human Pathway	# of reactions
hsa00250	Alanine, aspartate and glutamate metabolism	2

RefMet/Metabolite databases have links to MONA MS spectra

Example: https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=37135

RefMet database

InChIKey:

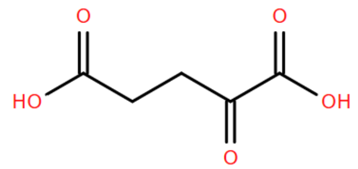
Mol. Formula

Name: Contains oxoglutaric acid

Super class(?)

Metabolite name | *MONA MS spectra*	PubChem CID
Oxoglutaric acid | *MS spectra*	51

Metabolite database



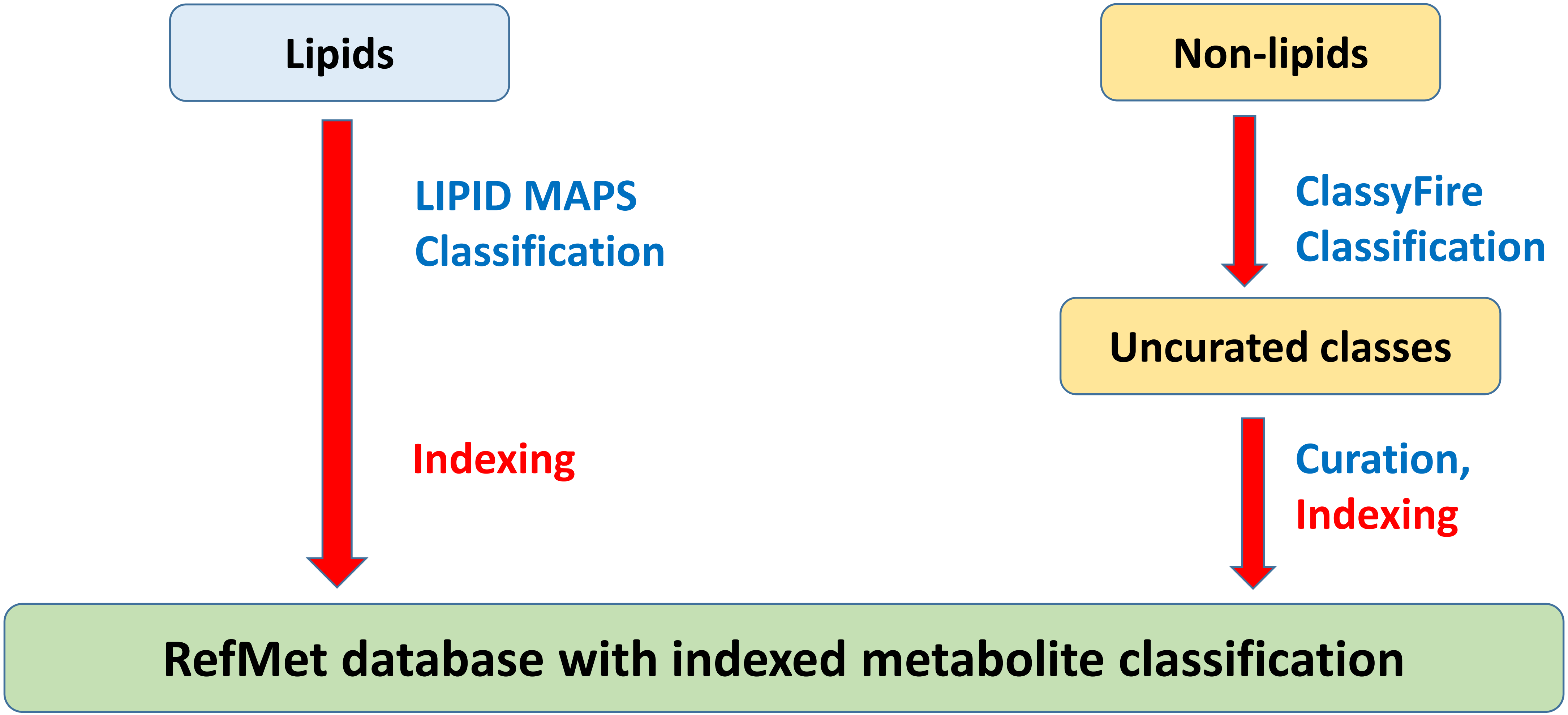
MW REGNO:	37135
PubChem CID:	51
Common Name:	Oxoglutaric acid
Systematic Name:	2-oxopentanedioic acid
Synonyms:	alpha-ketoglutaric acid; alpha-ketoglutarate; Oxoglutarate [PubChem Synonyms]
Exact Mass:	146.0215 (neutral) **Calculate m/z:** (Select m/z)
Formula:	$C_5H_6O_5$
InChIKey:	KPGXRSRHYNQIFN-UHFFFAOYSA-N
ClassyFire superclass:	Organic acids and derivatives
ClassyFire class:	Keto acids and derivatives
ClassyFire subclass:	Gamma-keto acids and [illegible]
ClassyFire direct parent:	Gamma-keto [illegible]es
ClassyFire alternative parents:	Short-c[illegible] and derivatives; Dicarboxylic acids and derivatives; Alpha-keto acids and derivatives; Alph Carboxy[illegible]; Organic oxides; Hydrocarbon derivatives;
MoNA MS spectra:	View spectra
Studies:	Available studies

MONA MS database records for REGNO 37135

Massbank ID	Metabolite	Instrument	Inst. type	MS type	Collision energy	Ion type	Ion mode	MS level
FiehnLib000378	Oxoglutaric acid	Leco Pegasus IV	-	EI	-	-	Positive	MS1
KZ000080	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	MS1
OUF00113	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	MS1
PR010210	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	MS1
HMDB00208_1231	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	-
HMDB00208_1263	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	-
KO001528	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	10 V	[M-H]-	Negative	MS2
KO001529	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	20 V	[M-H]-	Negative	MS2
KO001530	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	30 V	[M-H]-	Negative	MS2
KO001531	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	40 V	[M-H]-	Negative	MS2
KNA00530	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS1
KNA00700	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS1
KNA00531	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
KNA00533	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
KNA00701	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
KNA00702	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
PS037807	Oxoglutaric acid	TQD, Waters	-	ESI	10	-	-	-
HMDB00208_337	Oxoglutaric acid	TQD, Waters	Quattro_QQQ	ESI	10eV	-	Negative	-
HMD[illegible]38	Oxoglutaric acid	TQD, Waters	Quattro_QQQ	ESI	25eV	-	Negative	-
[illegible]339	Oxoglutaric acid	TQD, Waters	Quattro_QQQ	ESI	40eV	-	Negative	-
[illegible]B002[illegible]_998	Oxoglutaric acid	TQD, Waters	-	-	-	-	-	-

Listing of MONA spectra for metabolite

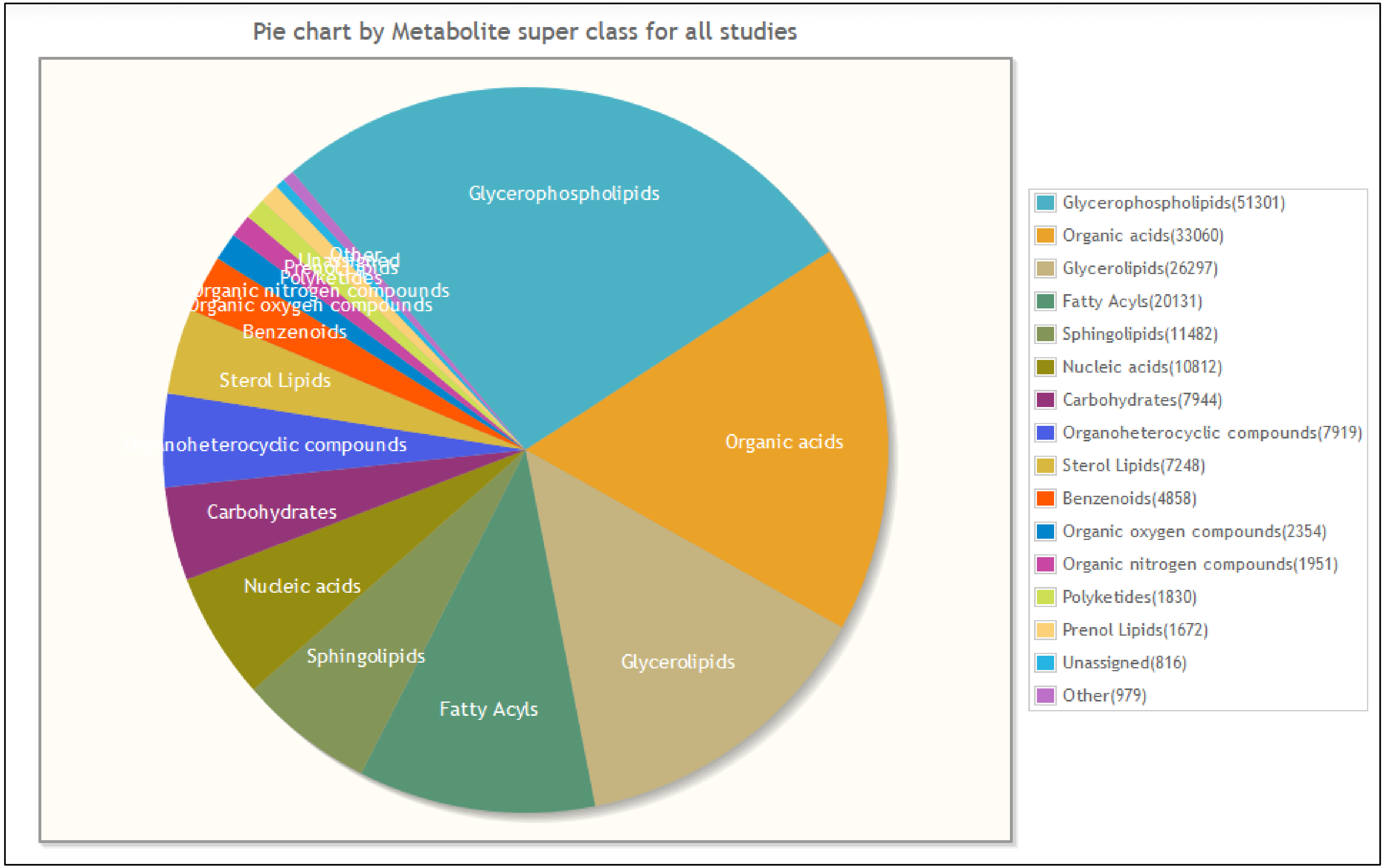
RefMet Metabolite Classification and indexing



