Metabolomics Databases

Xiuxia Du, Stephen Barnes

Outline

- Comprehensive metabolomics databases
- Compound databases
- Spectral databases
- Metabolic pathway databases
- Drug databases
- Disease & physiology databases
- Raw data databases

Comprehensive Metabolomics Database: HMDB 4.0

HMDB 4.0

- www.hmdb.ca

- Contain detailed information about small molecule metabolites found in the human body.

- Contain or link three kinds of data
  - Chemical data
  - Clinical data
  - Molecular biology/biochemistry data

- Contain four additional databases
  - DrugBank, T3DB, SMPDB, and FooDB

HMDB 4.0

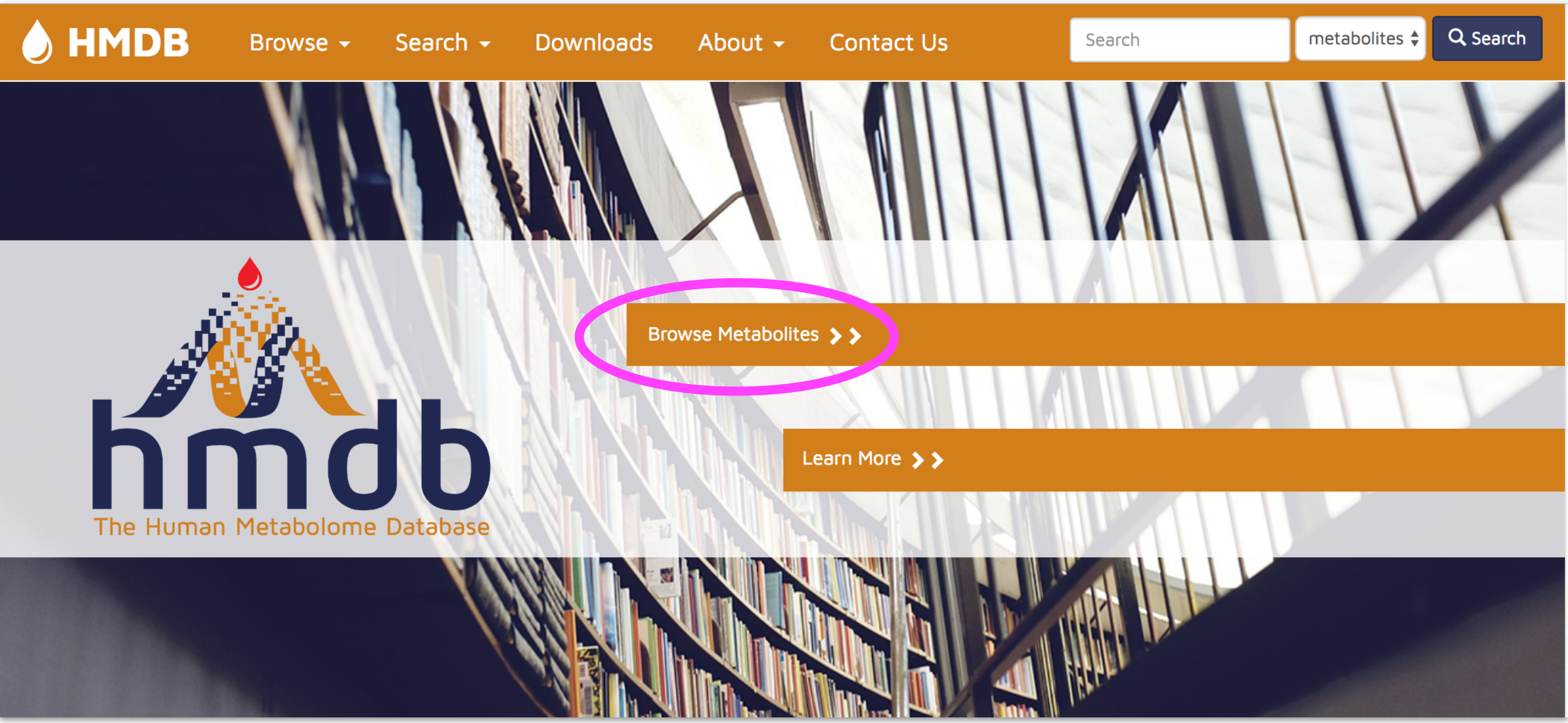
Table 1. Comparison between the coverage in HMDB 1.0, 2.0, 3.0 and HMDB 4.0

Category	HMDB 1.0	HMDB 2.0	HMDB 3.0	HMDB 4.0
Total number of metabolites	2180	6408	40 153	114 100
Number of detected & quantified metabolites	883	4413	16 714	18 557
Number of detected, not quantified metabolites	1297	1995	2798	3271
Number of expected metabolites	0	0	20 641	82 274
Number of predicted metabolites*	0	0	0	9548
Number of unique synonyms	27 700	43 882	199 668	1 231 398
Number of cmpds with expt. MS/MS spectra	390	799	1249	2265
Number of cmpds with expt. GC/MS spectra	0	279	1220	2544
Number of cmpds with expt. NMR spectra	385	792	1054	1494
Number of cmpds with pred. MS/MS spectra*	0	0	0	98 601
Number of cmpds with pred. GC/MS spectra*	0	0	0	26 880
Number of experimental NMR spectra	765	1580	2032	3840
Number of experimental MS/MS spectra	1180	2397	5776	22 198
Number of experimental GC/MS spectra	0	279	1763	7418
Number of predicted MS/MS spectra*	0	0	0	279 972
Number of predicted GC/MS spectra*	0	0	0	38 277
Number of metabolic pathway maps	26	58	442	25 570
Number of compounds with disease links	862	1002	3105	5498
Number of compounds with concentration data	883	4413	5027	7552
Number of predicted molecular properties	2	2	10	24
Number of metabolite-SNP interactions*	0	0	0	6777
Number of metabolite-drug interactions*	0	0	0	2497
No. of metabolites w. sex/diurnal/age variation*	0	0	0	2901
Number of metabolic reactions*	0	0	0	18,192
Number of defined ontology terms*	0	0	0	3150
Number of HMDB data fields	91	102	114	130

* New for HMDB 4.0

Wishart DS, Feunang YD, Marcu A, Guo AC, Liang K, Vazquez-Fresno R, Sajed T, Johnson D, Li C, Karu N et al: **HMDB 4.0: the human metabolome database for 2018.** *Nucleic Acids Res* 2018, 46(D1):D608-D617.

HMDB 4.0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The Human Metabolome Database

HMDB 4.0

Browsing metabolites

Filter by metabolite status (default all):

☑ Detected and quantified ☐ Detected but not quantified ☐ Expected but not quantified ☐ Predicted

Filter by biospecimen:

☐ Blood ☐ Urine ☐ Saliva ☐ Cerebrospinal Fluid ☐ Feces ☐ Sweat ☑ Breast Milk ☐ Bile ☐ Amniotic Fluid ☐ Other Biospecimens

Filter by origin:

☐ Exogenous ☐ Endogenous ☐ Food ☐ Plant ☐ Microbial ☐ Toxin/Pollutant ☐ Cosmetic ☐ Drug ☐ Drug Metabolite

Filter by subcellular location:

☐ Cell Membrane ☐ Cytoplasm ☐ Nucleus ☐ Mitochondria

Clear Apply Filter

Displaying metabolites **1 - 25** of **114100** in total

1 2 3 4 5 ... Next › Last »

HMDB 4.0

Filter by metabolite status (default all):

☑ Detected and quantified ☐ Detected but not quantified ☐ Expected but not quantified ☐ Predicted

Filter by biospecimen:

☐ Blood ☐ Urine ☐ Saliva ☐ Cerebrospinal Fluid ☐ Feces ☐ Sweat ☑ Breast Milk ☐ Bile ☐ Amniotic Fluid ☐ Other Biospecimens

Filter by origin:

☐ Exogenous ☐ Endogenous ☐ Food ☐ Plant ☐ Microbial ☐ Toxin/Pollutant ☐ Cosmetic ☐ Drug ☐ Drug Metabolite

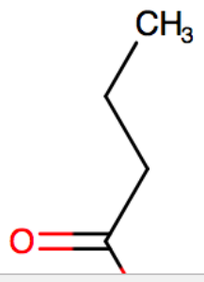
Filter by subcellular location:

☐ Cell Membrane ☐ Cytoplasm ☐ Nucleus ☐ Mitochondria

Clear Apply Filter

Displaying metabolites **1 - 25** of **101** in total

1 2 3 4 5 Next › Last »

HMDB ID / CAS Number	Name	Structure	Formula / Average Mass / Monoisotopic Mass	Biospecimen Location
HMDB0000039 107-92-6	Butyric acid		$C_4H_8O_2$ 88.1051 88.0524295	Urine

HMDB 4.0

Showing metabocard for Butyric acid (HMDB0000039)

Identification | Taxonomy | Ontology | Physical properties | Spectra | Biological properties | Concentrations | Links | References | XML

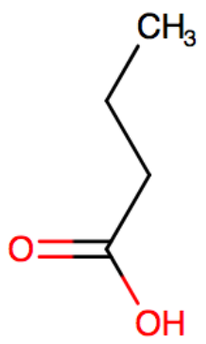
enzymes (16) | transporters (1) | Show 17 proteins

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	2018-05-20 20:40:09 UTC
HMDB ID	HMDB0000039
Secondary Accession Numbers	• HMDB00039

HMDB 4.0

Common Name	**Butyric acid**
Description	Butyric acid, a four-carbon fatty acid, is formed in the human colon by bacterial fermentation of carbohydrates (including dietary fiber), and putatively suppresses colorectal cancer (CRC). Butyrate has diverse and apparently paradoxical effects on cellular proliferation, apoptosis and differentiation that may be either pro-neoplastic or anti-neoplastic, depending upon factors such as the level of exposure, availability of other metabolic substrate and the intracellular milieu. In humans, the relationship between luminal butyrate exposure and CRC has been examined only indirectly in case-control studies, by measuring fecal butyrate concentrations, although this may not accurately reflect effective butyrate exposure during carcinogenesis. Perhaps not surprisingly, results of these investigations have been mutually contradictory. The direct effect of butyrate on tumorigenesis has been assessed in a no. of in vivo animal models, which have also yielded conflicting results. In part, this may be explained by methodology: differences in the amount and route of butyrate administration, which are likely to significantly influence delivery of butyrate to the distal colon. (PMID: 16460475) Butyric acid is a carboxylic acid found in rancid butter, parmesan cheese, and vomit, and has an unpleasant odor and acrid taste, with a sweetish aftertaste (similar to ether). Butyric acid is a fatty acid occurring in the form of esters in animal fats and plant oils. Interestingly, low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes. As a consequence, they find use as food and perfume additives. Butyrate is produced as end-product of a fermentation process solely performed by obligate anaerobic bacteria.
Structure	 MOL SDF 3D-SDF PDB SMILES InChI View 3D Structure

HMDB 4.0

Showing metabocard for Butyric acid (HMDB0000039)

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Show Metabolites with Similar Structures

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HMDB ID	HMDB0000039
Secondary Accession Numbers	• HMDB00039

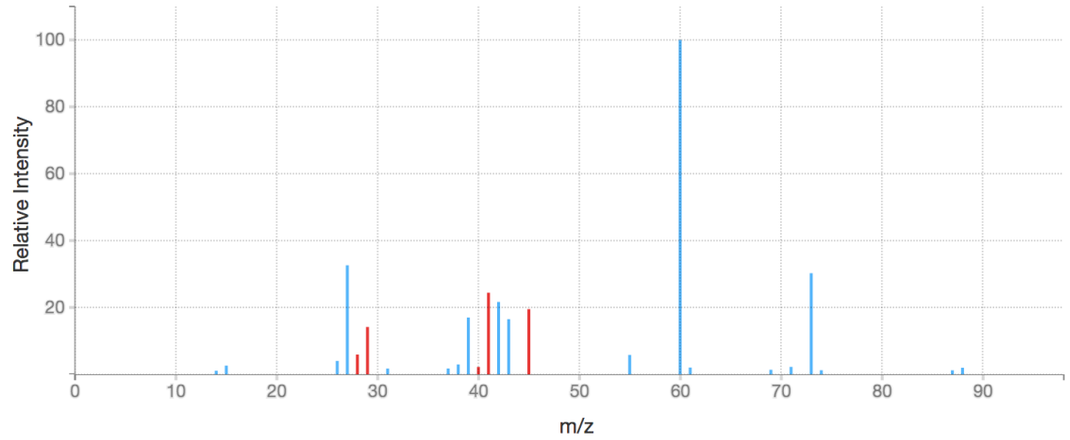
HMDB 4.0

GC-MS	GC-MS Spectrum - EI-B (Non-derivatized)	splash10-03dl-9000000000-032fc35b394786b5896a	View in MoNA
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (Non-derivatized) - 70eV, Positive	splash10-002f-9000000000-a7792b54320e7c859731	View in MoNA
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (1 TMS) - 70eV, Positive	splash10-00fr-9100000000-d125b331c4a6d37648a1	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 10V, Negative (Annotated)	splash10-000i-9000000000-7f461db56bfd8568ec71	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 25V, Negative (Annotated)	splash10-000i-9000000000-66f857fa612f773837bc	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 40V, Negative (Annotated)	splash10-000i-9000000000-e6689b2e6bf21570b934	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - EI-B (HITACHI RMU-7M) , Positive	splash10-03dl-9000000000-b2ffa7d67b2466dea94f	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - EI-B (HITACHI M-80B) , Positive	splash10-03dl-9000000000-7467bf19c64fd3f51105	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - LC-ESI-QQ (API3000, Applied Biosystems) 10V, Negative	splash10-000i-9000000000-9ae015043b014b3c93d9	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - LC-ESI-QQ (API3000, Applied	splash10-000i-9000000000-	View in MoNA

HMDB

GC-MS	GC-MS Spectrum - EI-B (Non-derivatized)
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (Non-derivatized) - 70eV, Positive
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (1 TMS) - 70eV, Positive
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 10V, Negative (Annotated)
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 25V, Negative (Annotated)
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 40V, Negative (Annotated)
LC-MS/MS	LC-MS/MS Spectrum - EI-B (HITACHI RMU-7M) , Positive
LC-MS/MS	LC-MS/MS Spectrum - EI-B (HITACHI M-80B) , Positive
LC-MS/MS	LC-MS/MS Spectrum - LC-ESI-QQ (API3000, Applied Biosystems) 10V, Negative
LC-MS/MS	LC-MS/MS Spectrum - LC-ESI-QQ (API3000, Applied

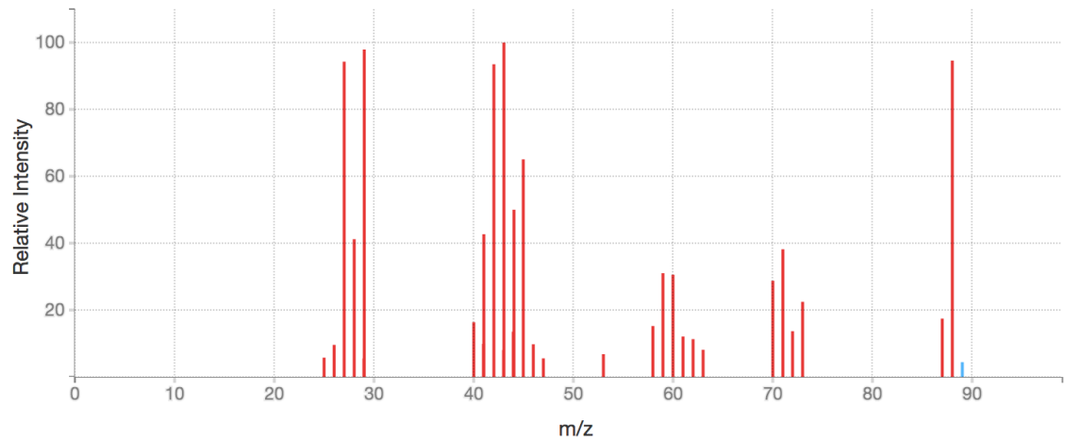
Spectrum View

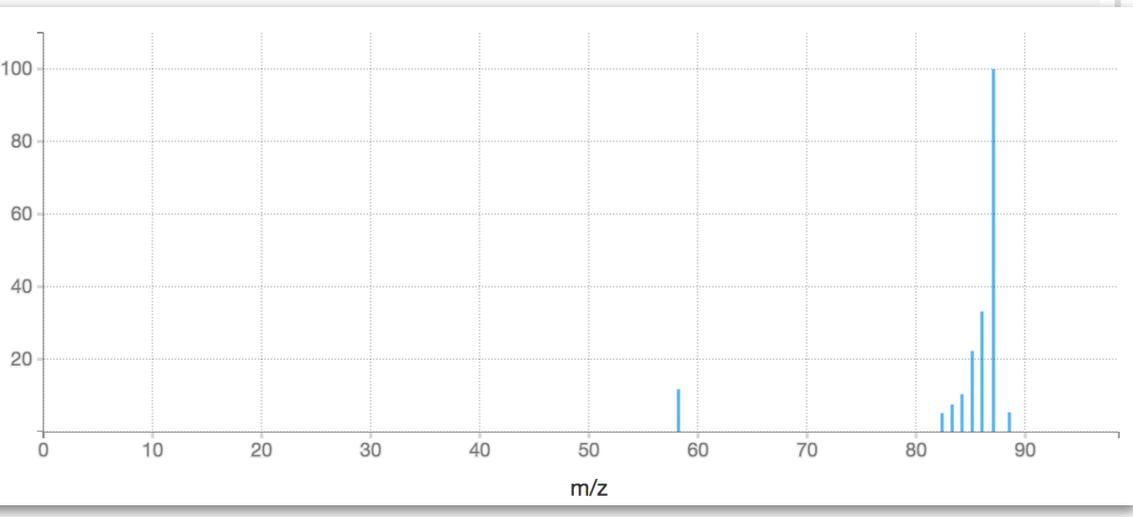


splash10-00fr-9100000000-

View in MoNA

Spectrum View





LC-MS Search | LC-MS/MS Search | GC-MS Search | 1D NMR Search | 2D NMR Search

Query Masses (Da)

175.01
238.19
420.16
780.32
956.25
1100.45

Enter one mass per line (maximum 700 query masses per request)

Ionization

Ion Mode

Positive

Adduct Type

Unknown
M+H
M-2H2O+H
M-H2O+H
M-H2O+NH4
M+Li
M+NH4

Hold Ctrl ( ) or C
select multiple add

Molecular Weight Tolerance ±

0.05

Da

Search

Load Example

LC-MS Search | LC-MS/MS Search | GC-MS Search | 1D NMR Search | 2D NMR Search

Parent Ion Mass (Da) 146.0

Parent Ion Mass Tolerance ± 0.1 Da

Ionization Positive

CID Energy Low

MS/MS Peak List (M/Z & Intensity)

```
40.948 0.174
56.022 0.424
84.37 53.488
101.50 8.285
102.401 0.775
129.670 100.000
146.966 20.070
```

Enter one peak per line

Mass/Charge (m/z) Tolerance ± 0.5 Da

Include predicted spectra?

