

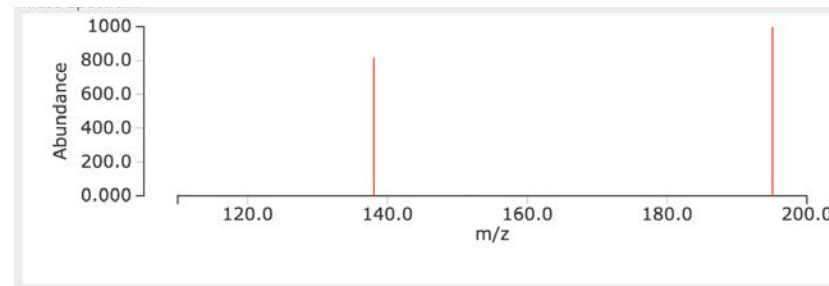
# **Databases for Metabolomics**

**ELIXIR Metabolomics Course  
Bari, Italy, April 2022**

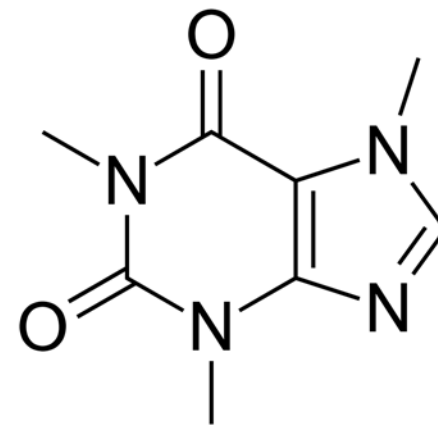
**Christoph Steinbeck, Friedrich-Schiller-University, Jena, Germany**

# What type of database are we talking about?

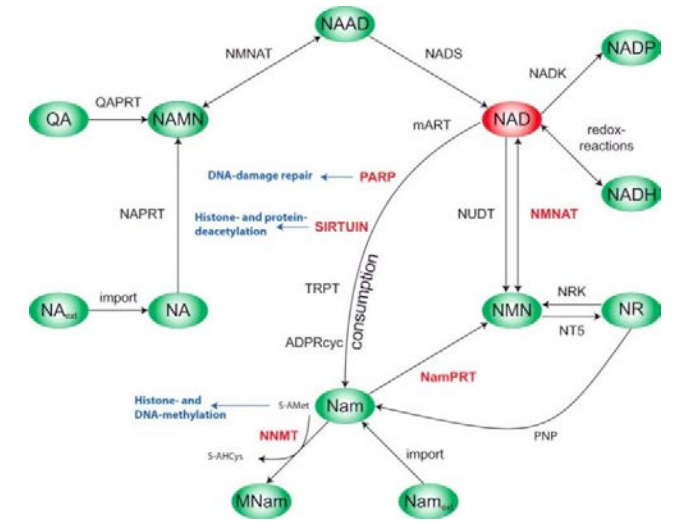
Metabolite Spectra  
(Spectral Databases)



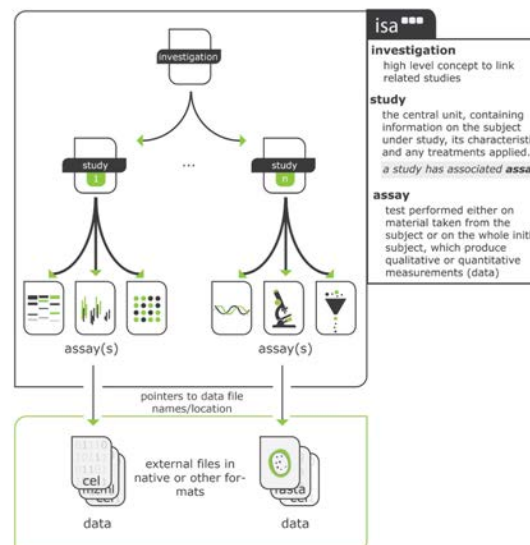
Metabolite structures  
(Structure Databases)



Role of metabolites in organisms  
(Pathway Databases)



Metabolomics studies  
(Metabolomics Repositories)



# MassBank Europe

[>> Search Spectra](#)[>> Learn More](#)

MassBank is a community effort and [you are invited to contribute](#). Please refer to our [contributor documentation](#) and get in touch via [github](#) or [email](#).

## News

**source (26.04.2022): <https://massbank.eu>**

Dear friends of MassBank,

**Update 05 January 2022:** A Happy and Healthy New Year 2022 to all our friends and contributors! We deployed the new Massbank system version 2.1.13 fixing [CVE-2021-44228](#).

**Update 14 December 2021:** We are excited to announce the new MassBank data release. We added 3251 new mass spectra of 304 compounds contributed kindly by Eawag, University of Antwerp, University of Athens, Mass Spectrometry Society of Japan, and INRAE France. The release version is [2021.12](#) with the DOI: [10.5281/zenodo.5775684](#). We also deployed the new Massbank system version 2.1.11 fixing for example [CVE-2021-44228](#).

**Update 3 September 2021:** MassBank Europe spectra annotations in [PubChem](#) are online now. What a great enhancement! MassBank Europe spectra go online via our new [MassBank ↔ PubChem deposition / annotation repository pipeline](#) with code developed by [LCSB-ECI](#). Find an example for [arsanilic acid](#) at PubChem. See also the related [tweet](#).

**Update 5 March 2021:** The new MassBank data release is available and deployed on MassBank Europe. We added 159 new mass spectra containing tentative mass spectra of pesticide metabolites. They include Markush structures for the first time, for example a mass spectra of the tentatively identified [atrazine-desamine](#). The release version is [2021.03](#) with the DOI: [10.5281/zenodo.4563726](#). The whole MassBank content is available in NIST msp format for integration in mass spectrometry software.

**Update 8 February 2021:** The new MassBank data release is available and deployed on MassBank Europe. The release version is [2021.02](#) with the DOI: [10.5281/zenodo.4506480](#). The whole MassBank content is available in NIST msp format for integration in mass spectrometry software. The [MassBank\\_NIST.msp](#) file contains all records to be used in vendors' software library search. We also provide a msp file in RIKEN format for integration in [MS DIAL](#). Enjoy and report your



Please Login to Analyze Data at GNPS

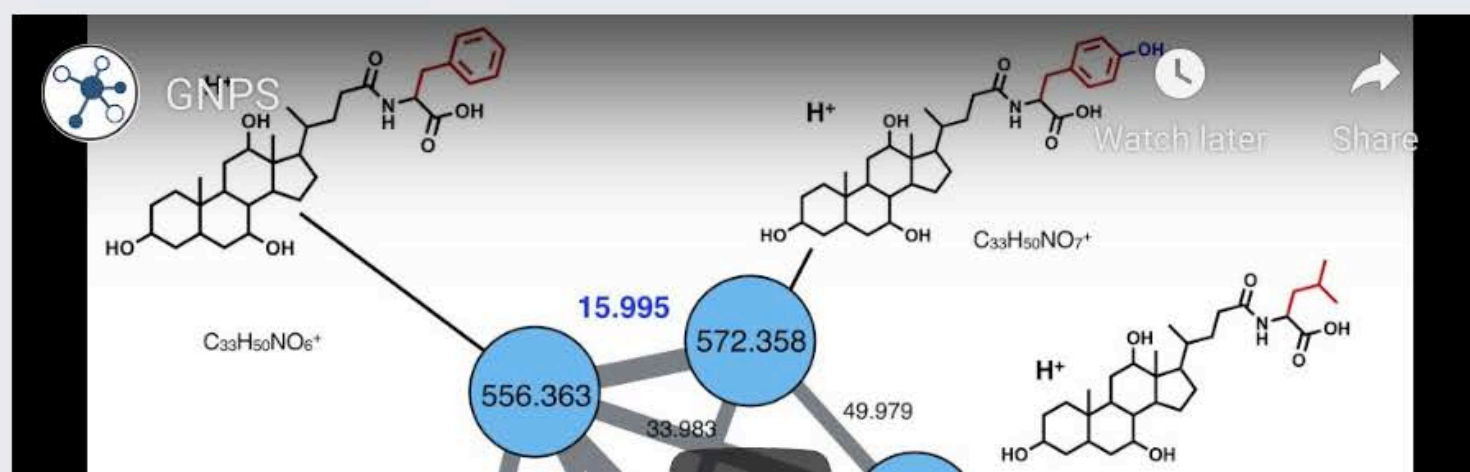
Login to Existing Account

Register New Account

source (26.04.2022): <https://gnps.ucsd.edu/>



GNPS is a web-based mass spectrometry ecosystem that aims to be an open-access knowledge base for community-wide organization and sharing of raw, processed, or annotated fragmentation mass spectrometry data (MS/MS). GNPS aids in identification and discovery throughout the entire life cycle of data; from initial data acquisition/analysis to post publication.



