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

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Comprehensive databases

- HMDB

HMDB: overview

Welcome to HMDB Version 3.6

The Human Metabolome Database (HMDB) is a freely available electronic database containing detailed information about small molecule metabolites found in the human body. It is intended to be used for applications in metabolomics, clinical chemistry, biomarker discovery and general education. The database is designed to contain or link three kinds of data: 1) chemical data, 2) clinical data, and 3) molecular biology/biochemistry data. The database contains 74,462 metabolite entries including both water-soluble and lipid soluble metabolites as well as metabolites that would be regarded as either abundant (> 1 uM) or relatively rare (< 1 nM). Additionally, 5,701 protein sequences are linked to these metabolite entries. Each MetaboCard entry contains more than 110 data fields with 2/3 of the information being devoted to chemical/clinical data and the other 1/3 devoted to enzymatic or biochemical data. Many data fields are hyperlinked to other databases (KEGG, PubChem, MetaCyc, ChEBI, PDB, UniProt, and GenBank) and a variety of structure and pathway viewing applets. The HMDB database supports extensive text, sequence, chemical structure and relational query searches. Four additional databases, DrugBank, T3DB, SMPDB and FooDB are also part of the HMDB suite of databases. DrugBank contains equivalent information on ~1600 drug and drug metabolites, T3DB contains information on ~3600 common toxins and environmental pollutants, SMPDB contains pathway diagrams for ~700 human metabolic and disease pathways, while FooDB contains equivalent information on ~28,000 food components and food additives.

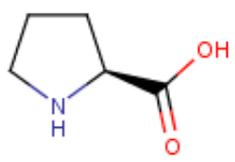
HMDB: one metabocard

Showing metabocard for L-Proline (HMDB00162)

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

enzymes (29) | transporters (1) | Show 30 proteins

Show Metabolites with Similar Structures

Record Information	
Version	3.6
Creation Date	2005-11-16 15:48:42 UTC
Update Date	2016-06-10 21:23:05 UTC
HMDB ID	HMDB00162
Secondary Accession Numbers	None
Metabolite Identification	
Common Name	**L-Proline**
Description	L-Proline is one of the twenty amino acids used in living organisms as the building blocks of proteins. Proline is sometimes called an imino acid, although the IUPAC definition of an imine requires a carbon-nitrogen double bond. 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.
Structure	

HMDB: one metabocard

Chemical Formula	$C_5H_9NO_2$
Average Molecular Weight	115.1305
Monoisotopic Molecular Weight	115.063328537
IUPAC Name	(2S)-pyrrolidine-2-carboxylic acid
Traditional Name	L-proline
CAS Registry Number	147-85-3
SMILES	OC(=O)[C@@H]1CCCN1
InChI Identifier	InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)/t4-/m0/s1
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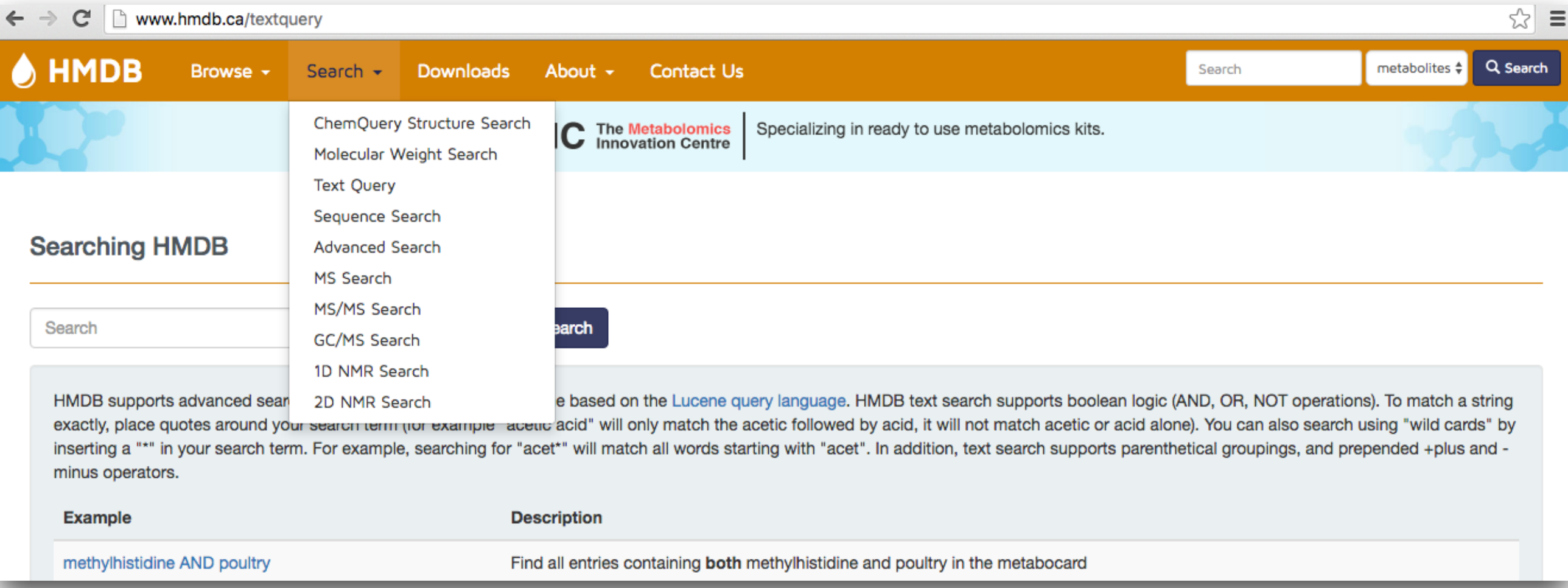
HMDB: searches

- Searches



HMDB: downloads

Protein/Gene Sequences (in FASTA Format)

Data Set	Released on	Protein Sequences	Gene Sequences
All Metabolite Metabolizing Enzymes	2017-07-16	Download	Download

Structures (in SDF Format)

Data Set	Released on	SDF File
Metabolite Structures	2017-07-16	Download

HMDB: downloads

Metabolite and Protein Data (in XML format)

Data Set	Released on	XML File
All Metabolites	2017-07-16	Download
All Proteins	2017-07-16	Download
Urine Metabolites	2017-07-16	Download
Serum Metabolites	2017-07-16	Download
CSF Metabolites	2017-07-16	Download
Saliva Metabolites	2017-07-16	Download
Feces Metabolites	2017-07-16	Download
Sweat Metabolites	2017-07-16	Download

HMDB: downloads

Spectra

Data Set	Download Link
Mass Spectra Image Files	Download
GC/MS Peak Lists	Download
NMR Spectra FIDS Files	Download
NMR Spectra Peaklist Files	Download
Spectra information (in XML format)	Download

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Compound databases

- PubChem
- ChemSpider
- ChEBI
- KEGG Glycan
- IIMDB

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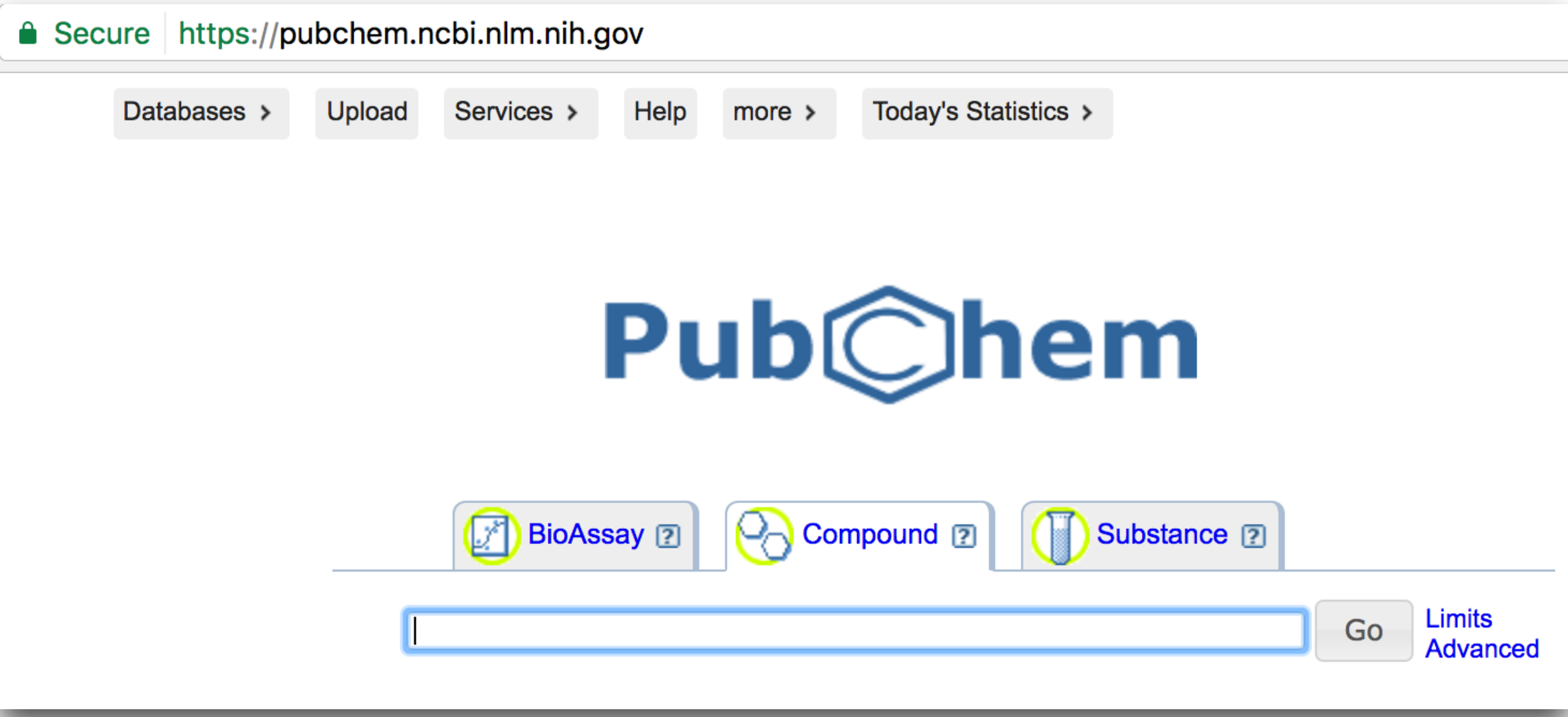
PubChem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https://pubchem.ncbi.nlm.nih.gov
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BioAssay
Compound
Substance
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Limits
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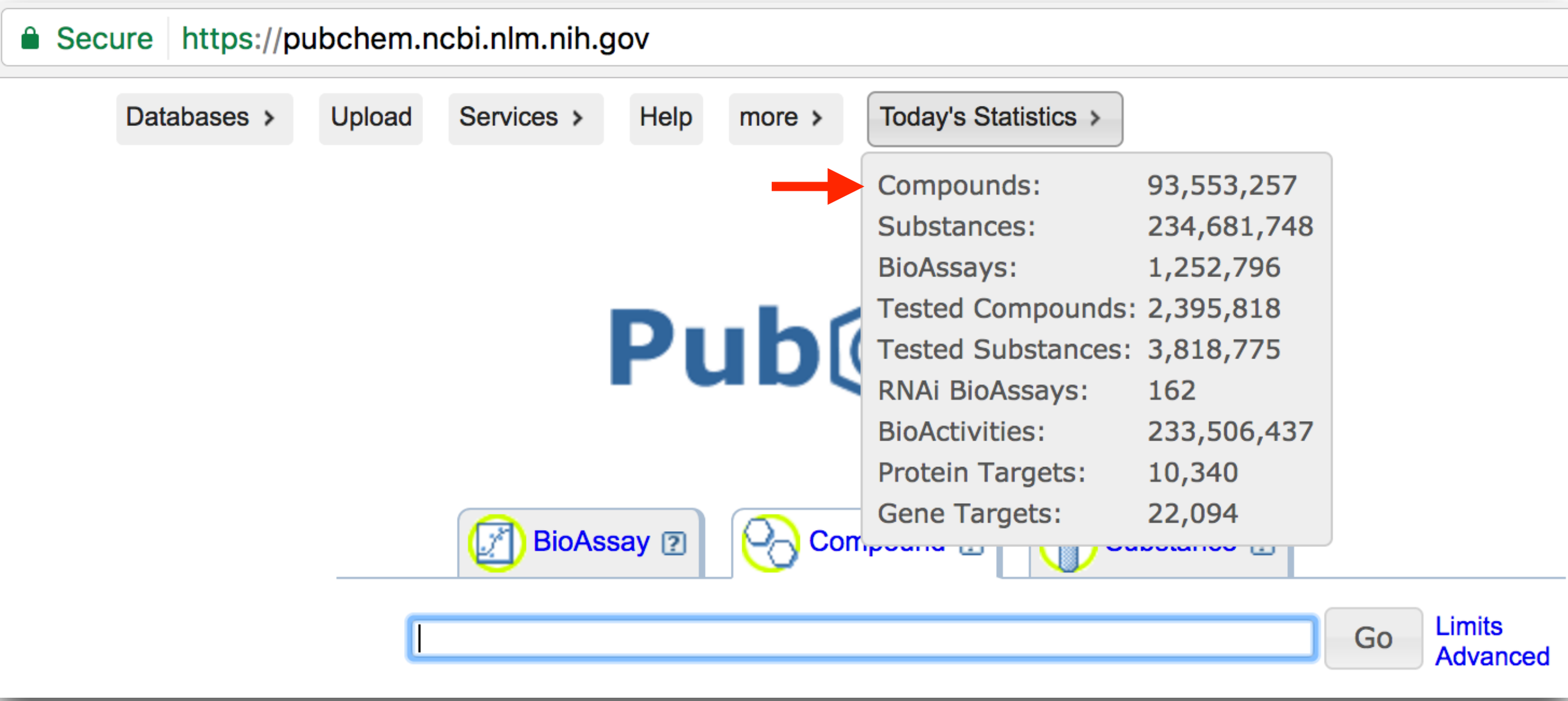
PubChem

