Knowledge that will change your world

Pathway software and databases

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Synopsis

- **Public and proprietary metabolite databases**
  - **Instrument manufacturers provide software and search tools for their proprietary databases**
  - **Usually a single copy of the software is provided**
  - **Sciex and Waters provide additional copies at >$35,000 for each**
  - **Metabolomics service companies have proprietary databases and do not allow investigators submitting samples to have access to them**
    - **This discourages deeper research to be performed on metabolomics data**

Public databases

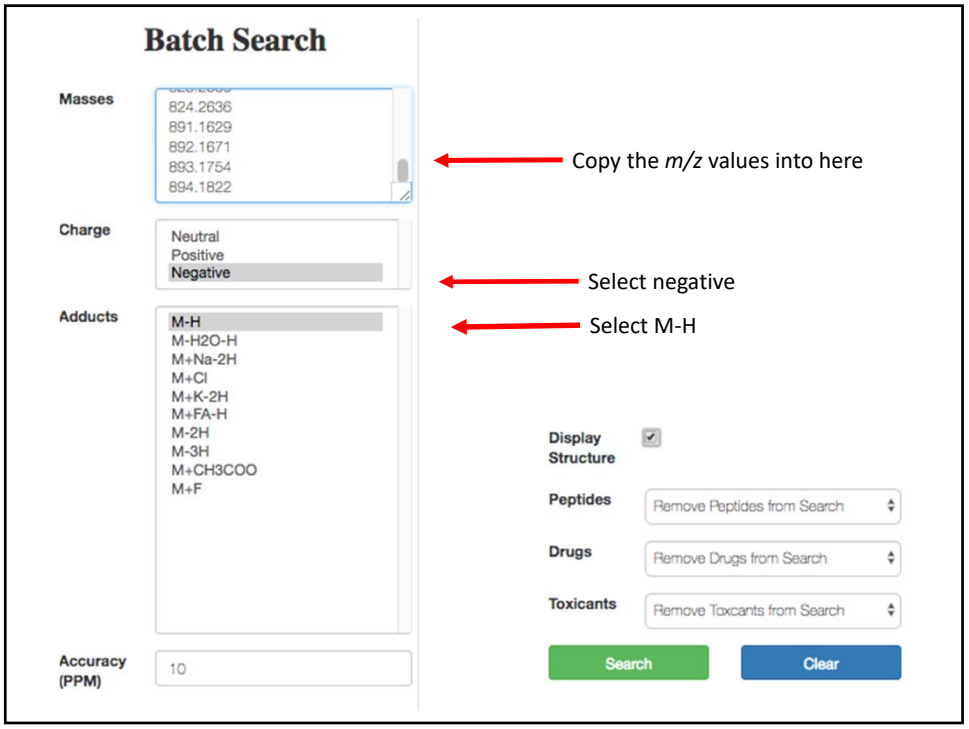
- North America
  - Metlin (https://metlin.scripps.edu/index.php)
  - Human metabolomics database http://www.hmdb.ca/
  - PubChem http://pubchem.ncbi.nlm.nih.gov/
  - Metabolomics Workbench (http://www.metabolomicsworkbench.org/data/index.php)
- Europe
  - ChemSpider (http://www.chemspider.com/)
  - Metabolights (https://www.ebi.ac.uk/metabolights/)
- Asia
  - Kyoto Encyclopedia of Genes and Genomes (KEGG) (http://www.genome.jp/kegg/)

Choosing the ions to search

- Go to the Download file from Metaboanalyst and open the file "plsda.vip"
- In Excel, highlight the whole file and sort according to Comp 1 (high to low)
- Copy the m/z values for those with comp1 values >2 and place them in a new sheet and save the file
- We'll search these in multiple databases

METLIN

Go to https://metlin.scripps.edu/ and login in with your email address and password



METLIN output 1

144.0477 m/z
(145.0535 - 145.0564 daltons): 0 Metabolites [M-H]⁻
186.1152 m/z
(187.1206 - 187.1243 daltons): 3 Metabolites [M-H]⁻

Show 10 entries Search:

METLIN ID	Mass	ΔPPM	Name	Formula	CAS	MS/MS	Structure
3322	187.1208	8	KAPA	C9H17NO3	4707-58-8	View	
5799	187.1208	8	N-n-Hexanoylglycine methyl ester	C9H17NO3		View	
69263	187.1208	8	(E)-2-Butenyl-4-methyl-threonine	C9H17NO3	81135-57-1	View	

No hits to 4-ethylphenol sulfate

201.0237 m/z

(202.029 - 202.033 daltons): 0 Metabolites $[M-H]^-$

202.0266 m/z

(203.0319 - 203.0359 daltons): 0 Metabolites $[M-H]^-$

203.0219 m/z

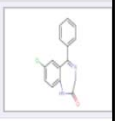
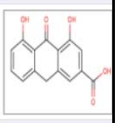
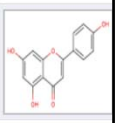
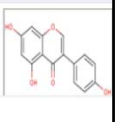
(204.0271 - 204.0312 daltons): 0 Metabolites $[M-H]^-$

Discovering genistein

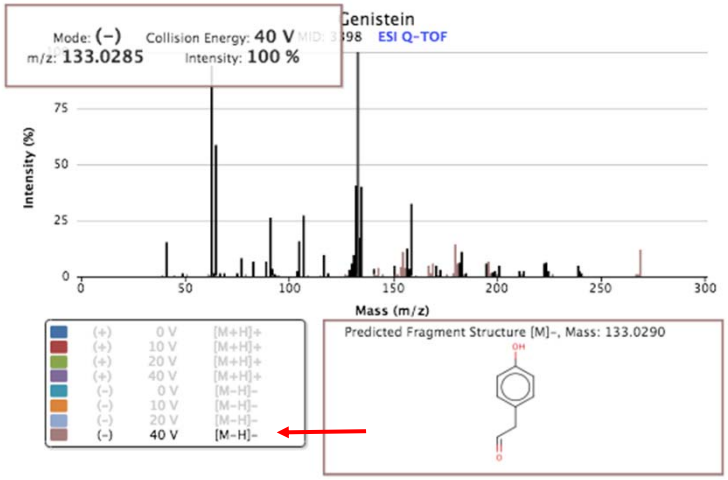
269.0471 m/z

(270.0517 - 270.0571 daltons): 30 Metabolites $[M-H]^-$

Show 10 entries Search:

METLIN ID	Mass	ΔPPM	Name	Formula	CAS	MS/MS	Structure
896	270.0560	6	N-Desmethyldiazepam (Nordazepam)	C15H11ClN2O	1088-11-5	View	
2412	270.0528	5	Rhein-9-anthrone	C15H10O5	480-09-1	View	
3397	270.0528	5	Apigenin	C15H10O5	520-36-5	View	
3398	270.0528	5	Genistein	C15H10O5	446-72-0	View	

MSMS of genistein



No 4-ethylphenol glucuronide

275.0969 m/z

(276.1014 - 276.1069 daltons): 0 Metabolites $[M-H]^-$

291.0916 m/z

(292.096 - 292.1018 daltons): 0 Metabolites $[M-H]^-$

292.0935 m/z

(293.0979 - 293.1037 daltons): 0 Metabolites $[M-H]^-$

297.1012 m/z

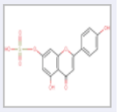
(298.1055 - 298.1114 daltons): 0 Metabolites $[M-H]^-$

METLIN identifies apigenin sulfate, but not genistein sulfate

349.0035 m/z

(350.0073 - 350.0143 daltons): 1 Metabolite [M-H]⁻

Show 10 entries Search:

METLIN ID	Mass	ΔPPM	Name	Formula	CAS	MS/MS	Structure
48862	350.0096	3	Apigenin 7-sulfate	C15H10O8S		View	

Genistein is the isoflavonoid isomer of the flavonoid, apigenin

The MSMS data is only for the positive ion.

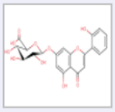
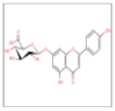
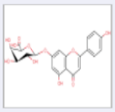
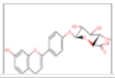
Genistein glucuronide is not listed

The MSMS data is only for the positive ion.