Search | Load Example

LC-MS Search | LC-MS/MS Search | GC-MS Search | 1D NMR Search | 2D NMR Search

GC/MS Peak list

```
70 54
71 63
72 296
77 86
81 260
87 87
88 240
89 128
90 12
101 73
102 83
103 348
105 82
106 11
115 98
```

Enter a mass (m/z) and a peak intensity corresponding to one peak on each line -- click the "Load Example" button for a standard input. Note also that if only the mass is entered, a default peak intensity of 100 is assumed.

Peak Tolerance ± (Da) 0.1

Include predicted spectra? ☐

Search | Load Example

LC-MS Search | LC-MS/MS Search | GC-MS Search | 1D NMR Search | 2D NMR Search

Spectra Library 1H NMR

Peak List

3.81
3.82
3.83
3.85
3.89
3.90
3.91
4.25
4.26
4.27
4.41
8.19
8.31

Enter one peak per line

Peak Tolerance ± 0.02

Search | Load Example

LC-MS Search | LC-MS/MS Search | GC-MS Search | 1D NMR Search | 2D NMR Search

Spectra Library 2D TOCSY

Peak List

```
3.76 2.126
3.76 2.446
3.76 3.76
2.446 2.126
2.446 2.446
2.446 3.76
2.126 2.126
2.126 2.446
2.126 3.76
```

One Co-ordinate per line with the numbers seperated by a space

X-axis Peak Tolerance ± 0.02

Y-axis Peak Tolerance ± 0.02

Search

Load Example

HMDB 4.0

Normal Concentrations

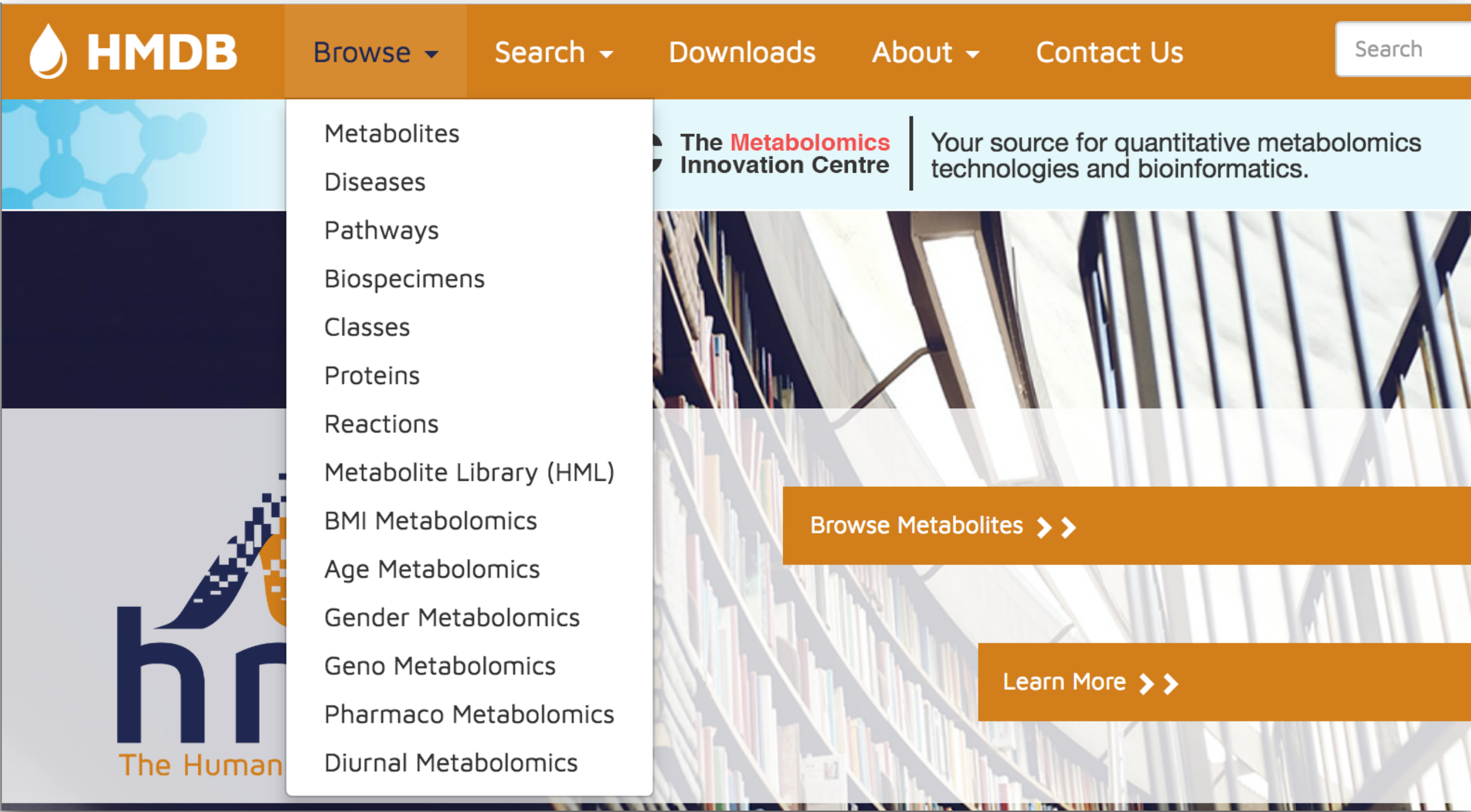
Biospecimen	Status	Value	Age	Sex	Condition	Reference	Details
Blood	Detected and Quantified	1.0 (0.3- 1.5) uM	Adult (>18 years old)	Both	Normal	Geigy Scientific ...	details
Breast Milk	Detected and Quantified	192 +/- 149 uM	Adult (>18 years old)	Female	Normal	24027187	details
Cerebrospinal Fluid (CSF)	Detected and	1.4 (0-2.8) uM	Adult (>18 years old)	Both	Normal	Geigy Scientific	details

Show more...

Abnormal Concentrations

Biospecimen	Status	Value	Age	Sex	Condition	Reference	Details
Feces	Detected but not Quantified		Children (1-13 years old)	Both	Autism	24130822	details
Feces	Detected but not Quantified		Children (1-13 years old)	Both	Pervasive Developmental Disorder Not Otherwise Specified	24130822	details

HMDB: 4.0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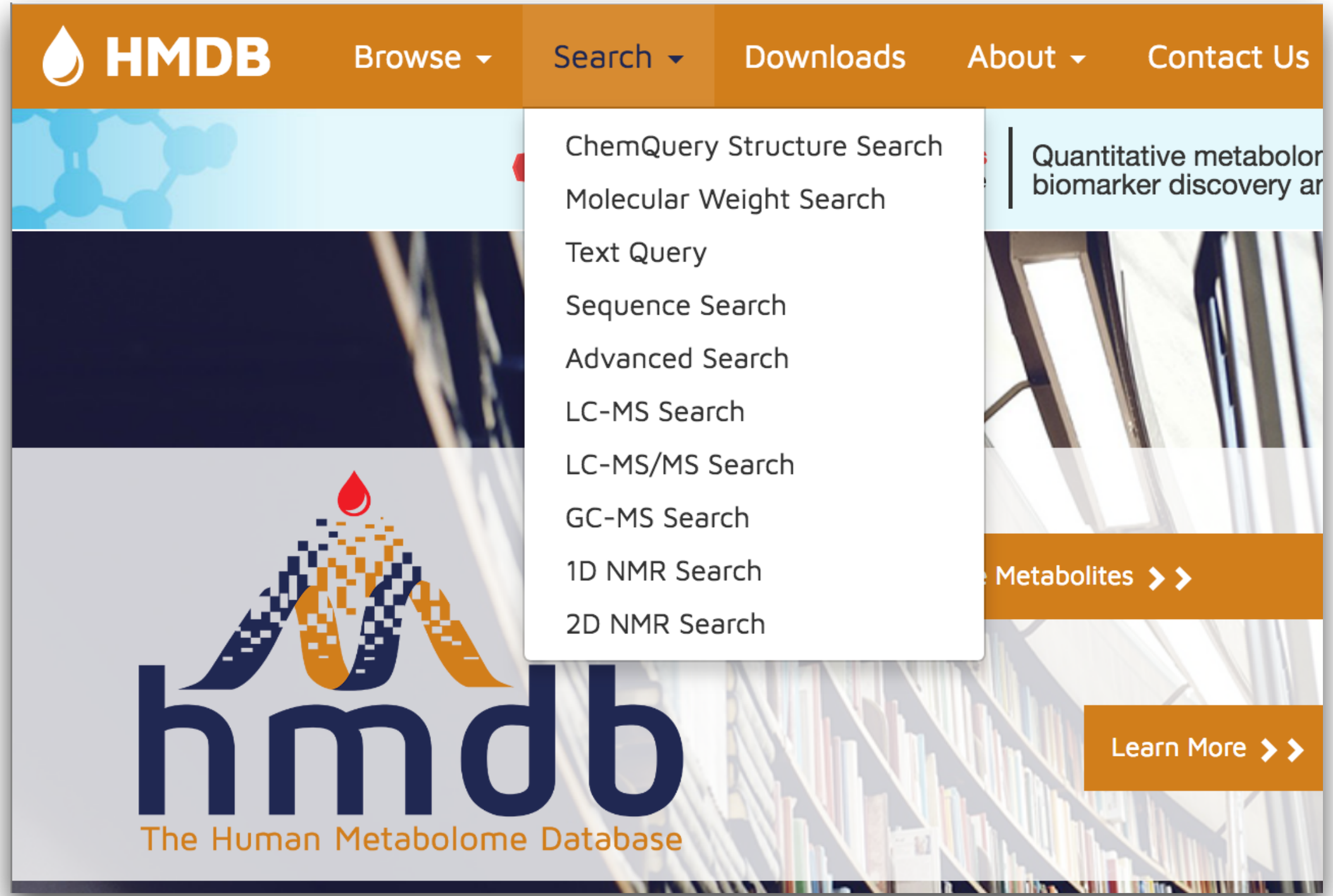
HMDB: 4.0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Metabolite and Protein Data (in XML format)

Data Set	Released on	XML File	File Size
All Metabolites	2018-07-08	Download	615 MB
All Proteins	2018-07-08	Download	26.7 MB
Urine Metabolites	2018-07-09	Download	26.2 MB
Serum Metabolites	2018-07-09	Download	197 MB
CSF Metabolites	2018-07-09	Download	8.23 MB
Saliva Metabolites	2018-07-09	Download	16.1 MB
Feces Metabolites	2018-07-09	Download	61.8 MB
Sweat Metabolites	2018-07-09	Download	3.12 MB

Spectra

Data Set	Released on	Download Link	File Size
Mass Spectra Image Files	2018-07-08	Download	166 MB
NMR Spectra FID Files	2018-07-08	Download	1.92 GB
Raw NMR Spectra Peaklist Files (TXT)	2018-07-08	Download	918 KB
Raw GC-MS Spectra Peaklist Files (TXT) - Predicted	2018-07-08	Download	23.1 MB
Raw MS-MS Spectra Peaklist Files (TXT) - Predicted	2018-07-08	Download	158 MB
Raw MS-MS Spectra Peaklist Files (TXT) - Experimental	2018-07-08	Download	2.29 MB
All Raw Spectra Peaklist Files (TXT)	2018-07-08	Download	1.04 GB
NMR Spectra Files (XML)	2018-07-08	Download	4.45 MB
GC-MS Spectra Files (XML) - Predicted	2018-07-08	Download	69.1 MB
GC-MS Spectra Files (XML) - Experimental	2018-07-08	Download	17.2 MB
MS-MS Spectra Files (XML) - Predicted	2018-07-08	Download	485 MB

DrugBank

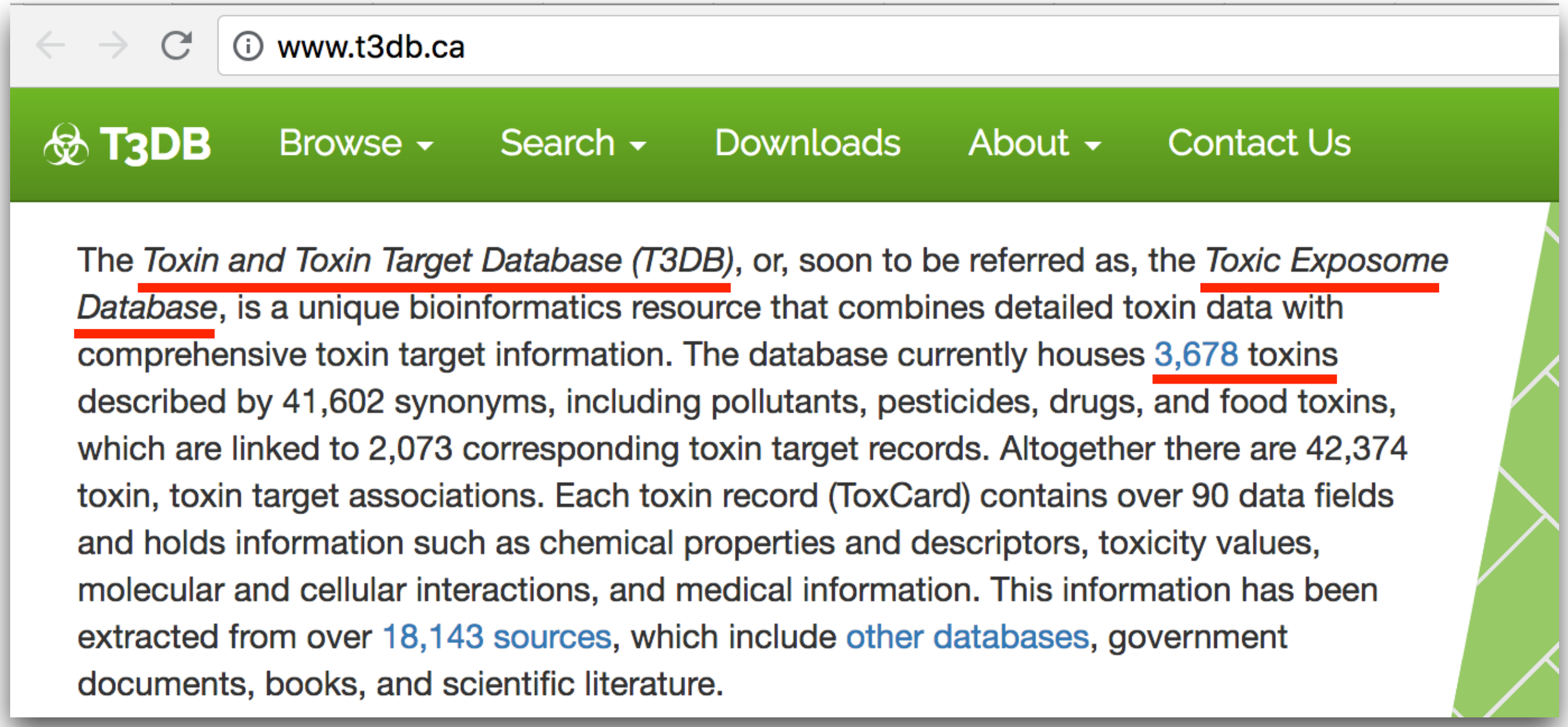
Secure | https://www.drugbank.ca

DRUGBANK

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug data with comprehensive drug target information.

> The latest release of DrugBank (version 5.1.1, released 2018-07-03) contains 11,678 drug entries including 2,625 approved small molecule drugs, 1,115 approved biotech (protein/peptide) drugs, 128 nutraceuticals and over 5,504 experimental drugs. Additionally, 5,128 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries. Each DrugCard entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data.

T3DB


www.t3db.ca
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The Toxin and Toxin Target Database (T3DB), or, soon to be referred as, the Toxic Exposome Database, is a unique bioinformatics resource that combines detailed toxin data with comprehensive toxin target information. The database currently houses 3,678 toxins described by 41,602 synonyms, including pollutants, pesticides, drugs, and food toxins, which are linked to 2,073 corresponding toxin target records. Altogether there are 42,374 toxin, toxin target associations. Each toxin record (ToxCard) contains over 90 data fields and holds information such as chemical properties and descriptors, toxicity values, molecular and cellular interactions, and medical information. This information has been extracted from over 18,143 sources, which include other databases, government documents, books, and scientific literature.