- Statistics (July 19, 2017)



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

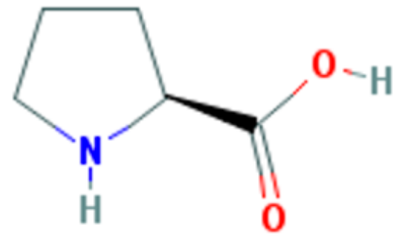
L-proline is a non-essential amino acid that is synthesized from GLUTAMIC ACID. It is an essential component of COLLAGEN and is important for proper functioning of joints and tendons.

PubChem

Contents

1 2D Structure

Search Download Get Image

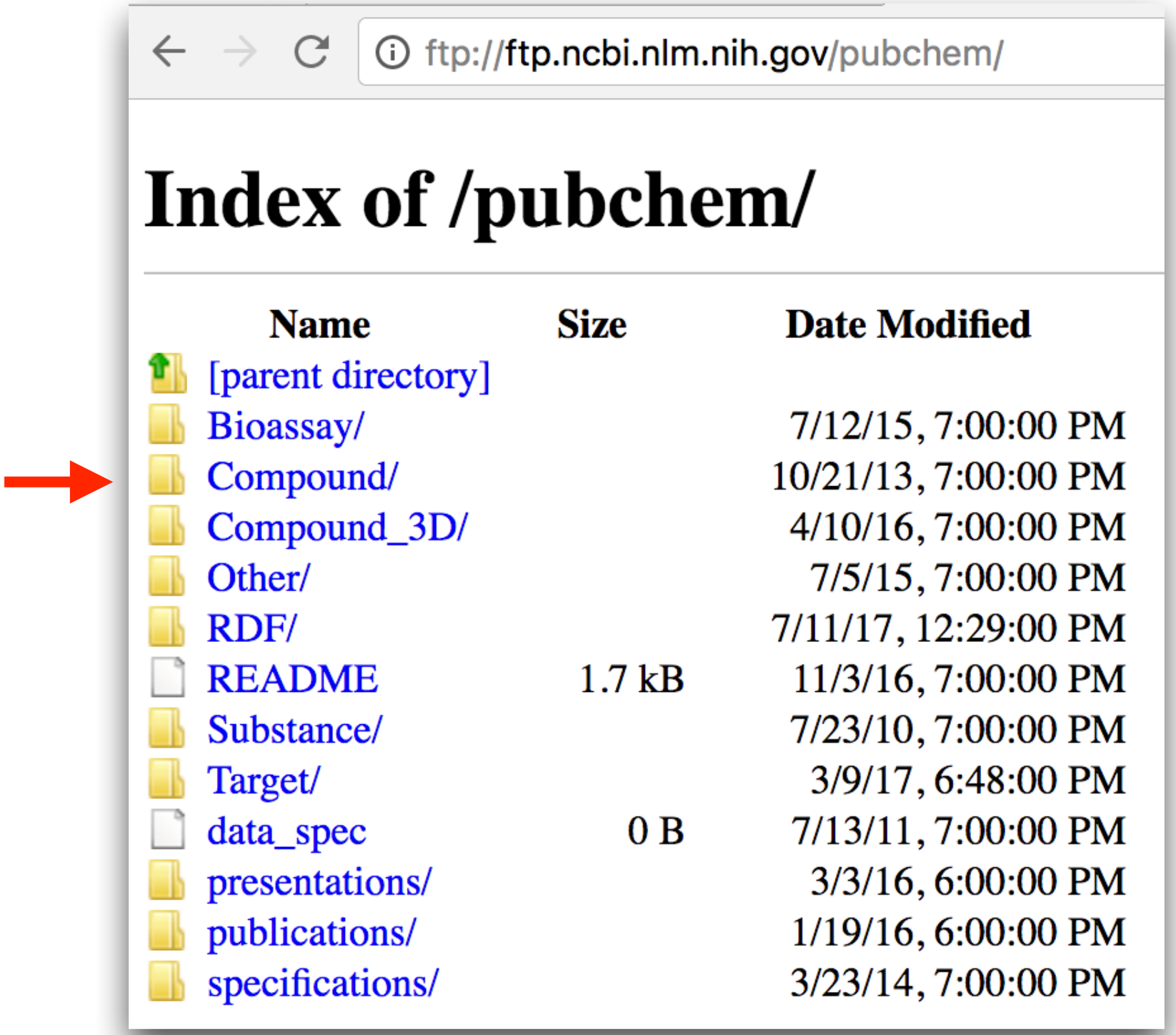


Magnify

2 3D Conformer

PubChem

- FTP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Compound/ 10/21/13, 7:00:00 PM
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Other/ 7/5/15, 7:00:00 PM
RDF/ 7/11/17, 12:29:00 PM
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Substance/ 7/23/10, 7:00:00 PM
Target/ 3/9/17, 6:48:00 PM
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publications/ 1/19/16, 6:00:00 PM
specifications/ 3/23/14, 7:00:00 PM

PubChem

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ChemSpider

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Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID

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ChemSpider

What is ChemSpider?

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- Database identifiers

Search by chemical structure

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your computer

Find important data

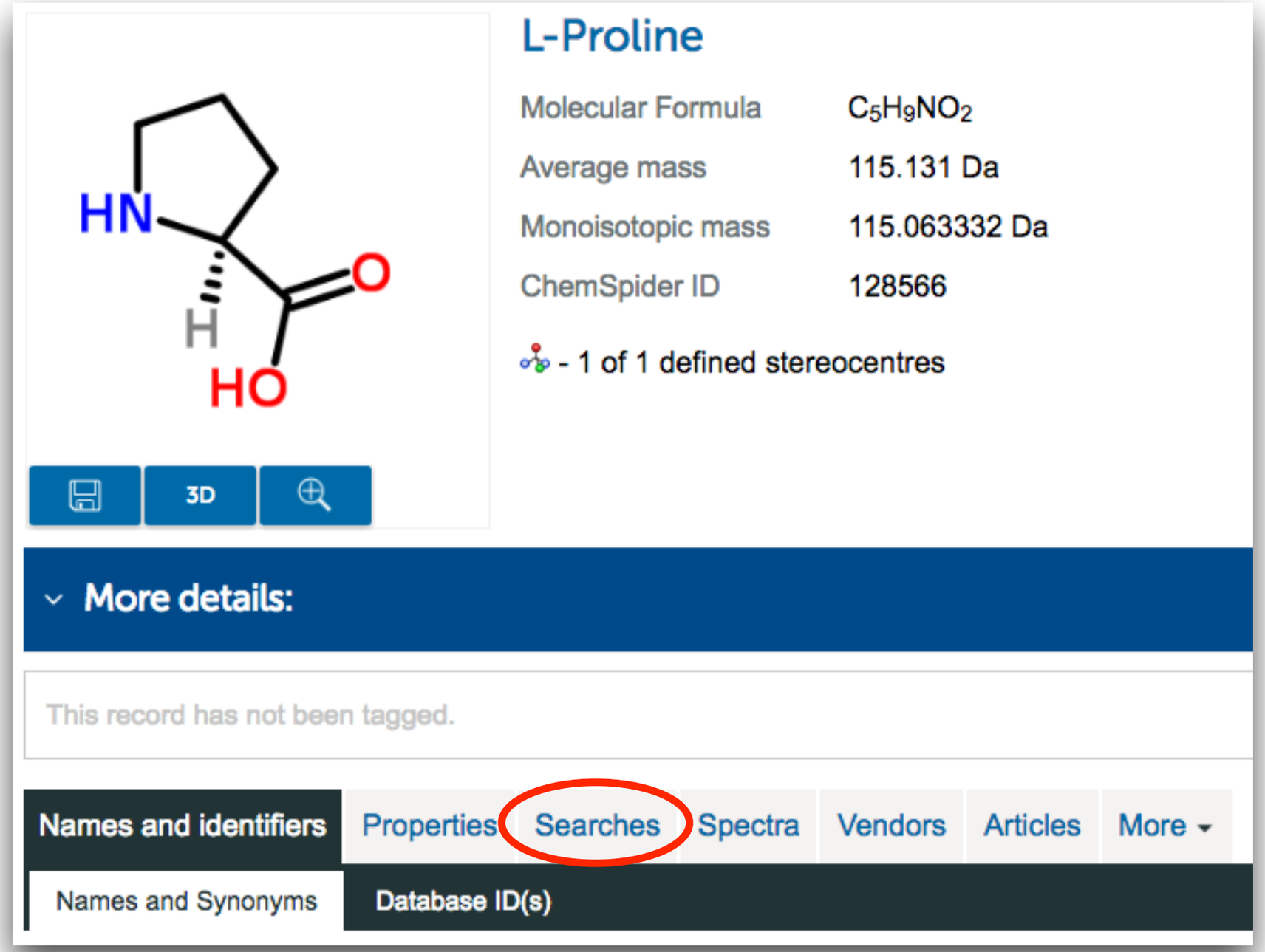
- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

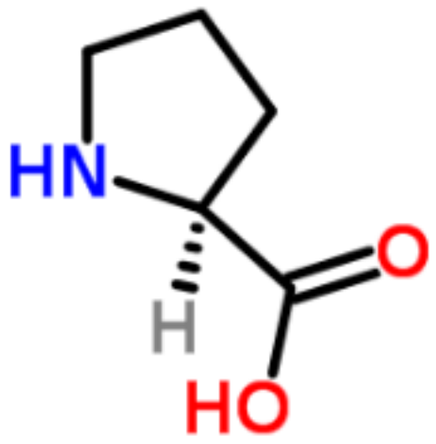
59 Million
chemical structures

487
Data sources

ChemSpider

- One compound





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:

This record has not been tagged.