445.0783 m/z

(446.0811 - 446.09 daltons): 14 Metabolites [M-H]⁻

Show 10 entries Search:

METLIN ID	Mass	ΔPPM	Name	Formula	CAS	MS/MS	Structure
48550	446.0849	1	5,7,2'-Trihydroxyflavone 7-glucuronide	C21H18O11		View	
48775	446.0849	1	Apigenin 7-glucuronide	C21H18O11		View	
48776	446.0849	1	Apigenin 7-galacturonide	C21H18O11		View	
48781	446.0849	1	Apigenin 4'-glucuronide	C21H18O11		View	

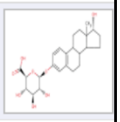
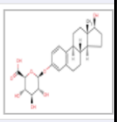
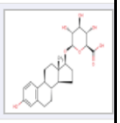
METLIN got E_2-glucuronide right

The MSMS data is only for the positive ion.

447.1991 m/z

(448.2019 - 448.2108 daltons): 12 Metabolites [M-H]⁻

Show 10 entries Search:

METLIN ID	Mass	ΔPPM	Name	Formula	CAS	MS/MS	Structure
43167	448.2097	7	17α-Estradiol 3-D-glucuronide	C24H32O8		View	
43169	448.2097	7	17β-Estradiol 3-(β-D-glucuronide)	C24H32O8		View	
43176	448.2097	7	17β-Estradiol 17-(β-D-glucuronide)	C24H32O8		NO	

No genistein glucuronide sulfate

523.069 m/z

(524.071 - 524.0815 daltons): 0 Metabolites [M-H]⁻

525.0362 m/z

(526.0382 - 526.0487 daltons): 0 Metabolites [M-H]⁻

526.041 m/z

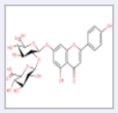
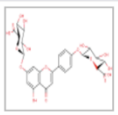
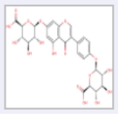
(527.043 - 527.0535 daltons): 0 Metabolites [M-H]⁻

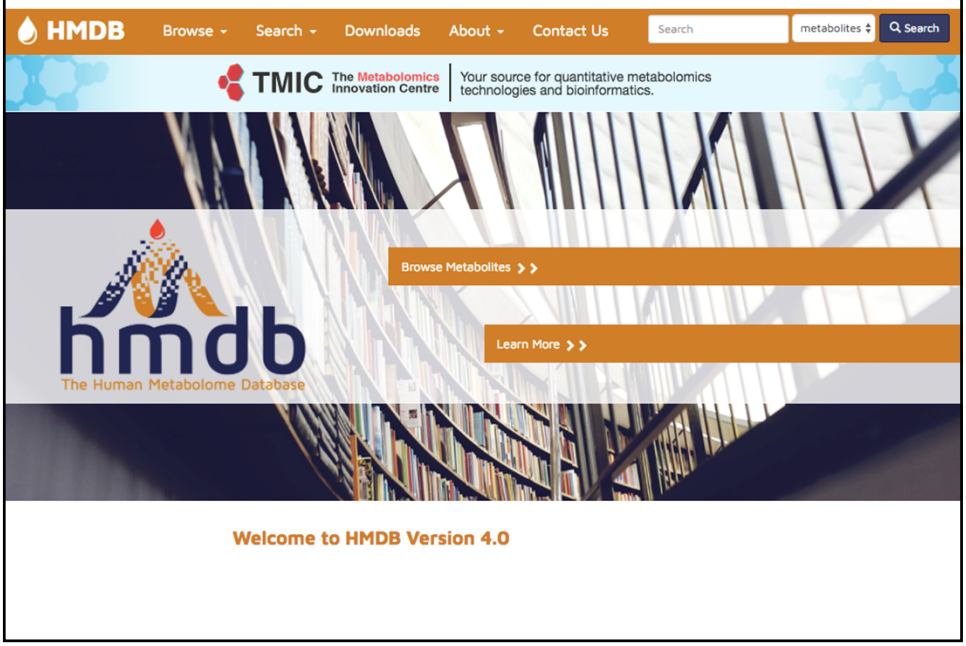
Did find genistein diglucuronide

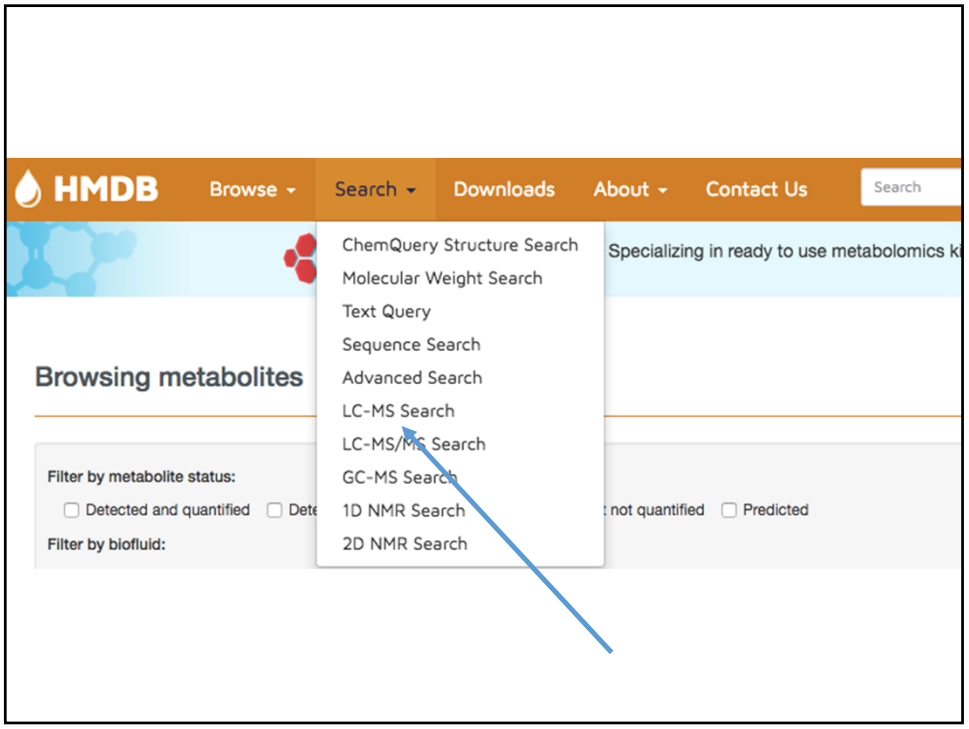
but the MSMS data is only for the positive ion.

(622.1149 - 622.1273 daltons): 3 Metabolites [M-H]⁻

Show 10 entries Search:

METLIN ID	Mass	ΔPPM	Name	Formula	CAS	MS/MS	Structure
48790	622.1170	6	Apigenin 7-glucuronosyl-(1->2)-glucuronide	C27H26O17		View	
48792	622.1170	6	Apigenin 7,4'-diglucuronide	C27H26O17		View	
96094	622.1170	6	Genistein 4',7-O-diglucuronide	C27H26O17		View	