Tweets by @GNPS\_UCSD

GNPS - UC San Diego Retweeted

**Ming Wang**  
@mingxunwang

Revival of a great initiative!

Just to make things a bit easier, the MS data has been deposited in @GNPS\_UCSD



- Perform **molecular networking** and **spectral library search** of LC-MS/MS data utilizing computational tools (See [Molecular Networking](#), [Spectral Library Search](#), etc).
- **Annotate/curate identified MS/MS spectra** in open-access GNPS reference spectral libraries.
- Annotate peptidic natural products in LC-MS/MS data with **DEREPLICATOR/VarQuest/DEREPLICATOR+** and **RiPPQuest**.
- Propagate in silico annotations in your LC-MS/MS data with **Network Annotation Propagation (NAP)**.
- **NEW!** Perform advanced molecular networking and spectral library search with **Feature-Based Molecular Networking**. See <https://doi.org/10.1101/812404>.
- **NEW!** Analyze **GC-MS data** with GNPS (See [GC-MS deconvolution](#), and [GC-MS library search/molecular networks](#)).
- **NEW!** Annotate your LC-MS/MS data with **MolNetEnhancer**. See <https://doi.org/10.1101/654459>.
- **NEW!** Search spectral Mass2Motifs in your LC-MS/MS data with **MS2LDA**.
- **NEW!** Give LC-MS/MS spectra biological/environmental context by searching against all public LC-MS/MS datasets (**MASST Search**). See <https://doi.org/10.1101/591016>.
- **NEW!** Find and co- or re-analyze public LC-MS/MS data via systematic sample information at **ReDU**. See <https://doi.org/10.1101/750471>.

# DESCRIPTION

## NIST Tandem Mass Spectral Library, 2020 release

- 31,000 compounds
- Twice as many as the 2017 release
- 186,000 precursor ions
- 1.3 million spectra

source (26.04.2022): <https://chemdata.nist.gov/>

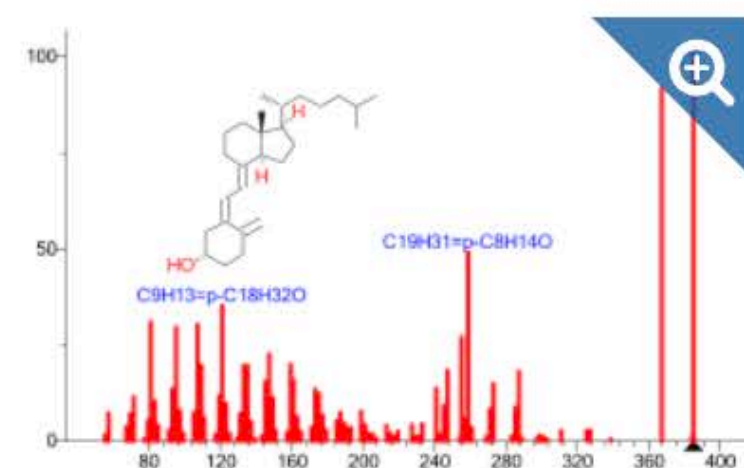
### Fragmentation methods

- 27,840 HRAM (high res accurate mass) compounds
- 29,890 QTOF, HCD, IT-HRAM, QqQ compounds
- 29,444 ion trap compounds (low res., up to MS<sup>4</sup>)
- 246 APCI HRAM “extractables and leachables”

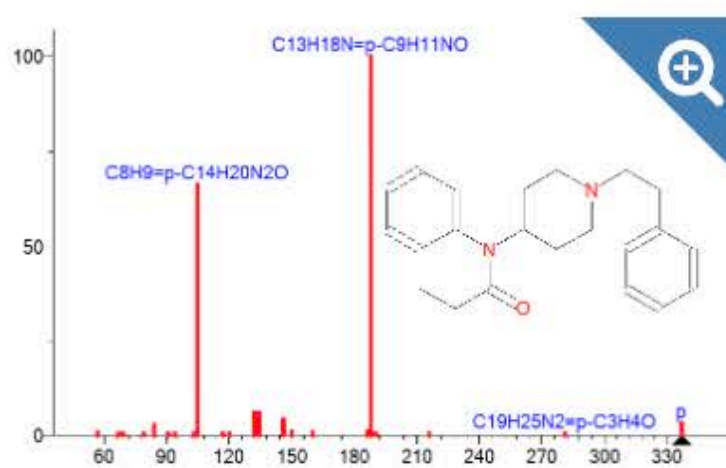
### Precursor ion types

- 26,575 protonated
- 12,589 deprotonated
- 10,032 water/ammonia loss
- 34,199 other in-source generated

### Wide variety of compounds



Vitamin D3 metabolite



Fentanyl drug



Malathion insecticide



## Search BMRB Metabolomics

### ► General search

Search for:

Enter search:

Experimental entries: ☒

Theoretical entries: ☐

Select the top  matches

Or upload batch file:  No file chosen

### ► Search by mass

### ► Search by structure

[Search 1D peak lists](#)

### ► Search 2D HSQC lists

### ► Solvent and field strength

[Help](#)

### Metabolomics data hosted at BMRB

- [What is metabolomics?](#)
- [All compounds hosted at BMRB](#)
- [Cell wall compounds from the USDA NMR database of lignin and cell wall model compounds](#)
- [\(NEW\) iNext screening library compounds](#)
- [Pathways of metabolism](#)
- [False standards](#)
- [Metabolic profiles of 47 marine bacteria](#)
- [Metabolic data by human gene](#)
- [Download all BMRB metabolomics entries as tar/gzip file](#)
- [Download relational database \(CSV, SQL\)](#)
- [Download entry data \(incl. raw NMR data\)](#)
- [Data upload](#)
- [Data policy](#)

### Other Metabolomics resources at BMRB



# Metlin

source (26.04.2022): <https://metlin.scripps.edu/>

Home  Simple Search Advanced Search MS2 To NL Converter  Logout [ christoph.... ]

Dear METLIN users,

Given the ongoing security and resource challenges of hosting METLIN academically, after ~20 years of service we have transitioned MS/MS data searching to a commercial (AWS) site, **METLIN Gen2**. Aspects of METLIN's searching capabilities will remain intact. However, through an exclusive arrangement with Scripps, the new **METLIN Gen2** subscription site will host new capabilities and data on 860,000 molecular standards (60 times bigger than the **METLIN.scripps.edu** site) with the following features:

**METLIN Gen2** features include:

- Searchable **MS<sup>2</sup>** data in both positive & negative ionization modes, at multiple collision energies, now comes as searchable composite spectra which brings together the **MS<sup>2</sup>** data from the multiple collision energies into one spectrum.
- New filters to include or exclude molecules you may not be interested in, such as peptides, drugs, toxicants, and/or halogenated species.
- MGF file batch searching that is enabled with above filters.
- A new **Neutral Loss** library exclusive to **METLIN Gen2** and generated from all 700,000 molecular standards, this also includes a MS<sup>2</sup> to NL converter, which allows you to convert your spectra from "Intensity vs  $m/z$ " to "Intensity vs  $\Delta m/z$ " for searching the full **Neutral Loss** library.