Names and identifiers | Properties | **Searches** | Spectra | Vendors | Articles | More

Search ChemSpider:

- Compounds with the same molecular formula
- Compounds with the same skeleton
- Use this molecule in a structure search

Search Google:

- Search Google Scholar (by synonym)
- Search Google for exact structure
- Search Google for structures with same skeleton

ChemSpider

- Compounds with the same molecular formula

Found 501 results

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

1 2 3 4 5

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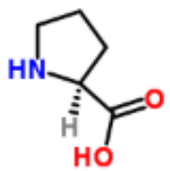
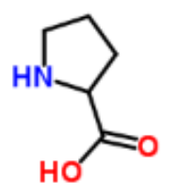
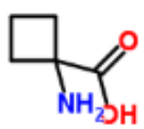
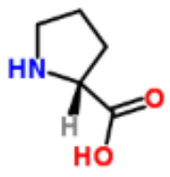
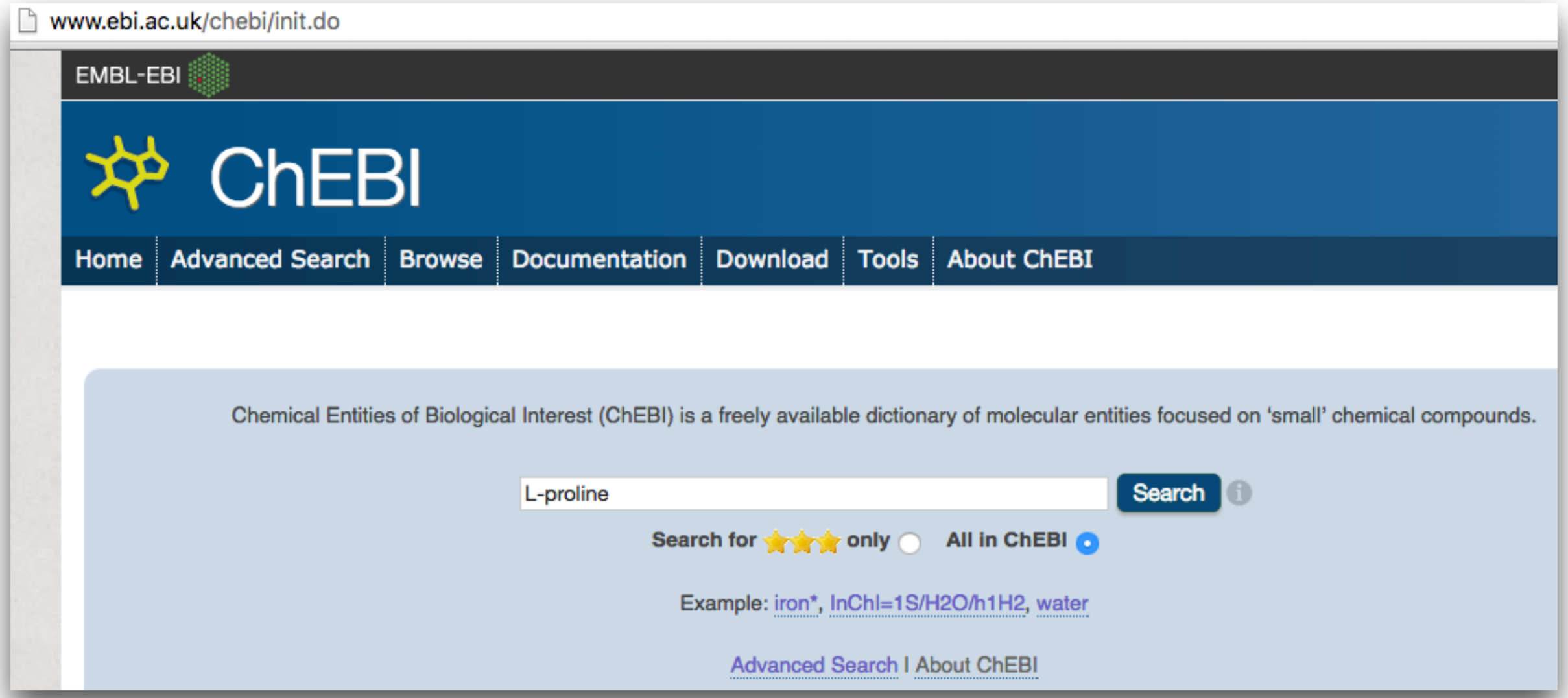
128566 - 1/1 defined		$C_5H_9NO_2$	115.1305	136	11954	28480	3548
594 - 0/1 defined		$C_5H_9NO_2$	115.1305	131	737	28034	3319
80908		$C_5H_9NO_2$	115.1305	110	185	8	5
8640 - 1/1 defined		$C_5H_9NO_2$	115.1305	103	293	701	268

ChEBI

- Chemical Entities of Biological Interest



ChEBI

- 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)

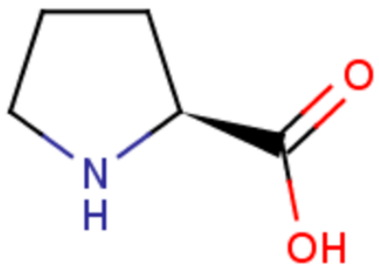
Molecules directly encoded by the genome (e.g. nucleic acids, proteins and peptides derived from proteins by cleavage) are *not* as a rule included in ChEBI.

ChEBI

- One compound

CHEBI:17203 - L-proline

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



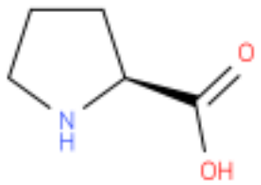
ChEBI Name	**L-proline**
ChEBI ID	**CHEBI:17203**
ChEBI ASCII Name	L-proline
Definition	Pyrrolidine in which the *pro-S* hydrogen at position 2 is substituted by a carboxylic acid group. L-Proline is the only one of the twenty DNA-encoded amino acids which has a secondary amino group α to the carboxyl 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
Supplier Information	eMolecules:524642, ZINC000000895360
Download	Molfile XML SDF

- Find compounds which contain this structure
- Find compounds which resemble this structure
- Take structure to the Advanced Search

more structures >>

Search Results for All in ChEBI

substructure



Edit Search

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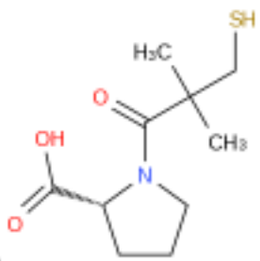

CHEBI:95254
Stars: ★★☆

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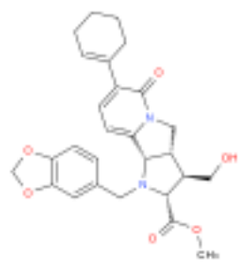
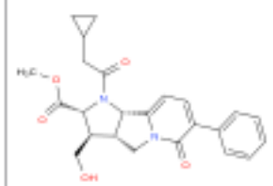


CHEBI:98944
Stars: ★★☆

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



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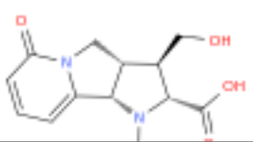


CHEBI:98447
Stars: ★★☆

(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: ★★☆

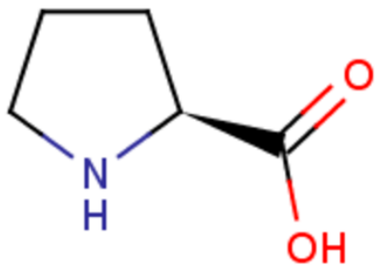
(2R,3R,3aS,9b
(hydroxymeth
tetrahydro-2H
acid

ChEBI

- One compound

CHEBI:17203 - L-proline

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



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Supplier Information	eMolecules:524642, ZINC000000895360
Download	Molfile XML SDF

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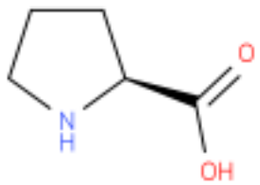
similar structures



Edit Search

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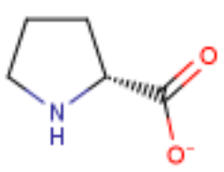
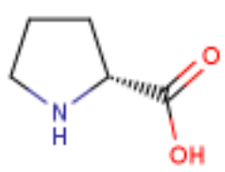
D-prolinate

CHEBI:32867
Stars: ★★★

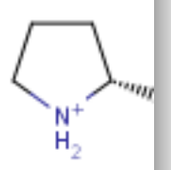


D-proline

CHEBI:16313
Stars: ★★★

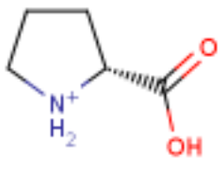


D-proline



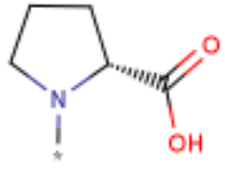
D-prolinium

CHEBI:32868
Stars: ★★★

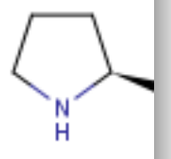


D-prolino group

CHEBI:32870
Stars: ★★★

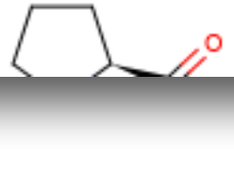


L-prolinat



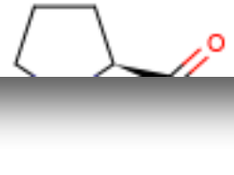
L-proline

CHEBI:17203
Stars: ★★★

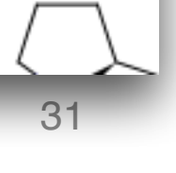


L-proline zwitterion

CHEBI:60039
Stars: ★★★



L-prolini



Outline

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

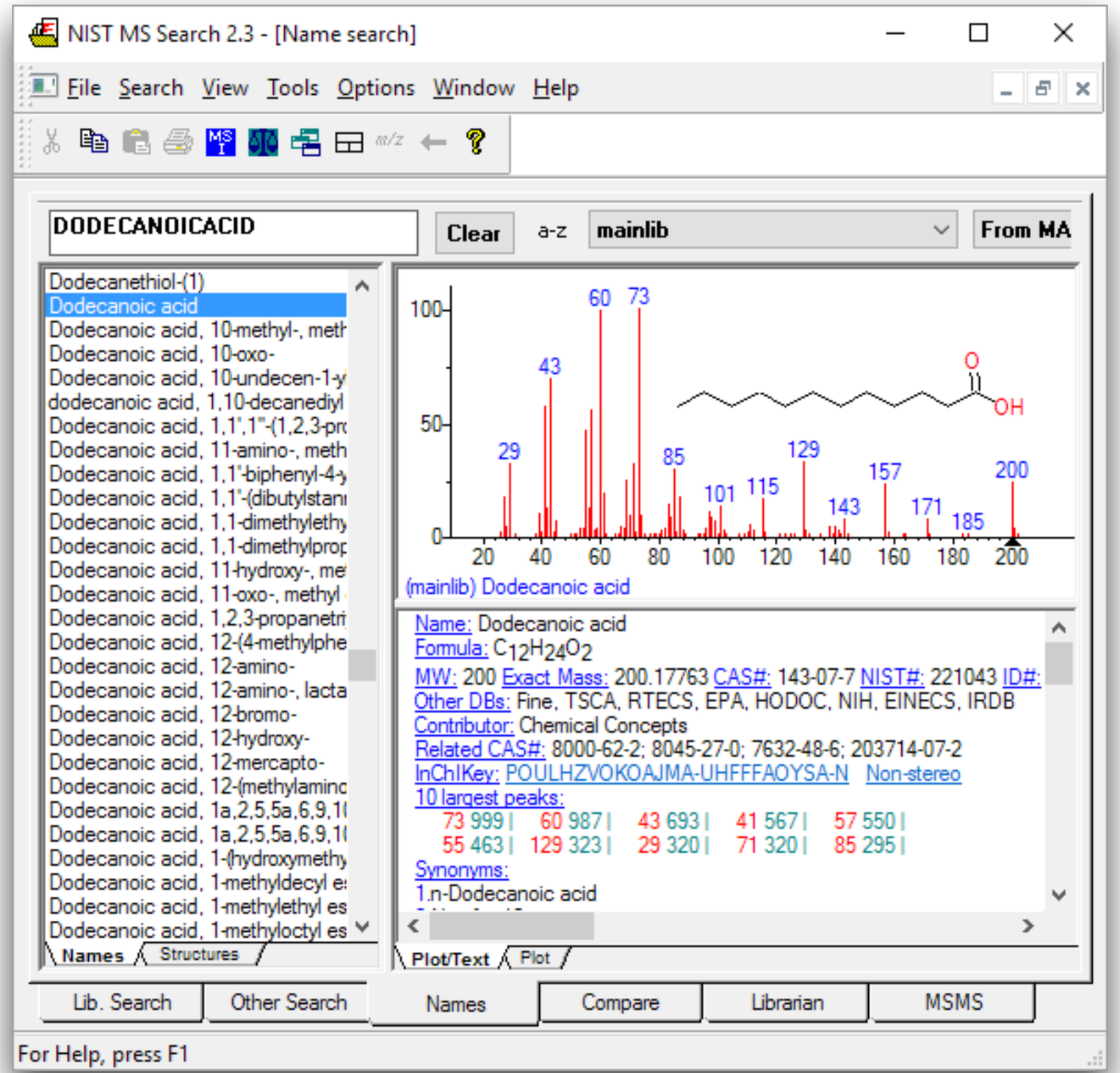
- Electron ionization mass spectral library
  - 306,622 spectra of 267,376 unique compounds