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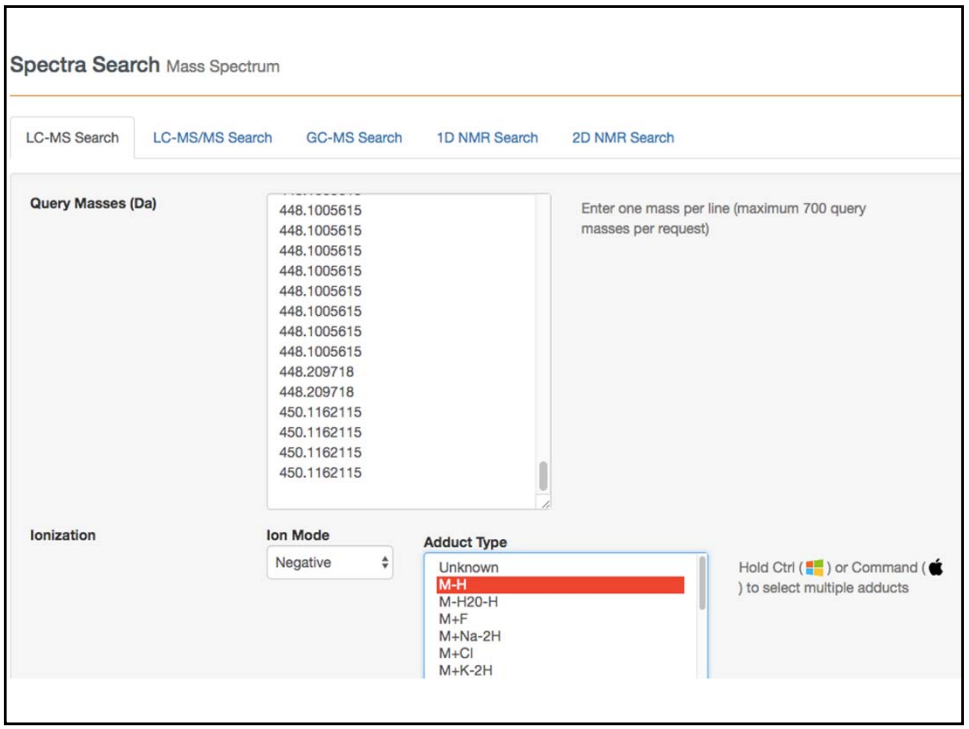
Molecular Weight Search
Text Query
Sequence Search
Advanced Search
LC-MS Search
LC-MS/MS Search
GC-MS Search
1D NMR Search
2D NMR Search
Specializing in ready to use metabolomics k
Browsing metabolites
Filter by metabolite status:
Detected and quantified
not quantified
Predicted
Filter by biofluid:


Spectra Search Mass Spectrum
LC-MS Search
LC-MS/MS Search
GC-MS Search
1D NMR Search
2D NMR Search
Query Masses (Da)
448.1005615
448.1005615
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448.209718
450.1162115
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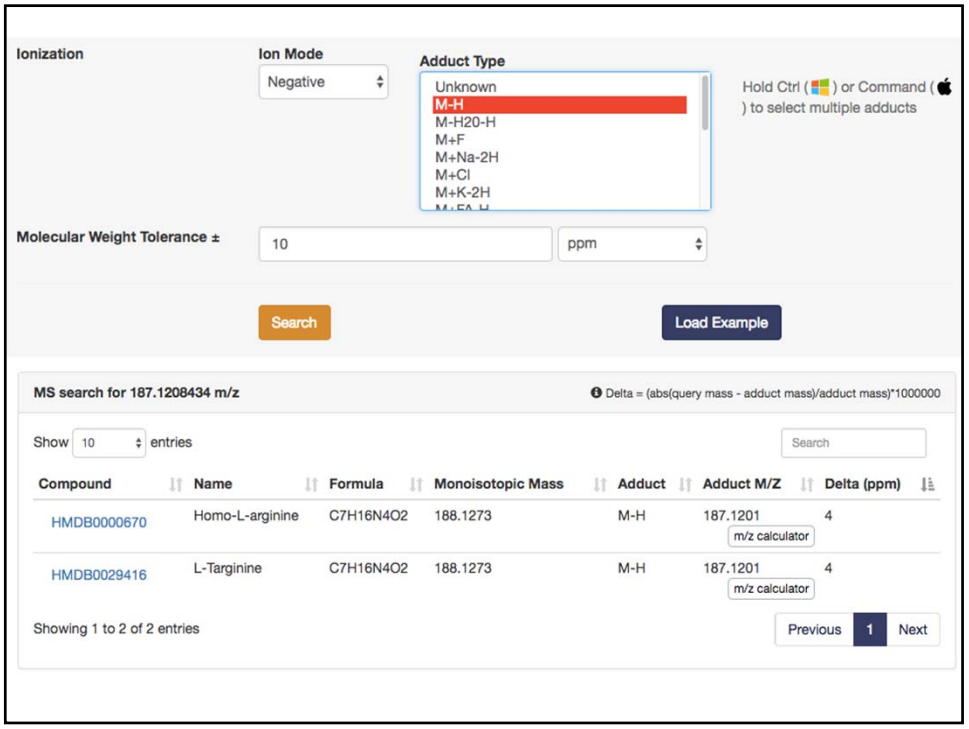
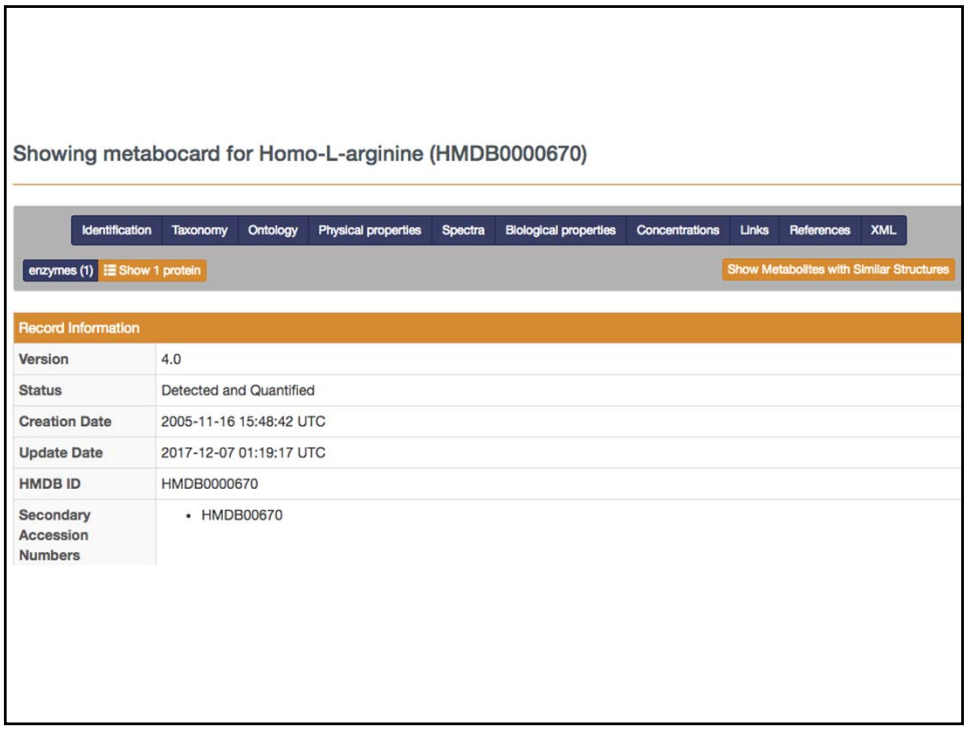
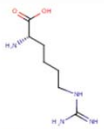
450.1162115
450.1162115
Enter one mass per line (maximum 700 query masses per request)
Ionization
Ion Mode
Negative
Adduct Type
Unknown
M-H
M-H20-H
M+F
M+Na-2H
M+Cl
M+K-2H
Hold Ctrl ( ) or Command ( ) to select multiple adducts


Ionization
Ion Mode
Negative
Adduct Type
Unknown
M-H
M-H20-H
M+F
M+Na-2H
M+Cl
M+K-2H
Hold Ctrl ( ) or Command ( ) to select multiple adducts
Molecular Weight Tolerance ±
10
ppm
Search
Load Example
MS search for 187.1208434 m/z
Delta = (abs(query mass - adduct mass)/adduct mass)*1000000
Show 10 entries
Search
Compound
Name
Formula
Monoisotopic Mass
Adduct
Adduct M/Z
Delta (ppm)
HMDB0000670
Homo-L-arginine
C7H16N4O2
188.1273
M-H
187.1201
m/z calculator
4
HMDB0029416
L-Targinine
C7H16N4O2
188.1273
M-H
187.1201
m/z calculator
4
Showing 1 to 2 of 2 entries
Previous
1
Next