Order

SERINE ADENOSINE TRIPHOSPHATE CHOLESTEROL  
PYRUVIC ACID UREA GALACTOSE CHOLINE  
TESTOSTERONE  
PYRUVIC ACID UREA GALACTOSE CHOLINE  
GLUCOSE  
NICOTINAMIDE  
SERINE  
PYRUVIC ACID UREA GALACTOSE CHOLINE  
TESTOSTERONE GLUCOSE PHOSPHATE  
GLUCOSE CHOLESTEROL ADENINE  
NICOTINAMIDE ADENINE PHOSPHATE  
SERINE TRYPTOPHAN PHOSPHATE  
**METLIN** Cloud

# Metlin

source (26.04.2022): <https://metlin.scripps.edu/>

Home  Simple Search Advanced Search MS2 To NL Converter ▾

Dear METLIN users,

Given the ongoing security and resource challenges over the past few years of service we have transitioned MS/MS data to **METLIN Gen2**. Aspects of METLIN's search capabilities and data on 860,000 molecular standards (available on the [METLIN.scripps.edu](https://metlin.scripps.edu) site) with the following

**METLIN Gen2** features include:

- Searchable **MS<sup>2</sup>** data in both positive & negative ionization modes, at multiple collision energies, now comes as searchable composite spectra which brings together the **MS<sup>2</sup>** data from the multiple collision energies into one spectrum.
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## METLIN Gen2 Feature Details

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## METLIN Gen2 Subscription Matrix

1-Day Demo	Academic Subscription
<b>\$0</b> 1-day trial Help center access Email support	<b>\$1,000/year</b> \$1,000 Annual renewal fee Help center access Email support
<a href="#">Request a Demo</a>	<a href="#">Request a Quote</a>
Company Subscription	Day Pass Access
<b>\$5,000/year</b> Multi-user discounts Annual renewal fee Help center access Email support	<b>\$100/day</b> Experience METLIN for the day Help center access Email support
<a href="#">Request a Quote</a>	<a href="#">Request a Day Pass</a>

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COMPOUND SUMMARY

# Caffeine

Cite

Download

CONTENTS

Title and Summary

1 Structures

2 Names and Identifiers

3 Chemical and Physical Properties

4 Spectral Information

5 Related Records

6 Chemical Vendors

7 Drug and Medication Information

8 Food Additives and Ingredients

9 Agrochemical Information

10 Pharmacology and Biochemistry

11 Use and Manufacturing

12 Identification

13 Safety and Hazards

14 Toxicity

15 Associated Disorders and Diseases

16 Literature

17 Patents

18 Biomolecular Interactions and Pathways

19 Biological Test Results

20 Taxonomy

21 Classification

22 Information Sources

PubChem CID

2519

Structure



[Find Similar Structures](#)

Chemical Safety



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula

C8H10N4O2

Synonyms

caffeine  
58-08-2  
1,3,7-Trimethylxanthine  
Guaranine  
Thein

[More...](#)

Molecular Weight

194.19

Dates

Modify	Create
2022-04-15	2004-09-16

Caffeine is a [methylxanthine](#) alkaloid found in the seeds, nuts, or leaves of a number of plants native to South America and East Asia that is structurally related to [adenosine](#) and acts primarily as an [adenosine](#) receptor antagonist with psychotropic and anti-inflammatory activities. Upon ingestion, caffeine binds to [adenosine](#) receptors in the central nervous system (CNS), which inhibits [adenosine](#) binding. This inhibits the [adenosine](#)-mediated downregulation of CNS activity; thus, stimulating the activity of the medullary, vagal, vasomotor, and respiratory centers in the brain. This agent also promotes neurotransmitter release that further stimulates the CNS. The anti-inflammatory effects of caffeine are due the nonselective competitive inhibition of phosphodiesterases (PDEs). Inhibition of PDEs raises the intracellular concentration of [cyclic AMP \(cAMP\)](#), activates protein kinase A, and inhibits leukotriene synthesis, which leads to reduced inflammation and innate immunity.

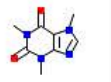


► [NCI Thesaurus \(NCIt\)](#)

Caffeine is [xanthine](#) alkaloid that occurs naturally in seeds, leaves and fruit of several plants and trees that acts as a natural pesticide. Caffeine is a major component of coffee, tea and chocolate and in humans acts as a central nervous system (CNS) stimulant. Consumption of caffeine, even in high doses, has not been associated with elevations in serum enzyme elevations or instances of clinically apparent liver injury.



COMPOUND SUMMARY

# Caffeine

PubChem CID	2519
Structure	<div>   </div> <p>2D 3D</p> <p><a href="#">Find Similar Structures</a></p>
Chemical Safety	 <p>Irritant</p> <p><a href="#">Laboratory Chemical Safety Summary</a></p>
Molecular Formula	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>
Synonyms	caffeine 58-08-2 1,3,7-Trimethylxanthine Guanine Thein <a href="#">More...</a>
Molecular Weight	194.19
Dates	Modify Create 2022-04-15 2004-09-16

Caffeine is a [methylxanthine](#) alkaloid found in the seeds, nuts, or leaves of a number of plants native to South America and East Asia that is structurally related to [adenosine](#) and acts primarily as an [adenosine](#) receptor antagonist with psychotropic and anti-inflammatory activities. Upon ingestion, caffeine binds to [adenosine](#) receptors in the central nervous system (CNS), which inhibits [adenosine](#) binding. This inhibits the [adenosine](#)-mediated downregulation of CNS activity; thus, stimulating the activity of the medullary, vagal, vasomotor, and respiratory centers in the brain. This agent also promotes neurotransmitter release that further stimulates the CNS. The anti-inflammatory effects of caffeine are due the nonselective competitive inhibition of phosphodiesterases (PDEs). Inhibition of PDEs raises the intracellular concentration of [cyclic AMP \(cAMP\)](#), activates protein kinase A, and inhibits leukotriene synthesis, which leads to reduced inflammation and innate immunity.

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Data Collection	Live Count	Description
<a href="#">Compounds</a>	111,263,473	Unique chemical structures extracted from contributed PubChem Substance records
<a href="#">Substances</a>	280,433,411	Information about chemical entities provided by PubChem contributors
<a href="#">BioAssays</a>	1,465,983	Biological experiments provided by PubChem contributors
<a href="#">Bioactivities</a>	294,716,876	Biological activity data points reported in PubChem BioAssays
<a href="#">Genes</a>	103,628	Genes tested in PubChem BioAssays and those involved in PubChem Pathways and identified in PubChem Patents
<a href="#">Proteins</a>	185,202	Proteins tested in PubChem BioAssays and those involved in PubChem Pathways and identified in PubChem Patents
<a href="#">Taxonomy</a>	112,645	Organisms of proteins/genes tested in PubChem BioAssays and those involved in PubChem Pathways and identified in PubChem Patents
<a href="#">Pathways</a>	238,908	Interactions between chemicals, genes, and proteins
<a href="#">Literature</a>	33,927,855	Scientific publications with links in PubChem
<a href="#">Patents</a>	41,796,860	Patents with links in PubChem
<a href="#">Data Sources</a>	856	Organizations contributing data to PubChem

14 Toxicity	▼
15 Associated Disorders and Diseases	
16 Literature	▼
17 Patents	▼
18 Biomolecular Interactions and Pathways	▼
19 Biological Test Results	▼
20 Taxonomy	
21 Classification	▼
22 Information Sources	

Natural Products Online is an open source project for Natural Products (NPs) storage, search and analysis. The present version hosts COCONUT, the COLleCtion of Open Natural ProDUcTs, one of the biggest and best annotated resources for NPs available free of charge and without any restriction.

## Latest updates: January 2022



### What's new?

- Improved taxonomic provenance
- Improved bibliography and references management
- Data described in the collaborative research consortium ChemBioSys added

## Component Browser

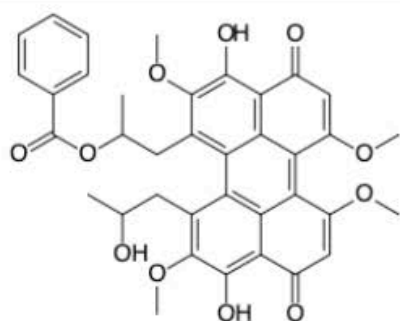
source (26.04.2022): <https://coconut.naturalproducts.net>

Cards

Table

There are 407,270 unique natural products in the database. They are sorted by their annotation level, starting with the best annotated.