SMPDB

smpdb.ca

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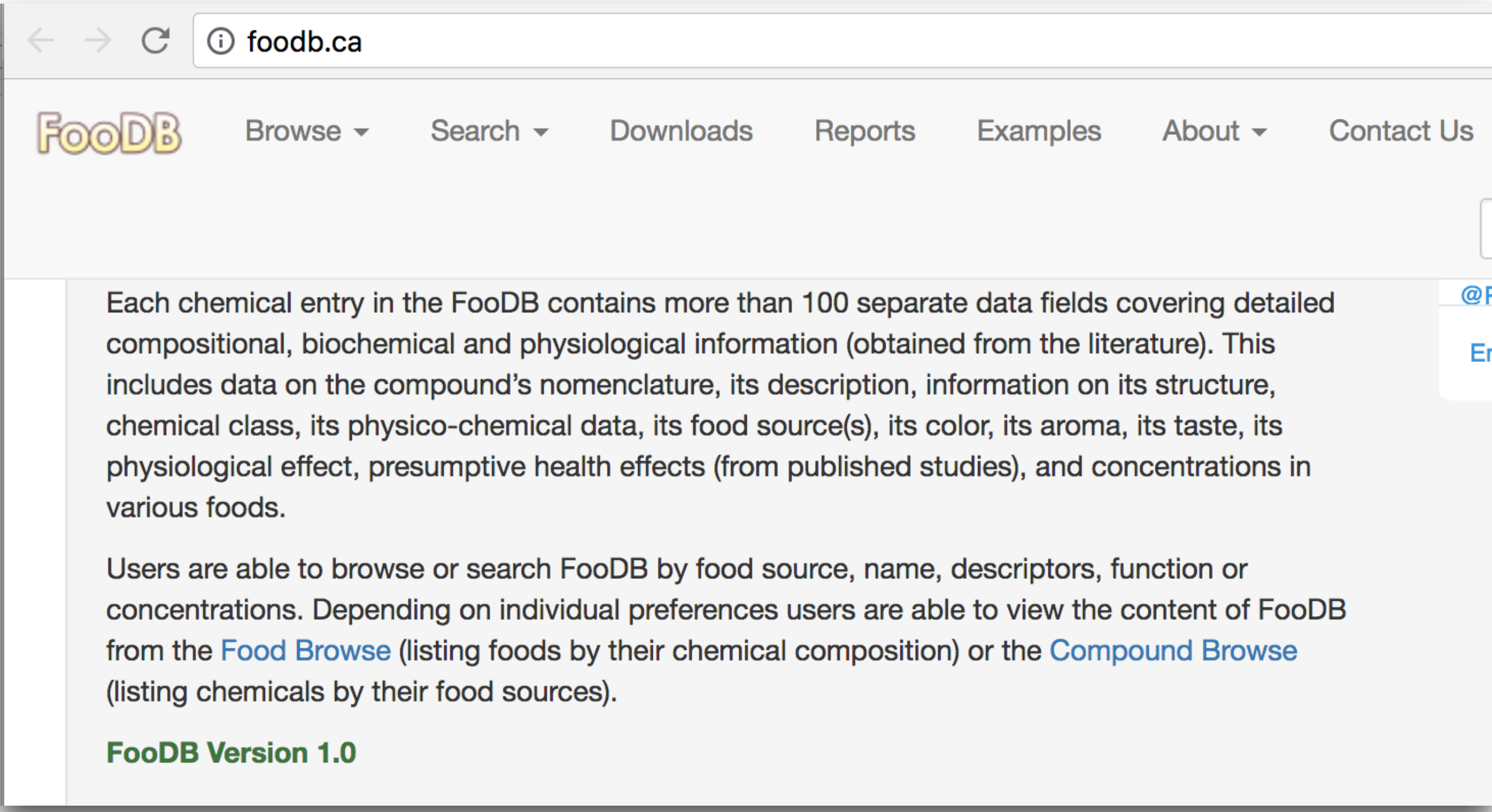
Small Molecule Pathway Database

Brought to you by the creators of the Human Metabolome Database (HMDB) and DrugBank:

SMPDB (The Small Molecule Pathway Database) is an interactive, visual database containing more than 30 000 small molecule pathways found in humans. The majority of these pathways are not found in any other pathway database. SMPDB is designed specifically to support pathway elucidation and pathway discovery in metabolomics, transcriptomics, proteomics and systems biology. It is able to do so, in part, by providing exquisitely detailed, fully searchable, hyperlinked diagrams of human metabolic pathways, metabolic disease pathways, metabolite signaling pathways and drug-action pathways. All SMPDB pathways include information on the relevant organs, subcellular compartments, protein_complex cofactors, protein_complex locations, metabolite locations, chemical structures and protein_complex quaternary structures. Each small molecule is hyperlinked to detailed descriptions contained in the HMDB or DrugBank and each protein_complex or enzyme complex is hyperlinked to UniProt. All SMPDB pathways are accompanied with detailed descriptions and references, providing an overview of the pathway, condition or processes depicted in each diagram. The database is easily browsed and supports full text, sequence and chemical structure searching. Users may query SMPDB with lists of metabolite names, drug names, genes/protein_complex names, SwissProt IDs, GenBank IDs, Affymetrix IDs or Agilent microarray IDs. These queries will produce lists of matching pathways and highlight the matching molecules on each of the pathway diagrams. Gene, metabolite and protein_complex concentration data can also be visualized through SMPDB's mapping interface. All of SMPDB's images, image maps, descriptions and tables are downloadable.

Get started now: ★ Browse Pathways ★

FooDB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Each chemical entry in the FooDB contains more than 100 separate data fields covering detailed compositional, biochemical and physiological information (obtained from the literature). This includes data on the compound's nomenclature, its description, information on its structure, chemical class, its physico-chemical data, its food source(s), its color, its aroma, its taste, its physiological effect, presumptive health effects (from published studies), and concentrations in various foods.
Users are able to browse or search FooDB by food source, name, descriptors, function or concentrations. Depending on individual preferences users are able to view the content of FooDB from the Food Browse (listing foods by their chemical composition) or the Compound Browse (listing chemicals by their food sources).
FooDB Version 1.0

Compound Databases

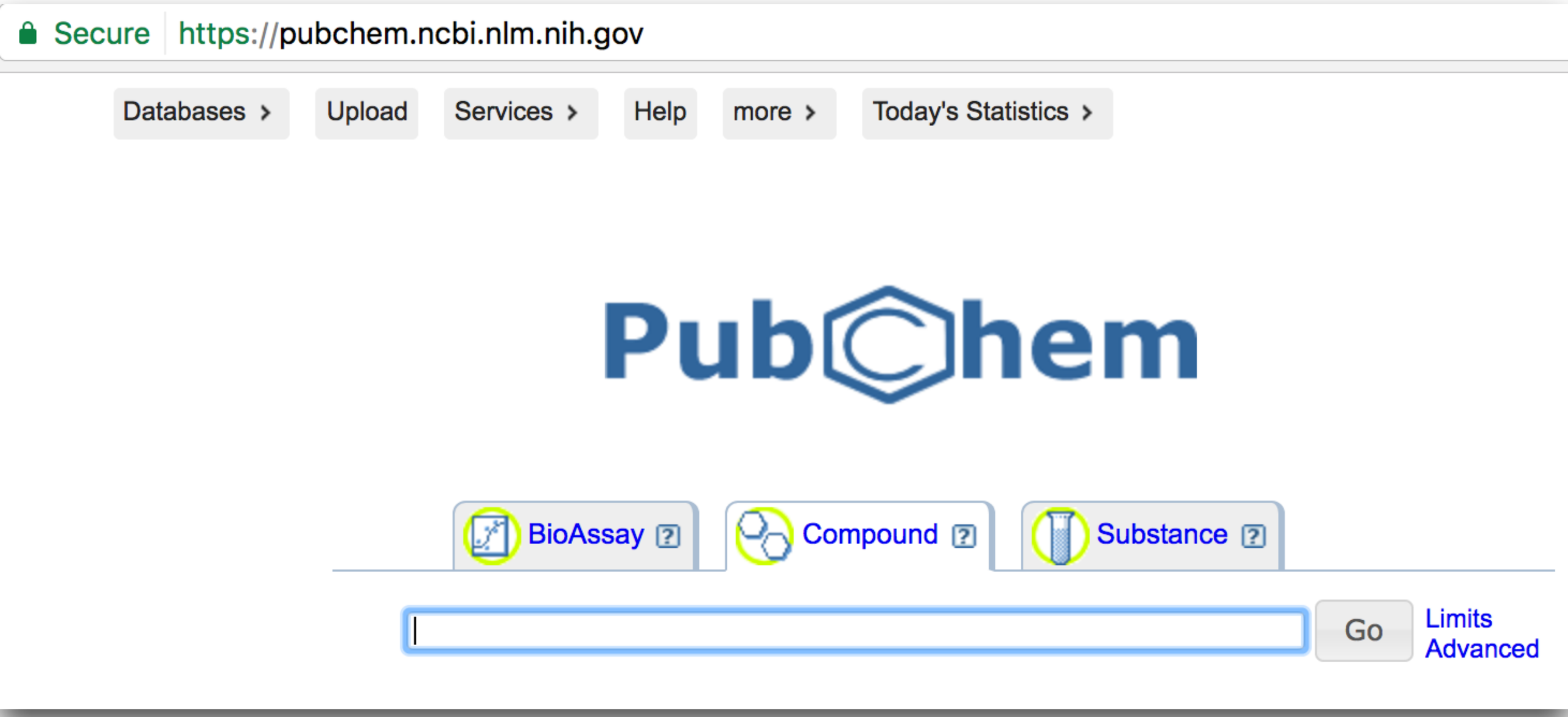
Compound databases

- PubChem
- ChemSpider
- ChEBI
- KEGG Glycan
- IIMDB

Compound databases

- PubChem
- ChemSpider
- ChEBI
- KEGG Glycan
- IIMDB

PubChem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BioAssay
Compound
Substance
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Limits
Advanced

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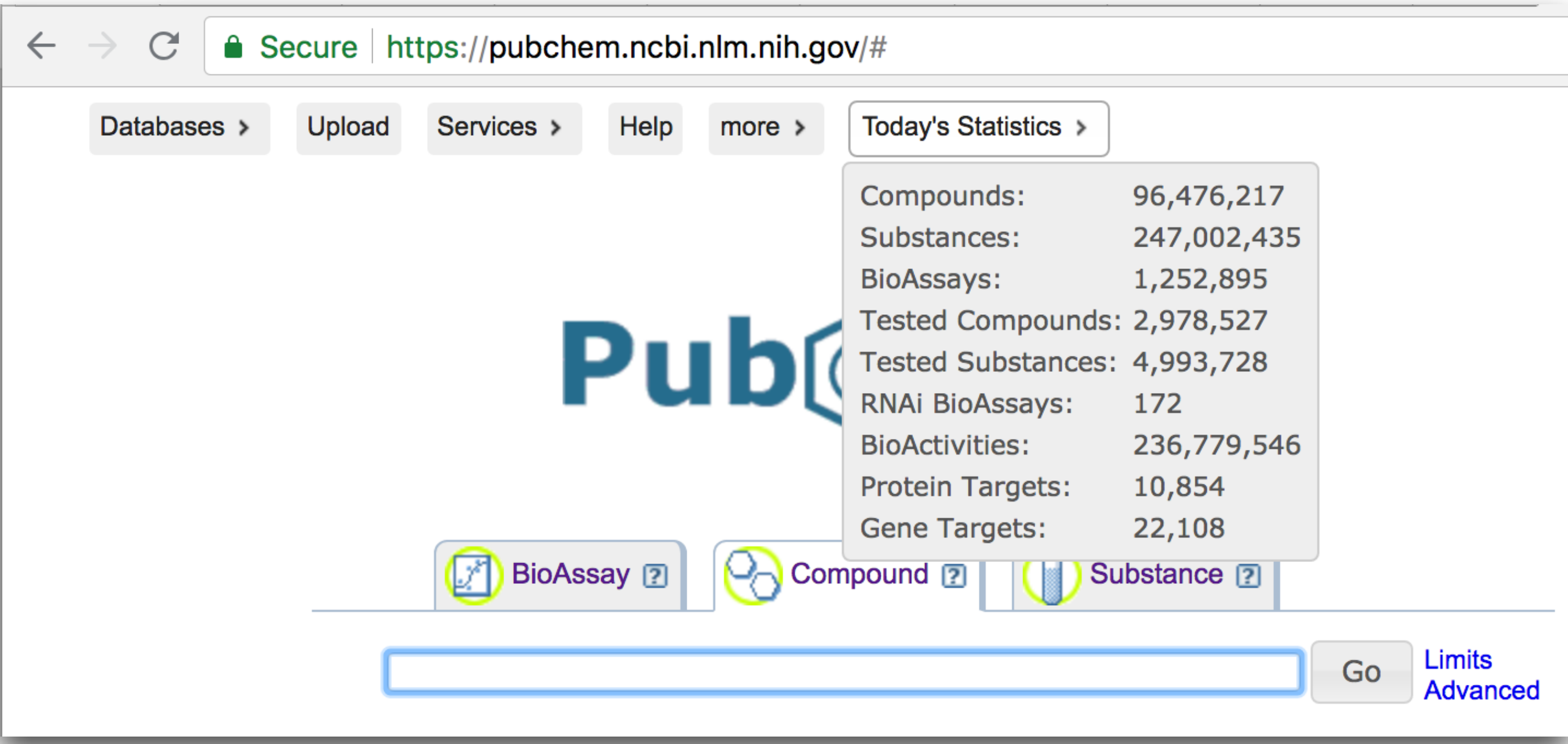
- Statistics (July 25, 2018)



PubChem

- Information on one compound

L-proline

Cite this Record

STRUCTURE VENDORS DRUG INFO PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID:	145742
Chemical Names:	L-proline; 147-85-3; Proline; L-(-)-Proline; 2-pyrrolidinecarboxylic acid; (-)-Proline More...
Molecular Formula:	$C_5H_9NO_2$
Molecular Weight:	115.132 g/mol
InChI Key:	ONIBWKKTOPOVIA-BYPYZUCNSA-N
Drug Information:	Drug Indication Therapeutic Uses FDA UNII

L-proline is a non-essential amino acid that is synthesized from GLUTAMIC ACID. It is an essential component of COLLAGEN and is important for proper functioning of joints and tendons.

PubChem

Contents

1 2D Structure

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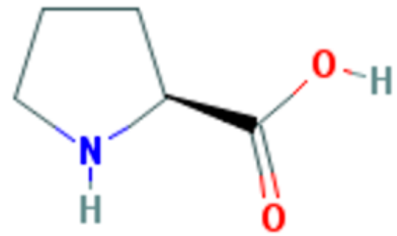

Magnify

2 3D Conformer

PubChem

Contents

5 Chemical and Physical Properties

5.1 Computed Properties

Property Name	Property Value
Molecular Weight	115.132 g/mol
Hydrogen Bond Donor Count	2
Hydrogen Bond Acceptor Count	3
Rotatable Bond Count	1
Complexity	103
CACTVS Substructure Key Fingerprint	AAADccBiMAAAAAAAAAAAAAAAAAAAW AAAAAAAAAAAAAAAAAAAAAHgAQCAA ACCjBgAQACALAAgAIAACQCAAAAAAAAA AAAIGIAAACABIAgCAEQAAEEACQAACYE QAAAAAAAAAAAAAAAAAAAAAAAAAAA AAAA==
Topological Polar Surface Area	49.3 A^2
Monoisotopic Mass	115.063 g/mol
Exact Mass	115.063 g/mol
XLogP3	-2.5
Compound Is Canonicalized	true
Formal Charge	0

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Compound_3D/		4/10/16, 7:00:00 PM
Other/		7/5/15, 7:00:00 PM
RDF/		6/11/18, 9:30:00 AM
README	1.7 kB	11/3/16, 7:00:00 PM
Substance/		7/23/10, 7:00:00 PM
Target/		3/9/17, 6:00:00 PM
data_spec	0 B	7/13/11, 7:00:00 PM
presentations/		3/3/16, 6:00:00 PM
publications/		1/19/16, 6:00:00 PM
specifications/		3/23/14, 7:00:00 PM

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README		
Substance/		
Target/		
data_spec		
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Extras/		10/23/17, 7:00:00 PM
Monthly/		7/1/18, 11:47:00 AM
README	4.1 kB	10/18/13, 7:00:00 PM
Weekly/		7/22/18, 9:50:00 AM

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Compound_3		
Other/		
RDF/		
README		
Substance/		
Target/		
data_spec		
presentations/		
publications/		1/19/16, 6:00:00 PM
specifications/		3/23/14, 7:00:00 PM

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SDF/		7/10/18, 7:37:00 AM
XML/		7/10/18, 7:37:00 AM

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Name		
Bioassay/		
Compound/		
Compound_3		
Other/		
RDF/		
README		
Substance/		
Target/		
data_spec		
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publications/		1/19/16, 6:00:00 PM
specifications/		3/23/14, 7:00:00 PM