- 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

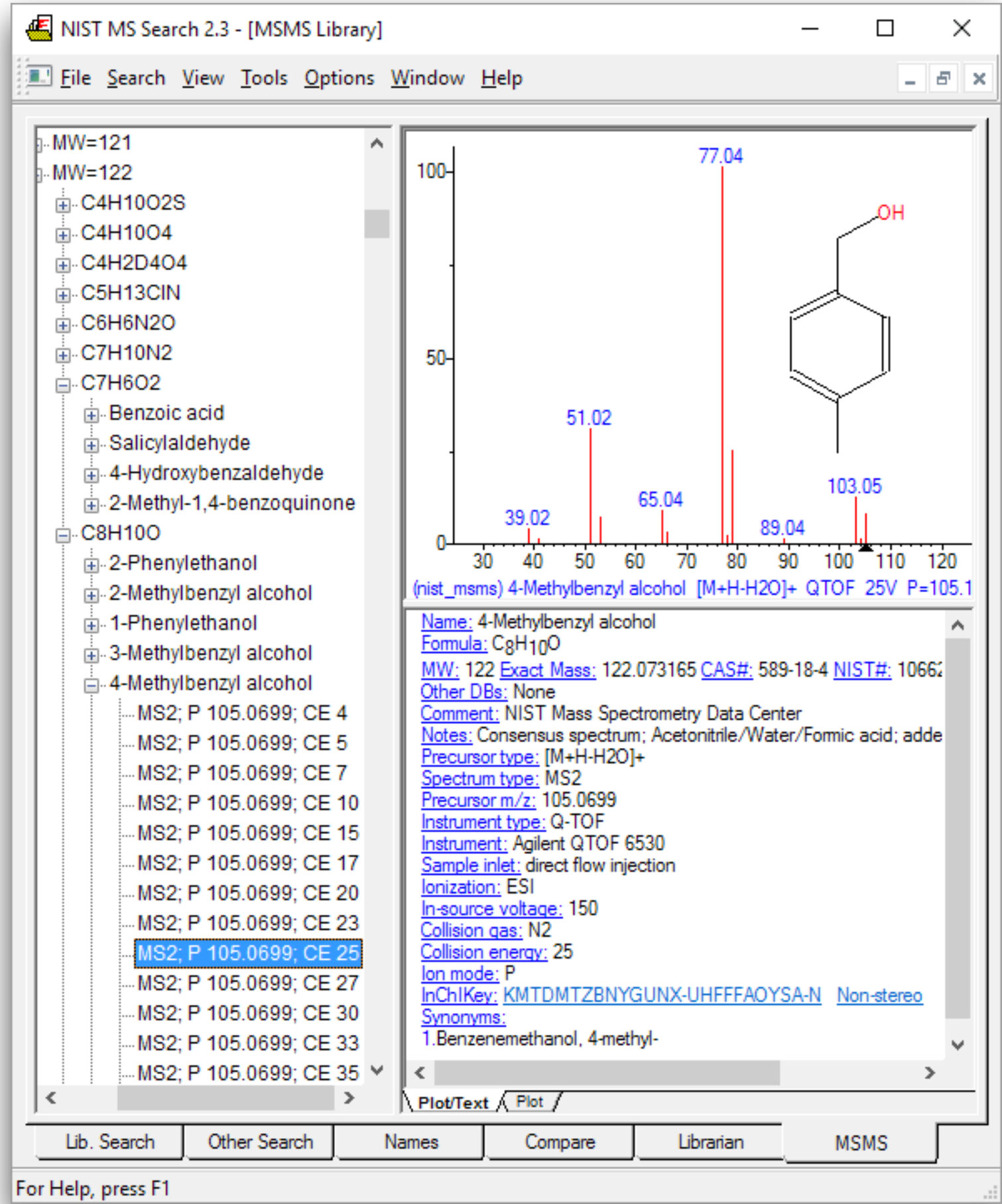
NIST 17 EI library



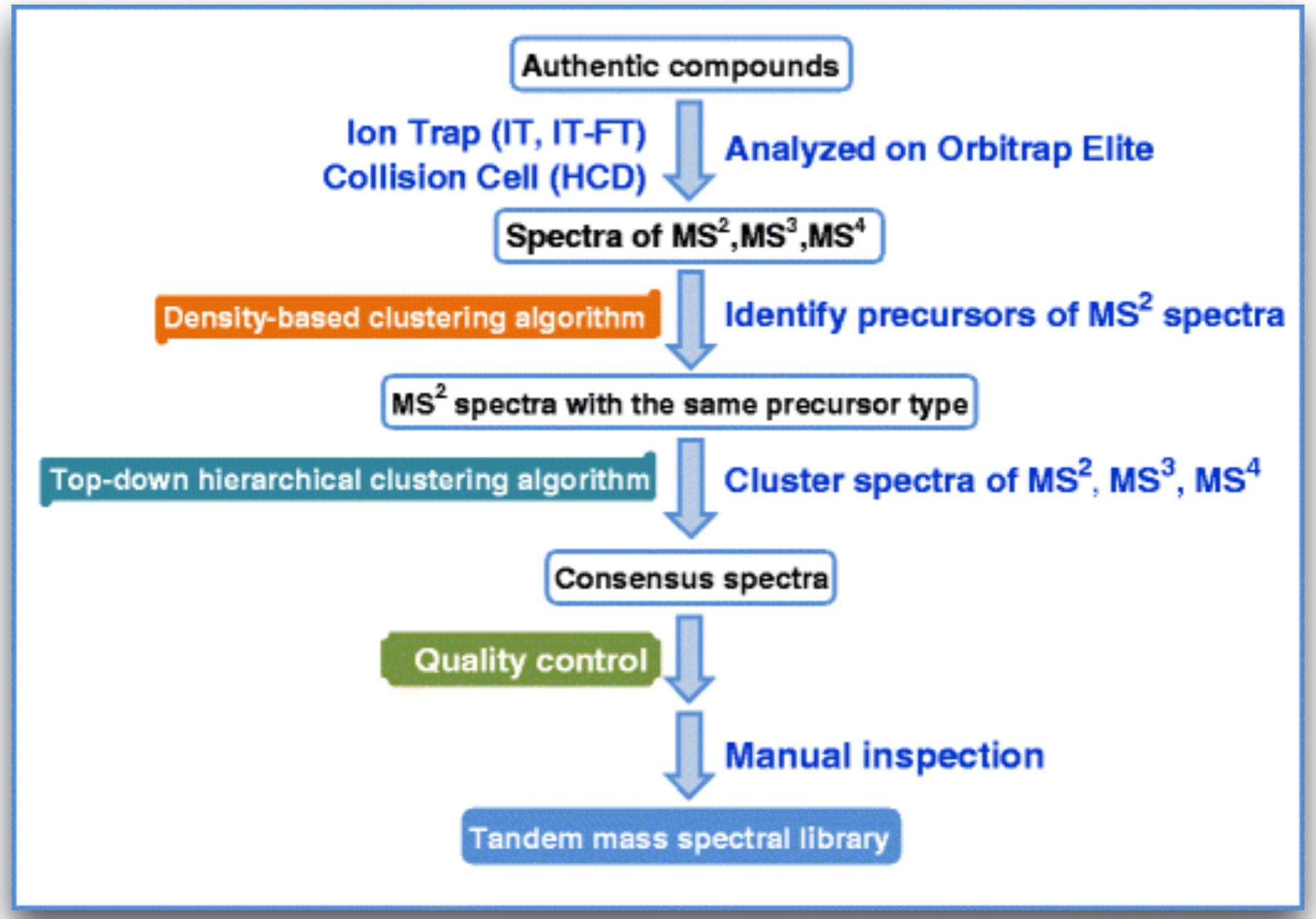
NIST 17 EI library

- 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

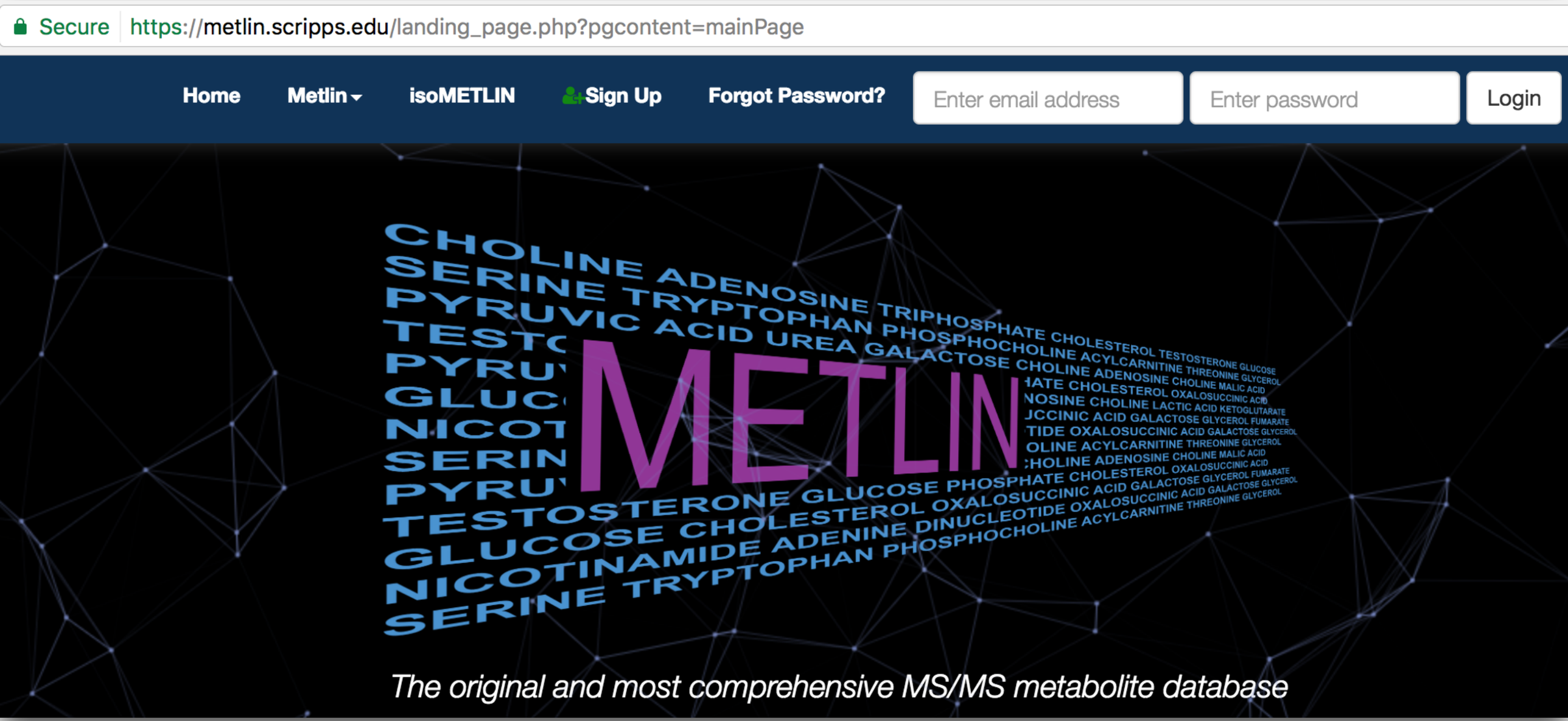
  [M-H]-, [M-2H]2-, [M-H-H2O]-, [M-H-NH3]-, [M-H+H2O]-, [M-H+NH3]-, [2M-H]-, [3M-H]-

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
Metlin
isoMETLIN
Sign Up
Forgot Password?
Enter email address
Enter password
Login
METLIN
The original and most comprehensive MS/MS metabolite database

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.