« < 1 2 3 4 5 6 7 8 9 10 ... 16969 > »



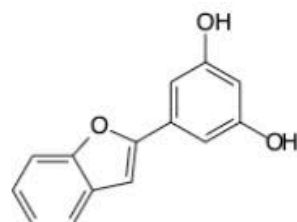
CNP0320385

Calphostin B

Mol. formula C<sub>37</sub>H<sub>34</sub>O<sub>11</sub>

Mol. weight 654.66

NP-likeness 1.34



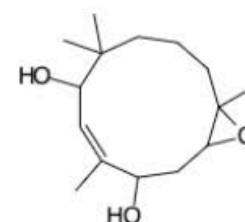
CNP0192622

Stemofuran A

Mol. formula C<sub>14</sub>H<sub>10</sub>O<sub>3</sub>

Mol. weight 226.23

NP-likeness 0.58



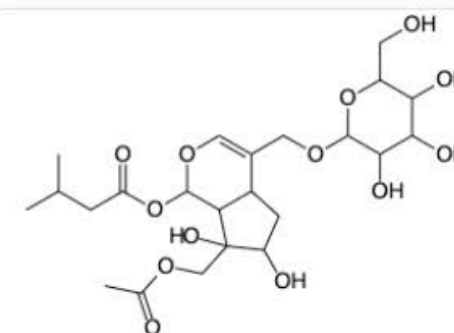
CNP0234206

Fexerol

Mol. formula C<sub>15</sub>H<sub>26</sub>O<sub>3</sub>

Mol. weight 254.37

NP-likeness 2.57



CNP0146144

Suspensolide E

Mol. formula C<sub>23</sub>H<sub>36</sub>O<sub>13</sub>

Mol. weight 520.53

NP-likeness 2.38

# 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 cellular location:






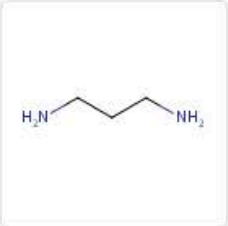
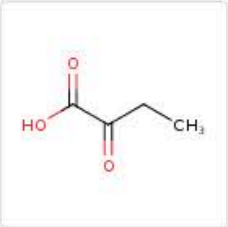
☐ Cell Membrane☐ Cytoplasm☐ Nucleus☐ Mitochondria

Clear

Apply Filter

Displaying metabolites 1 - 25 of 253245 in total

Export

HMDB ID 			Formula	
CAS Number	Name 	Structure	Average Mass 	Biospecimen Location
			Monoisotopic Mass 	
<div>HMDB0000001</div> <div>332-80-9</div>	1-Methylhistidine		C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>  169.1811 169.085126611	Blood Cerebrospinal Fluid (CSF) Feces Urine
<div>HMDB0000002</div> <div>109-76-2</div>	1,3-Diaminopropane		C <sub>3</sub> H <sub>10</sub> N <sub>2</sub>  74.1249 74.08439833	Blood Feces Urine
<div>HMDB0000005</div> <div>600-18-0</div>	2-Ketobutyric acid		C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>  102.0886 102.031694058	Blood Cerebrospinal Fluid (CSF) Saliva Urine





caffeine

Examples: [iron\\*](#), [InChI=1S/CH4O/c1-2/h2H,1H3](#), [caffeine](#)

Search

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[Home](#) [Advanced Search](#) [Browse](#) [Documentation](#) [Download](#) [Tools](#) [About ChEBI](#)
[Contact us](#) [Submit](#)
[ChEBI](#) > Search Results

# Search Results for All in ChEBI

[+ Show more data from EMBL-EBI](#)

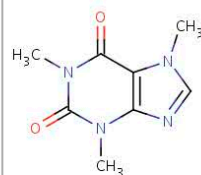
AND caffeine in All

source (26.04.2022): <https://ebi.ac.uk/chebi>[Edit Search](#)
[Download your results](#)

16 entries found, displaying 1 to 15.

1 2 &gt; &gt;&gt;

## caffeine



CHEBI:27732

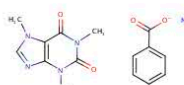
Stars: ★★ ★

Formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>

Mass: 194.19076

Charge: 0

## sodium caffeine benzoate



CHEBI:32140

Stars: ★★ ★

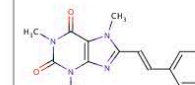
Formula:

C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>.C<sub>7</sub>H<sub>5</sub>O<sub>2</sub>.Na

Mass: 338.299

Charge: 0

## 8-(3-chlorostyryl)caffeine



CHEBI:53115

Stars: ★★ ★

Formula: C<sub>16</sub>H<sub>15</sub>ClN<sub>4</sub>O<sub>2</sub>

Mass: 330.76900

Charge: 0

## caffeine monohydrate



CHEBI:31332

Stars: ★★ ★

Formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>.H<sub>2</sub>O

Mass: 212.20604

Charge: 0

## Caffeine-trimethyl-13C3



CHEBI:178066

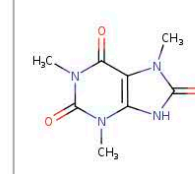
Stars: ★★ ★

Formula: C<sub>5</sub>[<sup>13</sup>C]3H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>

Mass: 197.171

Charge: 0

## 1,3,7-trimethyluric acid



CHEBI:691622

Stars: ★★ ★

Formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>3</sub>

Mass: 210.193

Charge: 0

## 3-methylxanthine

CHEBI:62205

Stars: ★★ ★

Definition:

A monomethylxanthine having the methyl group located at the 3-position. It is a metabolite of caffeine....

## 1-methylxanthine

CHEBI:68443

Stars: ★★ ★

Definition:

A monomethylxanthine having the methyl group located at the 1-position. It is a metabolite of caffeine in humans....

## 1,7-dimethylxanthine



CHEBI:25858

Stars: ★★ ★

Formula: C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>

Mass: 180.16400

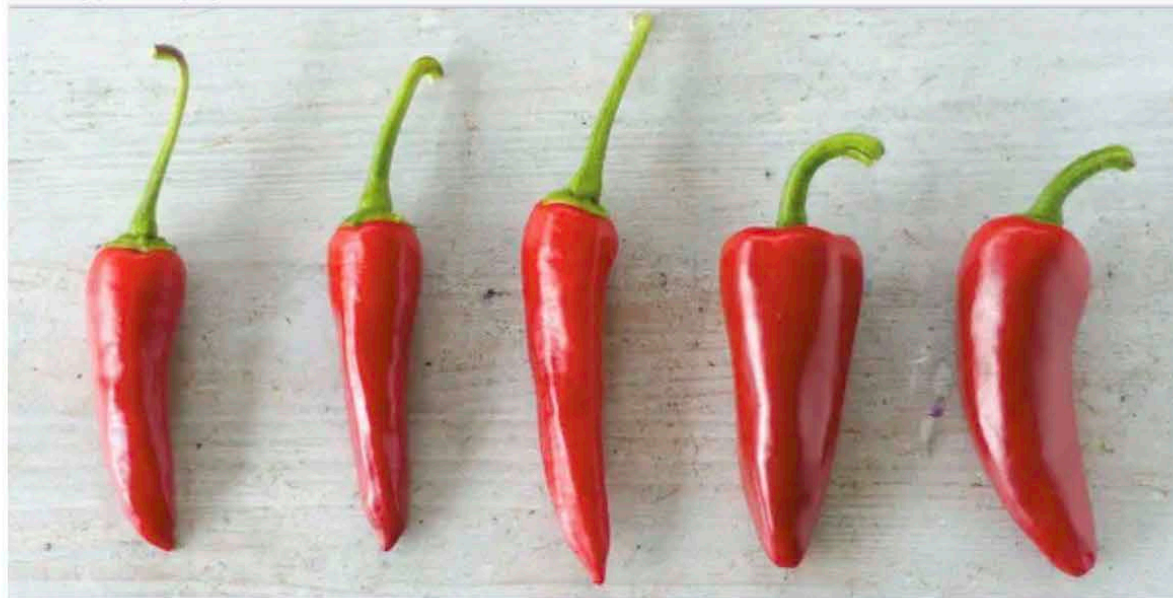
Charge: 0

[Change Current Database](#)Current Database: *MetaCyc*

Search in Current Database:



Vanillin goes with deserts. Chilli peppers go with salsa. But you can't have salsa without vanillin.

[Learn More](#)

Chili pepper by [hepp](#). Used under creative commons license

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## MetaCyc Metabolic Pathway Database

MetaCyc is a curated database of experimentally elucidated metabolic pathways from all domains of life. MetaCyc contains 2937 pathways from 3295 different organisms.

MetaCyc contains pathways involved in both primary and secondary metabolism, as well as associated metabolites, reactions, enzymes, and genes. The [goal](#) of MetaCyc is to catalog the universe of metabolism by storing a representative sample of each experimentally elucidated pathway.