Indexing of metabolite classes/subclasses facilitates logical ordering of data

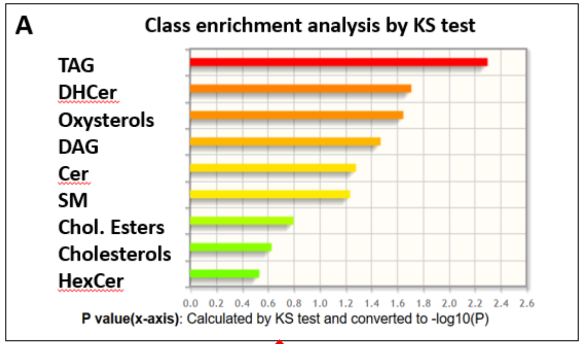
RefMet classification at superclass, main class and sub class levels available for each study in Analysis Toolbox

Example: see pie-charts at https://www.metabolomicsworkbench.org/data/stats_toolbox.php?STUDY_ID=ST001140



Central role of RefMet on the Metabolomics Workbench

Statistical/graphical analysis



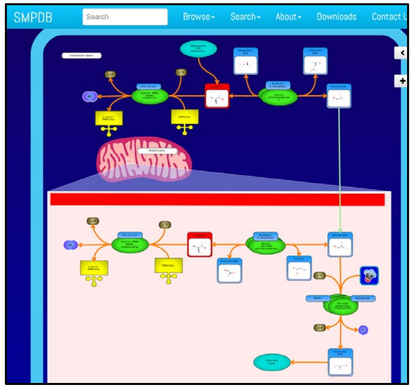
Metabolites detected in NMDR studies

Compare/contrast studies

Metabolite classification

RefMet (standardized names)

Biochemical pathways



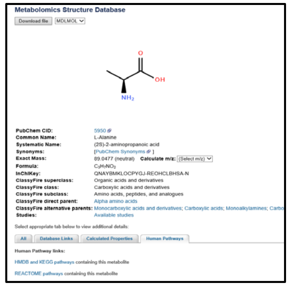
Summary reports/statistics

Search parameters: Source:Tuberculosis | Most significant ANOVA measurements

Refmet Name [Pathways]	Studies [Data Details]	RSD	Main Class	Sub Class
Gly-Phe [P]	3 [Data]	82.98	Amino acids and peptides	Dipeptides
Ile-Val [P]	3 [Data]	127.33	Amino acids and peptides	Dipeptides
Glucose [P]	3 [Data]	21.71	Monosaccharides	Monosaccharides
Gly-Leu [P]	3 [Data]	68.70	Amino acids and peptides	Dipeptides
Hippuric acid [P]	3 [Data]	62.78	Benzamides	Hippuric acids
Hypoxanthine [P]	3 [Data]	54.54	Purines	Hypoxanthines
Fumaric acid [P]	3 [Data]	35.16	TCA acids	TCA acids
Gluconic acid [P]	3 [Data]	55.19	Monosaccharides	Sugar acids
Glycochenodeoxycholic acid [P]	3 [Data]	87.48	Bile acids	C24 bile acids
Glycoursodeoxycholic acid [P]	3 [Data]	83.54	Bile acids	C24 bile acids
Heptylic acid [P]	3 [Data]	36.96	Fatty acids	Saturated FA
Hexadecanedioic acid [P]	3 [Data]	45.27	Fatty acids	Dicarboxylic acids
Histidine [P]	3 [Data]	20.54	Amino acids and peptides	Amino acids
Hydroxypropionic acid [P]	3 [Data]	37.18	Fatty acids	Hydroxy FA
DPA [P]	3 [Data]	69.31	Fatty acids	Unsaturated FA
Fructose [P]	3 [Data]	61.96	Monosaccharides	Monosaccharides
DHA [P]	3 [Data]	54.71	Fatty acids	Unsaturated FA
Gln-Leu [P]	3 [Data]	103.36	Amino acids and peptides	Dipeptides
Glutamic acid [P]	3 [Data]	43.21	Amino acids and peptides	Amino acids
Glycine [P]	3 [Data]	28.48	Amino acids and peptides	Amino acids
Glycodeoxycholate sulfate [P]	3 [Data]	94.56	Bile acids	C24 bile acids

MW metabolite structure database

Structure details



External datasharing via REST services and other portals

RefMet: What are the positive outcomes?

A unifying nomenclature and data integration tool for reporting metabolites detected by analytical methods.

Ability to perform comparative analysis across metabolomics studies.

Exact structures are linked to metabolite structure database.

Comprehensive chemical classification provides numerous advantages for data visualization/statistical analysis.

Integration with biochemical pathway tools enables mapping of RefMet names via systems biology approaches.

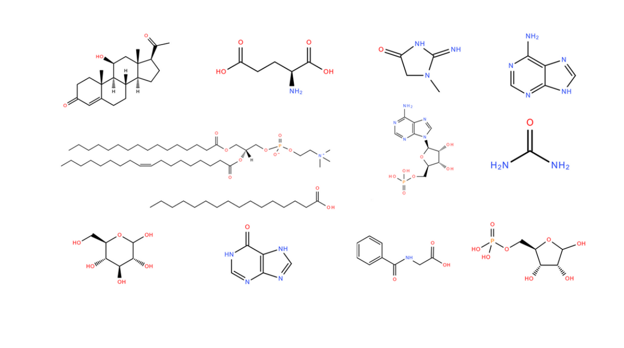
Metabolomics Workbench Metabolite structure database

~164,000 metabolite structures and annotations Linked to NMDR studies via RefMet

Metabolite Database

The **Metabolomics Workbench Metabolite Database** contains structures and annotations of biologically relevant metabolites. As of January, 2022, the database contains over 164,000 entries, collected from various public sources.

- **Browse the metabolite database**
- **Substructure search on metabolite database**
- **Text search on metabolite database**
- **Mass (m/z) search on metabolite database**

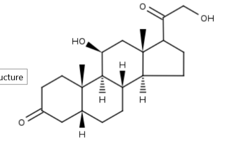


Browse the Metabolomics Workbench Metabolite Database

('Studies' link shows number of NMDR studies containing that metabolite)