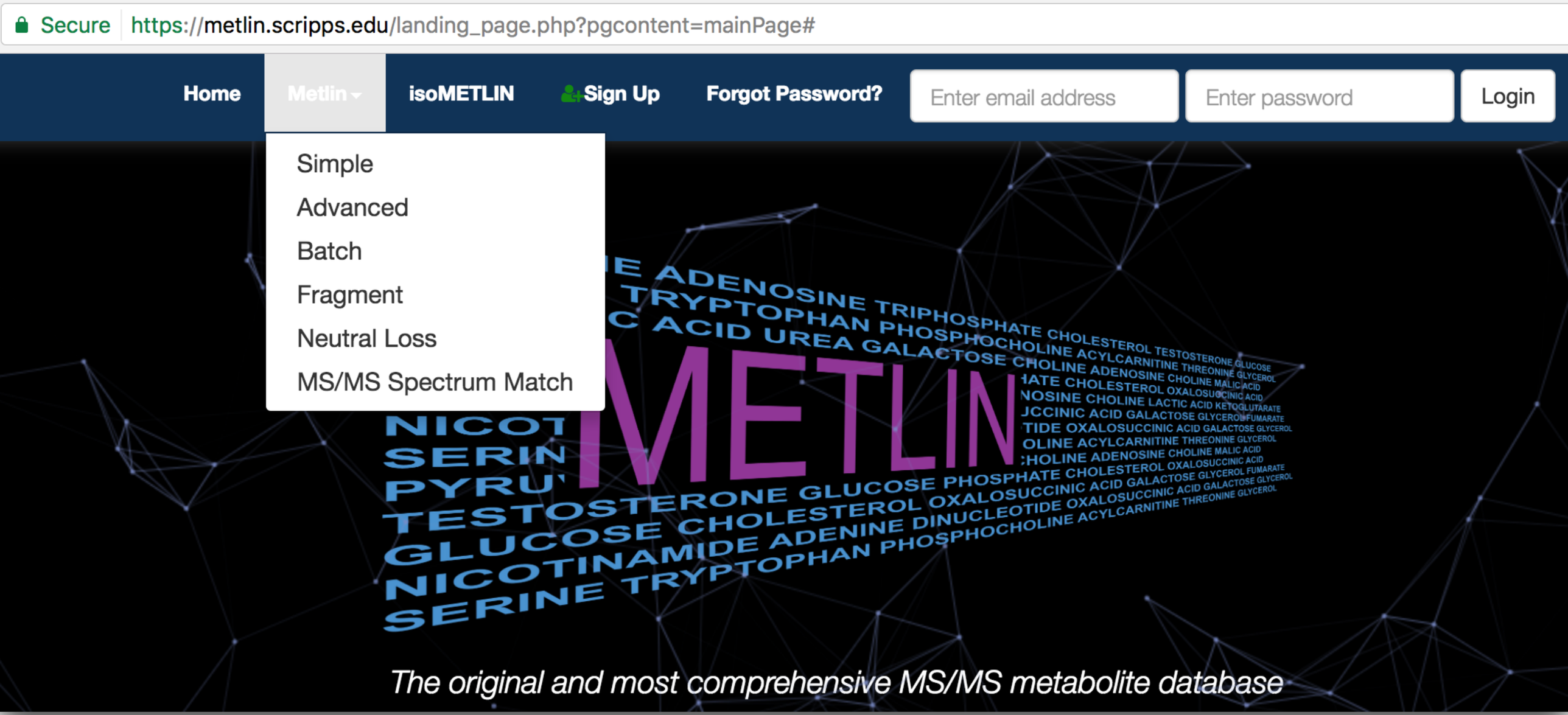
Tandem Mass Spectrometry

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.

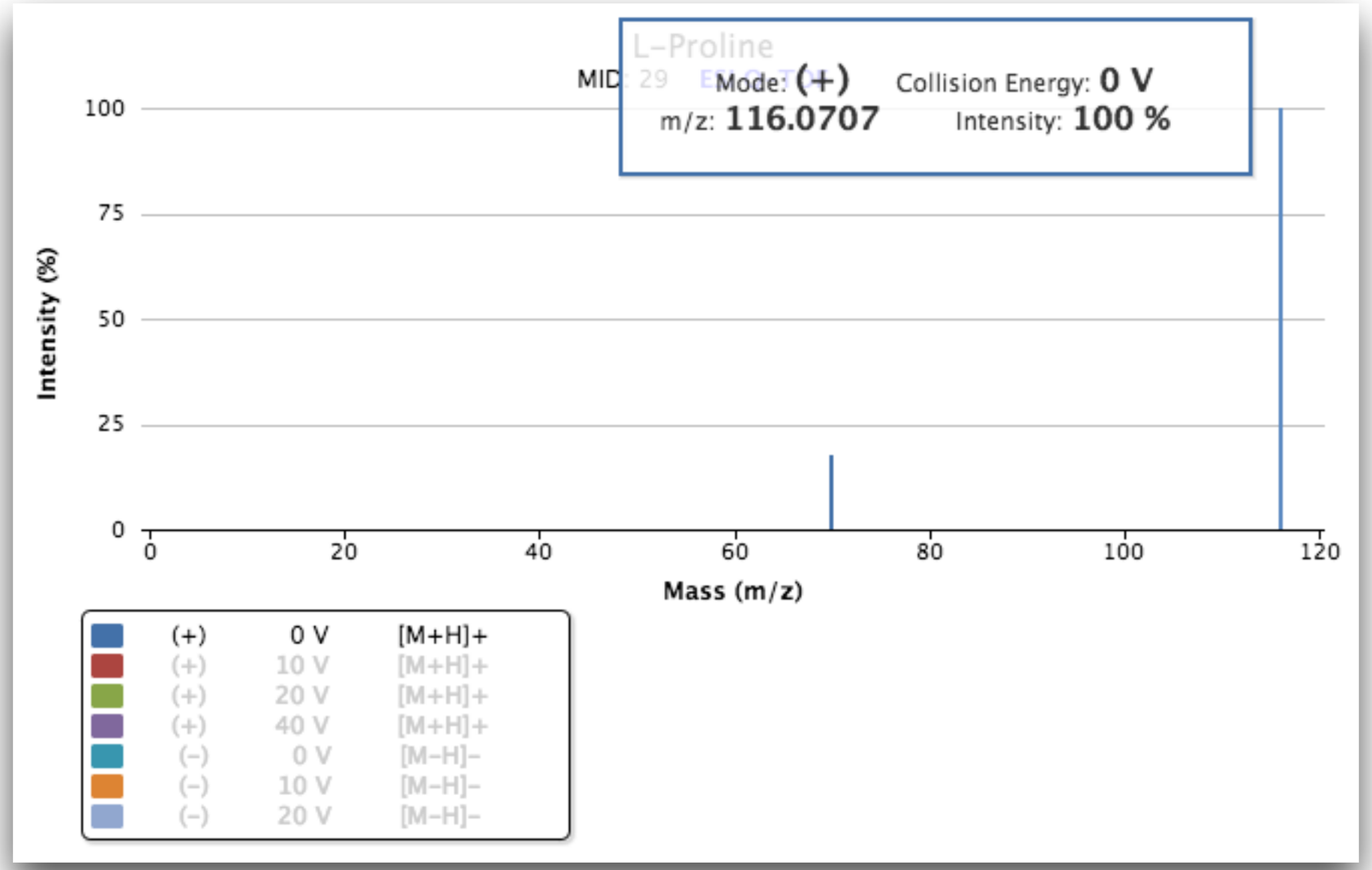
Metabolites

Created in 2004, METLIN now includes 961,829 molecules ranging from lipids, steroids, plant & bacteria metabolites, small peptides, carbohydrates, exogenous drugs/metabolites, central carbon metabolites and toxicants. Over 14,000 metabolites have been individually analyzed and another 200,000 has *in silico* MS/MS data.

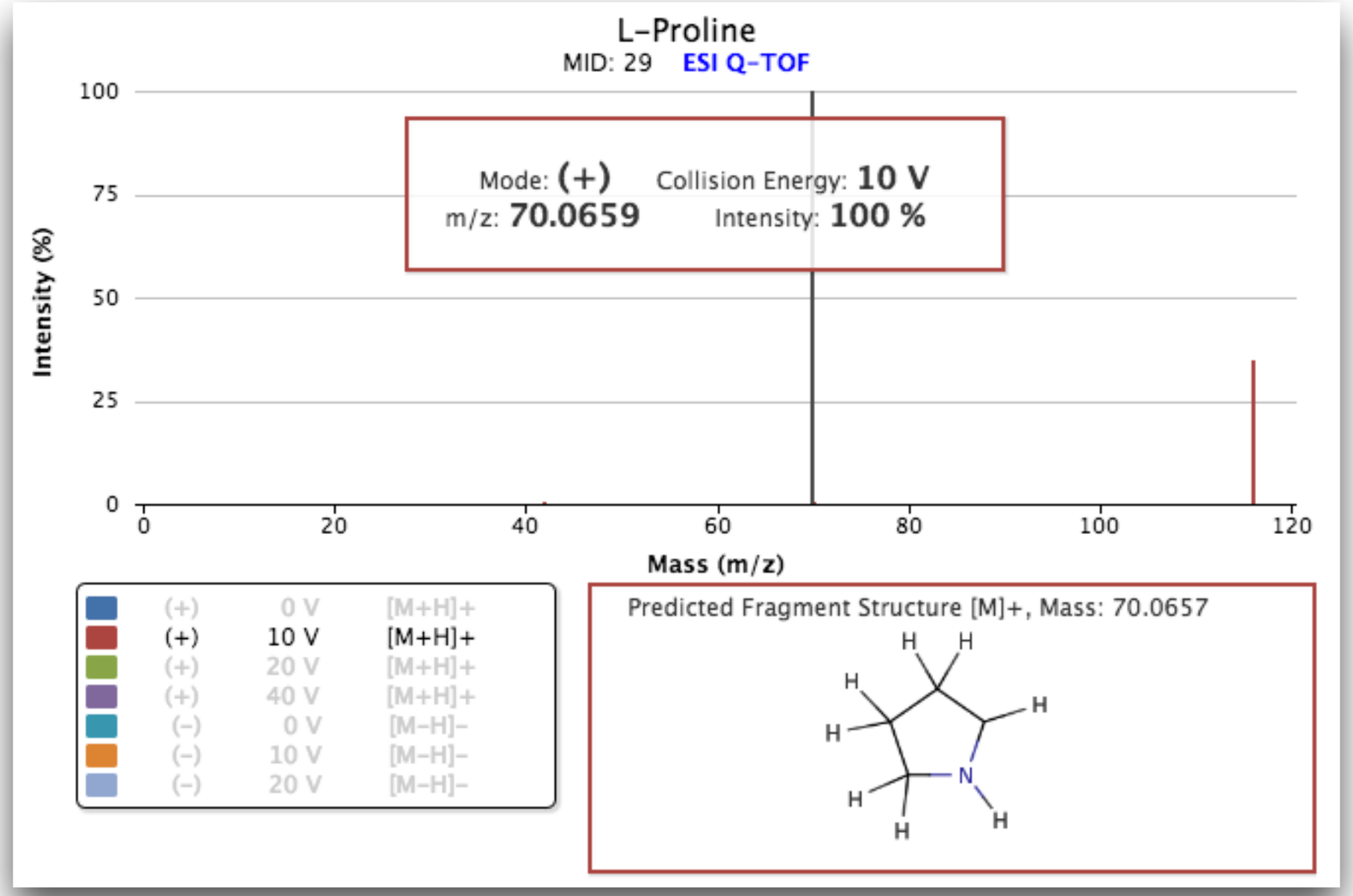
METLIN


Secure
https://metlin.scripps.edu/landing_page.php?pgcontent=mainPage#
Home
Metlin
isoMETLIN
Sign Up
Forgot Password?
Enter email address
Enter password
Login
Simple
Advanced
Batch
Fragment
Neutral Loss
MS/MS Spectrum Match
METLIN
The original and most comprehensive MS/MS metabolite database