MetaCyc [applications](#) include:

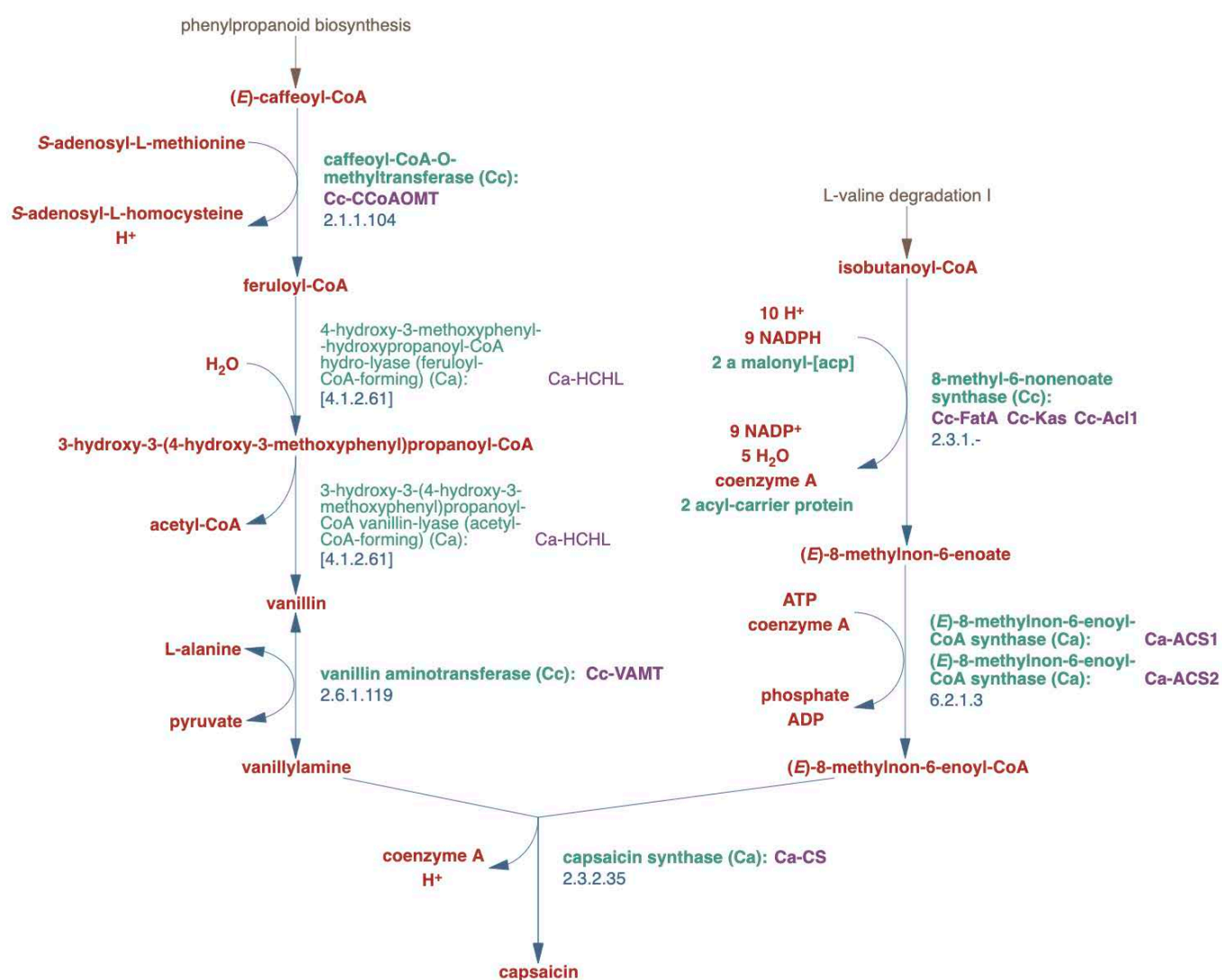
- Online encyclopedia of metabolism
- Predict metabolic pathways in sequenced genomes
- Support metabolic engineering via enzyme database
- Metabolite database aids metabolomics research

[Guide To MetaCyc](#)[Try Free](#)



## MetaCyc Pathway: capsaicin biosynthesis

Enzyme View: 


Detail Level: 


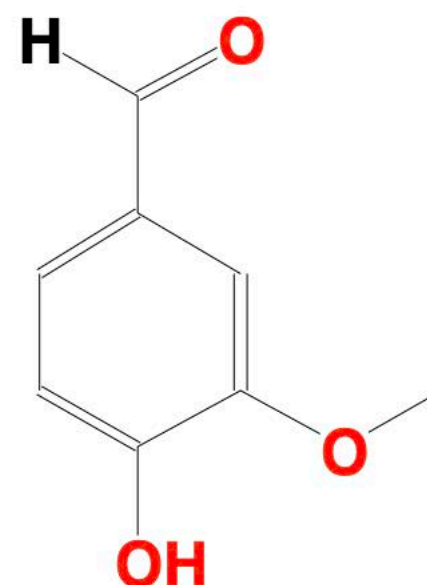
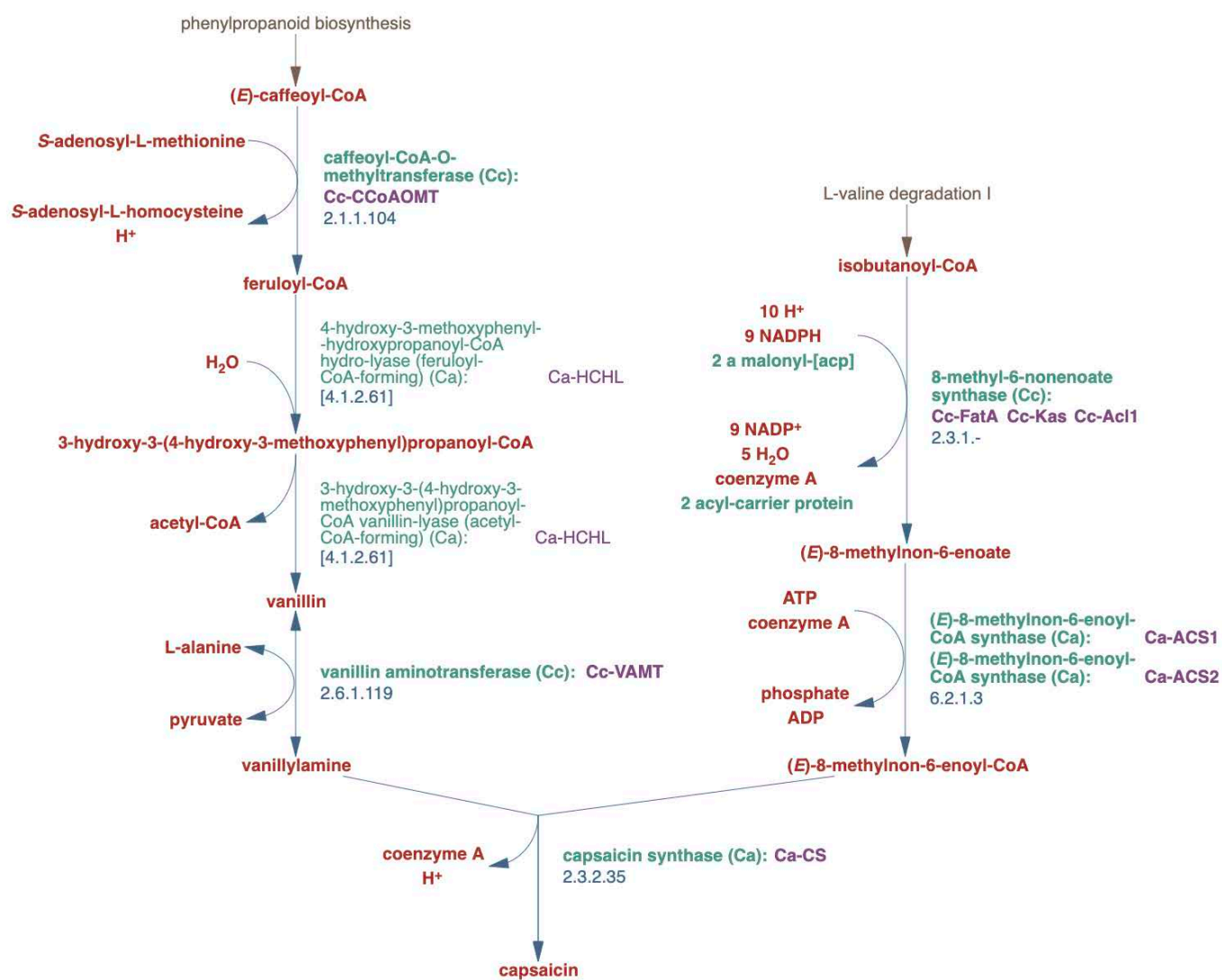
This view shows enzymes only for those organisms listed below, in the list of taxa known to possess the pathway. If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