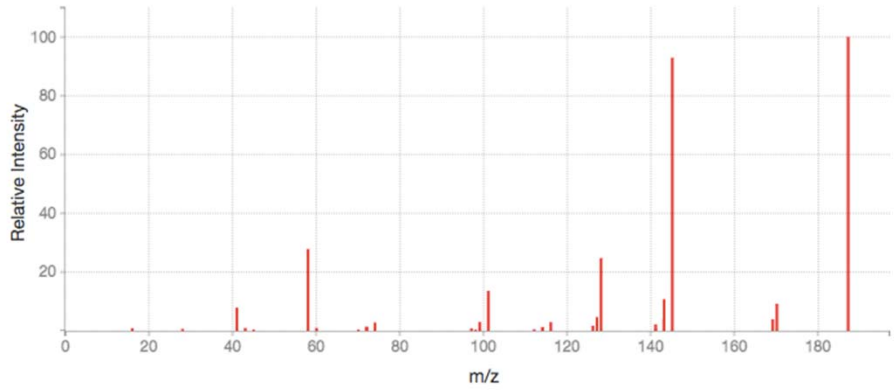

Showing metabocard for Homo-L-arginine (HMDB0000670)
Identification
Taxonomy
Ontology
Physical properties
Spectra
Biological properties
Concentrations
Links
References
XML
enzymes (1)
Show 1 protein
Show Metabolites with Similar Structures
Record Information
Version
4.0
Status
Detected and Quantified
Creation Date
2005-11-16 15:48:42 UTC
Update Date
2017-12-07 01:19:17 UTC
HMDB ID
HMDB0000670
Secondary Accession Numbers
HMDB00670

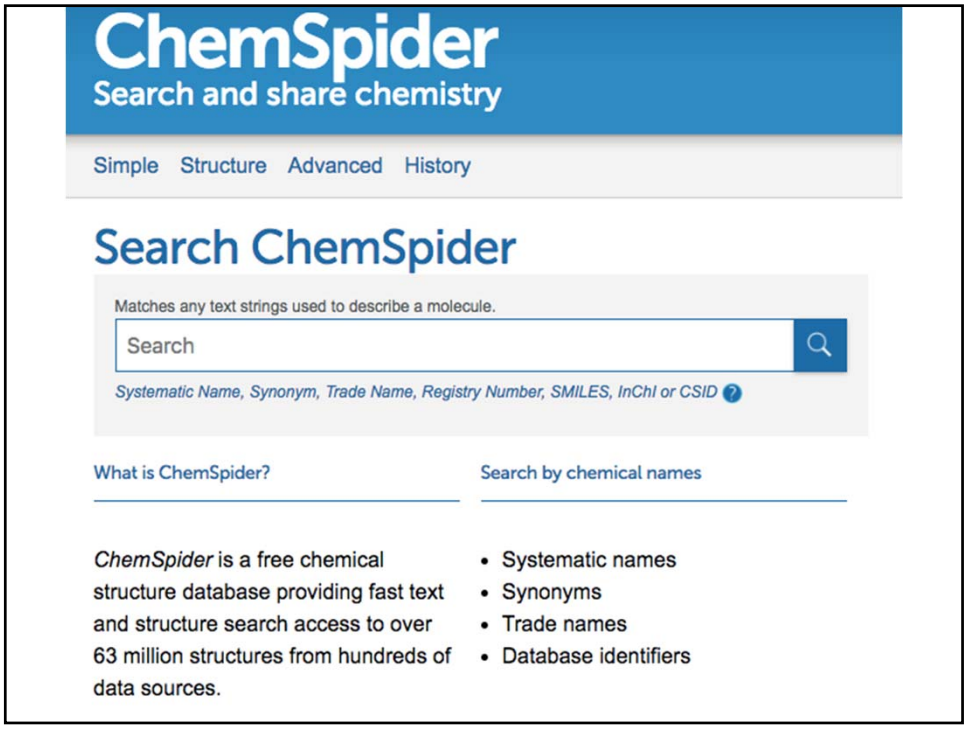
Spectrum View

Metabolite Identification	
Common Name	**Homo-L-arginine**
Description	L-homoarginine, also known as n6-(aminoiminomethyl)-L-lysine or n6-amidino-L-lysine, is a member of the class of compounds known as L-alpha-amino acids. L-alpha-amino acids are alpha amino acids which have the L-configuration of the alpha-carbon atom. L-homoarginine is slightly soluble (in water) and a moderately acidic compound (based on its pKa). L-homoarginine can be found primarily in blood, cerebrospinal fluid (CSF), and urine, as well as in human intestine and testes tissues. Within the cell, L-homoarginine is primarily located in the cytoplasm (predicted from logP). Moreover, L-homoarginine is found to be associated with cirrhosis and and the genetic disorder, hyperargininemia. Homoarginine is a guanidino compounds of guanidinoethanesulfonic acid It is an organ-specific uncompetitive inhibitor of human liver and bone alkaline phosphohydrolase (PMID 5063678).
Structure	 MOL SDF 3D-SDF PDB SMILES InChI View 3D Structure

Spectrum View

MSMS negative spectrum of homoarginine

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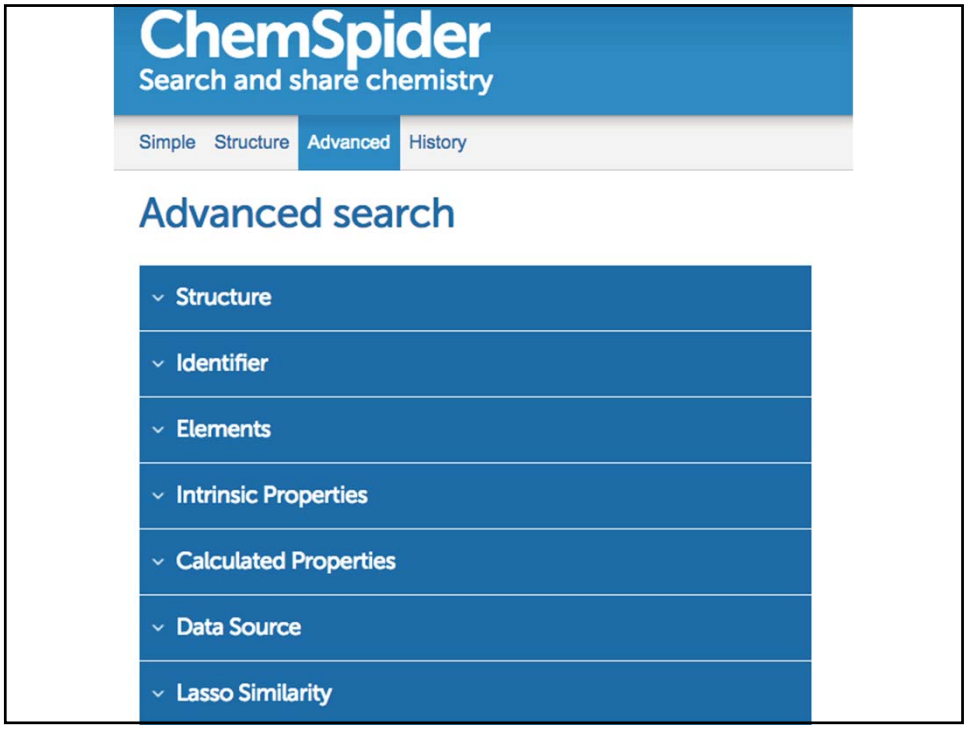
ChemSpider is a free chemical structure database providing fast text and structure search access to over 63 million structures from hundreds of data sources.
Systematic names
Synonyms
Trade names
Database identifiers


ChemSpider
Search and share chemistry
Simple Structure Advanced History
Advanced search
Structure
Identifier
Elements
Intrinsic Properties
Calculated Properties
Data Source
Lasso Similarity

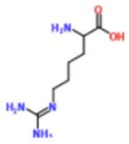
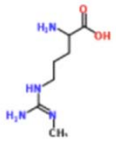
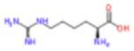
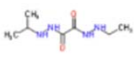
Monoisotopic Mass: 188.1273 ± 0.001

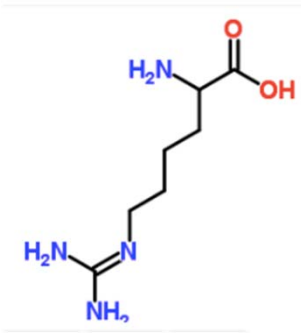
Search Hits Limit: 100 CLEAR FORM SEARCH