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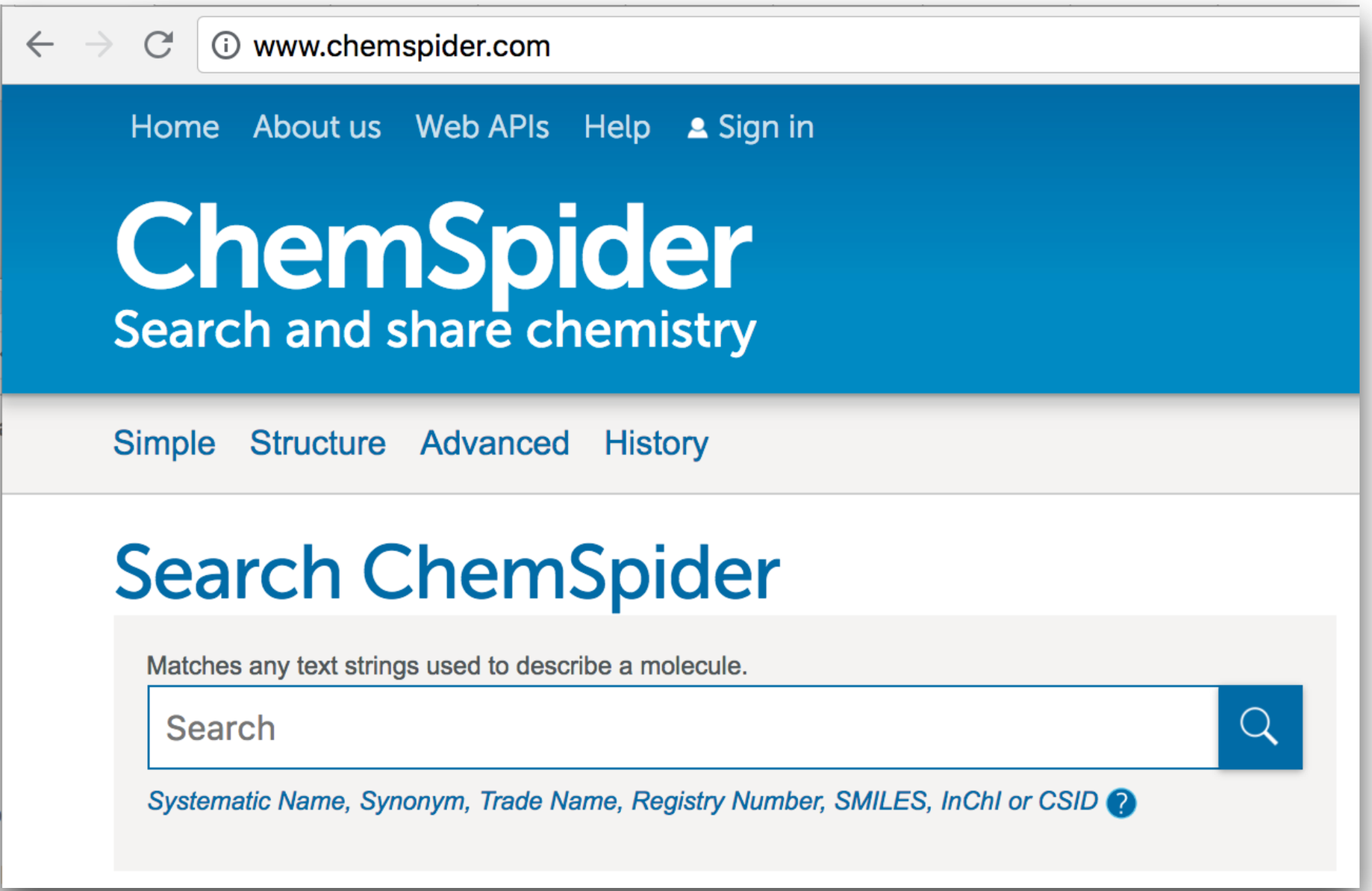
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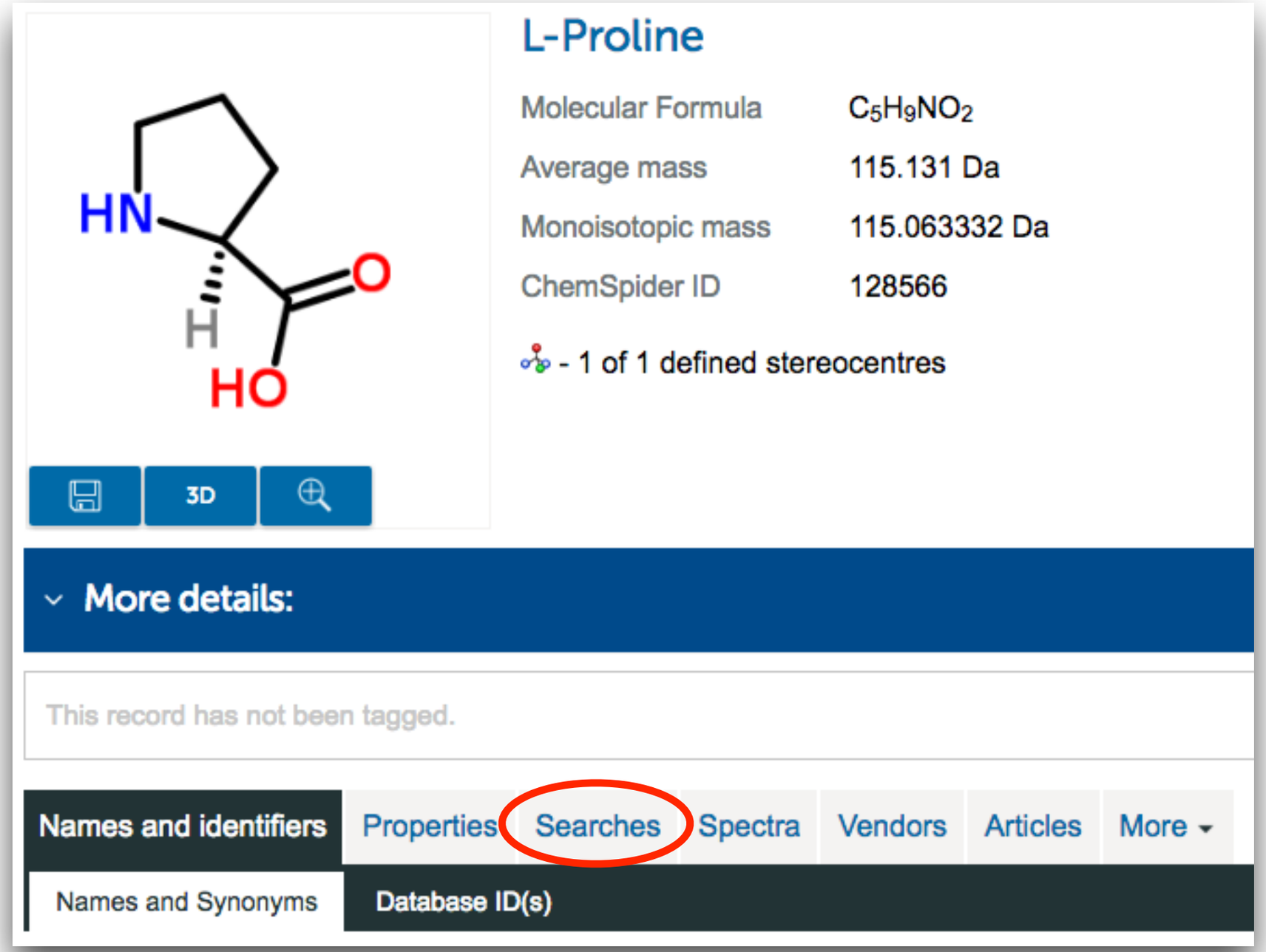

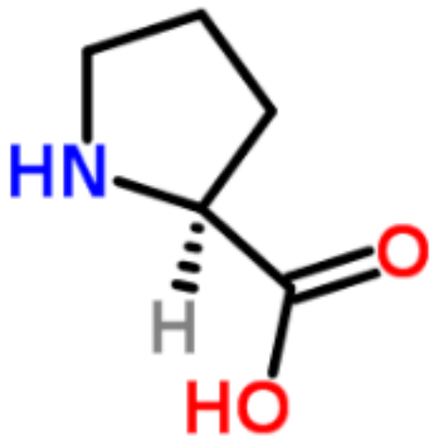

3D

L-Proline

Molecular Formula	$C_5H_9NO_2$
Average mass	115.131 Da
Monoisotopic mass	115.063332 Da
ChemSpider ID	128566

- 1 of 1 defined stereocentres

More details:

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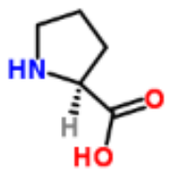
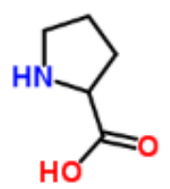
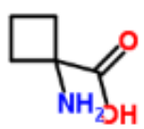
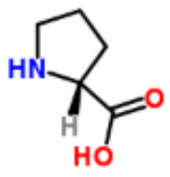
ChemSpider

- Compounds with the same molecular formula

Found 501 results

Search term: **MF = 'C_{5}H_{9}NO_{2}'**

1 2 3 4 5

ID	Structure	Molecular Formula	Molecular Weight	# of Data Sources	# of References	# of PubMed	# of RSC
128566 - 1/1 defined		$C_5H_9NO_2$	115.1305	136	11954	28480	3548
594 - 0/1 defined		$C_5H_9NO_2$	115.1305	131	737	28034	3319
80908		$C_5H_9NO_2$	115.1305	110	185	8	5
8640 - 1/1 defined		$C_5H_9NO_2$	115.1305	103	293	701	268

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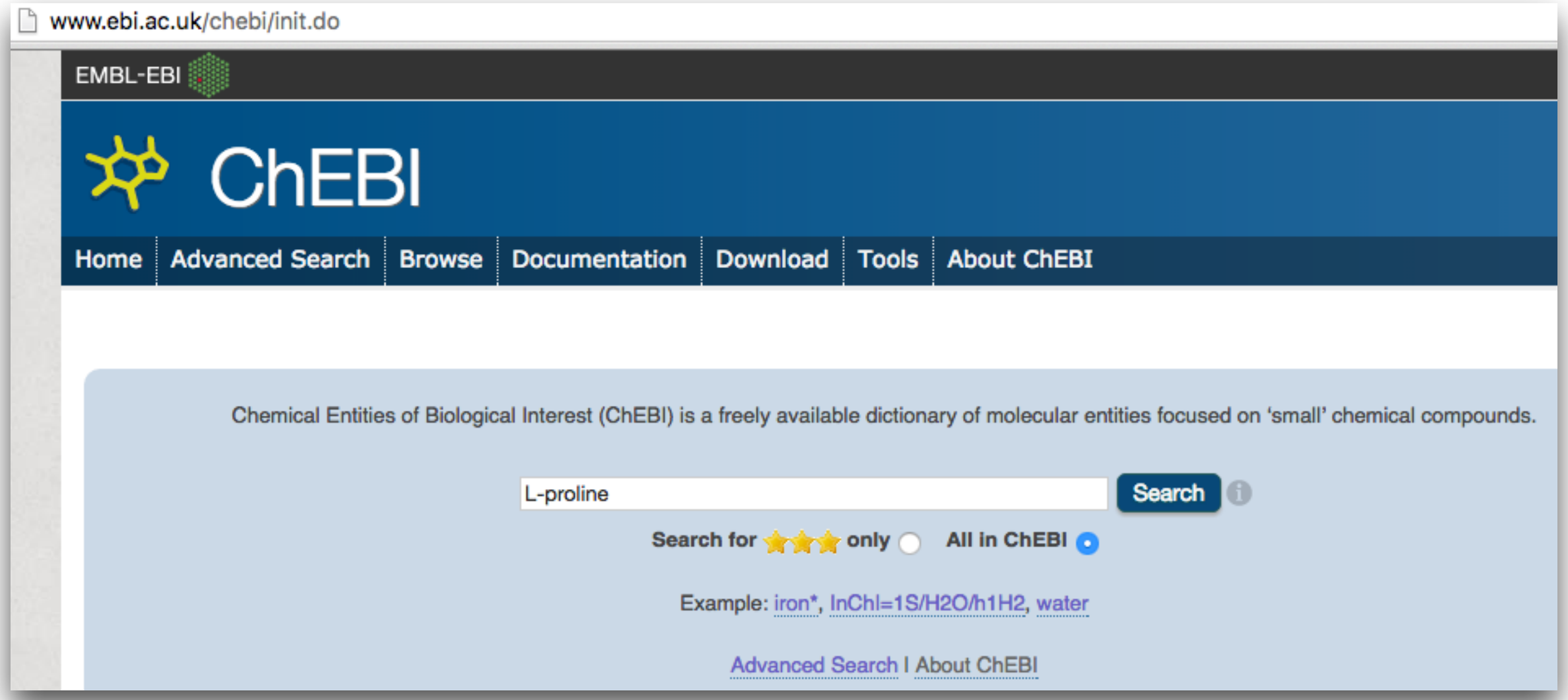

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- About

ChEBI > About ChEBI

1. Introduction

Chemical **E**ntities of **B**iological **I**nterest (**ChEBI**) is a freely available dictionary of molecular entities focused on 'small' chemical compounds. The term 'molecular entity' refers to any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc., identifiable as a separately distinguishable entity. The molecular entities in question are either products of nature or synthetic products used to intervene in the processes of living organisms.

ChEBI incorporates an ontological classification, whereby the relationships between molecular entities or classes of entities and their parents and/or children are specified.

ChEBI uses nomenclature, symbolism and terminology endorsed by the following international scientific bodies:

- International Union of Pure and Applied Chemistry (IUPAC)
- Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (NC-IUBMB)

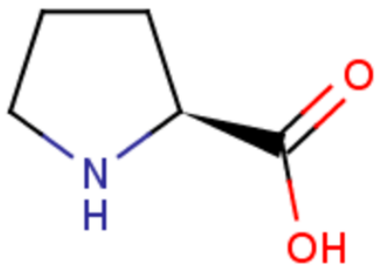
Molecules directly encoded by the genome (e.g. nucleic acids, proteins and peptides derived from proteins by cleavage) are *not* as a rule included in ChEBI.

ChEBI

- One compound

CHEBI:17203 - L-proline

Main | ChEBI Ontology | Automatic Xrefs | Reactions | Pathways | Models



ChEBI Name	**L-proline**
ChEBI ID	**CHEBI:17203**
ChEBI ASCII Name	L-proline
Definition	Pyrrolidine in which the *pro-S* hydrogen at position 2 is substituted by a carboxylic acid group. L-Proline is the only one of the twenty DNA-encoded amino acids which has a secondary amino group α to the carboxyl group. It is an essential component of collagen and is important for proper functioning of joints and tendons. It also helps maintain and strengthen heart muscles.
Stars	⭐⭐⭐ This entity has been manually annotated by the ChEBI Team.
Secondary ChEBI IDs	CHEBI:45159, CHEBI:45100, CHEBI:45040, CHEBI:42067, CHEBI:184637, CHEBI:6286, CHEBI:13154, CHEBI:21373
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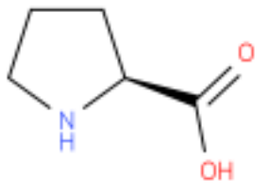

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314 entries found, displaying 1 to 15.

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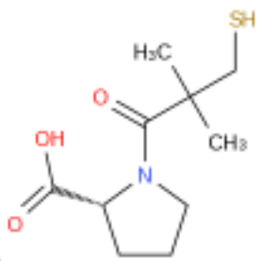
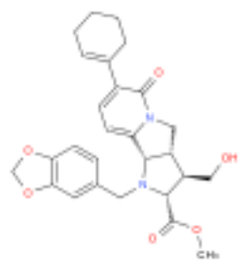


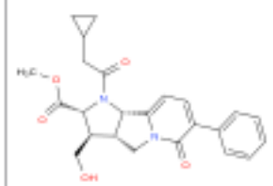
CHEBI:95254
Stars: ★★☆

(2R,3R,3aS,9bS)-1-(1,3-benzodioxol-5-ylmethyl)-7-(1-cyclohexenyl)-3-(hydroxymethyl)-6-oxo-3,3a,4,9b-tetrahydro-2H-pyrrolo[2,3-a]indolizine-2-carboxylic acid methyl ester

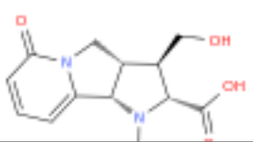


CHEBI:98944
Stars: ★★☆

(2R,3R,3aS,9b
(hydroxymeth
tetrahydro-2H
acid methyl es



(2R,3R,3aS,9bS)-1-(cyclopentylcarbamoyl)-3-(hydroxymethyl)-6-oxo-3,3a,4,9b-tetrahydro-2H-pyrrolo[2,3-a]indolizine-2-carboxylic acid



CHEBI:98447
Stars: ★★☆

(2R,3R,3aS,9bS)-1-(cyclopentylmethyl)-3-(hydroxymethyl)-7-(2-methoxyphenyl)-6-oxo-3,3a,4,9b-tetrahydro-2H-pyrrolo[2,3-a]indolizine-2-carboxylic acid methyl ester

CHEBI:131226
Stars: ★★☆

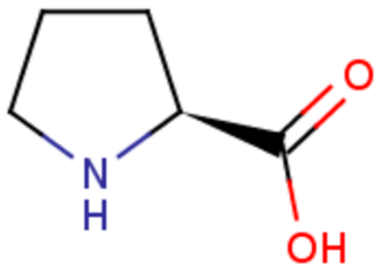
(2R,3R,3aS,9b
(hydroxymeth
tetrahydro-2H
acid

ChEBI

- One compound

CHEBI:17203 - L-proline

Main | ChEBI Ontology | Automatic Xrefs | Reactions | Pathways | Models



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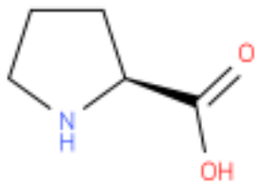

Edit Search

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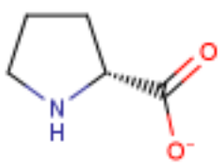
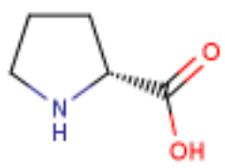
D-prolinate

CHEBI:32867
Stars: ★★★

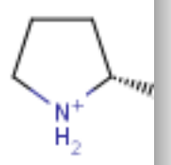


D-proline

CHEBI:16313
Stars: ★★★



D-proline



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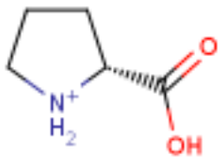
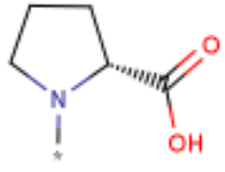
CHEBI:32868
Stars: ★★★



D-prolino group

CHEBI:32870
Stars: ★★★



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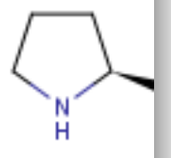
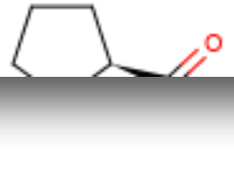


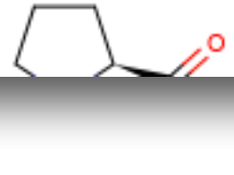
L-proline

CHEBI:17203
Stars: ★★★

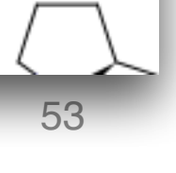


L-proline zwitterion

CHEBI:60039
Stars: ★★★



L-prolinium



Spectral Databases

Spectral databases

- NIST 14
- METLIN
- MassBank
- MoNA
- Gold Metabolome Database
- Feign GC-MS database
- HMDB
- BMRB
- Madison Metabolomics Consortium Database
- BML-NMR
- mzCloud

Spectral databases

- NIST 17
- METLIN
- MassBank
- MoNA
- Gold Metabolome Database
- Feign GC-MS database
- HMDB
- BMRB
- Madison Metabolomics Consortium Database
- BML-NMR
- mzCloud