Organisms known to possess this pathway include: [Capsicum annuum](#), [Capsicum chinense](#), [Capsicum frutescens](#), [Capsicum puberulum](#), [Capsicum](#)



## MetaCyc Pathway: capsaicin biosynthesis

Enzyme View: 

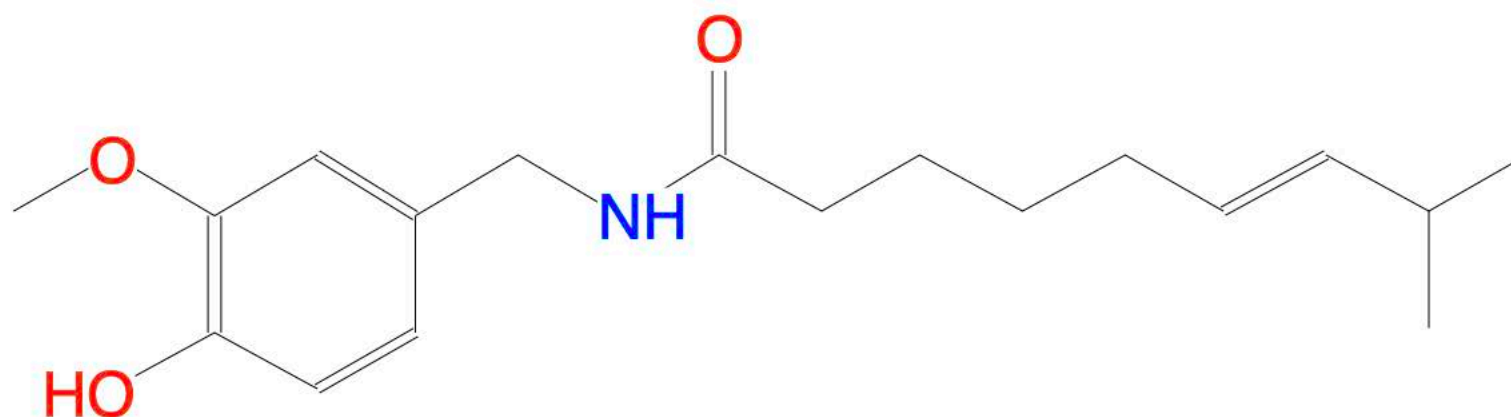
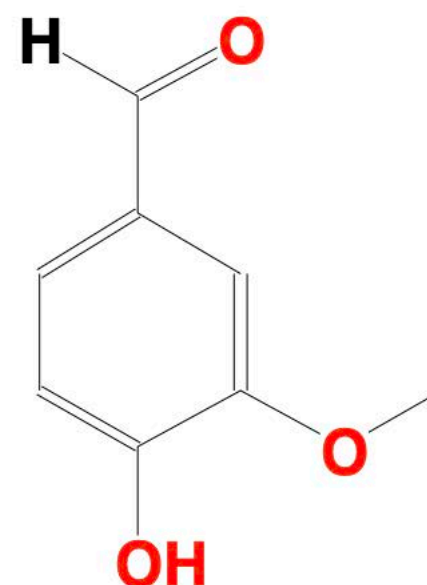
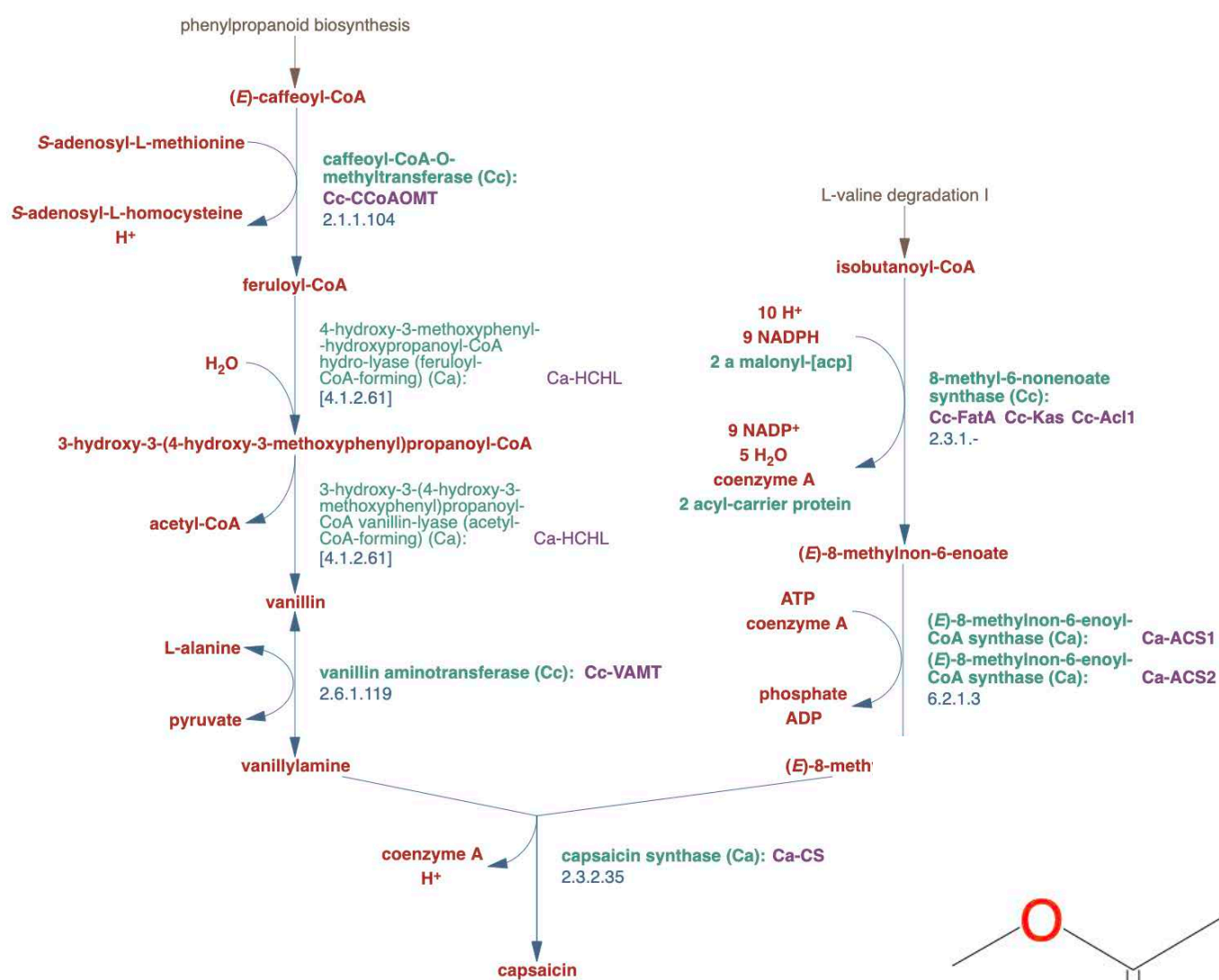

Detail Level: 


This view shows enzymes only for those organisms listed below, in the list of taxa known to possess the pathway. If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

Organisms known to possess this pathway include: [Capsicum annuum](#), [Capsicum chinense](#), [Capsicum frutescens](#), [Capsicum](#)

## MetaCyc Pathway: capsaicin biosynthesis

Enzyme View: 


Detail Level: 


This view shows enzymes only for those organisms listed below, in the list of taxa known to possess the pathway. If

an organism is known to possess this pathway but is not listed, you can click on the name to add it to the list.