FILTER

Found 378 results

Search term: **MM >= 188.1263 AND MM <= 188.1283 AND abs(Monoisotopic_Mass - 188.1273) as mass_defect**

ID	Structure	Molecular Formula	Molecular Weight
+ 3500 - 0/1 defined		$C_7H_{16}N_4O_2$	188.2275
+ 4213 - 0/1 defined		$C_7H_{16}N_4O_2$	188.2275
+ 8732 - 1/1 defined		$C_7H_{16}N_4O_2$	188.2275
+ 50797		$C_7H_{16}N_4O_2$	188.2275



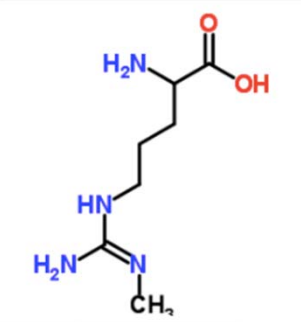
N6-amidino-Lysine

Molecular Formula $C_7H_{16}N_4O_2$

Average mass
188.227 Da

Monoisotopic mass
188.127319 Da

ChemSpider ID 3500



N^5-(N'-Methylcarbamimidoyl)ornithine

Molecular Formula $C_7H_{16}N_4O_2$

Average mass
188.227 Da

Monoisotopic mass
188.127319 Da

ChemSpider ID 4213

MetaboSearch

- **Find MetaboSearch using your browser**
  - **it's at http://omics.georgetown.edu/metabosearch.html**
  - **Note that this software has issues – do not attempt to download the metabolite data**
  - **Instead copy it and paste it to a Word file**
  - **Then copy the Word translated version to an Excel file**
    - **This creates tab separated data**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METABOSEARCH
Introduction
Mass-based search is an important step for metabolite identification in mass-spectrometry-based metabolomic analysis. The mass-to-charge ratio (m/z) value of a molecular ion of interest is searched against metabolite database(s). The metabolites having molecular weights within a specified tolerance to the query m/z value are retrieved from the databases as putative identifications. These putative identifications serve as a foundation for further metabolite verification. In addition to searching with m/z values only, the ion annotation information can be used to aid the mass-based search. Ion annotation groups the ions originating from the same metabolite together and annotates them as adducts/isotopes/in-source fragments. R package CAMERA (Collection of Algorithms for MEtabolite pRofile Annotation) was previously developed for ion annotation by Kuhl etc (Carsten Kuhl etc. CAMERA: Collection of annotation related methods for mass spectrometry data. R package version 1.10.0.). Using the ion annotation information, the appropriate mass values of ions can be calculated. Then the calculated mass values are searched against databases. This approach is expected to improve the accuracy for metabolite identification.
We developed MetaboSearch to perform mass-based metabolite search simultaneously against the four major metabolite databases: Human Metabolome DataBase (HMDB), Madison Metabolomics Consortium Database (MMCD), Metlin, and LipidMaps. The search results from these databases are integrated into a uniformly and non-redundant format based on IUPAC International Chemical Identifier (InChI) key. Chemical identifier information is provided by the software for effective reference to metabolites. Cross-referencing across multiple databases is performed when a particular identifier type is missing from a database. The comprehensive list of chemical identifiers includes PubChem Compound ID (CID), PubChem Substance ID (SID), HMDB ID, KEGG ID, InChI string, and InChI key. MetaboSearch performs mass-based search using a given list of m/z values. In addition, it can utilize ion annotation information for improved metabolite identification, as long as the ion annotation information is provided according to the CAMERA output format.
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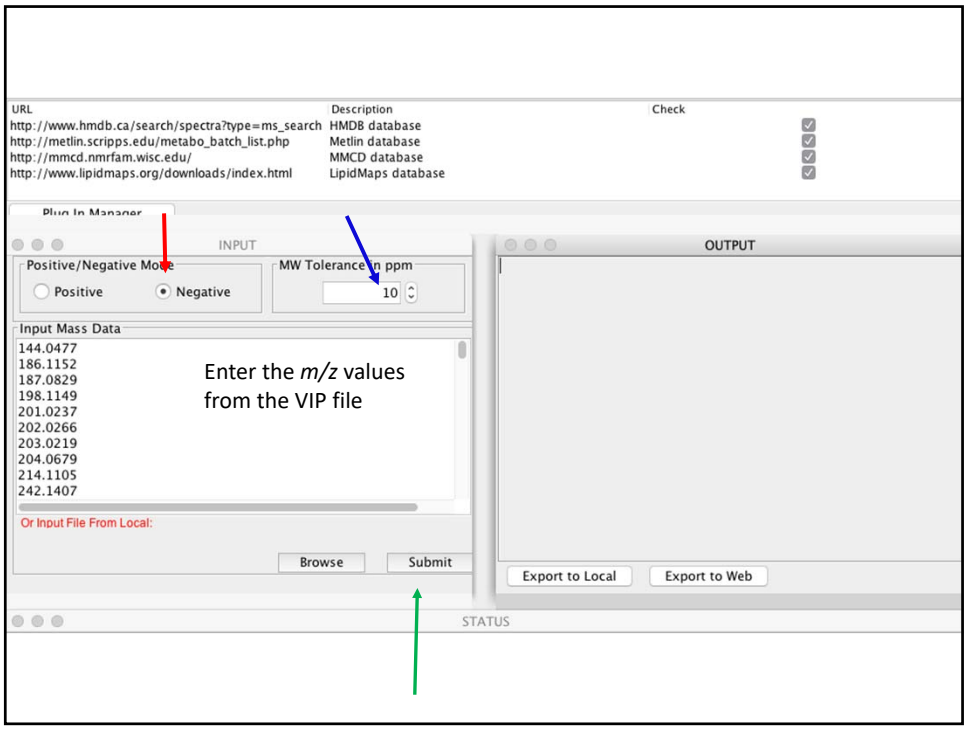
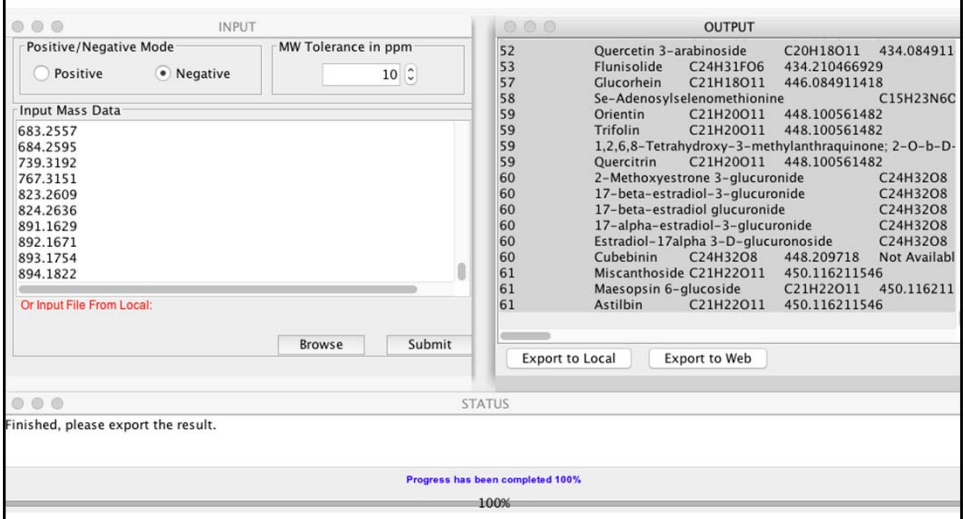

URL
Description
Check
http://www.hmdb.ca/search/spectra?type=ms_search HMDB database
http://metlin.scripps.edu/metabo_batch_list.php Metlin database
http://mmcd.nmrfam.wisc.edu/ MMCD database
http://www.lipidmaps.org/downloads/index.html LipidMaps database
INPUT
OUTPUT
Positive/Negative Mode
Positive
Negative
MW Tolerance in ppm
10
Input Mass Data
144.0477
186.1152
187.0829
198.1149
201.0237
202.0266
203.0219
204.0679
214.1105
242.1407
Enter the m/z values from the VIP file
Or Input File From Local:
Browse
Submit
Export to Local
Export to Web
STATUS