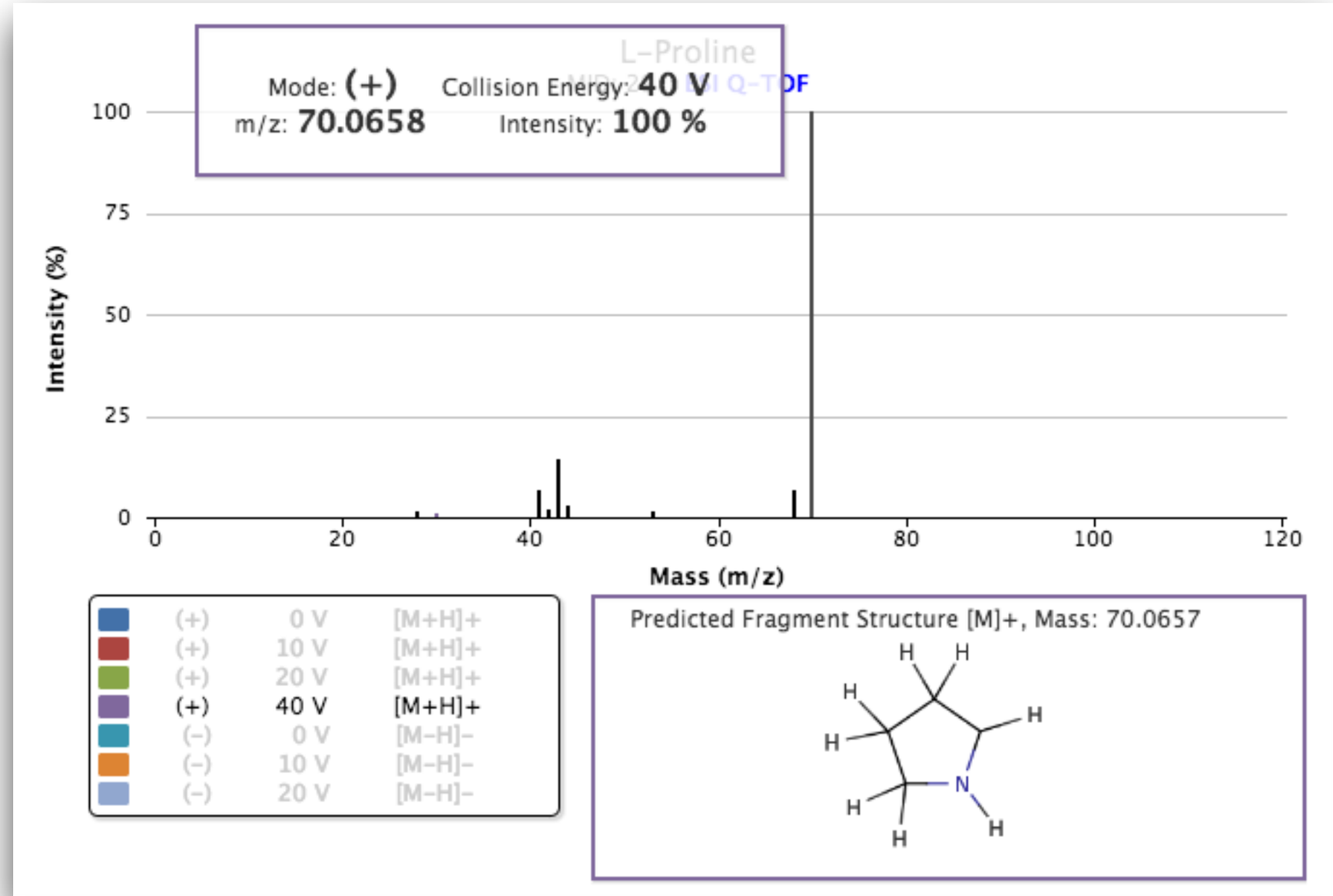
METLIN


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 %
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
H
N
H

MassBank

www.massbank.jp/?lang=en

MassBank

High Quality Mass Spectral Database

Database Service

- Spectrum Search
- Quick Search
- Peak Search
- Substructure Search
- Metabolite Prediction
- Spectral Browser
- Batch Service
- Browse Page
- Record Index

MassBank

Database Service

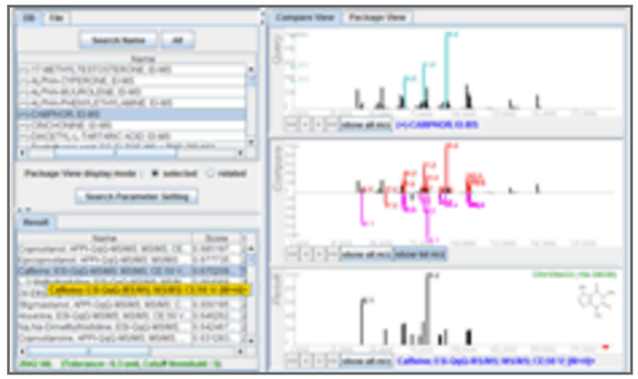
- Spectrum Search
- Quick Search
- Peak Search
- Substructure Search
- Metabolome Prediction
- Spectral Browser
- Batch Service
- Browse Page
- Record Index

Statistics

Publications

Database Service

Spectrum Search



Search similar spectra on a peak-to-peak basis

Retrieves spectra similar to user's spectrum in terms of the *m/z* value. This search is helpful to identify chemical compound by comparing similar spectra on a 3D-display.

Spectrum Search

User's Manual

Quick Search

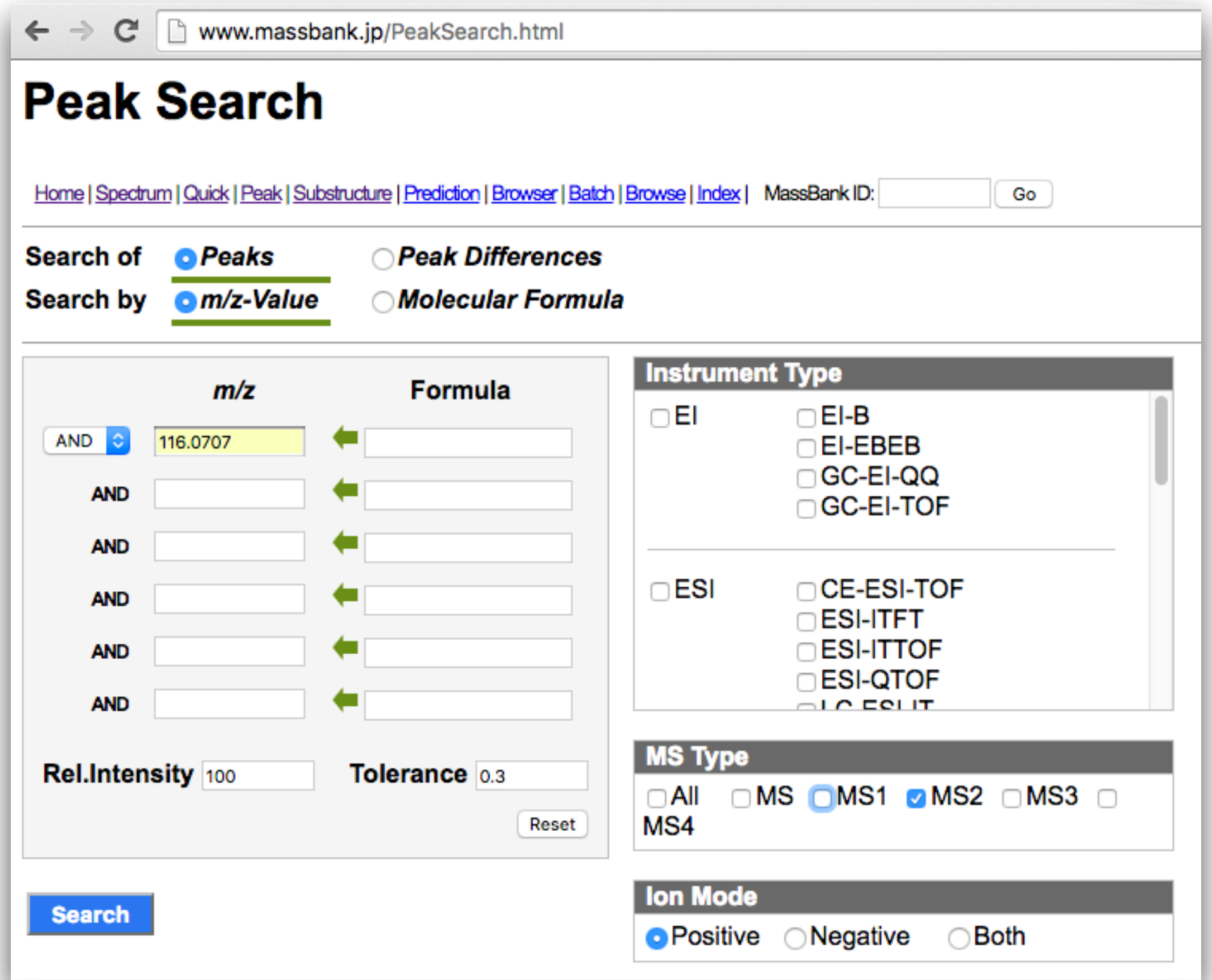
Keyword search of chemical compounds

Retrieves the chemical compound(s) specified by chemical name or molecular formula, and displays its spectra.

Quick Search

User's Manual

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**

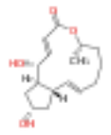
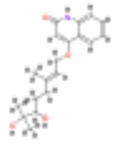
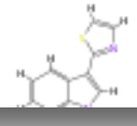
Edit / Resubmit Query

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

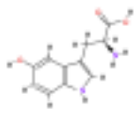
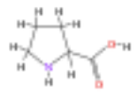
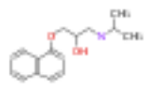
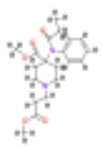
Open All Tree | Multiple Display | Spectrum Search

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**	
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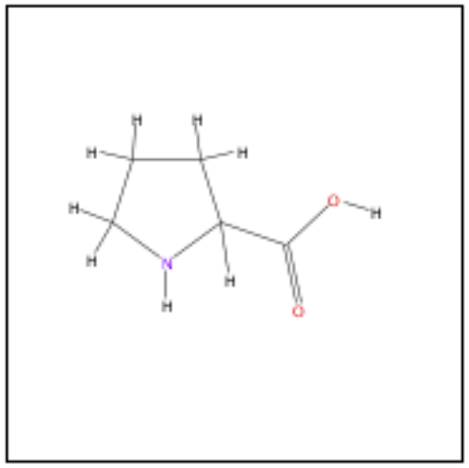
Proline; LC-ESI-QTOF; MS2; CE:15 eV; [M+H]+

Mass Spectrum Chemical Structure



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RECORD_TITLE: Proline; LC-ESI-QTOF; MS2; CE:15 eV; [M+H]+
DATE: 2016.01.19 (Created 2008.01.02, modified 2013.06.04)
AUTHORS: Boettcher C, Institute of Plant Biochemistry, Halle, Germany
LICENSE: CC BY-SA
COMMENT: IPB_RECORD: 261
COMMENT: CONFIDENCE: confident structure

CH$NAME: Proline
CH$NAME: pyrrolidine-2-carboxylic acid
CH$COMPOUND_CLASS: Natural Product; amino acid
CH$FORMULA: C5H9NO2
CH$EXACT_MASS: 115.06333
CH$SMILES: C1CC(NC1)C(=O)O
CH$IUPAC: InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)
CH$LINK: INCHIKEY ONIBWKKTOPOVIA-UHFFFAOYSA-N
CH$LINK: KEGG C00148
CH$LINK: PUBCHEM CID:614

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AC$INSTRUMENT_TYPE: LC-ESI-QTOF
AC$MASS_SPECTROMETRY: MS_TYPE MS2
AC$MASS_SPECTROMETRY: ION_MODE POSITIVE
AC$MASS_SPECTROMETRY: COLLISION_ENERGY 15 eV
AC$MASS_SPECTROMETRY: IONIZATION ESI

MS$FOCUSED_ION: PRECURSOR_TYPE [M+H]+

PK$SPLASH: splash10-01b9-8900000000-000cb5f6ae87b559450a
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MassBank

mona.fiehnlab.ucdavis.edu/spectra/splash/splash10-01b9-8900000000-000cb5f6ae87b559450a

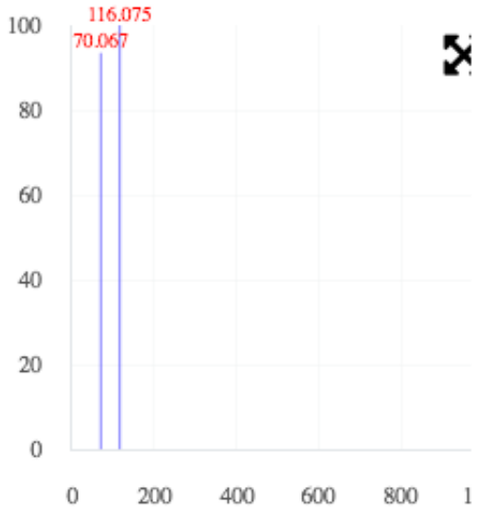
MoNA - MassBank of North America | Browse | Statistics | Resources | Download | Upload | Search...