MetaCyc  
Kegg  
HMDB  
YMDB  
Pubchem  
COCONUT  
MetaboLights  
Metabolomics Workbench  
GNPS  
NIST DB  
BMRB  
NP-DB review Maria

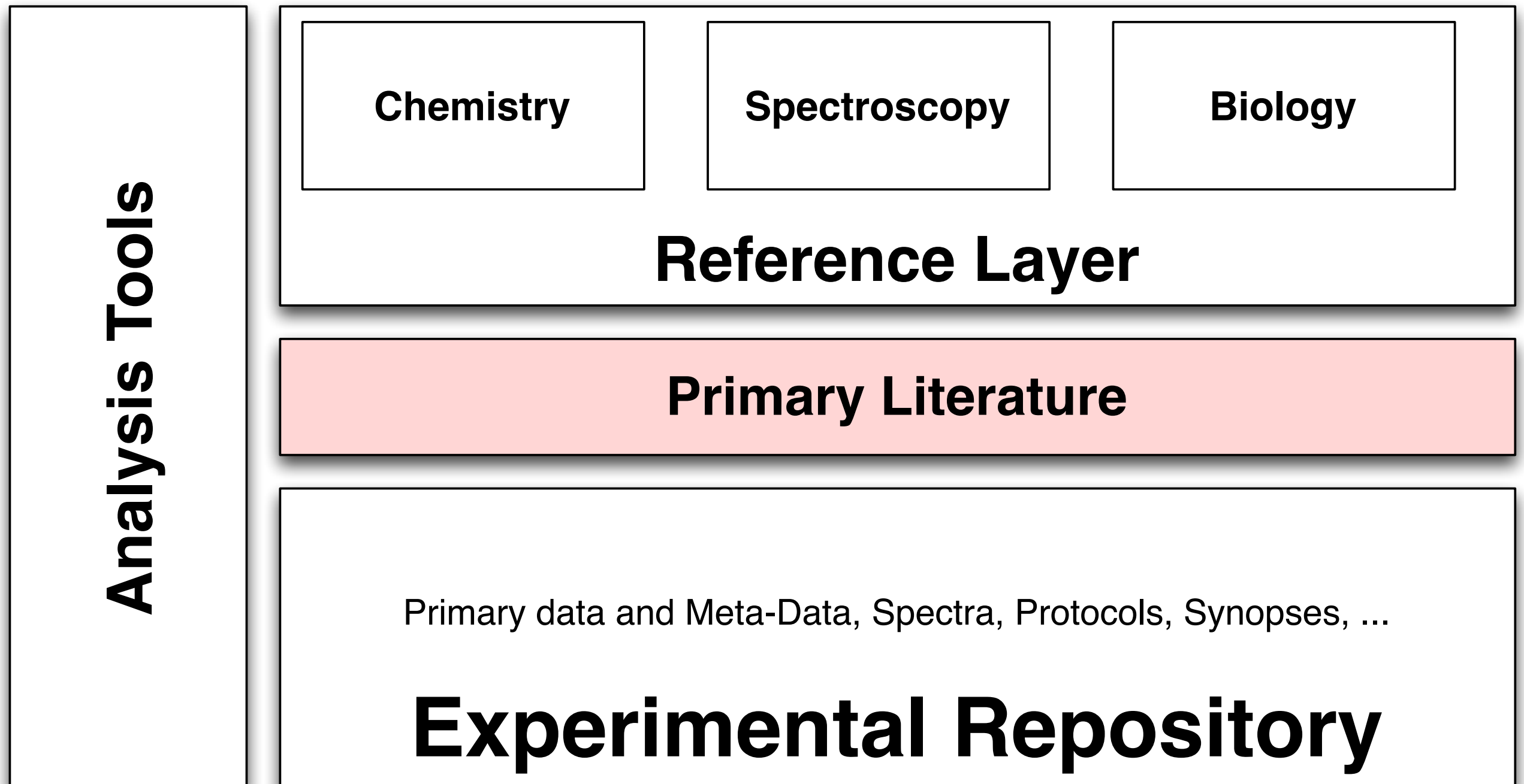


<http://www.ebi.ac.uk/metabolights>

# MetaboLights

open-access, cross-species, cross-application,  
long-term supported

# MetaboLights Datenbank





# MetaboLights Datenbank

## 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](#).

## Download



**Pre-packaged ISAcreator download.** To make it easy for new users, please download and just unzip our pre-packaged ISAcreator with plugin and configurations.



**Experiments.** All public MetaboLights experiments can be downloaded from our public [ftp archive](#). Please find zip archives under the "studies" folder. Each public study can be found in the corresponding MTBLS-id folder. Complete experiments can be opened with [ISAcreator](#) or you can extract the archives using your normal unzip program.

[Tweets by @MetaboLights](#)

### Submit a new study

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### Update an existing study

Use this option if you like to update a previously submitted study



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## Search results

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☐ compound

Technology



Organism



Organism Part



Validations Status Details



15 results, showing 1 to 10

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Page 1 of 2

### A metabolomics approach to unravel the regulating role of phytohormones towards carotenoid metabolism in *tomato* fruit. (Zeaxanthin metabolism)

Validations Status



Release date:

31-Aug-2014

Organism

Solanum lycopersicum

Study Factors

Phytohormones  
 Carotenoids

Study identifier

**MTBLS107**

Total Study size

**1.64GB**

Submitted by

Lieven van Meulebroek

### A metabolomics approach to unravel the regulating role of phytohormones towards carotenoid metabolism in *tomato* fruit. (alpha-carotene metabolism)

Validations Status



Release date:

31-Aug-2014

Organism

Solanum lycopersicum

Study Factors

Phytohormones

Study identifier

**MTBLS109**

Total Study size

**1.67GB**

Submitted by

Lieven van Meulebroek

[www.ebi.ac.uk/metabolights](http://www.ebi.ac.uk/metabolights)  
([metabolights.org](http://metabolights.org), [metabolights.eu](http://metabolights.eu))



# MTBLS36: Metabolic differences in ripening of *Solanum lycopersicum* 'Ailsa Craig' and three monogenic mutants

Authors: Paul Fraser , Graham Seymour , Charlie Hodgman , Mark Seymour , Aniko Kende , Dave Portwood , Charles Baxter , Stephan Beisen , Mark Earl

Submitted: 07-Feb-2014 , Release date: 07-Feb-2014 , Update date: 02-Jun-2016

Submitted by: [Stephan Beisen](#) | Study status: Public

[Share Study](#)

## Study Description

[View Metabolites](#)

[Download Study files](#)

Application of mass spectrometry enables the detection of metabolic differences between groups of related organisms. Differences in the metabolic fingerprints of wild-type *Solanum lycopersicum* and three monogenic mutants, ripening inhibitor (rin), non-ripening (nor) and Colourless non-ripening (Cnr), of tomato are captured with regard to ripening behaviour. A high-resolution tandem mass spectrometry system coupled to liquid chromatography produced a time series of the ripening behaviour at discrete intervals with a focus on changes post-anthesis. Internal standards and quality controls were used to ensure system stability. The raw data of the samples and reference compounds including study protocols have been deposited in the open metabolomics database MetaboLights via the metadata annotation tool Isatab to enable efficient re-use of the datasets, such as in metabolomics cross-study comparisons or data fusion exercises.

Study Design Description

Protocols

Samples

Assay

Study Files

Study Validation

Pathways

Organism(s)