Structure	Studies	Common Name	Systematic Name	PubChem CID	Formula	Exact mass
3055	2	10,11-DiHDPE	(+/-)-10,11-dihydroxy-4Z,7Z,13Z,16Z,19Z-docosapent...	16061145	$C_{22}H_{34}O_4$	362.2457
3050	2	10(11)-EpDPE	(+/-)-10(11)-epoxy-4Z,7Z,13Z,16Z,19Z-docosapentaen...	11638767	$C_{22}H_{32}O_3$	344.2351
2987	1	10,11-epoxy-chlorovulone I	methyl 9-oxo-10R-chloro-10,11S-epoxy-12S-hydroxy-5...	5283226	$C_{21}H_{29}ClO_5$	396.1704
586	2	10,12,15-octadecatrienoic acid	10,12,15-octadecatrienoic acid	5282824	$C_{18}H_{30}O_2$	278.2246
4884	1	10,22-Dimethyldotriacontane	10,22-Dimethyldotriacontane	6430363	$C_{34}H_{70}$	478.5478
52080	2	10-deacetyl-2-debenzoylbaccatin III	10-deacetyl-2-debenzoylbaccatin III	443489	$C_{22}H_{32}O_9$	440.2046
21306	3	10-Deoxymethynolide	(3R,4S,5S,7R,9E,11R,12R)-12-ethyl-4-hydroxy-3,5,7,...	5282031	$C_{17}H_{28}O_4$	296.1988
3042	8	(+/-)-10-HDoHE	(+/-)-10-hydroxy-4Z,7Z,11E,13Z,16Z,19Z-docosahexae...	11537494	$C_{22}H_{32}O_3$	344.2351
471	11	10-hendecenoic acid	10-undecenoic acid	5634	$C_{11}H_{20}O_2$	184.1463
1375	1	10-hydroxy-11-dodecenoic acid	10-hydroxy-11-dodecenoic acid	5312746	$C_{12}H_{22}O_3$	214.1569
1309	34	10-hydroxy capric acid	10-hydroxy-decanoic acid	74300	$C_{10}H_{20}O_3$	188.1412
84	1	10-methyl-heptadecanoic acid	10-methyl-heptadecanoic acid	5282600	$C_{18}H_{36}O_2$	284.2715
258	3	10-methyl-hexadecanoic acid	10-methyl-hexadecanoic acid	5312292	$C_{17}H_{34}O_2$	270.2559
1883	2	10-Nitrolinoleic acid	10-nitro,9Z,12Z-octadecadienoic acid	5282259	$C_{18}H_{31}NO_4$	325.2253
1885	9	10-nitrooleic acid	10-nitro-9E-octadecenoic acid	24836820	$C_{18}H_{33}NO_4$	327.2410
1585	6	10-oxo-decanoic acid	10-oxo-decanoic acid	79686	$C_{10}H_{18}O_3$	186.1256
3062	1	10S,17S-DiHDoHE	10S,17S-dihydroxy-4Z,7Z,11E,13Z,15E,19Z-docosahexa...	11667655	$C_{22}H_{32}O_4$	360.2301
701	27	10Z-heptadecenoic acid	10Z-heptadecenoic acid	5312435	$C_{17}H_{32}O_2$	268.2402
2687			+/-)-11,12-dihydroxy-5Z,8Z,14Z,17Z-eicosatetraeno...	16061121	$C_{20}H_{32}O_4$	336.2301
2616			1,12-dihydroxy-5Z,8Z,14Z-eicosatrienoic acid	5283146	$C_{20}H_{34}O_4$	338.2457
2358			+/-)-11(12)-epoxy-5Z,8Z,14Z,17Z-eicosatetraenoic ...	16061087	$C_{20}H_{30}O_3$	318.2195
2759			1,12-epoxy-5Z,8Z,14Z-eicosatrienoic acid	5283204	$C_{20}H_{32}O_3$	320.2351
1837			1-amino-undecanoic acid	17083	$C_{11}H_{23}NO_2$	201.1729
35467			1b,21-Dihydroxy-5b-pregnane-3,20-dione	44263339	$C_{21}H_{32}O_4$	348.2301
35347			1beta-hydroxyandrost-4-ene-3,17-dione	94141	$C_{19}H_{26}O_3$	302.1882
[illegible]			2S,3S,4S,5R,6R)-3,4,5-trihydroxy-6-{[(1S,2S,5R,7S...	53480452	$C_{25}H_{38}O_9$	482.2516
35447			1beta-hydroxypregn-4-ene-3,20-dione	101788	$C_{21}H_{30}O_3$	330.2195
2421			-oxo-11S,15S-dihydroxy-5Z,13E-prostadienoic acid	5283061	$C_{20}H_{32}O_5$	352.2250
2402			S,11S,15S-trihydroxy-5Z,13E-prostadienoic acid	5280886	$C_{20}H_{34}O_5$	354.2406
3233			1-Chloro-8E,10E-undecadien-1-ol	44256516	$C_{11}H_{19}ClO$	202.1124

11beta,21-Dihydroxy-5beta-pregnane-3,20-dione

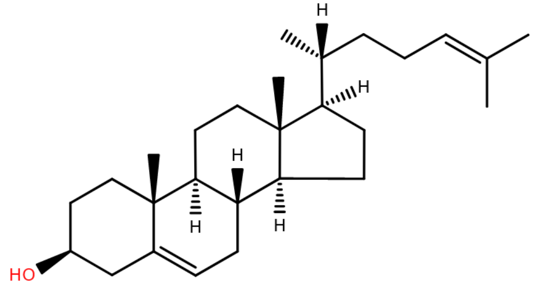


Show Structure

First | Previous | 1 | 2 | 3 | 4 | 5 | 6 | 7 | Next | Last   Go   Page 1 of 5528

Metabolomics Structure Database

Download file | MDLMOL



MW REGNO:	34376
Common Name:	Desmosterol
Systematic Name:	cholest-5,24-dien-3beta-ol
Synonyms:	[PubChem Synonyms]
Exact Mass:	384.3392 (neutral) **Calculate m/z:** (Choose adduct)
Formula:	$C_{27}H_{44}O$
InChIKey:	AVSXSVCZWQODGV-DPAQBDIFSA-N
LIPID MAPS Category:	Sterol Lipids [ST]
LIPID MAPS mainclass:	Sterols [ST01]
LIPID MAPS subclass:	Cholesterol and derivatives [ST0101]
MoNA MS spectra:	View MS spectra
SMILES:	CC(C)=CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C
Studies:	Available studies

Select appropriate tab below to view additional details:

All | Database Links | Calculated Properties | Human Pathways

External database links:

PubChem CID:	439577
LIPID MAPS ID:	LMST01010016
CHEBI ID:	17737
HMDB ID:	HMDB0002719
KEGG ID:	C01802
Chemspider ID:	388662
METLIN ID:	423
MetaCyc ID:	DESMOSTEROL-CPD
EPA CompTox DB:	DTXCID80810725

Text Search on Metabolomics Workbench Metabolite database

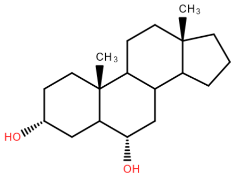
Metabolite name:	
Formula:	
Exact mass:	Tolerance (daltons): +/- 0.5
PUBCHEM_CID:	
LIPID MAPS ID:	
KEGG ID:	
ChEBI ID:	
HMDB ID:	
InChIKey:	Search with entire InChIKey to find exact match Search with 1st 14 characters of InChIKey to ignore stereochemistry and double-bond geometry
Lipid Category: ?	Sterol Lipids
Lipid Main class:	Sterols [ST01]
Lipid Sub class:	Furostanols and derivatives [ST0107]
Lipid level 4 class:	
Classyfire class:?	
Classyfire sub class:	
Sort by:	Common Name

Submit | Reset

Search Metabolomics Workbench Metabolite Database

100% | Clean | Arom | Arom

H C N O S P F Cl Br I Generic Groups



Name (Common, Systematic)		**Search type:**	Substructure
Sort by	Common Name	**Lower limit for Tanimoto:**	0.95
Records per page:	20	**Flags for Exact match:**	All(default)

Submit | Reset

Browse the Metabolomics Workbench Metabolite structure database

- **Browse the metabolite database**
- **Substructure search on metabolite database**
- **Text search on metabolite database**
- **Mass (m/z) search on metabolite database**

Click on "Studies" link to access studies reporting that metabolite

Compare metabolites in 2 of these studies:
Study A: ST000016 Study B: ST000017 Submit

List of Studies (Metabolite:10-Hydroxydecanoic acid)

Study_id	Study_title	Source	Species
ST000009	Mixed meal tolerance		Human
ST000010	Lung Cancer Cells 4	Lung	Human
ST000011	African Metabolomics		Human
ST000016	NPM-ALK metabolic regulation	Lymphoma cells	Human
ST000017	Rat HCR/LCR Stamina Study	Blood	Rat
ST000041	High PUFA diet in humans	Blood	Human
ST000042	BALF Control vs ALI by RPLC-MS	Lung	Human
ST000044	Pilot experiment looking for the existence of certain molecules in pancreatic cancer cells	Pancreas	Human
ST000046	Identification of altered metabolic pathways in Alzheimer's disease, mild cognitive impairment and cognitively normals using Metabolomics (plasma)	Blood	Human
ST000105	SCOR Metabolomics	Blood	Human
ST000106	IWMS Study 1:Weight comparison of obese and lean patients	Blood	Human
ST000286	Mouse skeletal myotube chronic low-frequency stimulation	Skeletal myotubes	Mouse
ST000291	LC-MS Based Approaches to Investigate Metabolomic Differences in the Urine of Young Women after Drinking Cranberry Juice or Apple Juice	Urine	Human
ST000403	Metabolomics-based elucidation of active metabolic pathways in erythrocytes and HSC-derived reticulocytes	Blood	[illegible]
ST000422	Type 1 Diabetes good glycemic control and controls samples	Blood	[illegible]

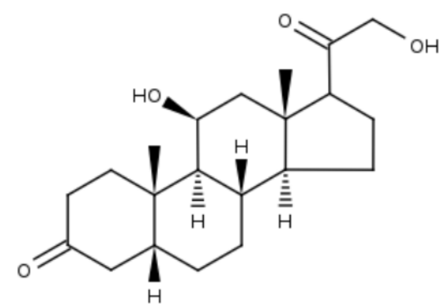
Click on "Structure" link to access metabolite detail page