NIST 17

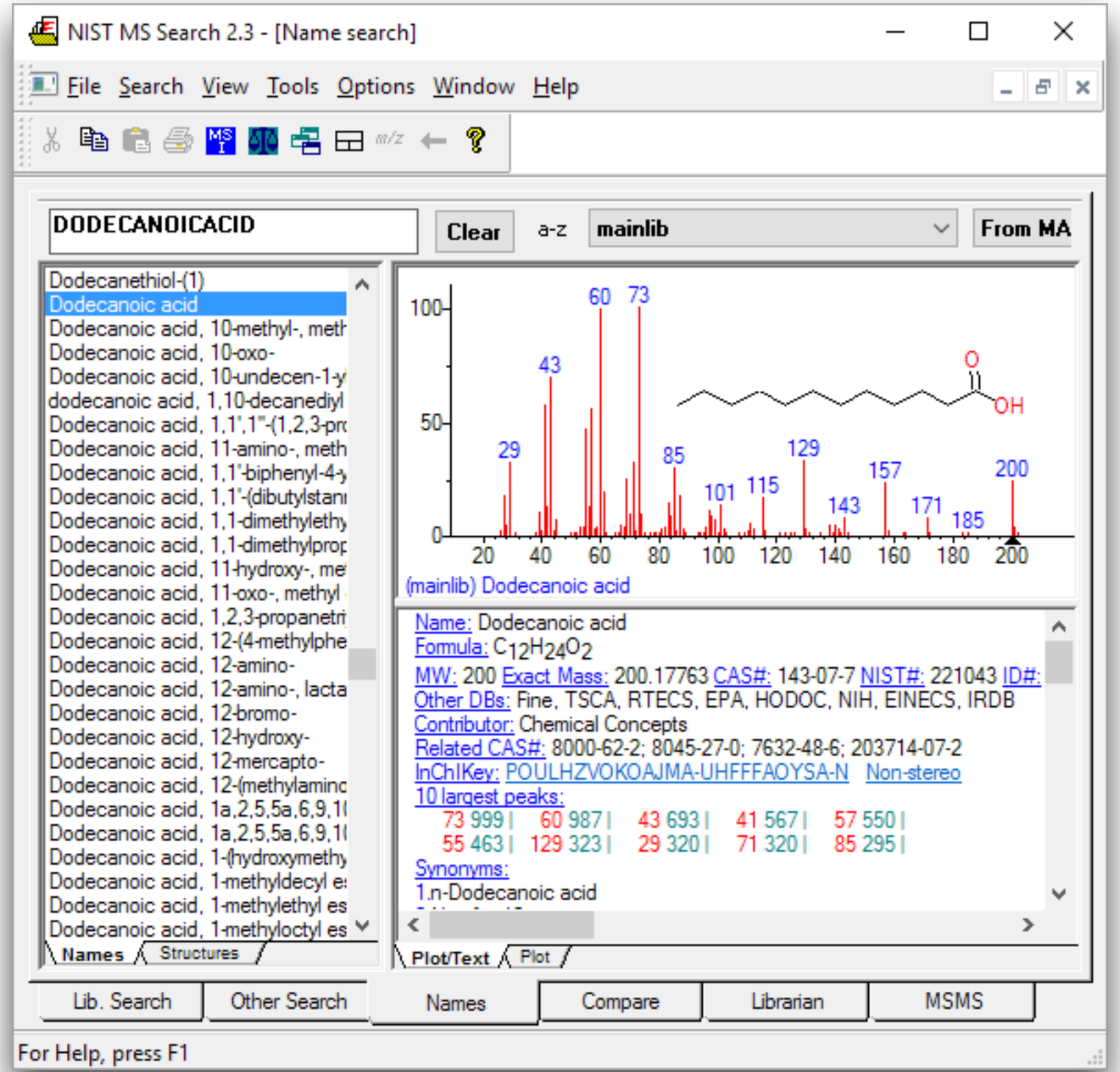
- Electron ionization mass spectral library
  - 306,622 spectra of 267,376 unique compounds

- MS/MS library: 652,475 spectra
  - 176,594 ion trap spectra for 120,346 different ions of 14,351 compounds
  - 475,881 collision cell spectra (QTOF and tandem quad) spectra for 39,158 different ions of 14,073 compounds

NIST 17

- New ways to identify unknowns
  - Hybrid search
  - Annotated recurring spectral libraries
  - High mass accuracy MS Interpreter

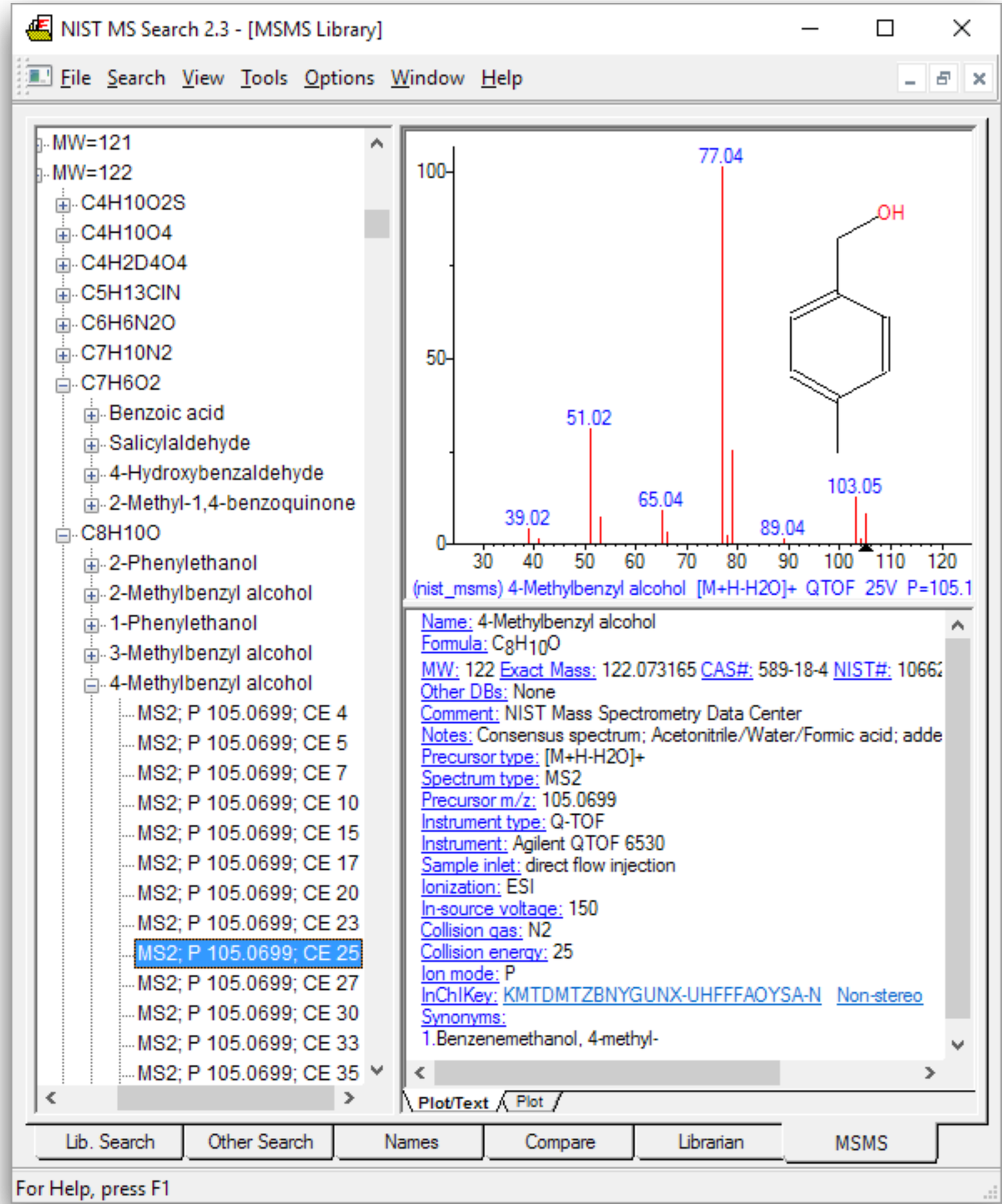
NIST 17 EI library



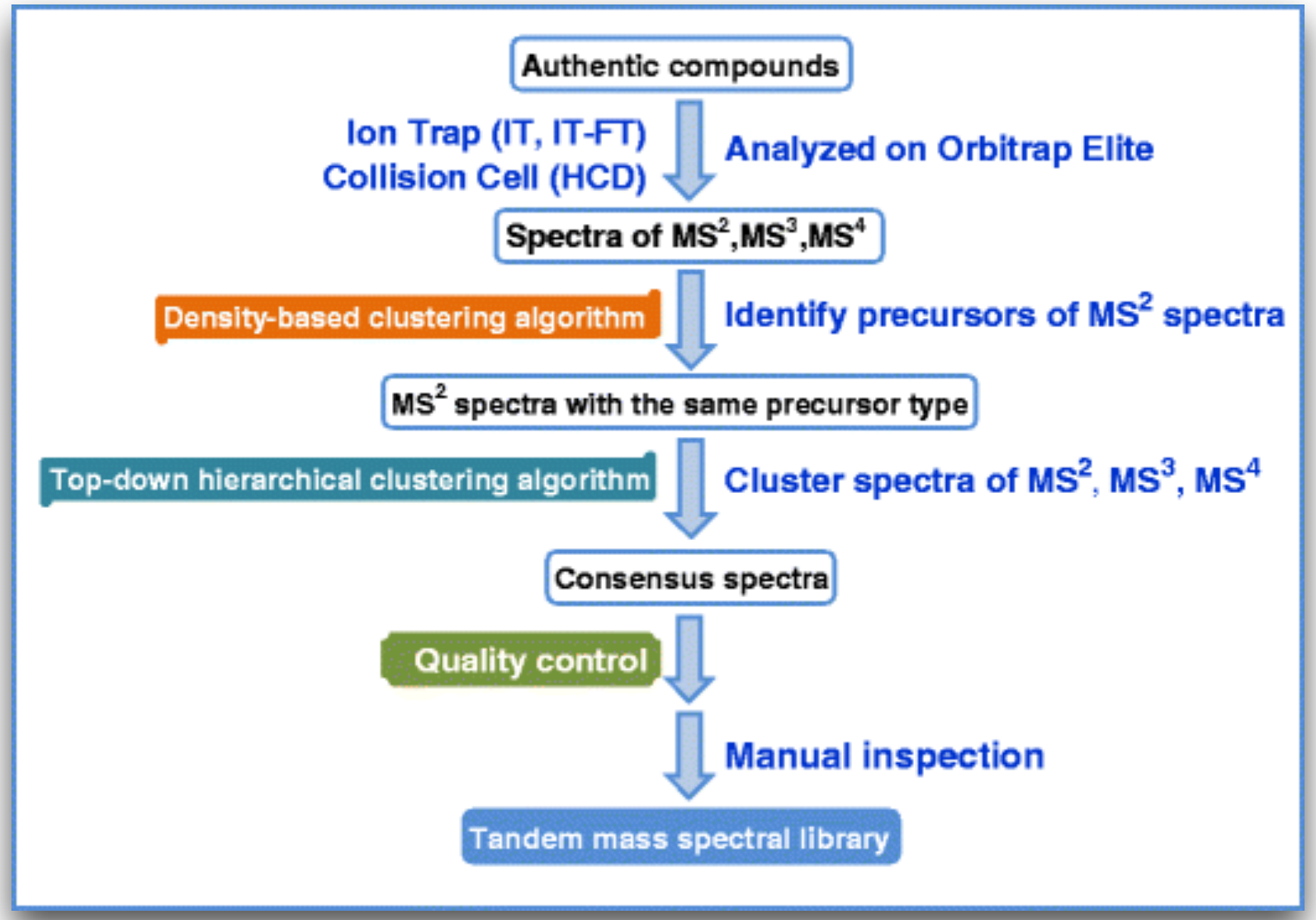
NIST 17 EI library

- Focuses on
  - Drugs, metabolites, and poisons
  - Pesticides and fungicides
  - Organics present in soil, water, and air
  - Amino acids, di- and tai-peptides
  - Common sample contaminants
  - Common analytical derivatives of the above

NIST 17
MS/MS library



NIST 17 MS/MS library



NIST 17 MS/MS library

- 13,045 precursor precursor ions

  [M+H]+, [M+2H]2+, [M+H-H2O]+, [M+H-NH3]+, [M+H-OH]+, [M+H+H2O]+, [M+NH4]+, [2M+H]+, [3M+H]+, [M+Na]+, [M-H+2Na]+, [M-2H+3Na]+, [M+K]+, [M-H+2K]+, [M-2H+3K]+, [M+Li]+, [M-H+2Li]+

- 6,001 negative precursors ions

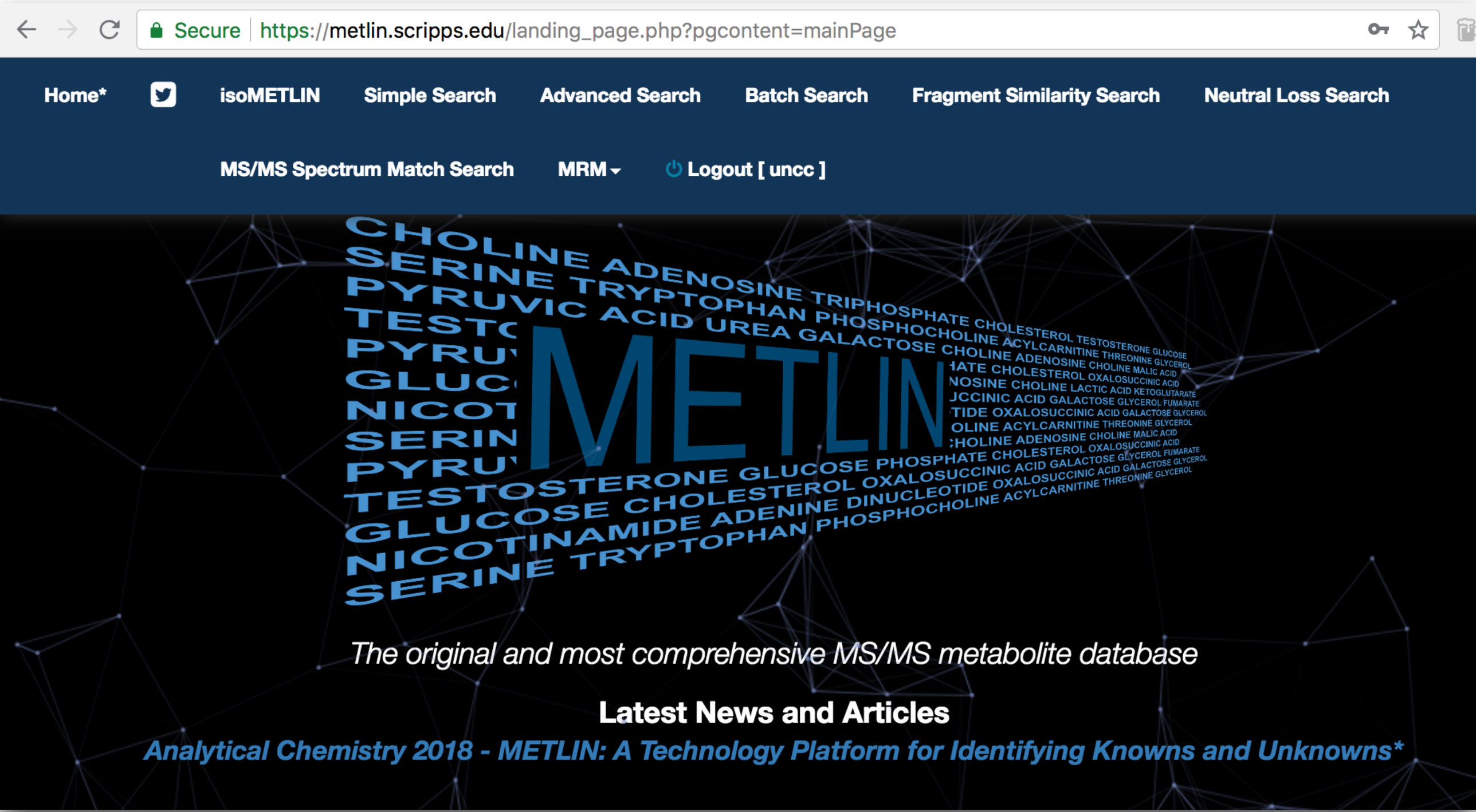
  [M-H]-, [M-2H]2-, [M-H-H2O]-, [M-H-NH3]-, [M-H+H2O]-, [M-H+NH3]-, [2M-H]-, [3M-H]-

NIST 17 MS/MS library

- MS3 and MS4 spectra of the most intense peaks in the MS2 and MS3 spectra, respectively

- New precursors:
  - In-source fragments
  - [M+H-neutral]+ and [M-H-neutral]-
  - Fragments from the original target compound within the ESI source

METLIN


Secure
https://metlin.scripps.edu/landing_page.php?pgcontent=mainPage
Home*
isoMETLIN
Simple Search
Advanced Search
Batch Search
Fragment Similarity Search
Neutral Loss Search
MS/MS Spectrum Match Search
MRM
Logout [uncc]
METLIN
The original and most comprehensive MS/MS metabolite database
Latest News and Articles
Analytical Chemistry 2018 - METLIN: A Technology Platform for Identifying Knowns and Unknowns*

METLIN

Metabolite Searching

METLIN has multiple searching capabilities including single, batch, precursor ion, neutral loss, accurate mass, and fragment searches. The popular similarity search algorithm for unknown characterization, another METLIN search option, originated on METLIN in 2008.

Tandem Mass Spectrometry

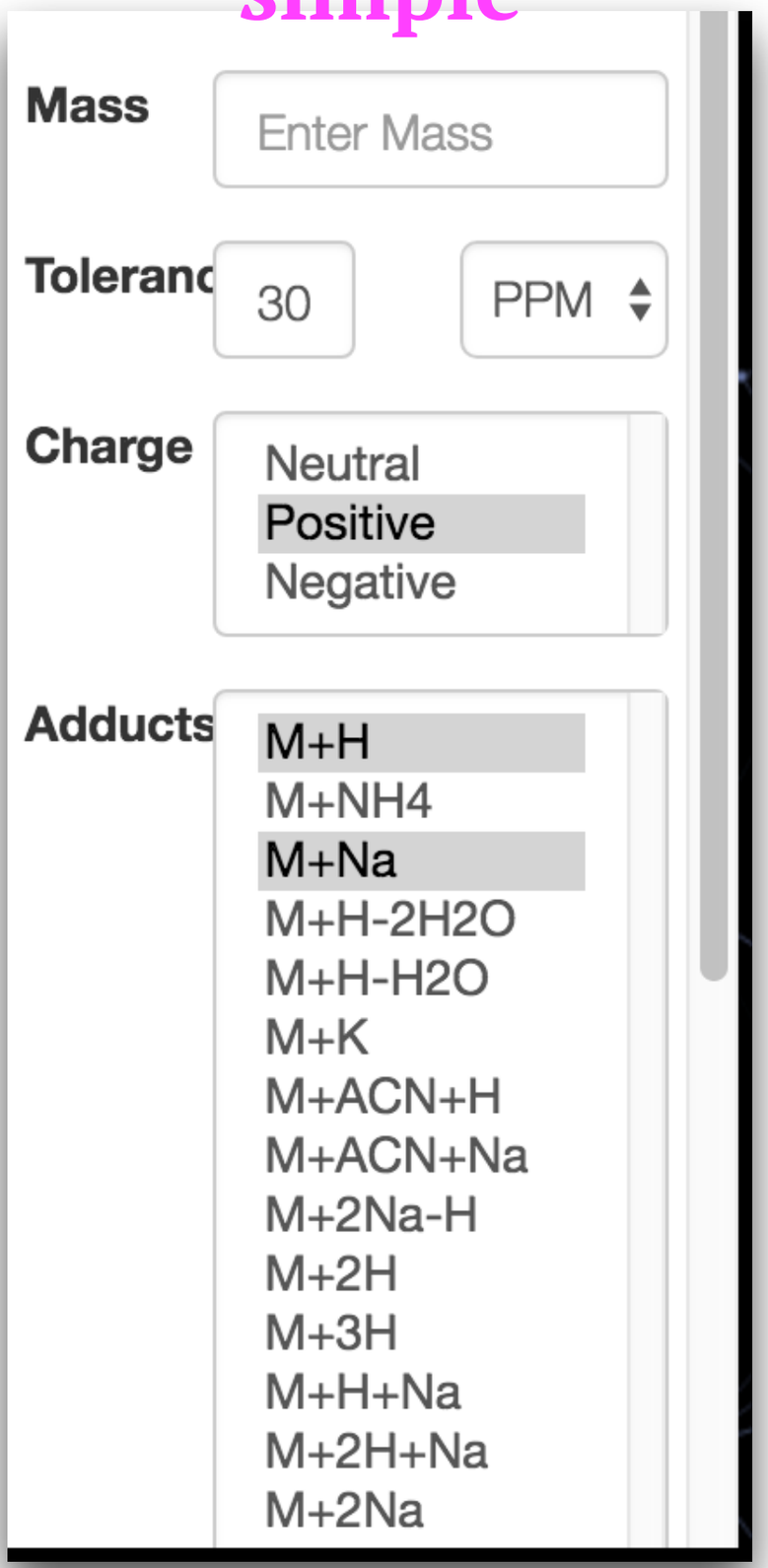
METLIN represents the largest MS/MS collection of data with the database generated at multiple collision energies and in positive and negative ionization modes. The data is generated on multiple instrument types including SCIEX, Agilent, Bruker and Waters QTOF mass spectrometers.