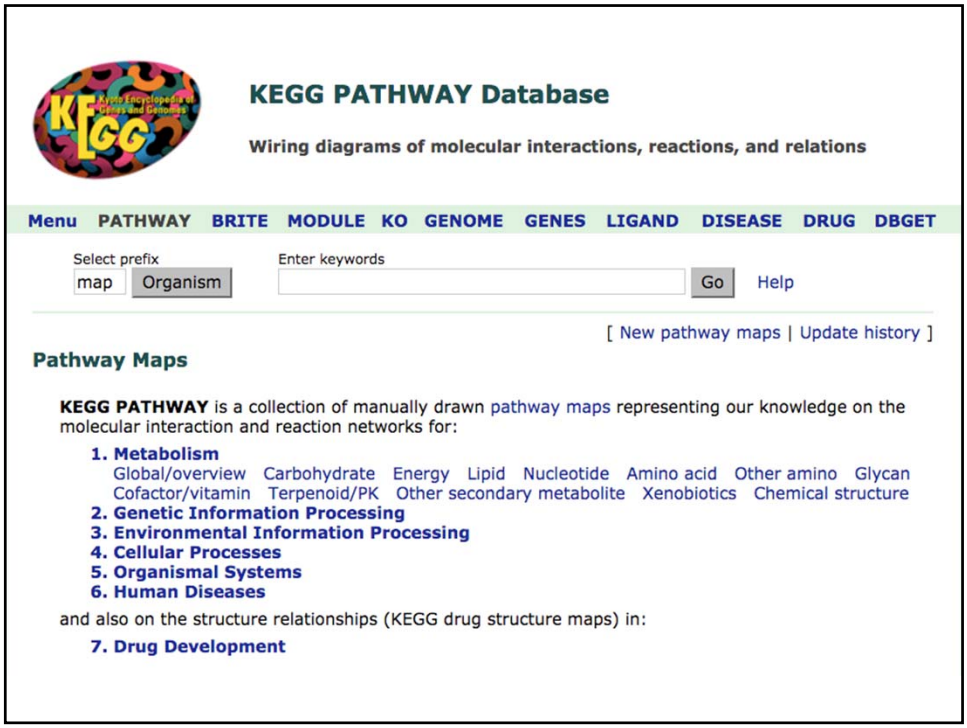
When the search is complete, copy the data in the output panel (command-A, command-C)
Open a new Word file – switch to Landscape mode – then copy again and transfer to Excel

QueryID	CQ_ID	Delta	Name	Formula	Mass	Comments	Kegg	Pubchem SI	Pubchem CI	HMDB
2	cq_08598	0.00163271	(E)-2-Butenyl-4-methyl-th	C9H17NO3	187.120843	[M-H]	C12029	14185	5282047	Not Available
2	cq_00742	0.00163271	8-Amino-7-oxononanoate	C9H17NO3	187.120843	[M-H]	C01092	770755	Not Available	Not Available
2	cq_10810	0.00163271	N-n-Hexanoylglycine met	C9H17NO3	187.120843	[M-H]	Not Availabl	7585459	338209	|HMDB0083
4	cq_07079	0.00133271	Tussilagine	C10H17NO3	199.120843	[M-H]	C10411	12597	185071	Not Available
4	cq_08968	0.00133271	Ecgonine methyl ester	C10H17NO3	199.120843	[M-H]	C12448	682364	104904	|HMDB0640
8	cq_01301	0.00128291	Indolelactate	C11H11NO3	205.073893	[M-H]	C02043	669834	92904	|HMDB0067
8	cq_03186	0.00128291	5-Methoxyindoleacetate	C11H11NO3	205.073893	[M-H]	C05660	161944	18986	|HMDB0409
8	cq_07406	0.00128291	Swietenidin B	C11H11NO3	205.073893	[M-H]	C10741	12924	5281851	Not Available
8	cq_06630	0.00128291	Gentianamine	C11H11NO3	205.073893	[M-H]	C09961	12147	442535	Not Available
9	cq_08597	0.00201809	2-Amino-9,10-epoxy-8-ox	C10H17NO4	215.115758	[M-H]	C12027	14184	443587	Not Available
9	cq_14007	0.00201809	3-CARBOXYMETHYL-4-ISC	C10H17NO4	215.115758	[M-H]	Not Availabl	Not Available	Not Available	Not Available
10	cq_17352	0.00091796	2-Ethylacrylylcarnitine	C12H21NO4	243.147058	[M-H]	Not Availabl	Not Available	Not Available	|HMDB0199
10	cq_17309	0.00091796	Tiglylcarnitine	C12H21NO4	243.147058	[M-H]	Not Availabl	Not Available	Not Available	|HMDB0236
11	cq_14779	0.002666	2-(OXALYL-AMINO)-4,5,6,	C10H10N2O5	270.031042	[M-H]	Not Availabl	Not Available	Not Available	Not Available
12	cq_11396	0.00131882	1-CHLORO-6-(4-HYDROXY	C16H11ClO2	270.044757	[M-H]	Not Availabl	Not Available	Not Available	Not Available
13	cq_05415	0.0015527	Sulphuretin;Sulfuretin	C15H10O5	270.052823	[M-H]	C08730	209227	67111	Not Available
13	cq_06706	0.0015527	5-Deoxykaempferol;3,7,4	C15H10O5	270.052823	[M-H]	C10037	742390	164918	Not Available
13	cq_06962	0.0015527	Aloe-emodin	C15H10O5	270.052823	[M-H];drug	C10294	153452	10207	Not Available
13	cq_16866	0.0015527	3,6,4'-Trihydroxyflavone;3	C15H10O5	270.052823	[M-H]	C15222	Not Available	Not Available	Not Available
13	cq_10153	0.0015527	3',4',7-Trihydroxyisoflavo	C15H10O5	270.052823	[M-H]	C14313	3881497	622984	Not Available
13	cq_07037	0.0015527	Lucidin	C15H10O5	270.052823	[M-H]	C10369	153404	10163	Not Available
13	cq_07011	0.0015527	Emodin	C15H10O5	270.052823	[M-H]	C10343	153905	Not Available	Not Available
13	cq_17542	0.0015527	Apigenin	C15H10O5	270.052823	[M-H]	Not Availabl	Not Available	5280443	|HMDB0212
13	cq_03743	0.0015527	Genistein;5,7,4'-Trihydro	C15H10O5	270.052823	[M-H];drug	C06563	153162	Not Available	Not Available
13	cq_06781	0.0015527	Norwogonin;5,7,8-Trihyd	C15H10O5	270.052823	[M-H]	C10113	163335	20510	Not Available
13	cq_07047	0.0015527	Norobtusifolin;2-Hydroxy	C15H10O5	270.052823	[M-H]	C10379	701155	442759	Not Available
13	cq_07044	0.0015527	Morindone	C15H10O5	270.052823	[M-H]	C10376	12562	442756	Not Available
13	cq_07065	0.0015527	Purpurin 1-methyl ether	C15H10O5	270.052823	[M-H]	C10397	12583	442766	Not Available