Browse the Metabolomics Workbench Metabolite Database

('Studies' link shows number of NMDR studies containing that metabolite)

Structure	Studies	Common Name	Systematic Name	PubChem CID	Formula	Exact mass
3055	2	10,11-DiHDPE	(+/-)-10,11-dihydroxy-4Z,7Z,13Z,16Z,19Z-docosapent...	16061145	$C_{22}H_{34}O_4$	362.2457
3050	2	10(11)-EpDPE	(+/-)-10(11)-epoxy-4Z,7Z,13Z,16Z,19Z-docosapentaen...	11638767	$C_{22}H_{32}O_3$	344.2351
2987	1	10,11-epoxy-chlorovulone I	methyl 9-oxo-10R-chloro-10,11S-epoxy-12S-hydroxy-5...	5283226	$C_{21}H_{29}ClO_5$	396.1704
586	2	10,12,15-octadecatrienoic acid	10,12,15-octadecatrienoic acid	5282824	$C_{18}H_{30}O_2$	278.2246
4884	1	10,22-Dimethyldotriacontane	10,22-Dimethyldotriacontane	6430363	$C_{34}H_{70}$	478.5478
52080	2	10-deacetyl-2-debenzoylbaccatin III	10-deacetyl-2-debenzoylbaccatin III	443489	$C_{22}H_{32}O_9$	440.2046
21306	3	10-Deoxymethynolide	(3R,4S,5S,7R,9E,11R,12R)-12-ethyl-4-hydroxy-3,5,7,...	5282031	$C_{17}H_{28}O_4$	296.1988
3042	8	(+/-)-10-HDoHE	(+/-)-10-hydroxy-4Z,7Z,11E,13Z,16Z,19Z-docosahexae...	11537494	$C_{22}H_{32}O_3$	344.2351
471	11	10-hendecenoic acid	10-undecenoic acid	5634	$C_{11}H_{20}O_2$	184.1463
1375	1	10-hydroxy-11-dodecenoic acid	10-hydroxy-11-dodecenoic acid	5312746	$C_{12}H_{22}O_3$	214.1569
1309	34	10-Hydroxydecanoic acid	10-hydroxy-decanoic acid	74300	$C_{10}H_{20}O_3$	188.1412
[illegible]	1	10-methyl-heptadecanoic acid	10-methyl-heptadecanoic acid	5282600	$C_{18}H_{36}O_2$	284.2715
258	3	10-methyl-hexadecanoic acid	10-methyl-hexadecanoic acid	5312292	$C_{17}H_{34}O_2$	270.2559
1883	2	10-Nitrolinoleic acid	10-nitro,9Z,12Z-octadecadienoic acid	5282259	$C_{18}H_{31}NO_4$	325.2253
1885	9	10-nitrooleic acid	10-nitro-9E-octadecenoic acid	24836820	$C_{18}H_{33}NO_4$	327.2410
1585	6	10-oxo-decanoic acid	10-oxo-decanoic acid	79686	$C_{10}H_{18}O_3$	186.1256
3062	1	10S,17S-DiHDoHE	10S,17S-dihydroxy-4Z,7Z,11E,13Z,15E,19Z-docosahexa...	11667655	$C_{22}H_{32}O_4$	360.2301
701	27	10Z-heptadecenoic acid	10Z-heptadecenoic acid	5312435	$C_{17}H_{32}O_2$	268.2402
2687			+/-)-11,12-dihydroxy-5Z,8Z,14Z,17Z-eicosatetraeno...	16061121	$C_{20}H_{32}O_4$	336.2301
2616			1,12-dihydroxy-5Z,8Z,14Z-eicosatrienoic acid	5283146	$C_{20}H_{34}O_4$	338.2457
2358			+/-)-11(12)-epoxy-5Z,8Z,14Z,17Z-eicosatetraenoic ...	16061087	$C_{20}H_{30}O_3$	318.2195
2759			1,12-epoxy-5Z,8Z,14Z-eicosatrienoic acid	5283204	$C_{20}H_{32}O_3$	320.2351
1837			1-amino-undecanoic acid	17083	$C_{11}H_{23}NO_2$	201.1729
35467			1b,21-Dihydroxy-5b-pregnane-3,20-dione	44263339	$C_{21}H_{32}O_4$	348.2301
35347			1beta-hydroxyandrost-4-ene-3,17-dione	94141	$C_{19}H_{26}O_3$	302.1882
40904			2S,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[[(1S,2S,5R,7S...	53480452	$C_{25}H_{38}O_9$	482.2516
35447			1beta-hydroxypregn-4-ene-3,20-dione	101788	$C_{21}H_{30}O_3$	330.2195
2421			-oxo-11S,15S-dihydroxy-5Z,13E-prostadienoic acid	5283061	$C_{20}H_{32}O_5$	352.2250
2402			S,11S,15S-trihydroxy-5Z,13E-prostadienoic acid	5280886	$C_{20}H_{34}O_5$	354.2406
3233			1-Chloro-8E,10E-undecadien-1-ol	44256516	$C_{11}H_{19}ClO$	202.1124

11beta,21-Dihydroxy-5beta-pregnane-3,20-dione



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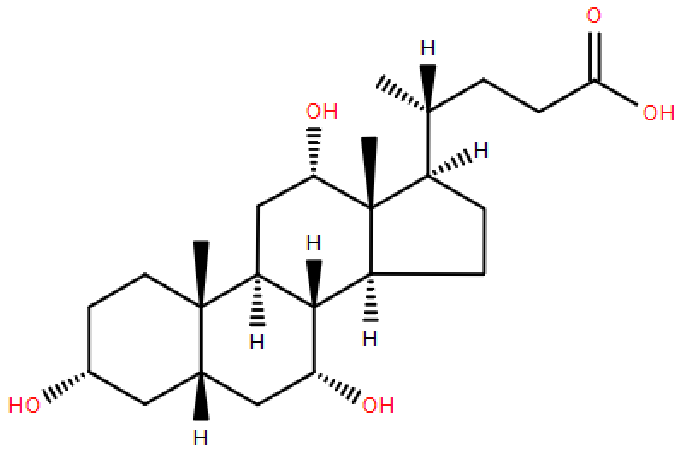
Metabolite Database : Molecule Detail View

Metabolomics Structure Database

Download file | MDLMOL



MW REGNO:	36243
PubChem CID:	221493
Common Name:	Cholic acid
Systematic Name:	3alpha,7alpha,12alpha-trihydroxy-5beta-cholan-24-oic acid
Synonyms:	Cholic Acid; CA [PubChem Synonyms]
Exact Mass:	408.2876 (neutral) **Calculate m/z:** (Select m/z)
Formula:	$C_{24}H_{40}O_5$
InChIKey:	BHQCQFFYRZLCQQ-OELDTZBJSA-N
LIPID MAPS Category:	Sterol Lipids
LIPID MAPS mainclass:	Bile acids and derivatives
LIPID MAPS subclass:	C24 bile acids, alcohols, and derivatives
MoNA MS spectra:	View spectra
Studies:	Available studies

All | Database Links | Calculated Properties | Human Pathways

External database links:

LIPID MAPS ID:	LMST04010001
CHEBI ID:	16359
HMDB ID:	HMDB0000619
KEGG ID:	C00695
Chemspider ID:	192176
METLIN ID:	206
BMRB ID:	bmse000650
MetaCyc ID:	CHOLATE

All | Database Links | Calculated Properties | Human Pathways

Human Pathway links:

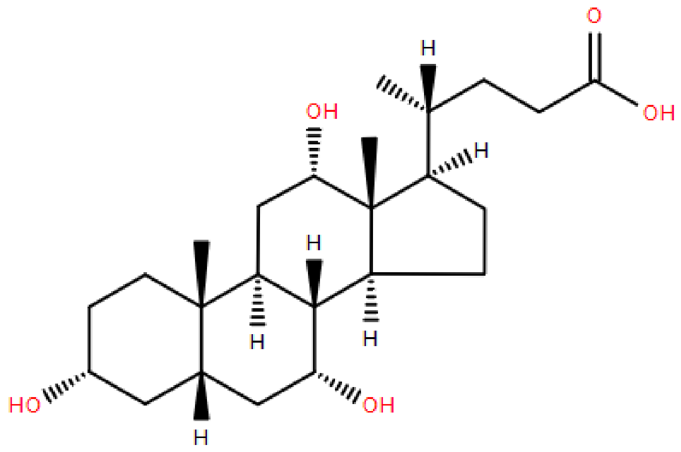
HMDB and KEGG pathways containing this metabolite

REACTOME pathways containing this metabolite

Metabolite Database : View MoNA MS spectra

Metabolomics Structure Database

Download file | MDLMOL



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LIPID MAPS mainclass:	Bile acids and derivatives
LIPID MAPS subclass:	C24 bile acids, alcohols, and derivatives
MoNA MS spectra:	View spectra
Studies:	Available studies