*Solanum lycopersicum*

blank

Study Design Description

GO:leaf development

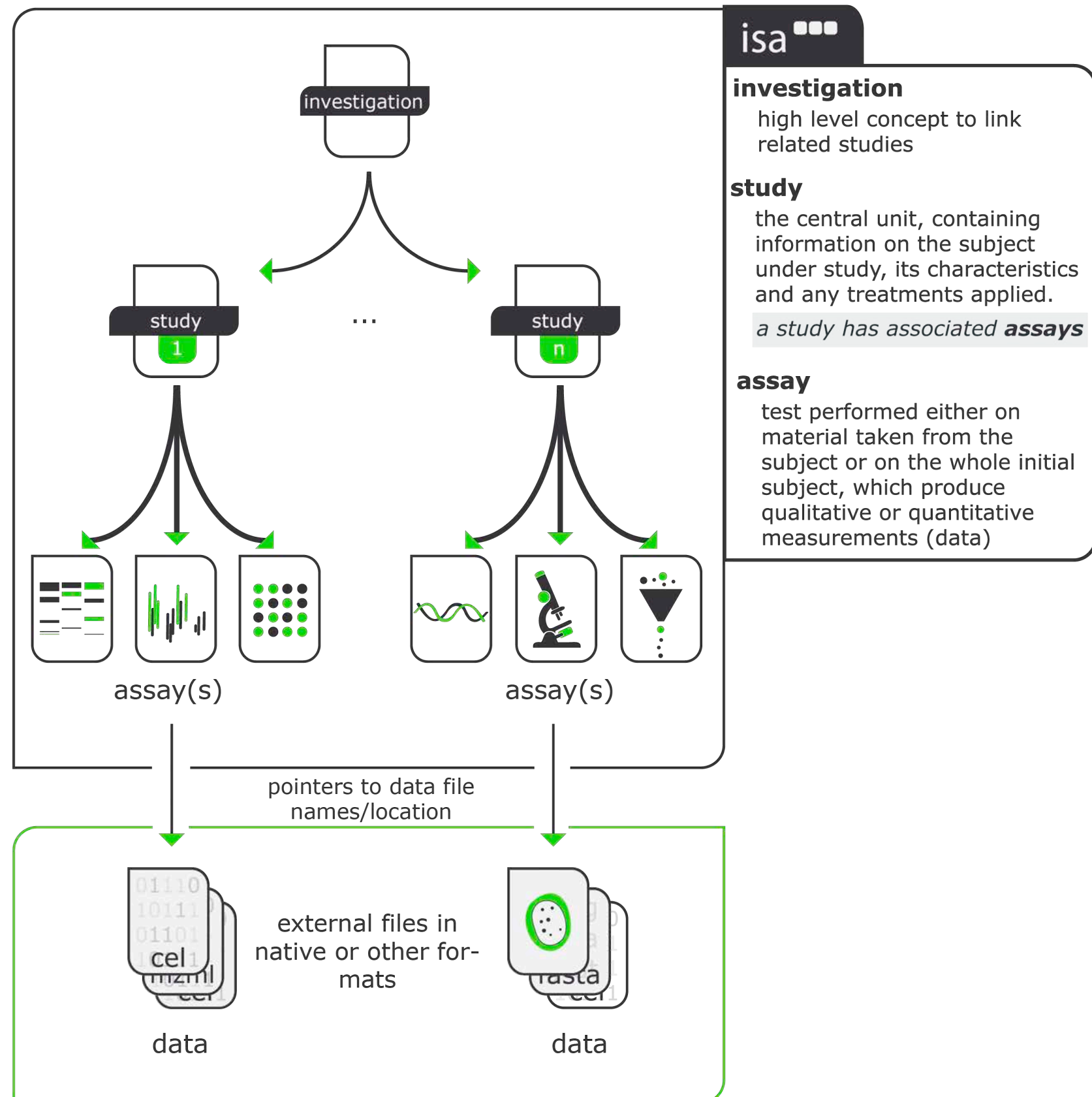
CHMO:ultra-performance liquid chromatography-mass spectrometry

CHMO:tandem mass spectrometry

[www.ebi.ac.uk/metabolights](http://www.ebi.ac.uk/metabolights)  
([metabolights.org](http://metabolights.org), [metabolights.eu](http://metabolights.eu))



# Structuring research data with ISA



# Multi-Omics Studies



BioStudies – one package for all the data supporting a study

The BioStudies database holds descriptions of biological studies, links to data from these studies in other databases at EMBL-EBI or outside, as well as data that do not fit in the structured archives at EMBL-EBI. The database can accept a wide range of types of studies described via a simple format. It also enables manuscript authors to submit supplementary information and link to it from the publication.

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- [Mutation analysis in a population-based cohort of boys with Duchenne or Becker muscular dystrophy](#) [S-EPMC5882193]
- [Blinatumomab versus Chemotherapy for Advanced Acute Lymphoblastic Leukemia](#) [S-EPMC5881572]
- [Calculation of Relative Binding Free Energy in the Water-Filled Active Site of Oligopeptide-Binding Protein A](#) [S-EPMC5881882]



BioStudies is part of the ELIXIR infrastructure

BioStudies is a recommended ELIXIR Deposition Database [Learn more >](#)

# Multi-Omics Studies



BioSamples stores and supplies descriptions and metadata about biological samples used in research and development by academia and industry. Samples are either 'reference' samples (e.g. from [1000 Genomes](#), [HipSci](#), [FAANG](#)) or have been used in an assay database such as the [European Nucleotide Archive \(ENA\)](#) or [ArrayExpress](#).

## Info

- [Help pages](#) about how to search BioSamples, how to submit data, and FAQ.
- [Programmatic access](#) to query and download data using web services.
- Contact us by emailing [biosamples@ebi.ac.uk](mailto:biosamples@ebi.ac.uk)

## Data Content



European Bank for induced pluripotent Stem Cells

[www.ebisc.org](http://www.ebisc.org)

[search for EBiSC samples](#)

EBiSC has been designed to address the increasing demand for quality-controlled, disease-relevant, research-grade iPSC lines, data and cell services.



[www.faang.org](http://www.faang.org)

[search for FAANG samples](#)

Functional Annotation of Animal Genomes. A coordinated international action to accelerate genome to phenome research.



[www.hipsci.org](http://www.hipsci.org)

[search for HipSci samples](#)

HipSci brings together diverse constituents in genomics, proteomics, cell biology and clinical genetics to create a UK national iPS cell resource and use it to carry out cellular genetic studies.



BioSamples Database is part of the ELIXIR infrastructure

BioSamples is an Elixir Deposition Database [Learn more >](#)



## Tweets by @OmicsDI



Omics Discovery Retweeted



**Yasset Perez-Riverol**  
@ypriverol

what do you use for proteomics downstream analysis:

40% Perseus

35% Limma (+ scripts)

25% MSstats

167 votes • Final results



Sep 23, 2020

Omics Discovery Retweeted

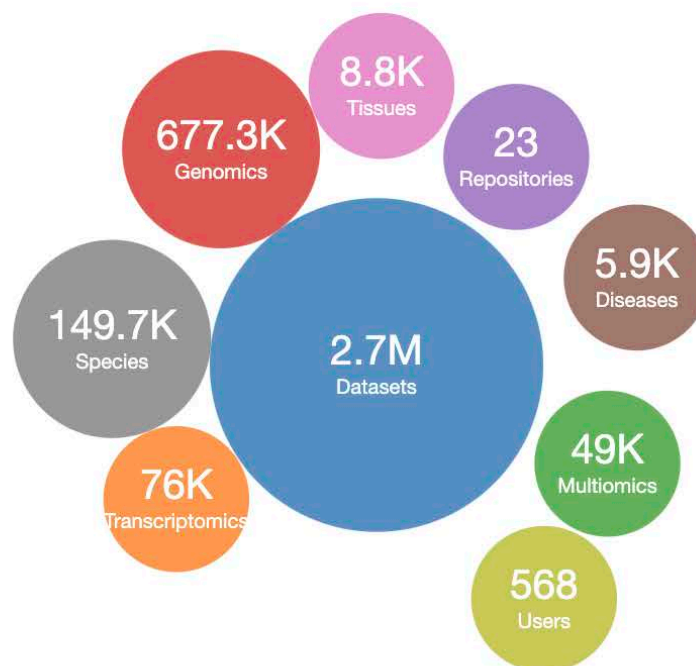


**Yasset Perez-Riverol**  
@ypriverol

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## Statistics



## About

The Omics Discovery Index (OmicsDI) provides a knowledge discovery framework across heterogeneous omics data (genomics, proteomics, transcriptomics and metabolomics). [Read More.](#)

### Publications

- Perez-Riverol Y, et al. Discovering and linking public omics data sets using the Omics Discovery Index. Nat Biotechnol. 2017 May 9;35(5):406-409. doi: <https://doi.org/10.1038/nbt.3790>.
- Perez-Riverol Y, et al. Quantifying the impact of public omics data. Biorxiv. <https://doi.org/10.1101/282517>.

OmicsDI project has been developed on [GitHub](#), you can check or contribute to our development [here](#).

The frontend is based on [Angular](#), [D3.js](#).



## OmicsDI is part of the ELIXIR infrastructure

OmicsDI is an Elixir interoperability service. [Learn more >](#)



### OmicsDI Databases

PRIDE  
 PeptideAtlas  
 MassIVE  
 JPOST Repository  
 Physiome Model Repository

EGA  
 EVA  
 ENA  
 LINCS  
 PAXDB  
 Cell Collective

MetaboLights  
 Metabolomics Workbench  
 MetabolomeExpress  
 GNPS  
 BioModels  
 FAIRDOMHub

ArrayExpress  
 dbGaP  
 ExpressionAtlas  
 GEO  
 NODE

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# The Large Omics Repositories

Genomik	Transkriptomik
Proteomik	Metabolomik

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