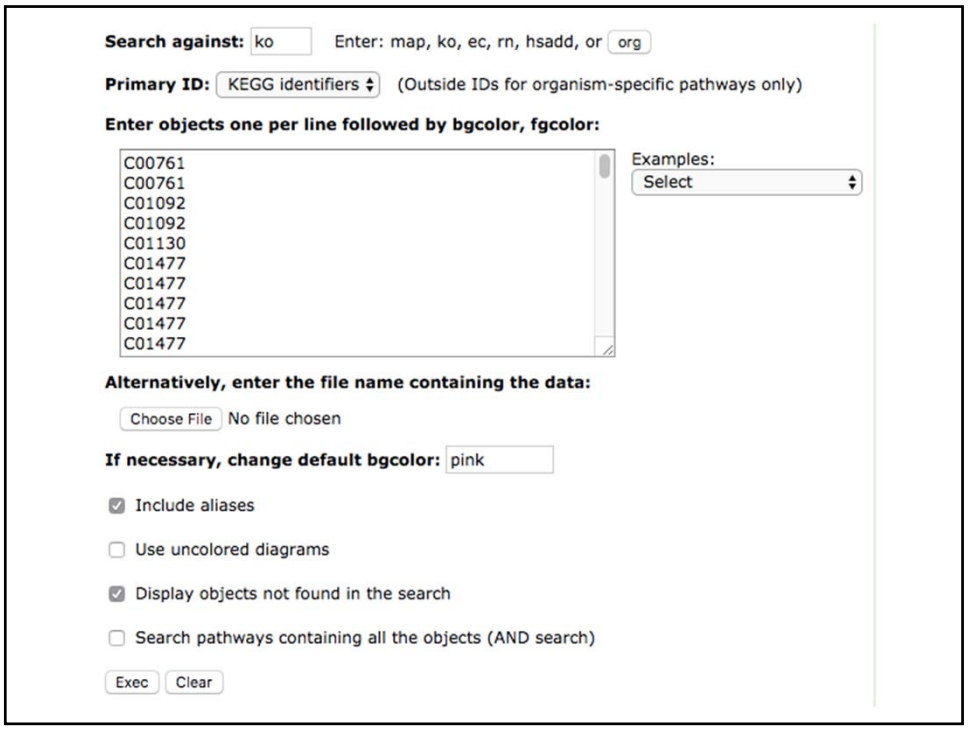
Copy to a new sheet, sort according to the KEGG column and then copy the values

Going to the KEGG Pathway website

- http://www.genome.jp/kegg/pathway.html
- We'll take the compounds detected in MetaboSearch that have KEGG identifiers
- These can be mapped to pathways




Pathway Mapping
KEGG PATHWAY mapping is the process to map molecular datasets, especially large-scale datasets in genomics, transcriptomics, proteomics, and metabolomics, to the KEGG pathway maps for biological interpretaion of higher-level systemic functions.
Search Pathway - basic pathway mapping tool
Search&Color Pathway - advanced pathway mapping tool
Color Pathway - selected pathway map coloring tool


Search against: ko
Enter: map, ko, ec, rn, hsadd, or org
Primary ID: KEGG identifiers
(Outside IDs for organism-specific pathways only)
Enter objects one per line followed by bgcolor, fgcolor:
C00761
C00761
C01092
C01092
C01130
C01477
C01477
C01477
C01477
C01477
Examples:
Select
Alternatively, enter the file name containing the data:
Choose File
No file chosen
If necessary, change default bgcolor: pink
Include aliases
Use uncolored diagrams
Display objects not found in the search
Search pathways containing all the objects (AND search)
Exec
Clear

Pathway Search Result

Following object(s) was/were not found cpd:C01130 cpd:C01821 cpd:C02822 cpd:C03357 cpd:C03502 cpd:C04300 cpd:C04888 cpd:C05691 cpd:C06817 cpd:C06979 cpd:C07005 cpd:C07310 cpd:C07486 cpd:C08160 cpd:C08174 cpd:C08183 cpd:C08598 cpd:C08730 cpd:C08951 cpd:C09011 cpd:C09013 cpd:C09116 cpd:C09261 cpd:C09359 cpd:C09486 cpd:C09553 cpd:C09795 cpd:C09800 cpd:C09803 cpd:C09961 cpd:C10023 cpd:C10025 cpd:C10037 cpd:C10042 cpd:C10052 cpd:C10053 cpd:C10069 cpd:C10092 cpd:C10113 cpd:C10114 cpd:C10294 cpd:C10343 cpd:C10359 cpd:C10369 cpd:C10376 cpd:C10379 cpd:C10397 cpd:C10411 cpd:C10741 cpd:C10753 cpd:C11237 cpd:C11593 cpd:C11930 cpd:C11931 cpd:C12027 cpd:C12029 cpd:C12656 cpd:C12699 cpd:C12848 cpd:C14313 cpd:C14625 cpd:C15218 cpd:C15222 cpd:C17449

Sort by the pathway list

Show all objects

- ko01110 Biosynthesis of secondary metabolites (10)
- ko01100 Metabolic pathways (5)
- ko00944 Flavone and flavonol biosynthesis (5)
- ko00943 Isoflavonoid biosynthesis (4)
- ko00950 Isoquinoline alkaloid biosynthesis (2)
- ko00902 Monoterpenoid biosynthesis (2)
- ko00941 Flavonoid biosynthesis (2)
- ko00380 Tryptophan metabolism (2)
- ko00140 Steroid hormone biosynthesis (2)

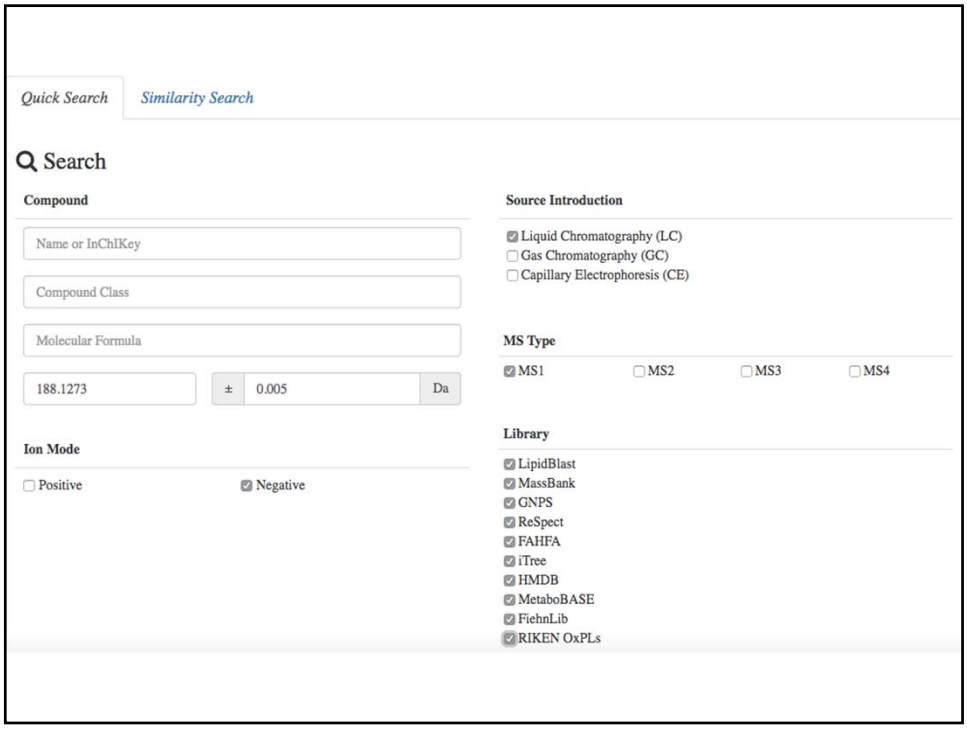
http://mona.fiehnlab.ucdavis.edu/

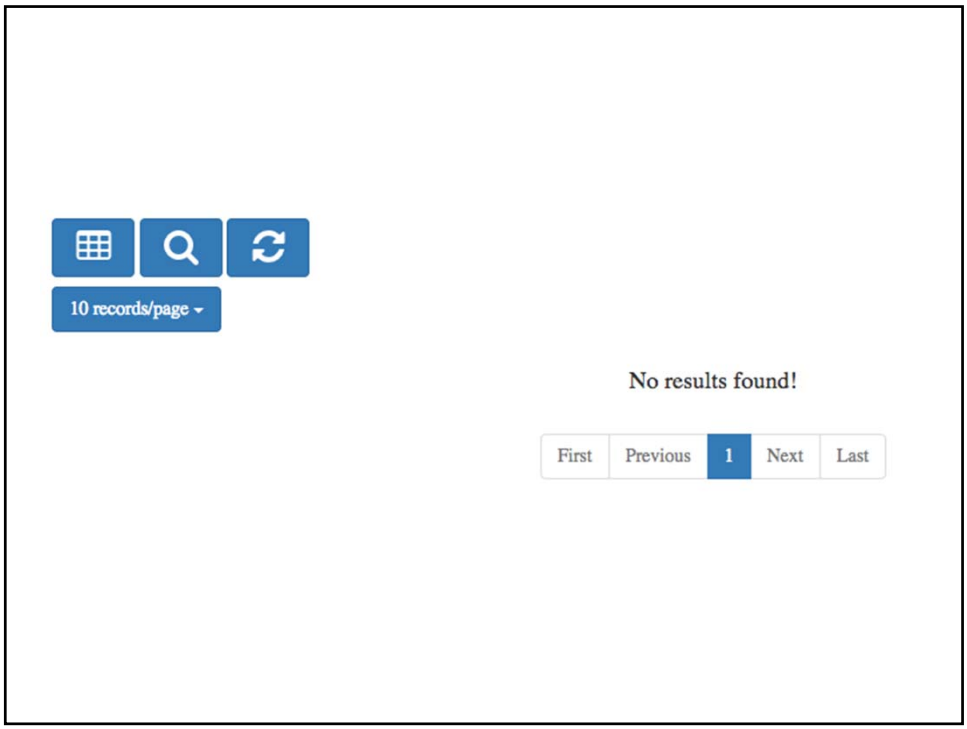
Welcome to MoNA!