MoNA MS database records for Cholic acid

Massbank ID	Instrument	Inst. type	MS type	Collision energy	Ion type	Ion mode	MS level
NU000191	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000192	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000193	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000194	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000195	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
UF415353	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	35 (nominal)	[M-H]-	negative	MS2
UF422[illegible]3	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	35 (nominal)	[M-H]-	negative	MS2
UF4[illegible]	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF4153[illegible]	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF422951	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF422954	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF415352	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	80 (nominal)	[M-H]-	negative	MS2
UF422952	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	80 (nominal)	[M-H]-	negative	MS2
MT000010	LTQ XL, Thermo Finnigan	LC-ESI-IT	ESI	40	[M-H]-	negative	MS2
PT206683	[illegible]of Premier, Waters	LC-Q-TOF/MS	ESI	30 V	[M-H]-	negative	MS2
PT206680	[illegible]emier, Waters	LC-Q-TOF/MS	ESI	Ramp 5-45 V	[M-H]-	negative	MS2
PS066807	TQD[illegible]	Flow-injection QqQ/MS	ESI	10	[M-H]-	negative	MS2
PS066808	TQD, Wa[illegible]	Flow-injection QqQ/MS	ESI	20	[M-H]-	negative	MS2
PS066809	TQD, Waters	Flow-injection QqQ/MS	ESI	30	[M-H]-	negative	MS2
PS066810	TQD, Waters	Flow-injection QqQ/MS	ESI	40	[M-H]-	negative	MS2
PS066811	TQD, Waters	Flow-injection QqQ/MS	ESI	50	[M-H]-	negative	MS2
PS066801	TQD, Waters	Flow-injection QqQ/MS	ESI	10	[M+H]+	positive	MS2
PS066802	TQD, Waters	Flow-injection QqQ/MS	ESI	20	[M+H]+	positive	MS2
PS066803	TQD, Waters	[illegible]w-injection QqQ/MS	ESI	30	[M+H]+	positive	MS2
PS066804	TQD, Waters	[illegible]jection QqQ/MS	ESI	40	[M+H]+	positive	MS2
PR100738	UPLC Q-Tof Premier, Waters	LC[illegible]TOF	ESI	30 V	[M-H]-	negative	MS2
PR100737	UPLC Q-Tof Premier, Water						
BML00989	Agilent 1200 RRLC; Agilent						
BML00997	Agilent 1200 RRLC; Agilent						
BML01005	Agilent 1200 RRLC; Agilent						
BML80931	Agilent 1200 RRLC; Agilent						
BML80933	Agilent 1200 RRLC; Agilent						
BML00963	Agilent 1200 RRLC; Agilent						
BML00972	Agilent 1200 RRLC; Agilent						
BML80930	Agilent 1200 RRLC; Agilent						
VF-NPL-QTOF003408	Agilent 6530 Q-TOF						
VF-NPL-QTOF[illegible]409	Agilent 6530 Q-TOF						
VF-NPL-QTO[illegible]0	Agilent 6530 Q-TOF						
VF-NPL-[illegible]02099	Agilent 6530 Q-TOF						

Spectrum UF415353 for Cholic acid

CLEAN

Rating: ★★★★★

Originally submitted to the MassBank High Quality Mass Spectral Database

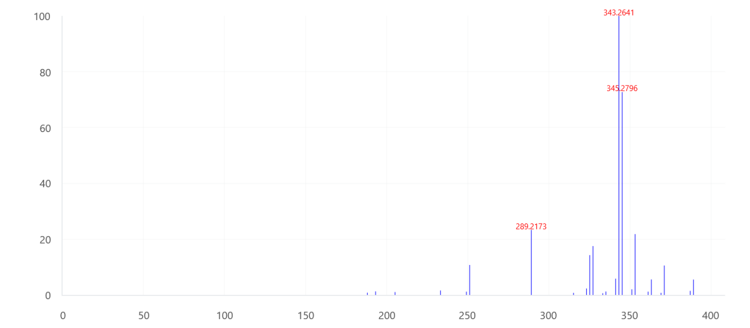
MassBank

LC-MS

SPLASH: splash10-0007-0019000000-285d3d0d87f5471b419a

Submitter: Tobias Schulze

Mass Spectrum



Ion Table / Peak Table

Text search on the Metabolomics Workbench Metabolite structure database

- Browse the metabolite database
- Substructure search on metabolite database
- Text search on metabolite database
- Mass (m/z) search on metabolite database

Text Search on Metabolomics Workbench Metabolite database

Metabolite name:

Formula:

Exact mass: Tolerance (daltons): +/- 0.5

PUBCHEM_CID:

LIPID MAPS ID:

KEGG ID:

ChEBI ID:

HMDB ID:

InChIKey:

Search with entire InChIKey to find exact match
Search with 1st 14 characters of InChIKey to ignore stereochemistry and double-bond geometry

Lipid Category: ? Sterol Lipids

Lipid Main class: Sterols [ST01]

Lipid Sub class: Furostanols and derivatives [ST0107]

Lipid level 4 class:

Classyfire class: ?

Classyfire sub class:

Sort by: Common Name

Submit Reset

Structure	Studies	Common Name	Systematic Name	PubChem	Formula	Exact mass
192367	-	16,22-epoxy-20beta,23S-dihydroxycholest-1-ene-3-on...		-	$C_{27}H_{42}O_4$	430.3083
127732	-	22-O-Methyl-Capsicoside D		76316014	$C_{63}H_{106}O_{33}$	1390.6616
127730	-	22-O-Methylcapsicoside G		76323354	$C_{64}H_{108}O_{34}$	1420.6722
140950	-	22-O-Methylparvispinoside A		11521008	$C_{57}H_{96}O_{29}$	1244.6037
135036	-	22-O-Methylparvispinoside B		11521005	$C_{57}H_{96}O_{28}$	1228.6088
127376	-	(22R,25R)-Spirosol-5-en-3beta-yl O-alpha-L-rhamnop...		76325952	$C_{47}H_{75}NO_{17}$	925.5035
188545	-	(22S)-24-Methyl-5alpha-furostane-3alpha,20beta,23,...	[(1R,2S,4S,6S,7R,8R,9S,12S,13S,16R,18S)-6-(1,3-dih...	-	$C_{30}H_{50}O_6$	506.3607
122452	-	2-({4,5-dihydroxy-6-[(4-hydroxy-6-{[6-hydroxy-7,9,...		46906324	$C_{57}H_{94}O_{26}$	1194.6033
122383	-	2-[(4-hydroxy-6-{[6-hydroxy-7,9,13-trimethyl-6-(3-...		441899	$C_{51}H_{84}O_{22}$	1048.5454
139501	-	(25R)-26-[(beta-D-glucopyranosyl)oxy]-2alpha-hydro...		10898575	$C_{63}H_{104}O_{34}$	1404.6409
139959	-	(25R)-26-[(beta-D-glucopyranosyl)oxy]-2alpha-hydro...		21603528	$C_{62}H_{100}O_{33}$	1372.6147
127378	-	(25R)-26-O-(beta-D-Glucopyranosyl)-furost-5-en-3be...		76307877	$C_{50}H_{82}O_{22}$	1034.5298
127377	-	(25R)-26-O-(beta-D-Glucopyranosyl)furost-5-en-3bet...		441885	$C_{51}H_{84}O_{23}$	1064.5403
140857	-	(25S)-3beta,5beta,22R-22-methoxy-urostan-3,26-diol...		44584284	$C_{58}H_{98}O_{29}$	1258.6194
66777	-	26-desglucoprotodioscin	(3beta,22R,25R)-22,26-dihydroxyfurost-5-en-3-yl al...	71581120	$C_{45}H_{74}O_{17}$	886.4926
139374	-	26-O-beta-D-glucopyranosyl-(25R)-5alpha-furost-3be...		44566638	$C_{56}H_{94}O_{28}$	1214.5932
35082	-	26-O-[beta-D-glucopyranosyl]-25R-furostan-3beta,22...	26-O-[beta-D-glucopyranosyl]-25R-furostan-3beta,22...	25041237	$C_{33}H_{56}O_9$	596.3924
140342	-	(2S,3R,4R,5R,6S)-2-{[(2R,3R,4S,5R,6R)-5-hydroxy-6-...		44566783	$C_{52}H_{86}O_{23}$	1078.5560
35088	-	3-O-(Rhaa1-2Glcb)-26-O-(Glcb)-(25R)-furosta-5,20(2...	3-O-(Rhaa1-2Glcb)-26-O-(Glcb)-(25R)-furosta-5,20(2...	52931425	$C_{45}H_{72}O_{17}$	884.4770
35092	-	3-O-(Rhaa1-4(Rhaa1-2)Glcb)-26-O-(Glcb)-(25R)-furos...	3-O-(Rhaa1-4(Rhaa1-2)Glcb)-26-O-(Glcb)-(25R)-furos...	52931429	$C_{51}H_{84}O_{22}$	1048.5454
35093	-	3-O-(Rhaa1-4Rhaa1-4(Rhaa1-2)Glcb)-26-O-(Glcb)-22R-...	3-O-(Rhaa1-4Rhaa1-4(Rhaa1-2)Glcb)-26-O-(Glcb)-22R-...	52931430	$C_{58}H_{96}O_{26}$	1208.6190
35084	-	3-O-(Rhaa1-4Rhaa1-4(Rhaa1-2)Glcb)-26-O-(Glcb)-3bet...	3-O-(Rhaa1-4Rhaa1-4(Rhaa1-2)Glcb)-26-O-(Glcb)-3bet...	52931420	$C_{57}H_{92}O_{27}$	1208.5826
35085	-	3-O-(Rhaa1-4Rhaa(Rhaa1-2)Glcb)-26-O-(Glcb)-22-meth...	3-O-(Rhaa1-4Rhaa(Rhaa1-2)Glcb)-26-O-(Glcb)-22-meth...	52931421	$C_{58}H_{96}O_{26}$	1208.6190
174627	-	(4S,8R,9S,13R)-6-hydroxy-7,9,13-trimethyl-6-(3-met...	(4S,8R,9S,13R)-6-hydroxy-7,9,13-trimethyl-6-(3-met...	-	$C_{27}H_{42}O_3$	414.3134
174628	-	(4S,8R,9S,13R)-6-hydroxy-7,9,13-trimethyl-6-(3-met...	(4S,8R,9S,13R)-6-hydroxy-7,9,13-trimethyl-6-(3-met...	-	$C_{27}H_{40}O_3$	412.2977
55128	-	5alpha-furostan	5alpha-furostan	6857522	$C_{27}H_{46}O$	386.3549
53792	-	5beta-furostan	5beta-furostan	6857456	$C_{27}H_{46}O$	386.3549
69001	-	Asparasaponin I	(3S,5S,8S,9S,10R,13S,14S)-3-[(2R,3R,4S,5S,6R)-4,5-...	118701252	$C_{51}H_{84}O_{22}$	1048.5454
158212	-	Asperfloroid		-	$C_{28}H_{40}O_7$	488.2774
163148	-	Asperflosterol		-	$C_{28}H_{42}O_7$	490.2931