Metabolites

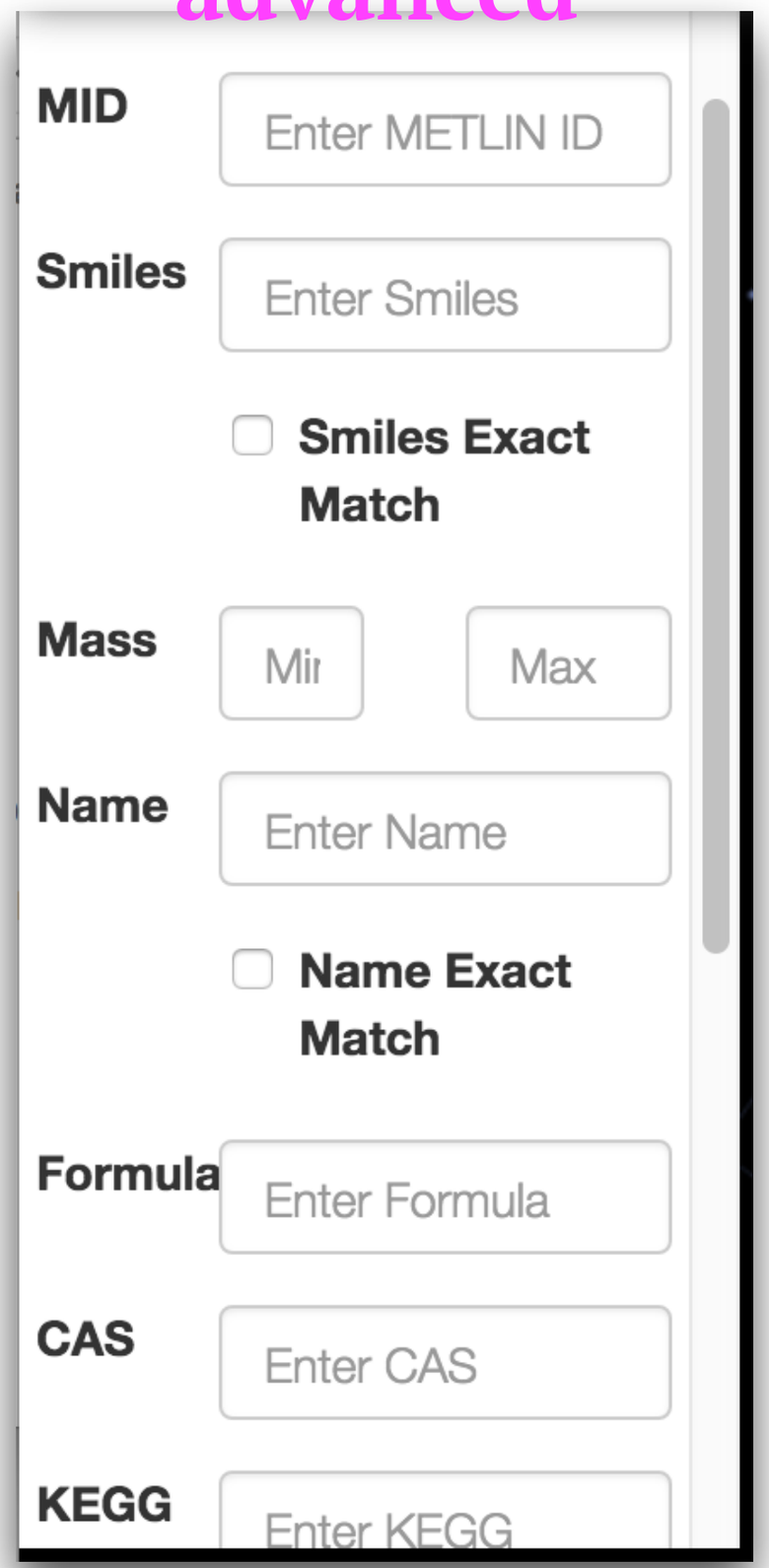
Created in 2003, METLIN now includes over a million molecules ranging from lipids, steroids, plant & bacteria metabolites, small peptides, carbohydrates, exogenous drugs/metabolites, central carbon metabolites and toxicants. The metabolites and other small molecules have been individually analyzed to provide both empirical and *in silico* MS/MS data.