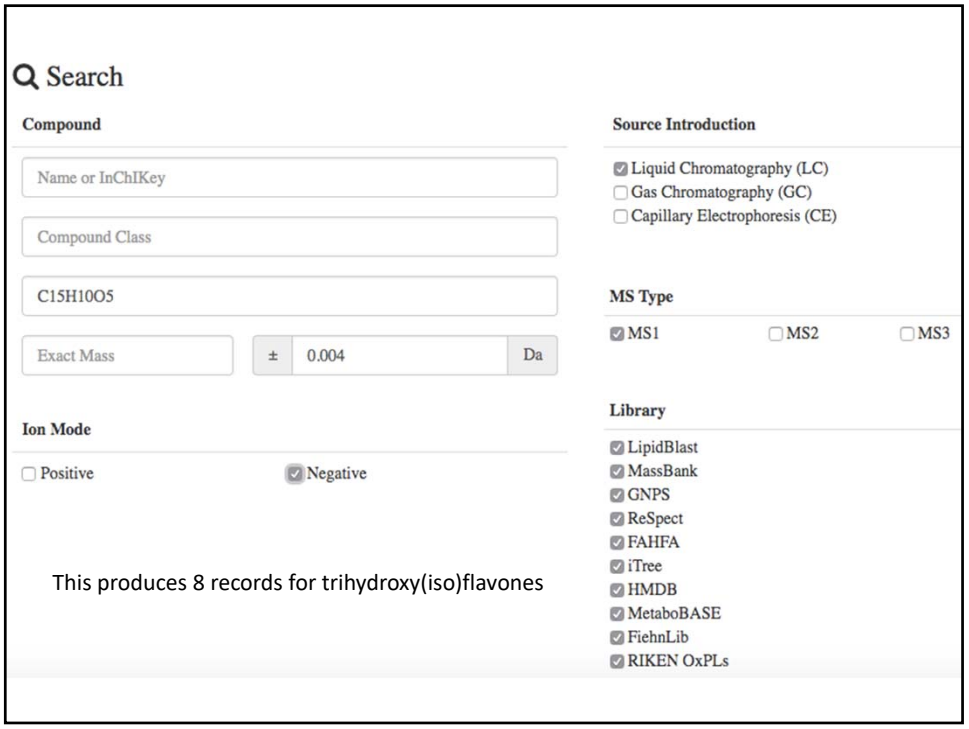
MassBank of North America (MoNA) is a metadata-centric, auto-curating repository designed for efficient storage and querying of mass spectral records. It intends to serve as a the framework for a centralized, collaborative database of metabolite mass spectra, metadata and associated compounds. MoNA currently contains over 200,000 mass spectral records from experimental and in-silico libraries as well as from user contributions.

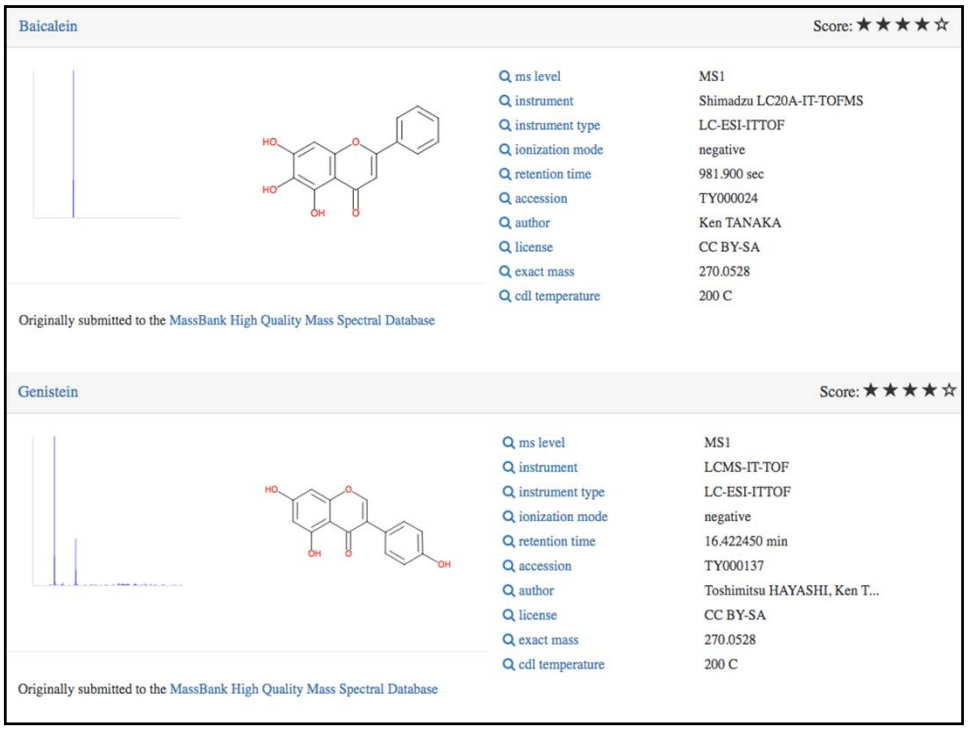
MoNA has recently been redesigned, with significant improvements to server-side architecture, query structure, and search speed. We are actively improving and adding features, so please be patient as functionality is added. If you notice any major issues, feel free to report them using the issue tracker linked below.

Search Spectra | Browse Spectra | Issue Tracker


Quick Search
Similarity Search
Search
Compound
Name or InChIKey
Compound Class
Molecular Formula
188.1273
±
0.005
Da
Ion Mode
Positive
Negative
Source Introduction
Liquid Chromatography (LC)
Gas Chromatography (GC)
Capillary Electrophoresis (CE)
MS Type
MS1
MS2
MS3
MS4
Library
LipidBlast
MassBank
GNPS
ReSpect
FAHFA
iTree
HMDB
MetaboBASE
FiehnLib
RIKEN OxPLs


10 records/page
No results found!
First
Previous
1
Next
Last


Search
Compound
Name or InChIKey
Compound Class
C15H10O5
Exact Mass
±
0.004
Da
Ion Mode
Positive
Negative
This produces 8 records for trihydroxy(iso)flavones
Source Introduction
Liquid Chromatography (LC)
Gas Chromatography (GC)
Capillary Electrophoresis (CE)
MS Type
MS1
MS2
MS3
Library
LipidBlast
MassBank
GNPS
ReSpect
FAHFA
iTree
HMDB
MetaboBASE
FiehnLib
RIKEN OxPLs


Baicalein
Score: ★★★★☆
ms level MS1
instrument Shimadzu LC20A-IT-TOFMS
instrument type LC-ESI-ITTOF
ionization mode negative
retention time 981.900 sec
accession TY000024
author Ken TANAKA
license CC BY-SA
exact mass 270.0528
cdl temperature 200 C
Originally submitted to the MassBank High Quality Mass Spectral Database
Genistein
Score: ★★★★☆
ms level MS1
instrument LCMS-IT-TOF
instrument type LC-ESI-ITTOF
ionization mode negative
retention time 16.422450 min
accession TY000137
author Toshimitsu HAYASHI, Ken T...
license CC BY-SA
exact mass 270.0528
cdl temperature 200 C
Originally submitted to the MassBank High Quality Mass Spectral Database