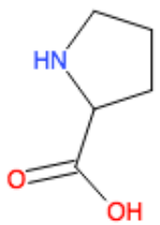
display generated query

1

Proline

Score: ★★★★★★★★★★☆





accession	PB000450
authors	Boettcher C, Institute of...
collision energy	15 eV
compound class	Natural Product; amino ac...
exact mass	115.0633
instrument	API QSTAR Pulsar i
instrument type	LC-ESI-QTOF
ion mode	positive
ionization	ESI
license	CC BY-SA
mass accuracy	8754.0881
mass error	-1007.2745
ms level	MS2
origin	PB000450.txt
precursor type	[M+H]+

Originally submitted to the MassBank Spectral Database as PB000450

MoNA

mona.fiehnlab.ucdavis.edu

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

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

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

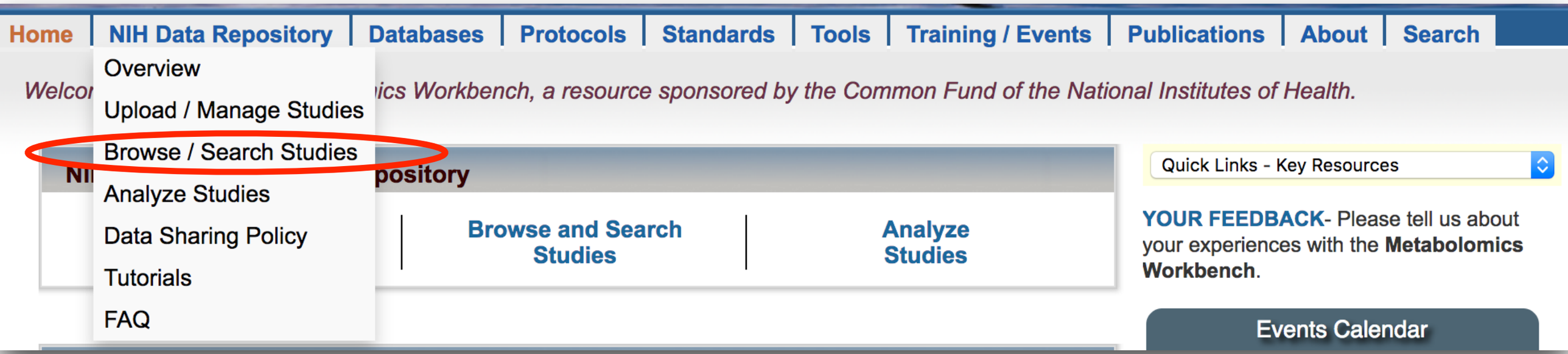
- Metabolomics Workbench
- MetaboLights

Raw data databases

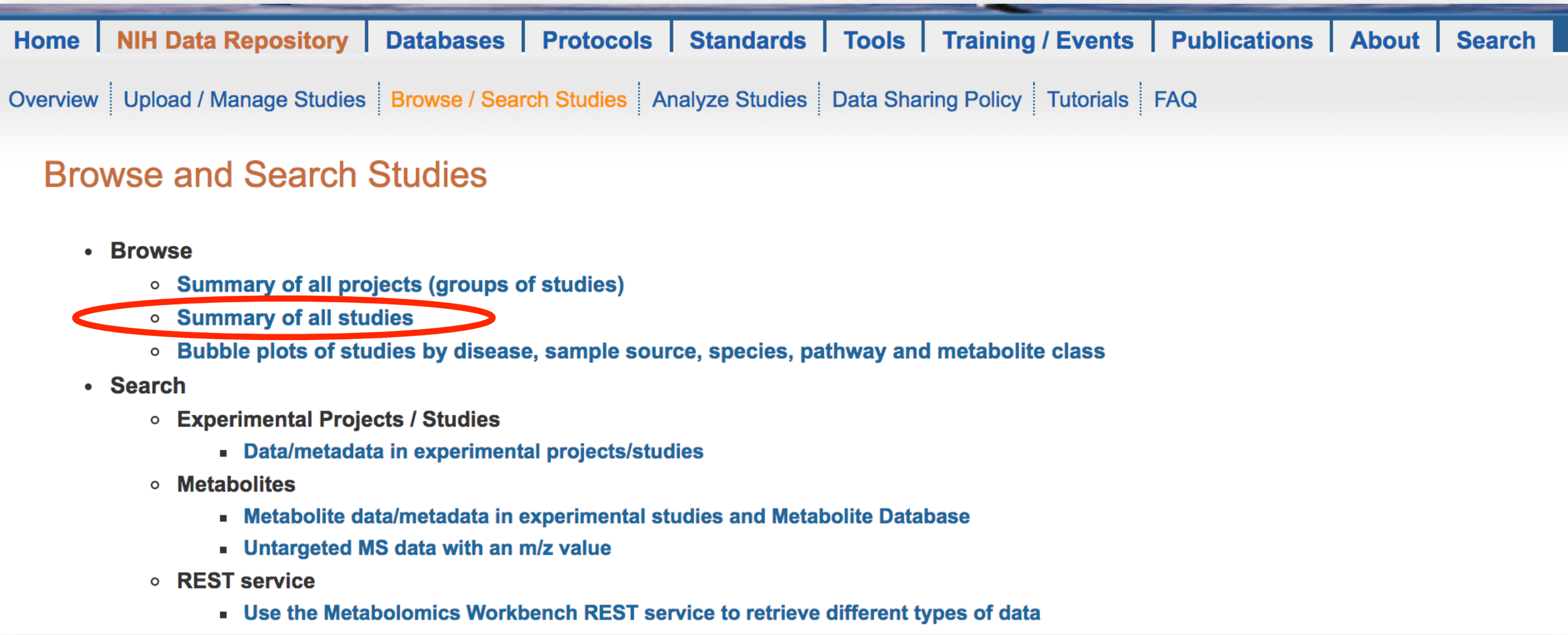
- Metabolomics Workbench
  - Funded by the NIH Common Fund Metabolomics Program
  - Serve as a national and international repository for metabolomics data and metadata
  - Provide access to raw data, metabolite standards, protocols .....

Metabolomics workbench

Metabolomics workbench



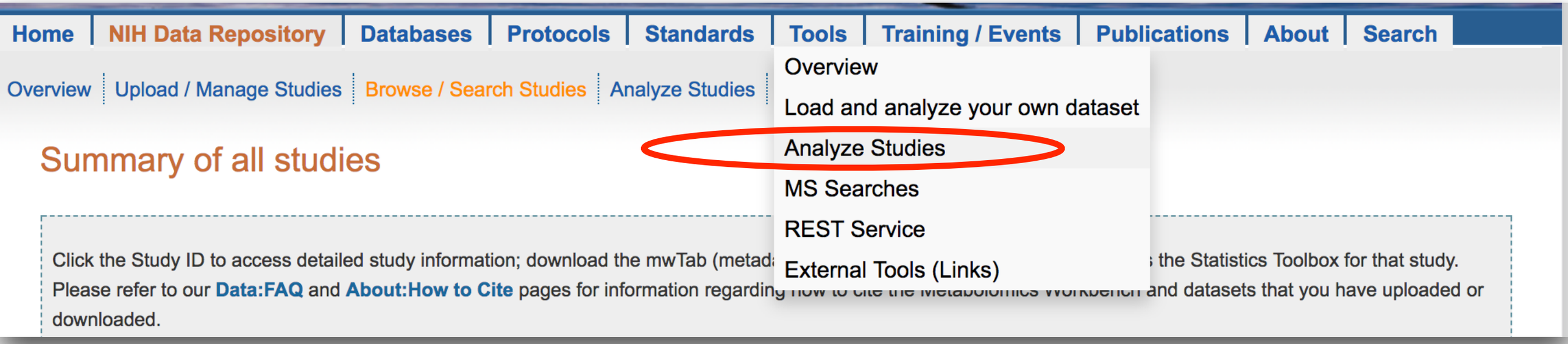
Metabolomics workbench



Metabolomics workbench

Study ID	Study Title	Species	Institute	Analysis	Release Date	Version	Samples	Download (* : Contains raw data)
ST000001	Fatb Induction Experiment (FatBIE)	Arabidopsis thaliana	University of California, Davis	MS	2013-02-14	1	24	Uploaded data (476K)
ST000002	Intestinal Samples II pre/post transplantation	Homo sapiens	University of California, Davis	MS	2013-02-22	1	12	Uploaded data (664K)
ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	Mus musculus	University of California, Davis	MS	2013-02-15	1	18	Uploaded data (5.3G)*
ST000004	Lipidomics studies on NIDDK / NIST human plasma samples	Homo sapiens	LIPID MAPS	MS	2013-03-17	1	8	Uploaded data (48K)
ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Mus musculus	LIPID MAPS	MS	2013-03-22	1	696	Uploaded data (56K)
ST000006	White Wine Study	Vitis vinifera	University of California, Davis	MS	2013-03-23	1	102	Uploaded data (532K)
ST000007	Rice Infection Study	Oryza sativa	University of California, Davis	MS	2013-03-24	1	60	Uploaded data (1.7M)
ST000008 (Availability TBA)	Metabolomics Analysis of Population Genetics (PopGen) for Response to Cholera Vaccination)	Homo sapiens	University of North Carolina	NMR	-	-	112	Not available
ST000009	Mixed meal tolerance	Homo sapiens	University of Michigan	MS	2013-04-26	1	228	Uploaded data (8.0M)
ST000010	Lung Cancer Cells 4	Homo sapiens	University of Michigan	MS	2013-05-03	1	78	Uploaded data (2.0M)
ST000011	African Metabolomics	Homo sapiens	University of Michigan	MS	2013-05-04	1	80	Uploaded data (2.2M)

Metabolomics workbench



Metabolomics workbench

Analyze Studies

MS/NMR studies identifying named metabolites

Normalization and averaging

- Metabolite averages per experimental factor for studies
- Normalize study data
- Relative log abundance plots

Clustering and correlation

- Hierarchial or heatmap cluster analysis
- Clustered correlation analysis
- Network analysis on correlated metabolites

Univariate analysis

- Volcano plot analysis

Multivariate analysis

- Principal component analysis
- Linear discriminant analysis
- Partial least-squares discriminant analysis

Classification and feature analysis

- OPLS-DA analysis and VIP projection
- Random Forest analysis and VIP projection

Mapping metabolites to biochemical pathways

Metabolomics workbench

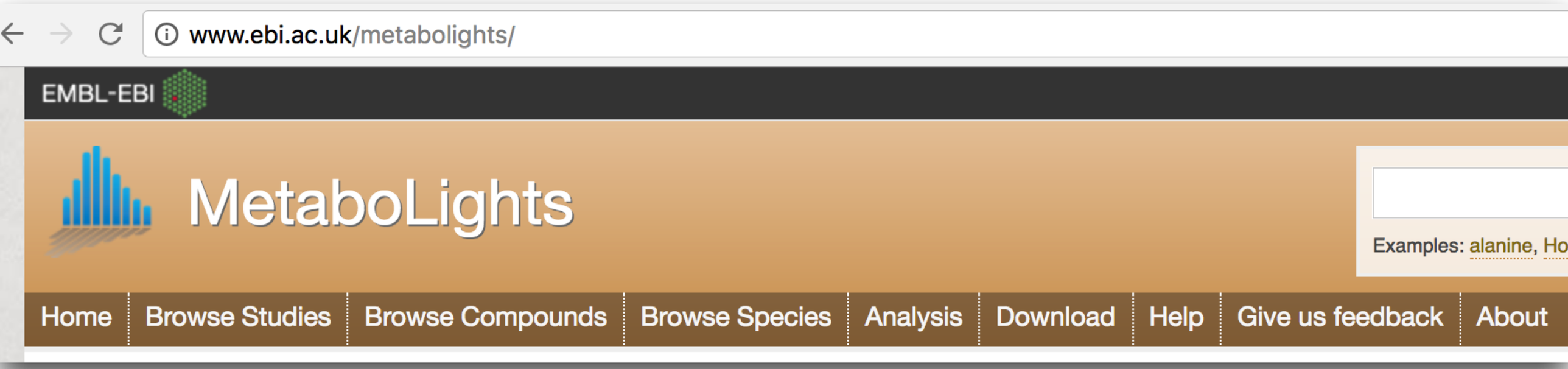
Principal Component Analysis on MS studies

This analysis uses the "prcomp" function of the R statistics environment
Click on links below to perform analysis.