METLIN: search

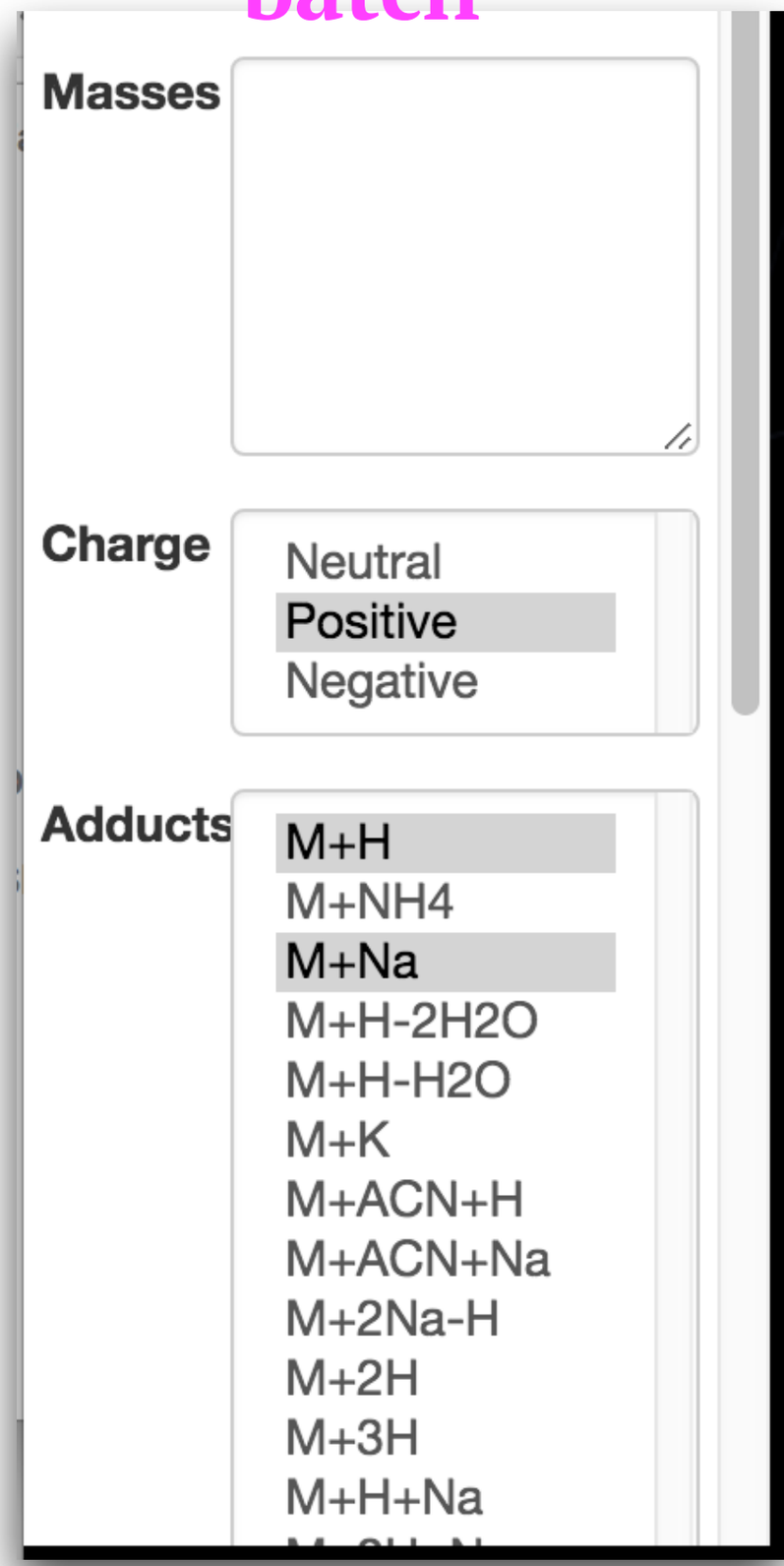
simple



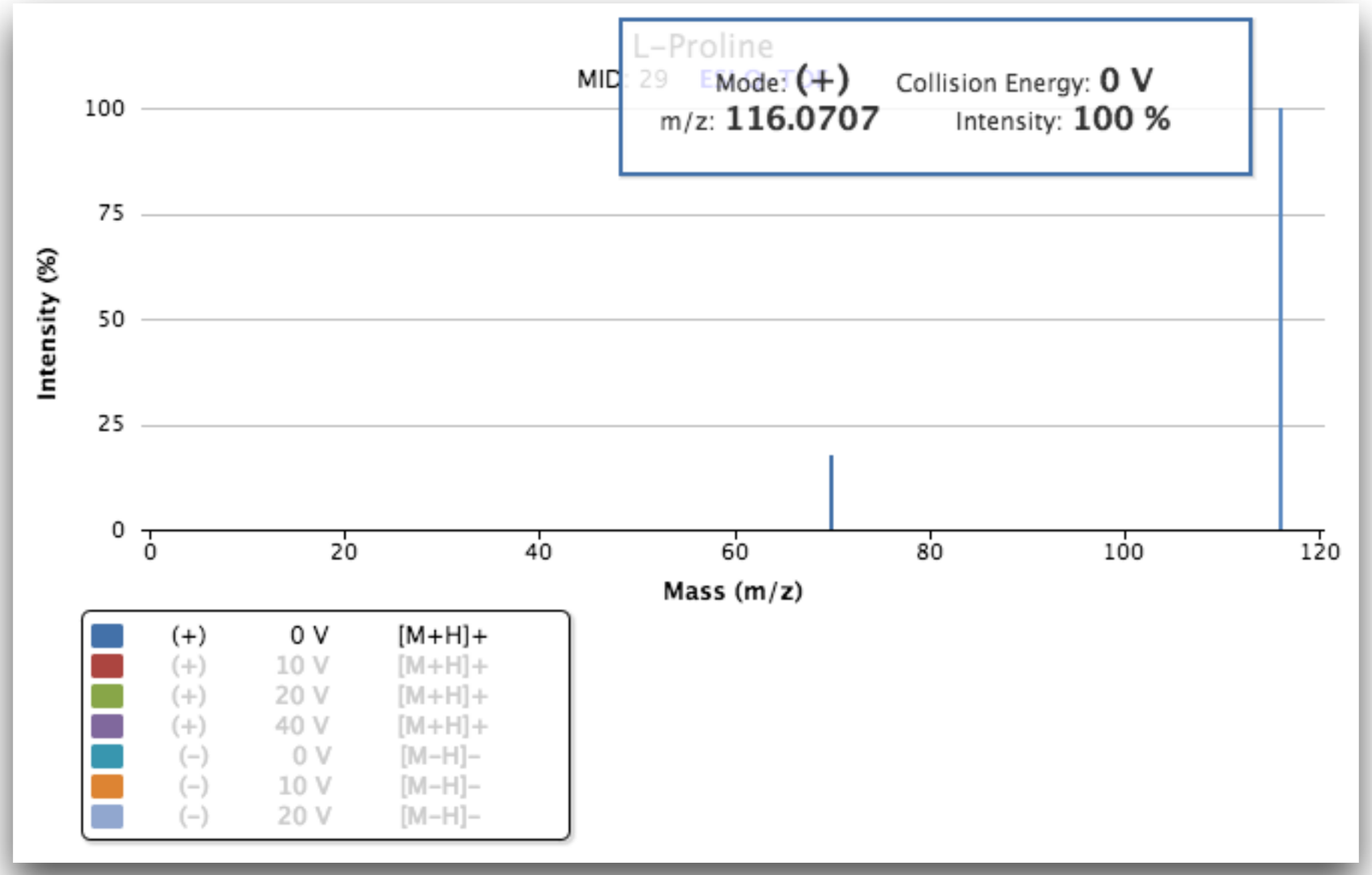
advanced



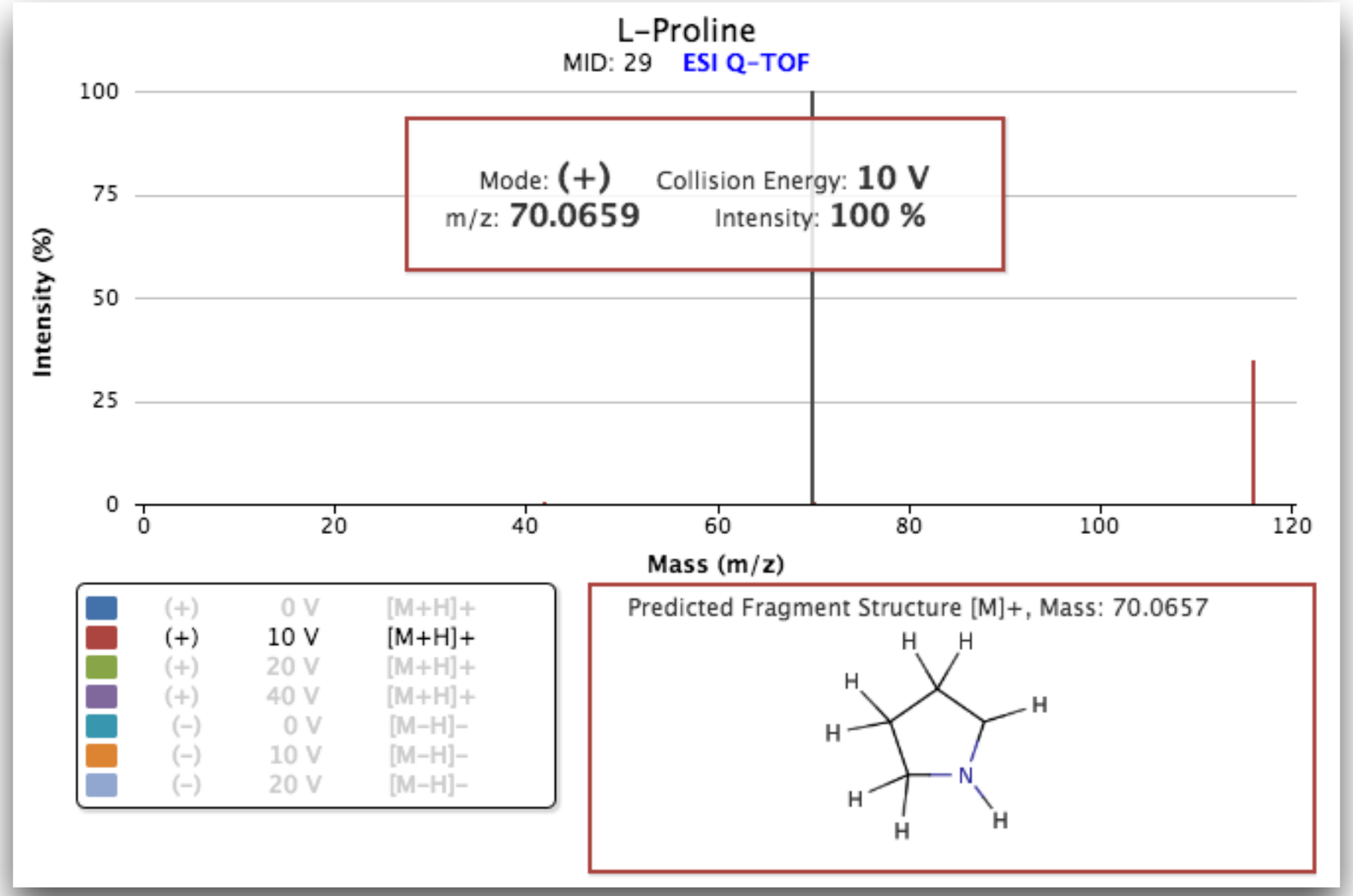
batch



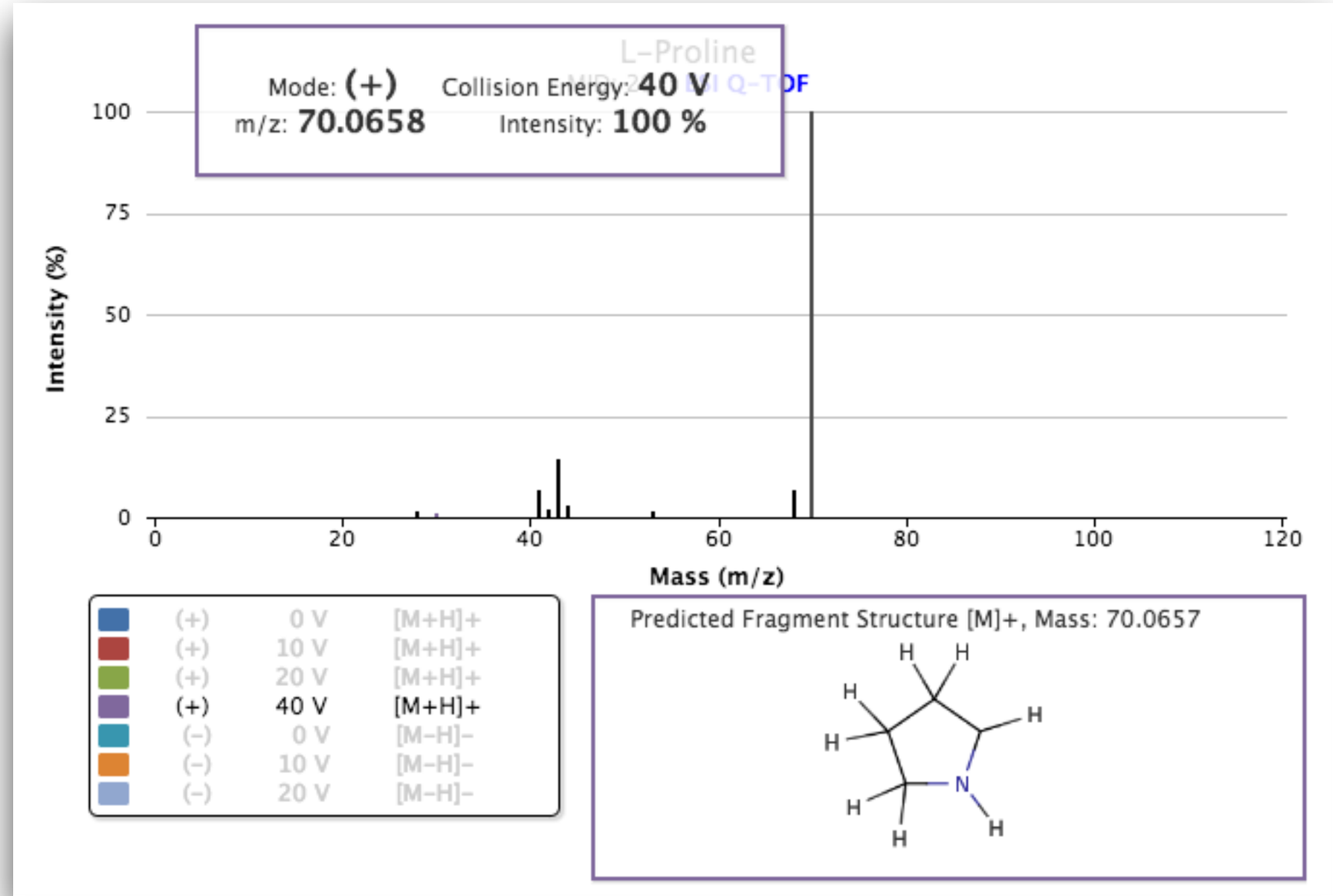
METLIN


L-Proline
Mode: (+)
Collision Energy: 0 V
m/z: 116.0707
Intensity: 100 %
Intensity (%)
100
75
50
25
0
0
20
40
60
80
100
120
Mass (m/z)
(+) 0 V [M+H]+
(+) 10 V [M+H]+
(+) 20 V [M+H]+
(+) 40 V [M+H]+
(-) 0 V [M-H]-
(-) 10 V [M-H]-
(-) 20 V [M-H]-

METLIN


L-Proline
MID: 29 ESI Q-TOF
Mode: (+) Collision Energy: 10 V
m/z: 70.0659 Intensity: 100 %
Intensity (%)
100
75
50
25
0
0
20
40
60
80
100
120
Mass (m/z)
(+) 0 V [M+H]+
(+) 10 V [M+H]+
(+) 20 V [M+H]+
(+) 40 V [M+H]+
(-) 0 V [M-H]-
(-) 10 V [M-H]-
(-) 20 V [M-H]-
Predicted Fragment Structure [M]+, Mass: 70.0657
H
H
H
H
H
N
H
H
H

METLIN


L-Proline
Mode: (+)
Collision Energy: 40 V
m/z: 70.0658
Intensity: 100 %
100
75
50
25
0
Intensity (%)
0
20
40
60
80
100
120
Mass (m/z)
(+) 0 V [M+H]+
(+) 10 V [M+H]+
(+) 20 V [M+H]+
(+) 40 V [M+H]+
(-) 0 V [M-H]-
(-) 10 V [M-H]-
(-) 20 V [M-H]-
Predicted Fragment Structure [M]+, Mass: 70.0657
H
H
H
H
H
H
N
H

MassBank

Secure | https://massbank.eu/MassBank/

MassBank norman High Resolution Mass Spectral Database

Home | Quick Search | Peak Search | Record Index | Statistics | Imprint/Data privacy MassBank ID: Go

European MassBank (NORMAN MassBank)

Quick Search

Peak Search

Record Index

- WEB-API WSDL

MassBank

Secure | https://massbank.eu/MassBank/QuickSearch.html

Quick Search

Home | Quick Search | Peak Search | Record Index | Statistics | Imprint/Data privacy MassBank ID: Go

Search by Keyword **Search by Peak**

Compound Name proline

AND **Exact Mass** **Tolerance** 0.3

AND **Formula**

(e.g. C6H7N5, C5H*N5, C5*)

Reset

Search

Instrument Type

- EI
  - EI-B
  - EI-EBEB
  - GC-EI-Q
  - GC-EI-QQ
  - GC-EI-TOF
- ESI
  - CE-ESI-TOF
  - ESI-FTICR
  - ESI-ITFT

MS Type

All MS MS1 MS2 MS3 MS4

Ion Mode

Positive Negative Both

MassBank

Quick Search Results

mass calculator use

Home | Quick Search | Peak Search | Record Index | Statistics | Imprint/Data privacy MassBank ID: Go

Search Parameters :

Compound Name: **proline**

Instrument Type: **CE-ESI-TOF , ESI-ITTOF , LC-ESI-IT , LC-ESI-Q , LC-ESI-QQ , UPLC-ESI-QTOF , ESI-FTICR , ESI-QTOF , LC-ESI-ITFT , LC-ESI-QFT , LC-ESI-QTOF , ESI-ITFT , HPLC-ESI-TOF , LC-ESI-ITTOF , LC-ESI-QIT , LC-ESI-TOF**

MS Type: **All**

Ion Mode: **Positive**

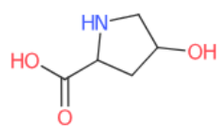
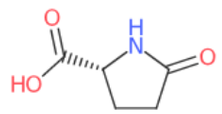
Edit / Resubmit Query

Results : 78 Hit. **(1 - 78 Displayed)**

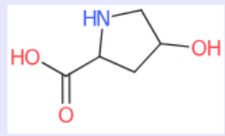
Open All Tree

First Prev ***1*** Next Last (Total ***1*** Page)

▼ Results End

	Name	Formula / Structure	ExactMass	ID
☐	**4-Hydroxy-L-proline** 5 spectra	**C5H9NO3** 	**131.05824**	
☐	**D-5-Oxoproline** 5 spectra	**C5H7NO3** 	**129.04259**	

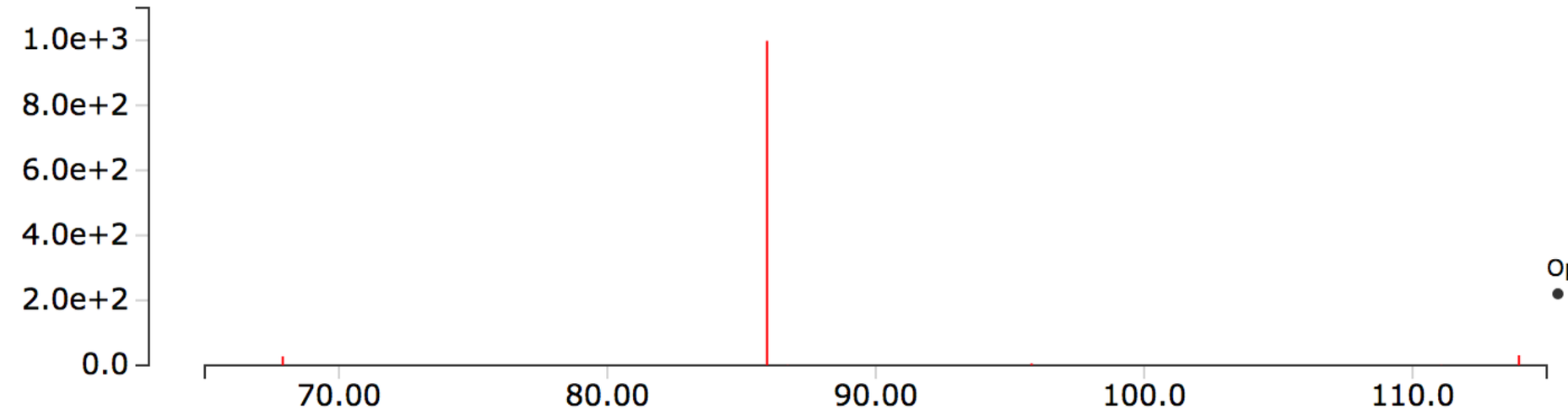
MassBank

	Name	Formula / Structure	ExactMass	ID
☐	⊟ 4-Hydroxy-L-proline 5 spectra	C5H9NO3 	131.05824	
☐	LC-ESI-ITFT; MS2; m/z:132.07; POS			KNA00040
☐	LC-ESI-ITFT; MS2; m/z:132.07; POS			KNA00297
☐	LC-ESI-ITFT; MS2; m/z:133.07; POS			KNA00298
☐	LC-ESI-ITFT; MS; POS			KNA00037
☐	LC-ESI-ITFT; MS; POS			KNA00296

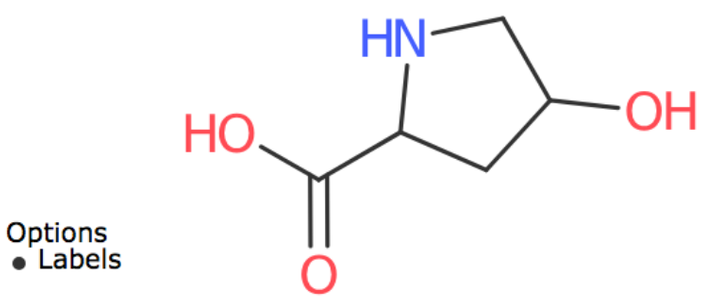
MassBank Record: KNA00040

4-Hydroxy-L-proline; LC-ESI-ITFT; MS2; m/z:132.07; POS

Mass Spectrum



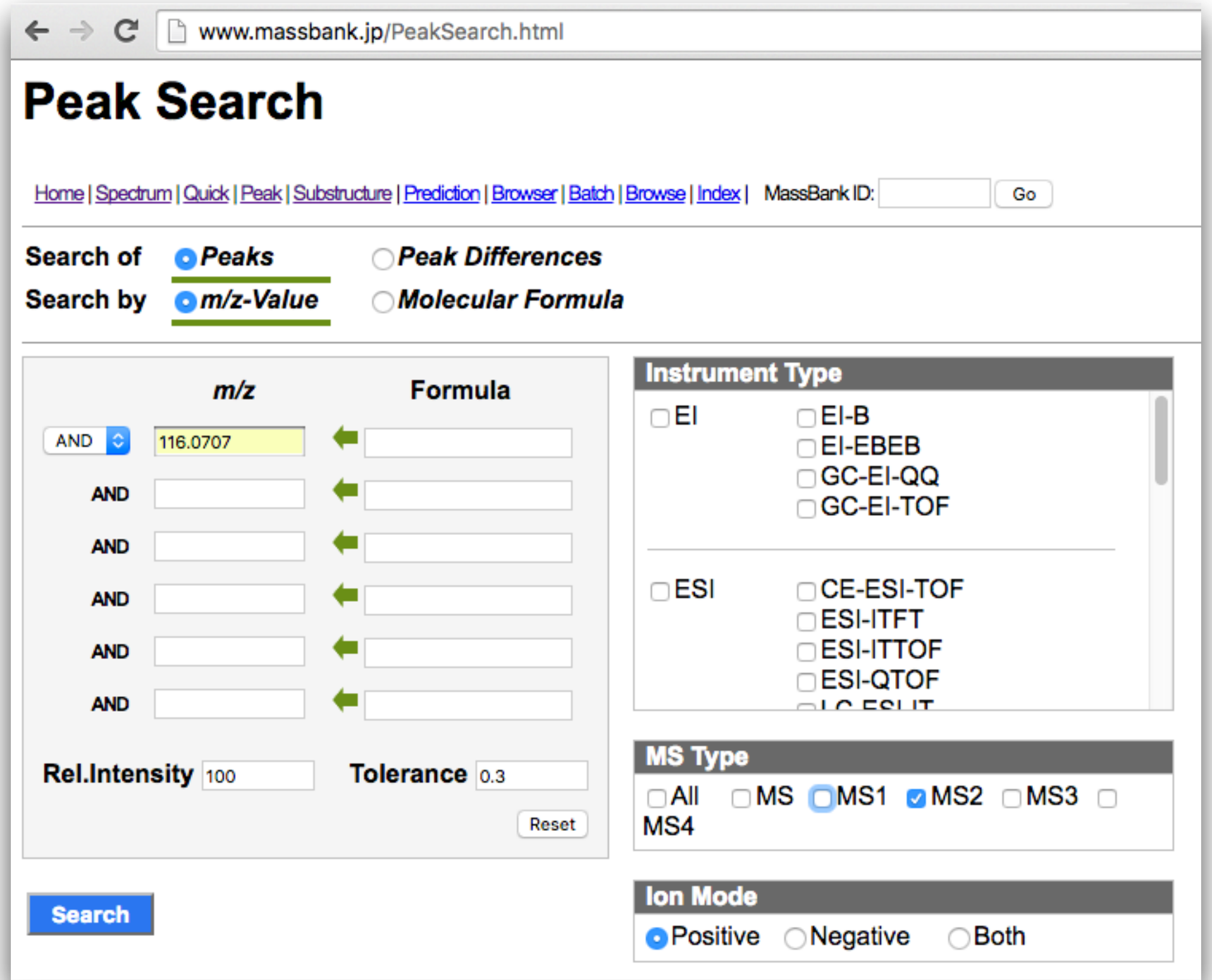
Chemical Structure



ACCESSION: KNA00040
RECORD_TITLE: 4-Hydroxy-L-proline; LC-ESI-ITFT; MS2; m/z:132.07; POS
DATE: 2016.01.19 (Created 2009.11.17, modified 2011.08.03)
AUTHORS: Takahashi H, Kanaya S, Ogasawara N, Graduate School of Information Science, NAIST
LICENSE: CC BY-SA

CH$NAME: 4-Hydroxy-L-proline
CH$NAME: L-Hydroxyproline
CH$COMPOUND_CLASS: Natural Product
CH$FORMULA: C5H9NO3
CH$EXACT_MASS: 131.05824
CH$SMILES: OC(C1)CC(N1)C(O)=O
CH$IUPAC: InChI=1S/C5H9NO3/c7-3-1-4(5(8)9)6-2-3/h3-4,6-7H,1-2H2,(H,8,9)/t3?,4-/m0/s1
CH$LINK: CAS 51-35-4

MassBank


www.massbank.jp/PeakSearch.html
Peak Search
Home | Spectrum | Quick | Peak | Substructure | Prediction | Browser | Batch | Browse | Index | MassBank ID: Go
Search of Peaks Peak Differences
Search by m/z-Value Molecular Formula
m/z
Formula
AND 116.0707
AND
AND
AND
AND
AND
Rel.Intensity 100
Tolerance 0.3
Reset
Search
Instrument Type
EI
EI-B
EI-EBEB
GC-EI-QQ
GC-EI-TOF
ESI
CE-ESI-TOF
ESI-ITFT
ESI-ITTOF
ESI-QTOF
MS Type
All MS MS1 MS2 MS3 MS4
Ion Mode
Positive Negative Both

MassBank

Peak Search Results (Peaks by *m/z* value)

Home | Spectrum | Quick | Peak | Substructure | Prediction | Browser | Batch | Browse | Index | MassBank ID: Go

Search Parameters :
m/z: **116.0707** Rel.Int: **100** Tol.(unit): **0.3**

Instrument Type: **LC-ESI-QTOF**
MS Type: **MS2**
Ion Mode: **Positive**

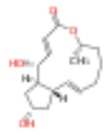
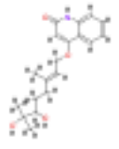
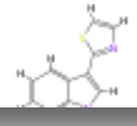
Edit / Resubmit Query

Results : 113 Hit. **(41 - 81 Displayed)**

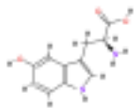
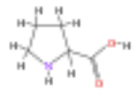
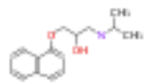
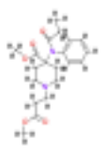
Open All Tree | Multiple Display | Spectrum Search

First Prev 1 **2** 3 Next Last (Total **3** Page)