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Lipid classification example

Text search on the Metabolomics Workbench Metabolite structure database

- Browse the metabolite database
- Substructure search on metabolite database
- Text search on metabolite database
- Mass (m/z) search on metabolite database

Text Search on Metabolomics Workbench Metabolite database

Metabolite name:

Formula:

Exact mass: Tolerance (daltons): +/- 0.5

PUBCHEM_CID:

LIPID MAPS ID:

KEGG ID:

ChEBI ID:

HMDB ID:

InChIKey: BHQCQFFYRZLCQQ

Search with entire InChIKey to find exact match

Search with 1st 14 characters of InChIKey to ignore stereochemistry and double-bond geometry

Lipid Category: ?

Lipid Main class:

Lipid Sub class:

Lipid level 4 class:

Classyfire class:?

Classyfire sub class:

Sort by: Common Name

Submit Reset

Database search results for " BHQCQFFYRZLCQQ "

Structure	Studies	Common Name	Systematic Name			
36334	-	3alpha,7alpha,12beta-Trihydroxy-5alpha-cholan-24-o...	3alpha,7alpha,12beta			
36326	-	3alpha,7alpha,12beta-Trihydroxy-5beta-cholanoic ac...	3alpha,7alpha,12beta			
36337	-	3alpha,7beta,12alpha-Trihydroxy-5alpha-Cholanoic a...	3alpha,7beta,12alpha			
36338	-	3alpha,7beta,12beta-Trihydroxy-5alpha-cholan-24-oi...	3alpha,7beta,12beta-			
36330	-	3alpha,7beta,12beta-Trihydroxy-5beta-cholanoic aci...	3alpha,7beta,12beta-			
36335	-	3beta,7alpha,12alpha-Trihydroxy-5alpha-Cholanoic a...	3beta,7alpha,12alpha			
36336	-	3beta,7alpha,12beta-Trihydroxy-5alpha-cholan-24-oi...	3beta,7alpha,12beta-Trihydroxy-5alpha-cholan-24-oi...	5283876	$C_{24}H_{40}O_5$	408.2876
36328	-	3beta,7alpha,12beta-Trihydroxy-5beta-cholan-24-oic...	3beta,7alpha,12beta-Trihydroxy-5beta-cholan-24-oic...	5283871	$C_{24}H_{40}O_5$	408.2876
36339	-	3beta,7beta,12alpha-Trihydroxy-5alpha-Cholanoic ac...	3beta,7beta,12alpha-Trihydroxy-5alpha-cholan-24-oi...	5283879	$C_{24}H_{40}O_5$	408.2876
36331	-	3beta,7beta,12alpha-Trihydroxy-5beta-cholanoic aci...	3beta,7beta,12alpha-Trihydroxy-5beta-cholan-24-oic...	5283873	$C_{24}H_{40}O_5$	408.2876
36340	-	3beta,7beta,12beta-Trihydroxy-5alpha-cholan-24-oic...	3beta,7beta,12beta-Trihydroxy-5alpha-cholan-24-oic...	5283880	$C_{24}H_{40}O_5$	408.2876
36332	-	3beta,7beta,12beta-Trihydroxy-5beta-cholan-24-oic ...	3beta,7beta,12beta-Trihydroxy-5beta-cholan-24-oic ...	1762378	$C_{24}H_{40}O_5$	408.2876
36333	2	Allocholic acid	3alpha,7alpha,12alpha-trihydroxy-5alpha-cholan-24-...	160636	$C_{24}H_{40}O_5$	408.2876
36243	156	Cholic acid	3alpha,7alpha,12alpha-trihydroxy-5beta-cholan-24-o...	221493	$C_{24}H_{40}O_5$	408.2876
36327	-	Isocholic acid	3beta,7alpha,12alpha-Trihydroxy-5beta-cholan-24-oi...	5283870	$C_{24}H_{40}O_5$	408.2876
36329	10	Ursocholic acid	3alpha,7beta,12alpha-trihydroxy-5beta-cholan-24-oi...	122340	$C_{24}H_{40}O_5$	408.2876

InChIKey example:Search on 1st 14 characters of InchIKey for cholic acid returns enantiomers, diastereomers

Text search on the Metabolomics Workbench Metabolite structure database

- Browse the metabolite database
- Substructure search on metabolite database
- Text search on metabolite database
- Mass (m/z) search on metabolite database

Text Search on Metabolomics Workbench Metabolite database

Metabolite name: cholic

Formula:

Exact mass: Tolerance (daltons): +/- 0.5

PUBCHEM_CID:

LIPID MAPS ID:

KEGG ID:

ChEBI ID:

HMDB ID:

InChIKey:

Search with entire InChIKey to find exact match

Search with 1st 14 characters of InChIKey to ignore stereochemistry and double-bond geometry

Lipid Category: ?

Lipid Main class:

Lipid Sub class:

Lipid level 4 class:

Classyfire class: ?

Classyfire sub class:

Sort by: Common Name

Submit Reset

Database search results for " CHOLIC "