PCA	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Fatty acid/eicosanoid MS quantitative analysis with deuterated standards
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Phospholipid MS quantitative analysis with odd-chain standards
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Sphingolipid MS quantitative analysis with C12 standards
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Sterol MS quantitative analysis with deuterated standards
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Prenol/Cardiolipin MS quantitative analysis with odd-chain(CL) or staable analog standards
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Triacylglycerol MS quantitative analysis with deuterated standards

Raw data databases

- MetaboLights



MetaboLights

MetaboLights: a database for metabolomics experiments and derived information

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.We will provide search services around spectral similarities and chemical structures.

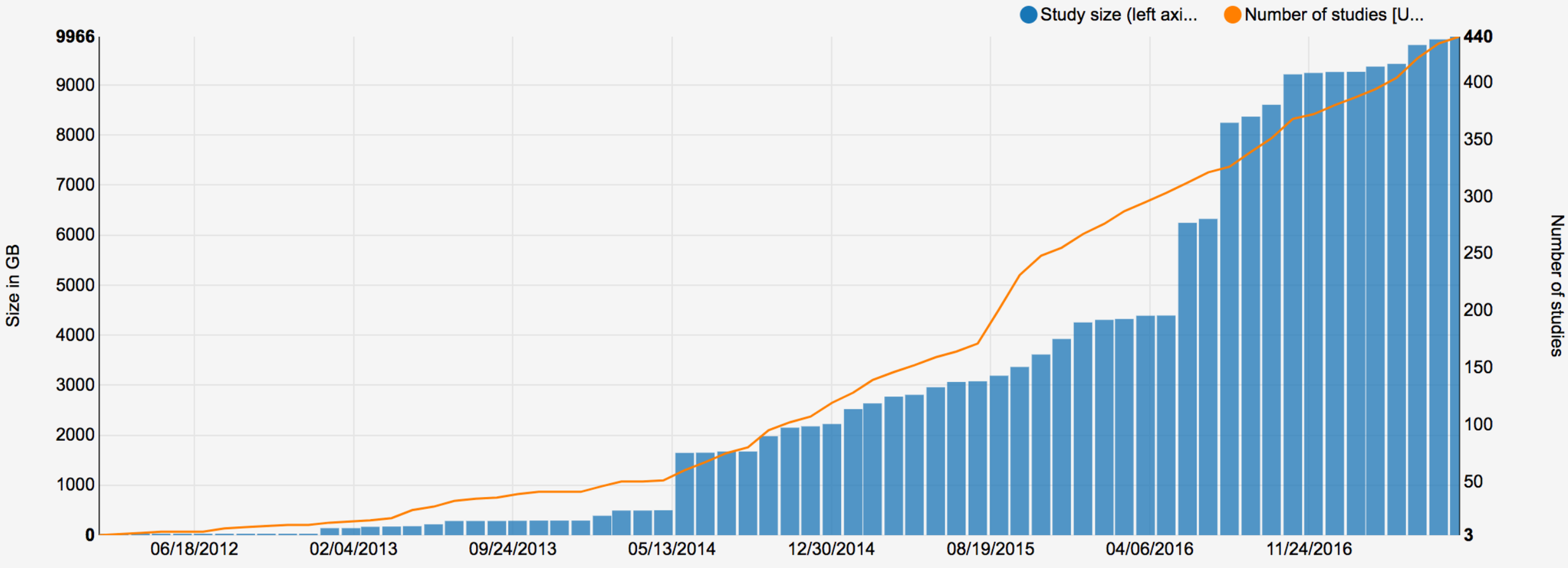
We offer user-submission tools and have strong reporting capabilities. We will utilise and further develop de-facto standard formats where various components are encapsulated, such as the encoded spectral and chromatographic data, and associated information about the chemical structure, as well as metadata describing assays and the study as a whole.

MetaboLights semantic quality will be based on various controlled vocabularies linking data to existing resources such as BRENDA (tissue ontology) and other established ontologies. We are dedicated to collaborate closely with major parties in world-wide metabolomics communities, such as the Metabolomics Society and the associated Metabolomics Standards Initiative (MSI).

MetaboLights

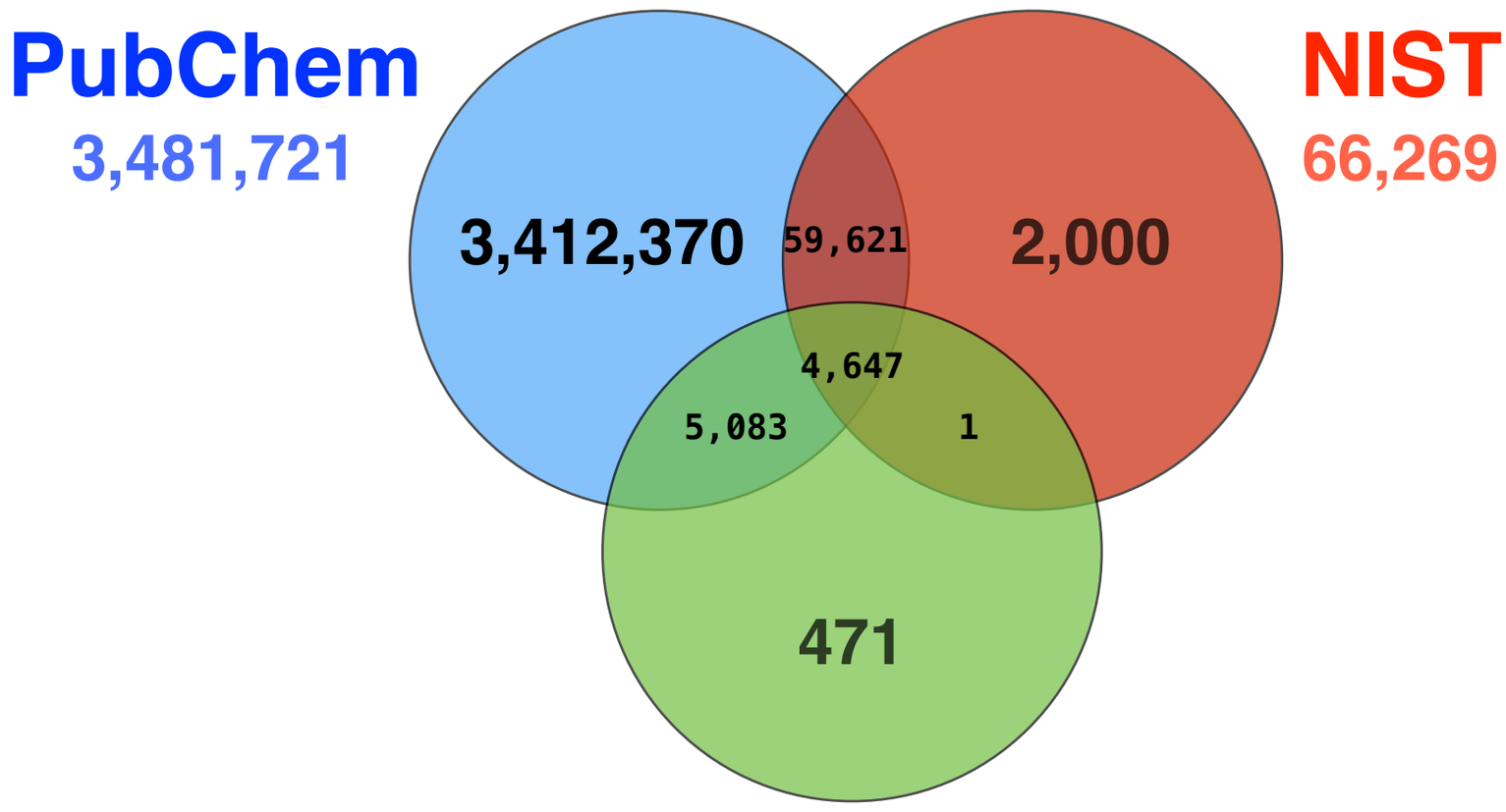
MetaboLights Statistics

Data growth over time



PubChem, NIST, and HMDB, again

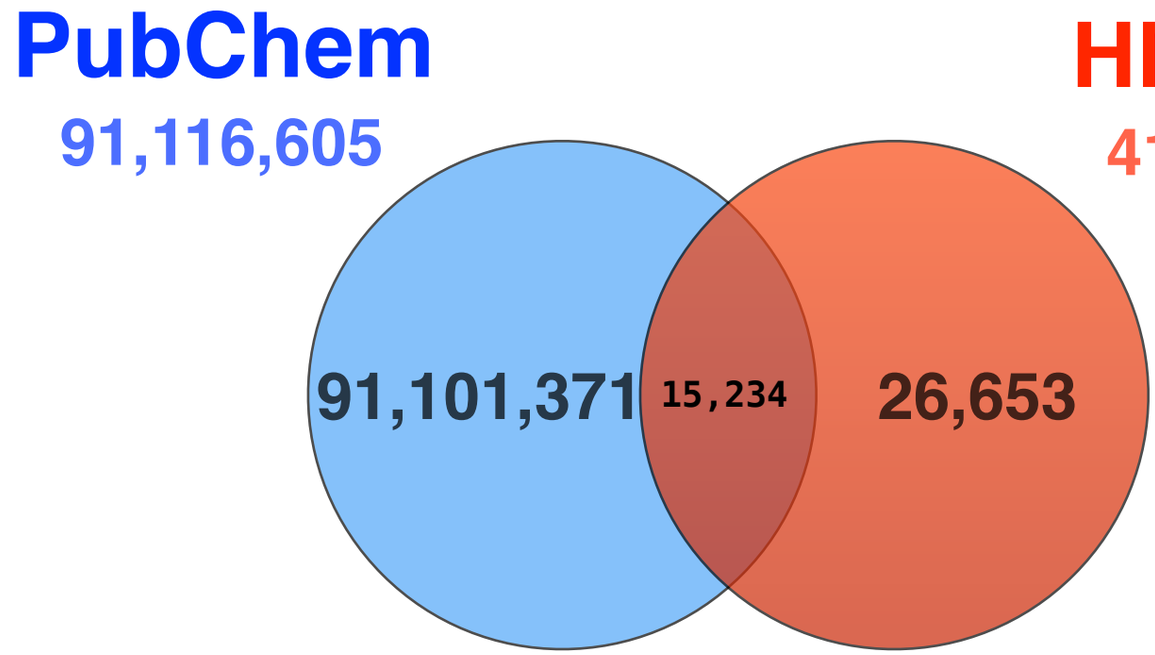
- In terms of unique molecular formula



based on database version in 2016

PubChem, NIST, and HMDB, again

- In terms of unique InChi Key



based on database version in 2016

Acknowledgement

- Aleksandr Smirnov, Ph.D.

Thank you!