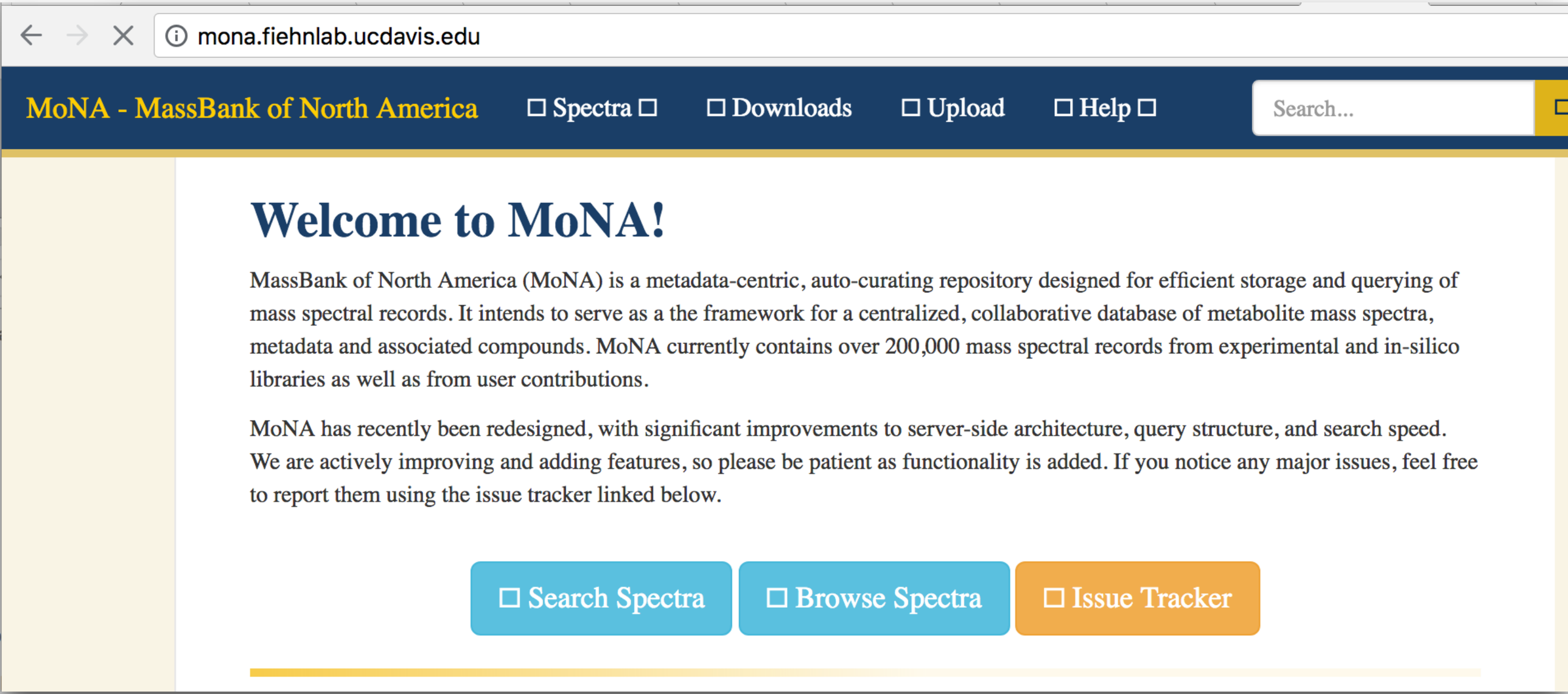
▼ Results End

Name	Formula / Structure	ExactMass	ID
Brefeldin-A 1 spectrum	**C16H24O4** 	**280.16746**	
Bucharaine 1 spectrum	**C19H25NO4** 	**331.17836**	
Camalexin 2 spectra	**C11H8N2S** 	**200.04082**	

MassBank

⊞ **Oxitriptan 1** 1 spectrum	**C11H12N2O3** 	**220.08479**	
⊟ **Proline** 2 spectra LC-ESI-QTOF; MS2; CE:10 eV; [M+H]+ LC-ESI-QTOF; MS2; CE:15 eV; [M+H]+	**C5H9NO2** 	**115.06333**	PB000449 PB000450
⊞ **Propranolol** 1 spectrum	**C16H21NO2** 	**259.15720**	
⊞ **Remifentanil** 4 spectra	**C20H28N2O5** 	**376.19982**	
⊞ **S-Lactoylglutathione** 1 spectrum	**C13H21N3O8S** 	**379.10494**	

MoNA


mona.fiehnlab.ucdavis.edu
MoNA - MassBank of North America
Spectra
Downloads
Upload
Help
Search...
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

mona.fiehnlab.ucdavis.edu/spectra/search

MoNA - MassBank of North America | Spectra | Downloads | Upload | Help | Search...

Search

Compound

Name or InChIKey

Compound Class

Molecular Formula

Exact Mass ± 0.5 Da

Source Introduction

- [ ] Liquid Chromatography (LC)
- [ ] Gas Chromatography (GC)
- [ ] Capillary Electrophoresis (CE)

MS Type

- [ ] MS1
- [ ] MS2
- [ ] MS3
- [ ] MS4

Ion Mode

- [ ] Positive
- [ ] Negative

Library

- [ ] LipidBlast
- [ ] MassBank
- [ ] GNPS
- [ ] ReSpect
- [ ] HMDB
- [ ] FAHFA
- [ ] iTree
- [ ] Fiehn HILIC
- [ ] MetaboBASE
- [ ] FiehnLib
- [ ] RIKEN OxPLs

Add Additional Tags to Query

Search Reset

Metabolic pathway databases

- KEGG
- MetaCyc
- HumanCyc
- BioCyc
- Reactome
- WikiPathways

Drug databases

- DrugBank
- Therapeutic target databases
- PharmGKB
- STITCH
- SuperTarget

Disease & physiology databases

- OMIM
- METAGENE
- OMMBID

Raw data databases

- Metabolomics Workbench
- MetaboLights

MetaboLights

European Bioinformatics Institute [GB] | https://www.ebi.ac.uk/metabolights/

EMBL-EBI | About us | Training | Research | Services

MetaboLights

Examples: Alanine, Hor

Home | Browse Studies | Browse Compounds | Browse Species | More

MetaboLights

MetaboLights is a database for Metabolomics experiments and derived information. The database is cross-species, cross-technique and covers metabolite structures and their reference spectra as well as their biological roles, locations and concentrations, and experimental data from metabolic experiments. MetaboLights is the recommended Metabolomics repository for a number of leading journals.

More about us

MetaboLights

What is MetaboLights?

Select Language

Powered by Google Tr

MetaboLights is the first general purpose, open access repository for metabolomics studies, their raw experimental data and associated metadata, maintained by one of the major open access data providers in molecular biology (Figure 1).

The identification and quantification of metabolites can provide unique insights into the metabolic processes that are taking place in the cellular environment. Metabolic profiles taken from body fluids have the potential to act as biomarkers for many different diseases, an approach that has already shown value in, for example, heart disease and diabetes, the effects of diet and interactions with the environment.

MetaboLights consists of two distinct layers:

1) a **repository**, enabling the metabolomics community to share findings, data and protocols for any form of metabolomics study;

2) a **reference layer** of curated knowledge about metabolite structures and their reference spectra, as well as their biological roles, locations, concentrations, and raw data from metabolic experiments.

MetaboLights

What can I do with MetaboLights?

Select Langua

Powered by Google

With MetaboLights you can:

- Find metabolites and related metablomics studies by searching a wide range of associated `metadata`.
- Filter your search results on species, techniques and metabolites.
- Submit public or private studies.
- Receive a stable and unique `accession` number that can be used as a publication reference.
- Share private studies with collaborators/peer reviewers.
- Download public `metabolomics` studies for futher analysis.
- Retrieve molecular information from `ChEBI` or other linked compound databases.

MetaboLights

What can I do with MetaboLights?

Select Langua

Powered by Google

With MetaboLights you can:

- Find metabolites and related metablomics studies by searching a wide
- Filter your search results on species, techniques and metabolites.
- Submit public or private studies.
- Receive a stable and unique `accession` number that can be used as a
- Share private studies with collaborators/peer reviewers.
- Download public `metabolomics` studies for futher analysis.
- Retrieve molecular information from `ChEBI` or other linked compound

MetaboLights: Quick tour

- What is MetaboLights?
- What can I do with MetaboLights?
- **Searching and visualising data in MetaboLights**
- Getting data from MetaboLights
- Submitting data to MetaboLights
- Your feedback
- Get help and support on MetaboLights

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MetaboLights / Search

Filter your results

Type
- [x] study
- [ ] compound

Technology

Organism

Organism Part

387 results , showing 1 to 10

« ‹ Page 1 of 39 › »

Imaging with Mass Spectrometry of Bacteria on the Exoskeleton of Fungus-Growing Ants

Study Identifier	MTBLS471	Organism	Acromyrmex octospinosus
Study Size	13.47GB	Study Factors	Infection, Replicate
Submitted by	Kellen DeLaney		

MetaboLights

Home | Browse Studies | Browse Compounds | Browse Species | More | Submit Study | Login

MetaboLights / Search

Filter your results

Type

- compound

Compound features

- Species
- Pathways
- Reactions
- NMR
- MS

Technology

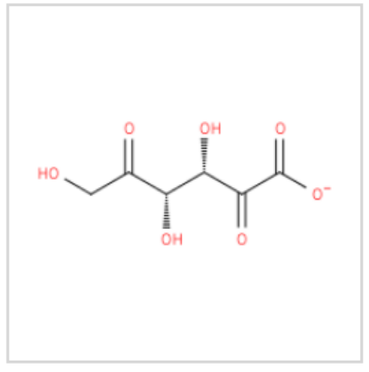
Organism

Organism Part

25920 results , showing 1 to 10

« ‹ Page 1 of 2592 › »

2,5-didehydro-D-gluconate



COMPOUND ACCESSION

MTBLC11449

DESCRIPTION

Conjugate base of 2,5-didehydro-D-gluconic acid.

1-(1-adamantyl)-3-[8-[[1-(2-furanylmethyl)-5-

MetaboLights

Home | Browse Studies | Browse Compounds | Browse Species | More | Su

MetaboLights / Species search

Species selection page

Find some direct links to some common model organisms and a wider list of all the organisms we have information about.

Taxonomy Search

Start typing the first 3 letters of the species name

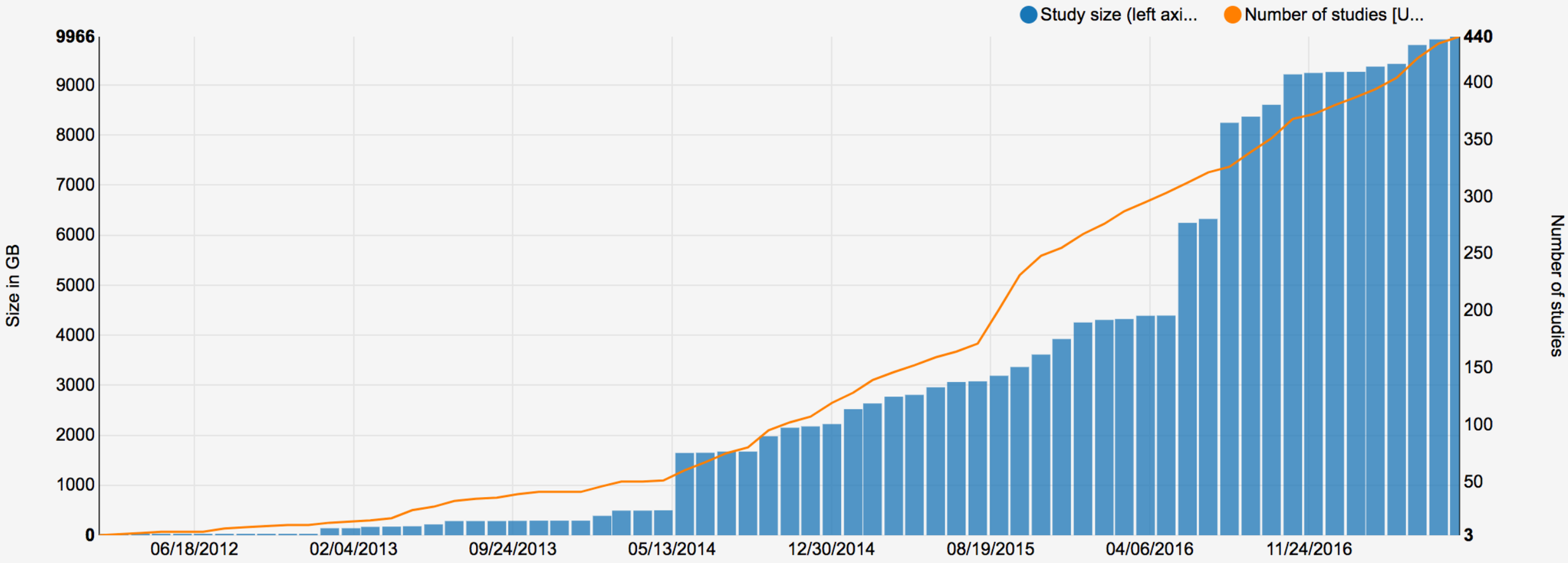
Model organisms

- Homo sapiens (Human)
- Mus musculus (Mouse)
- Arabidopsis thaliana (thale cress)
- Escherichia coli
- Saccharomyces cerevisiae (Baker's yeast)
- Caenorhabditis elegans

MetaboLights

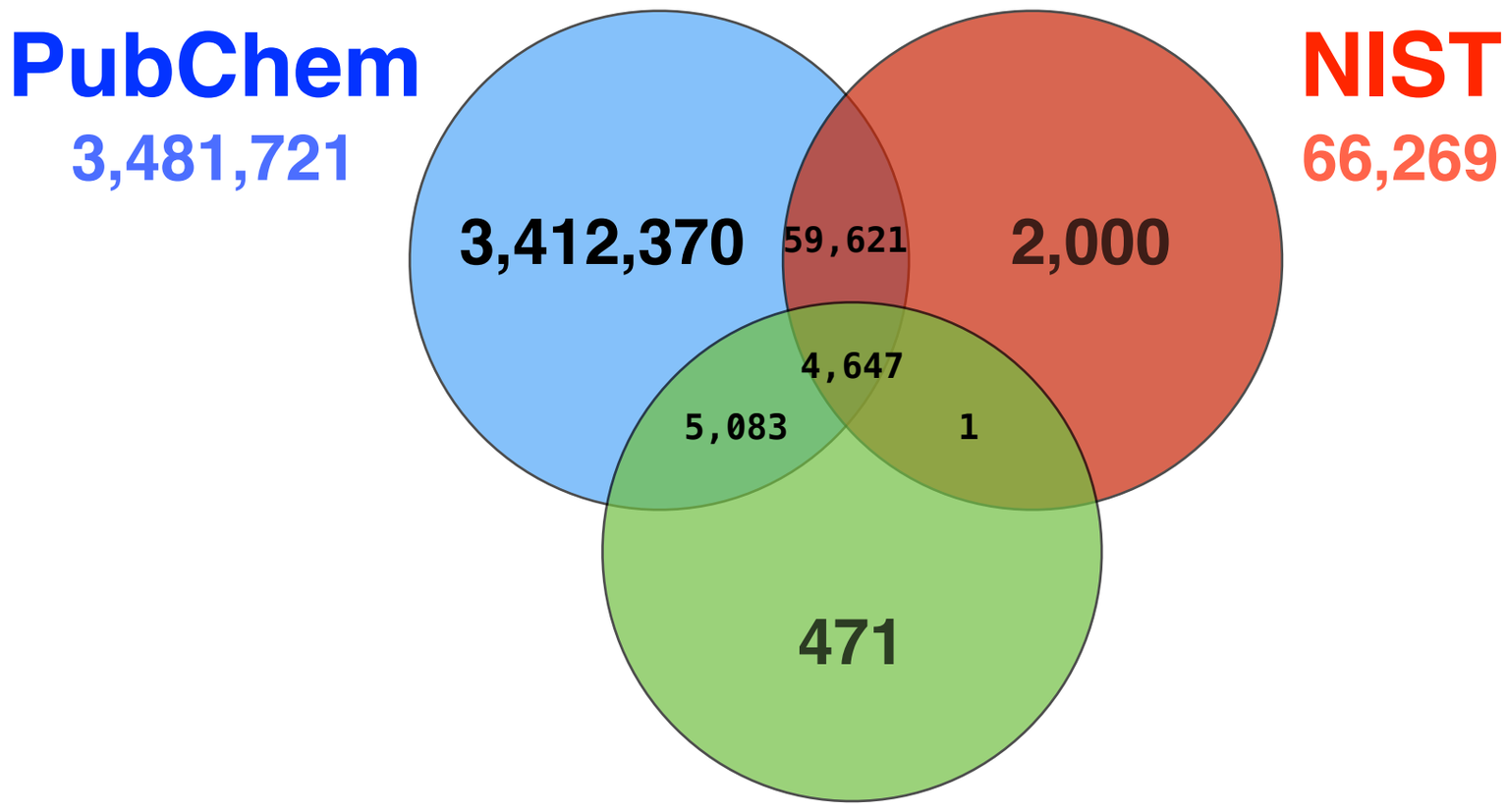
MetaboLights Statistics

Data growth over time



PubChem, NIST, and HMDB, again

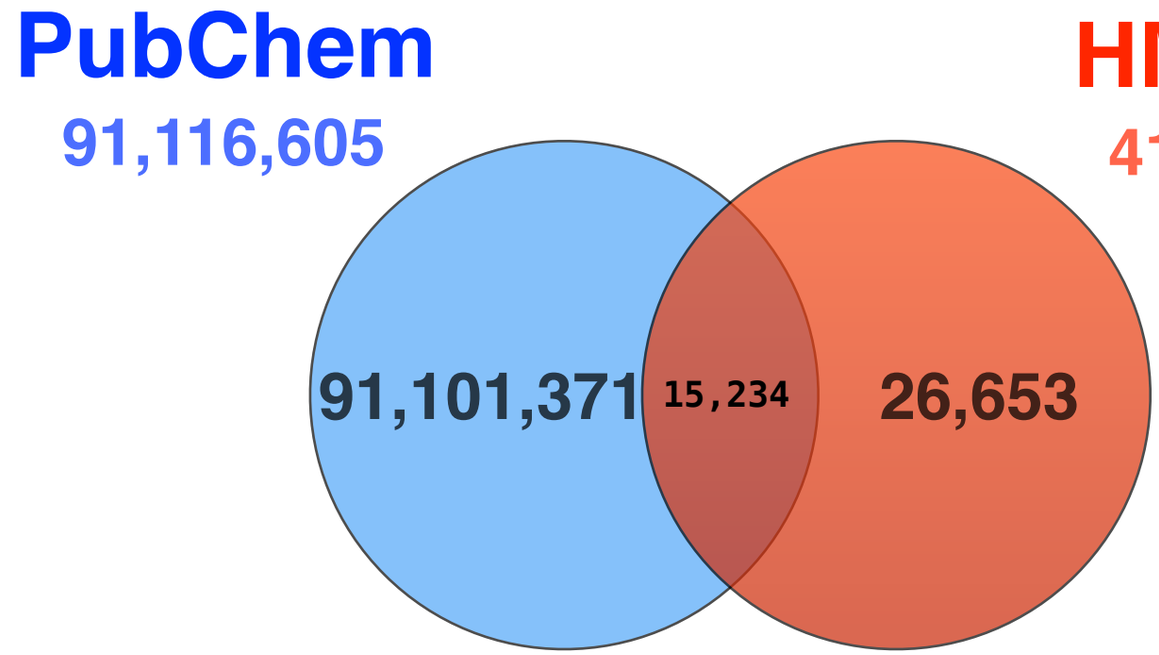
- In terms of unique molecular formula



based on database version in 2016

PubChem, NIST, and HMDB, again

- In terms of unique InChi Key



based on database version in 2016

Thank you!