Structure	Studies	Common Name	Systematic Name	PubChem		
36417	2	12-Ketochenodeoxycholic acid	3alpha,7alpha-dihydroxy-12-oxo-5beta-cholan-24-oic...	94235		
36396	3	12-Ketolithocholic acid	3alpha-hydroxy-12-oxo-5beta-cholan-24-oic acid	3080612		
36355	-	1beta-Hydroxycholic acid	1beta,3alpha,7alpha,12alpha-tetrahydroxy-5beta-cho...	5283893		
72130	-	(23S)-methylcholic acid	(23S)-methyl-3alpha,7alpha,12alpha-trihydroxy-5bet...	17756586		
36431	6	3-Dehydrocholic acid	7alpha,12alpha-Dihydroxy-3-oxo-5beta-cholan-24-oic...	5283956		
36674	-	3-Oxocholic acid	3-oxo-7alpha,12alpha-dihydroxy-5beta-cholan-24-oic...	44263354		
36677	-	3-Sulfodeoxycholic acid	3alpha-sulfooxy-12alpha-hydroxy-5beta-cholan-24-oi...	44263355		
87192	-	6,7-Diketolithocholic acid	3alpha-hydroxy-6,7-dioxo-5beta-cholan-24-oic acid	137333800		
36913	-	6alpha-Glucuronosylhyodeoxycholic acid	3alpha,6alpha-dihydroxy-5beta-cholan-24-oic acid 6...	443097		
36425	16	7-Ketodeoxycholic acid	3alpha,12alpha-dihydroxy-7-oxo-5beta-cholan-24-oic...	188292		
36391	5	7-ketolithocholic acid	3alpha-Hydroxy-7-oxo-5beta-cholan-24-oic acid	444262		
36675	-	7-Sulfocholic acid	7alpha-sulfooxy-3alpha,12alpha-dihydroxy-5beta-cho...	459070		
198434	-	Alanine conjugated chenodeoxycholic acid	2-[[(4R)-4-[(3R,5S,7R,8R,9S,10S,13R,14S,17R)-3,7-d...	145740400		
198435	-	Alanine conjugated cholic acid	2-[[(4R)-4-[(3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-3...	145740353		
36680	-	Alloavicholic acid	3alpha,7alpha,16alpha-trihydroxy-5alpha-cholan-24-...	12079222		
36278	1	Allochenodeoxycholic acid	3alpha,7alpha-dihydroxy-5alpha-cholan-24-oic acid	5283827		
36333	2	Allocholic acid	3alpha,7alpha,12alpha-trihydroxy-5alpha-cholan-24-...	160636		
36286	1	Allodeoxycholic acid	3alpha,12alpha-dihydroxy-5alpha-cholan-24-oic acid	5283833		
37229	2	Allolithocholic acid	3alpha-hydroxy-5alpha-cholan-24-oic acid	5283803		
198492	-	alpha-Hyocholic acid	(4R)-4-[(3R,5R,6R,7S,8S,9S,10R,13R,14S)-3,6,7-trih...	131750324		
36308	37	alpha-Muricholic acid	3alpha,6beta,7alpha-trihydroxy-5beta-cholan-24-oic...	5283852		
198493	-	alpha-Muricholic acid 7-sulfate	(4R)-4-[(3R,5R,6S,7S,8S,9S,10R,13R,14S,17R)-3,6-di...	155920197		
198602	-	Asparagine conjugated chenodeoxycholic acid	4-amino-2-[[(4R)-4-[(3R,5S,7R,8R,9S,10S,13R,14S,17...	145740366		
198603	-	Asparagine conjugated cholic acid	4-amino-4-oxo-2-[[(4R)-4-[(3R,5S,7R,8R,9S,10S,12S,...	145740402	$C_{28}H_{46}N_2O_7$	522.3305
198604	-	Aspartate conjugated chenodeoxycholic acid	2-[[(4R)-4-[(3R,5S,7R,8R,9S,10S,13R,14S,17R)-3,7-d...	145740501	$C_{28}H_{45}NO_7$	507.3196
36348	-	Avicholic acid	3alpha,7alpha,16alpha-trihydroxy-5beta-cholan-24-o...	5283886	$C_{24}H_{40}O_5$	408.2876
36678	-	Avideoxycholic acid	3alpha,16alpha-dihydroxy-5beta-cholan-24-oic acid	52931517	$C_{24}H_{40}O_4$	392.2927
36309	35	beta-Muricholic acid	3alpha,6beta,7beta-trihydroxy-5beta-cholan-24-oic ...	5283853	$C_{24}H_{40}O_5$	408.2876
36881	-	Bisnorcholic acid	24-dinor-3alpha,7alpha,12alpha-trihydroxy-5beta-ch...	9547705	$C_{22}H_{36}O_5$	380.2563
198645	-	Bisnorlithocholic acid	2-[(3R,5R,8R,9S,10S,13S,14S,17R)-3-hydroxy-10,13-d...	101012649	$C_{22}H_{36}O_3$	348.2664

First Previous 1 2 3 4 5 6 7 Next Last Go Page 1 of 7

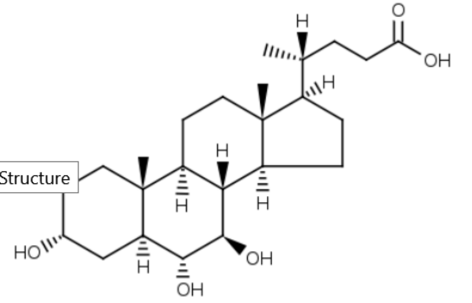
Metabolite name example

Structure search on Metabolomics Workbench Metabolite structure database

- Browse the metabolite database
- Substructure search on metabolite database
- Text search on metabolite database
- Mass (m/z) search on metabolite database

Structure	PubChem CID	Name	Systematic Name		
36894	5284308	24-Nor-5beta-chol-22-ene-3alpha,6alpha-diol	24-Nor-5beta-chol-22-ene-3alpha,6alpha-dic		
36888	5284303	24-Nor-5beta-cholane-3alpha,6alpha,23-triol	24-Nor-5beta-cholane-3alpha,6alpha,23-triol		
36492	5284006	2chi,3alpha,6alpha,7alpha-Tetrahydroxy-5beta-chola...	2chi,3alpha,6alpha,7alpha-Tetrahydroxy-5be		
36322	189059	3alpha,6alpha,12alpha-Trihydroxy-5beta-cholan-24-o...	3alpha,6alpha,12alpha-Trihydroxy-5beta-cho		
36514	5284027	3alpha,6alpha,12alpha-Trihydroxy-7-oxo-5beta-chola...	3alpha,6alpha,12alpha-Trihydroxy-7-oxo-5be		
36359	5283897	3alpha,6alpha,7alpha,12alpha-Tetrahydroxy-5beta-ch...	3alpha,6alpha,7alpha,12alpha-Tetrahydroxy		
36798		beta-ch...	3alpha,6alpha,7alpha,12alpha-Tetrahydroxy		
36750		beta-ch...	3alpha,6alpha,7alpha,12alpha-Tetrahydroxy		
36314		an-24-o...	3alpha,6alpha,7alpha-Trihydroxy-5alpha-cho		
36365		lpha-ch...	3alpha,6alpha,7beta,12alpha-Tetrahydroxy-5		
36360		eta-cho...	3alpha,6alpha,7beta,12alpha-Tetrahydroxy-5		
36315		n-24-oi...	3alpha,6alpha,7beta-Trihydroxy-5alpha-chol		
36655		n-24-oic...	3alpha,6alpha-Dihydroxy-12-oxo-5beta-cholan-24-oic...	$C_{24}H_{38}O_5$	406.2719
362		c Acid	3alpha,6alpha-Dihydroxy-5alpha-cholan-24-oic Acid	$C_{24}H_{40}O_4$	392.2927
176736		S)-3,6-d...	[(3R,6S,10R,13S,17R)-6-acetyloxy-17-[(2S,3S)-3,6-d...	$C_{31}H_{52}O_6$	520.3764
198057			-	$C_{29}H_{52}O_4$	464.3866
36547			5beta-Cholane-3alpha,6alpha,24-triol	$C_{24}H_{42}O_3$	378.3134
36414			3alpha,6alpha-Dihydroxy-7-oxo-5beta-cholan-24-oic ...	$C_{24}H_{38}O_5$	406.2719
36913	443097	6alpha-Glucuronosylhyodeoxycholic acid	3alpha,6alpha-dihydroxy-5beta-cholan-24-oic acid 6...	$C_{30}H_{48}O_{10}$	568.3247
34791	15542699	6alpha-Hydroxycastasterone	campestan-2alpha,3alpha,6alpha,22R,23R-pentol	$C_{28}H_{50}O_5$	466.3658

3alpha,6alpha,7beta-Trihydroxy-5alpha-cholan-24-oic Acid



Show Structure

First | Previous | 1 | 2 | 3 | 4 | 5 | 6 | Next | Last

Go

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Search Metabolomics Workbench Metabolite Database

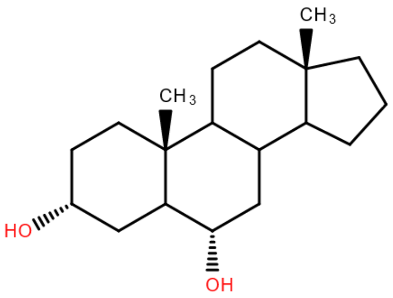
100%

Arom Arom

Clean

H C N O S P F Cl Br I

Generic Groups



Name (Common, Systematic)

Search type: Substructure

Sort by: Common Name

Lower limit for Tanimoto: 0.95

Records per page: 20

Flags for Exact match: All(default)

Submit | Reset

Mass (m/z) search on Metabolomics Workbench Metabolite structure database

- Browse the metabolite database
- Substructure search on metabolite database
- Text search on metabolite database
- **Mass (m/z) search on metabolite database**

Choose database to search, m/z tolerance, ion adducts. Enter list of ions or upload a peaklist

Input Mass	Matched Mass	Delta	Name	Formula	Ion	Examples
496.4773	496.4724	.0049	Cer(d14:1(4E)/17:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d15:1(4E)/16:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d16:1(4E)/15:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d17:1(4E)/14:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d18:1(4E)/13:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d19:1(4E)/12:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d20:1(4E)/11:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(d21:1(4E)/10:0)	C31H62NO3	[M+H]+	Structure
496.4773	496.4090	.0683	CMNPD22584	C26H52N6O3	[M+H]+	Structure
496.4773	496.4090	.0683	CMNPD22586	C26H52N6O3	[M+H]+	Structure
496.4773	496.3996	.0777	Orlistat	C29H54NO5	[M+H]+	Structure
496.4773	496.3897	.0876	Lycoperine A	C31H50N3O2	[M+H]+	Structure
496.4773	496.3857	.0916	Rhodopeptin C2	C26H50N5O4	[M+H]+	Structure
496.4773	496.3857	.0916	Rhodopeptin C3	C26H50N5O4	[M+H]+	Structure
496.4773	496.3761	.1012	1-O-(15'-Methylhexadecyl)-Sn-Glycero-3-Phosphoc...	C25H55NO6P	[M+H]+	Structure
496.4773	496.3761	.1012	PC(O-17:0/0:0)	C25H55NO6P	[M+H]+	Structure
496.4773	496.3761	.1012	PE(O-20:0/0:0)	C25H55NO6P	[M+H]+	Structure
496.4773	496.3745	.1028	Xefoampeptide B	C27H50N3O5	[M+H]+	Structure
496.4773	496.3421	.1352	Dysoxyhainanin A	C31H46NO4	[M+H]+	Structure
496.4773	496.3398	.1375	1-(2-methoxy-6Z-octadecenyl)-sn-glycero-3-phosp...	C24H51NO7P	[M+H]+	Structure
496.4773	496.3398	.1375	PC(0:0/16:0)	C24H51NO7P	[M+H]+	Structure
496.4773	496.3398	.1375	PC(16:0/0:0)	C24H51NO7P	[M+H]+	Structure
496.4773	496.3398	.1375	PC(16:0/0:0)[rac]	C24H51NO7P	[M+H]+	Structure
496.4773	496.3398	.1375	PC(O-14:0/2:0)	C24H51NO7P	[M+H]+	Structure
496.4773	496.3398	.1375	PE(19:0/0:0)	C24H51NO7P	[M+H]+	Structure
496.4773	496.3269	.1504	Cordil	C27H46NO7	[M+H]+	Structure
496.4773	496.3170	.1603	Acidiphilamide C	C29H42N3O4	[M+H]+	Structure
496.4773	496.3130	.1643	Syringolin B	C24H42N5O6	[M+H]+	Structure
496.4773	496.3057	.1716	zoanthamine	C30H42NO5	[M+H]+	Structure
496.4773	496.3034	.1739	PC(11:0/4:0)	C23H47NO8P	[M+H]+	Structure
496.4773	496.3034	.1739	PC(13:0/2:0)	C23H47NO8P	[M+H]+	Structure
496.4773	496.3034	.1739	PE(14:0/4:0)	C23H47NO8P	[M+H]+	Structure
496.4773	496.3034	.1739	PE(16:0/2:0)	C23H47NO8P	[M+H]+	Structure
496.4773	496.2970	.1803	Mibefradil	C29H39N3O3F	[M+H]+	Structure
496.4773	496.2905	.1868	14-acetyldelcosine	C26H42NO8	[M+H]+	Structure
496.4773	496.2840	.1933	Acidiphilamide E	C25H42N3O5S	[M+H]+	Structure
496.4773	496.2806	.1967	Nerfilin I	C28H38N3O5	[M+H]+	Structure
496.4773	496.2806	.1967	Tefinostat	C28H38N3O5	[M+H]+	Structure
496.4773	496.2806	.1967	YM-51084	C28H38N3O5	[M+H]+	Structure
496.4773	496.4724	.0049	Cer(t14:0/17:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t15:0/16:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t16:0/15:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t17:0/14:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t18:0/13:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t19:0/12:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t20:0/11:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4724	.0049	Cer(t21:0/10:0)	C31H62NO3	[M+H-H2O]+	Structure
496.4773	496.4261	.0512	Dendrogenin A	C32H54N3O	[M+H-H2O]+	Structure
496.4773	496.3996	.0777	21-Carboxy-heneicosanoyl-carnitine	C29H54NO5	[M+H-H2O]+	Structure
496.4773	496.3785	.0988	Daphnilongeridine	C32H50NO3	[M+H-H2O]+	Structure
496.4773	496.3269	.1504	2-(Acetylamino)-2-deoxy-3-O-[1-(methoxycarbonyl...	C27H46NO7	[M+H-H2O]+	Structure
496.4773	496.3246	.1527	Maraviroc	C29H40N5F2	[M+H-H2O]+	Structure
496.4773	496.3034	.1739	1-(2-methoxy-13-methyl-pentadecanyl)-sn-glycero...	C23H47NO8P	[M+H-H2O]+	Structure
496.4773	496.3034	.1739	1-(2-methoxy-14-methyl-pentadecanyl)-sn-glycero...	C23H47NO8P	[M+H-H2O]+	Structure
496.4773	496.3034	.1739	1-(2-methoxy-hexadecanyl)-sn-glycero-3-phosphos...	C23H47NO8P	[M+H-H2O]+	Structure
496.4773	496.3017	.1756	Arbumycin	C25H42N3O7	[M+H-H2O]+	Structure
496.4773	496.2918	.1855	azumamide A	C27H38N5O4	[M+H-H2O]+	Structure
496.4773	496.3994	.0779	lissodendoric acid B	C30H53N2O2Na	[M+Na]+	Structure
496.4773	496.3609	.1164	CMNPD12512	C26H51NO6Na	[M+Na]+	Structure
496.4773	496.3431	.1342	N-nervonoyl taurine	C26H51NO4SNa	[M+Na]+	Structure
496.4773	496.3397	.1376	(7Z,10Z,13Z,16Z,19Z)-docosapentaenoylcarnitine	C29H47NO4Na	[M+Na]+	Structure
496.4773	496.3397	.1376	Clupanodonyl carnitine	C29H47NO4Na	[M+Na]+	Structure
496.4773	496.3397	.1376	Docosa-4,7,10,13,16-pentaenoyl carnitine	C29H47NO4Na	[M+Na]+	Structure
496.4773	496.3397	.1376	Fiscpropionate D	C29H47NO4Na	[M+Na]+	Structure
496.4773	496.3397	.1376	Fiscpropionate E	C29H47NO4Na	[M+Na]+	Structure
496.4773	496.3305	.1468	Vestaine B1	C25H49N2O4SNa	[M+Na]+	Structure

Search: (i) a computationally generated database of lipid species, (ii) a reference set of metabolite species (RefMet), or (iii) the Metabolomics Workbench Metabolite database with a list of precursor ions

A computationally generated database composed of major classes of lipid species has been generated from a list of commonly occuring acyl/alkyl chains (listed below). Chain positions and double bond regiochemistry and geometry are not specified. Search the database by entering a list of precursor ion m/z values in the text box, optionally restrict the search to certain lipid classes and then select an appropriate ion type and mass tolerance range.

- ○ Option 1: **Search a computationally generated database of lipids** (optionally restrict search by lipid class below)
- ○ Option 2: **Search RefMet, a reference set of metabolite species**
- ◉ Option 3: **Search the Metabolomics Workbench Metabolite database** (search includes all metabolites)

Optionally restrict lipid search by class (Option 1 only):

- ☐ : Tri(acyl|alkyl)glycerols (TG)
- ☐ : Di(acyl|alkyl)glycerols (DG)
- ☐ : Mono(acyl|alkyl)glycerols (MG)
- ☐ : Monogalactosyldiacylglycerols (MGDG)
- ☐ : Monogalactosyldiacylglycerols (DGDG)
- ☐ : Sulfoquinovosyldiacylglycerols (SQDG)
- ☐ : Phosphtatidylcholines (PC)
- ☐ : Phosphtatidic acids (PA)
- ☐ : Phosphtatidylserines (PS)
- ☐ : Phosphtatidylethanolamines (PE)
- ☐ : Phosphtatidylglycerols (PG)
- ☐ : Phosphtatidylinositols (PI)
- ☐ : Phosphtatidylinositol phosphates (PIP)
- ☐ : Cardiolipins (CL)
- ☐ : Sphingoid bases (LCB)
- ☐ : Ceramides (Cer)
- ☐ : Ceramide phosphates (CerP)
- ☐ : PI-Ceramides(PI-Cer)
- ☐ : PE-Ceramides(PE-Cer)
- ☐ : Sphingomyelins (SM)
- ☐ : Hexosyl ceramides (HexCer)
- ☐ : Dihexosyl ceramides (Hex2Cer)
- ☐ : Sulfatides (SHexCer)
- ☐ : Mannosyl-PI-Ceramides (MIPC)
- ☐ : Mannosyl-di-PI-ceramides (M(IP)2C)
- ☐ : Fatty acids/esters (FA)
- ☐ : Acyl carnitines (CAR)
- ☐ : Sterols,inc. bile acids (ST)
- ☐ : Cholesterol esters (CE)

Mass Tolerance (+/- m/z) +/- 0.2 m/z

Ion adducts (choose at least one with appropriate polarity)

Positive mode:
☑ [M+H]+ ☑ [M+H-H2O]+ ☑ [M+Na]+ ☑ [M+NH4]+ ☑ [M+K]+ ☐ [M+2H]2+ ☐ [M+2Na]2+ ☐ [M+2Na-H]+ ☐ [M+H-EtnP]+ ☐ [M+H-SerP]+ ☐ [M+H-Hexose]+

Negative mode:
☐ [M-H]- ☐ [M+Cl]- ☐ [M+HCOO]- ☐ [M+OAc]- ☐ [M-CH3]- ☐ [M+Na-2H]- ☐ [M+K-2H]- ☐ [M-2H]2- ☐ [M-3H]3- ☐ [M-H-Ser]-

Neutral:
☐ Neutral

Lipid even chains only ☐

Sort by Delta

Submit Reset

List of precursor ions :

496.4773
520.4013
522.3777
524.4802
675.6826
676.6461
689.6807
701.6923
703.6888
704.6431
705.6451
706.6284
717.7772
718.5522
729.7747

Or upload a peaklist file
Browse... No file selected.