Metabolomics Workbench and the National Metabolomics Data Repository

Lina Aboulmouna, Eoin Fahy, Mano Maurya, Srini Ramachandran,
Neela Srinivasan, Sumana Srinivasan, Shankar Subramaniam
University of California San Diego

Kevin Coakley, Christine Kirkpatrick
San Diego Supercomputer Center

NIH Common Fund's National Metabolomics Data Repository
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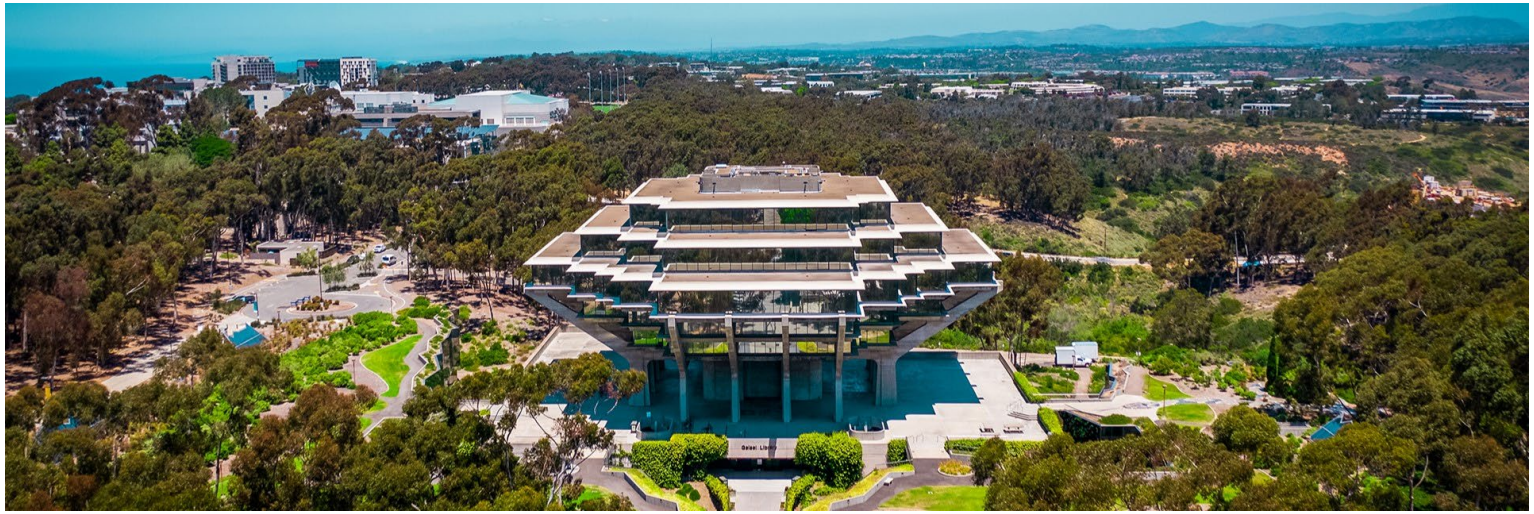
Overview of the Metabolomics Workbench

The National Institutes of Health (NIH) Common Fund Metabolomics Program was developed with the goal of increasing national capacity in metabolomics by supporting the development of next generation technologies, promoting data/metadata sharing and collaboration and providing training and mentoring opportunities.
In support of this effort, the Metabolomics Workbench website was created at the University of California, San Diego in 2013. The Metabolomics Workbench houses the National Metabolomics Data Repository (NMDR) which serves as a national and international center for metabolomics data and metadata and provides analysis tools and access to metabolite standards, protocols and other resources to the global community.



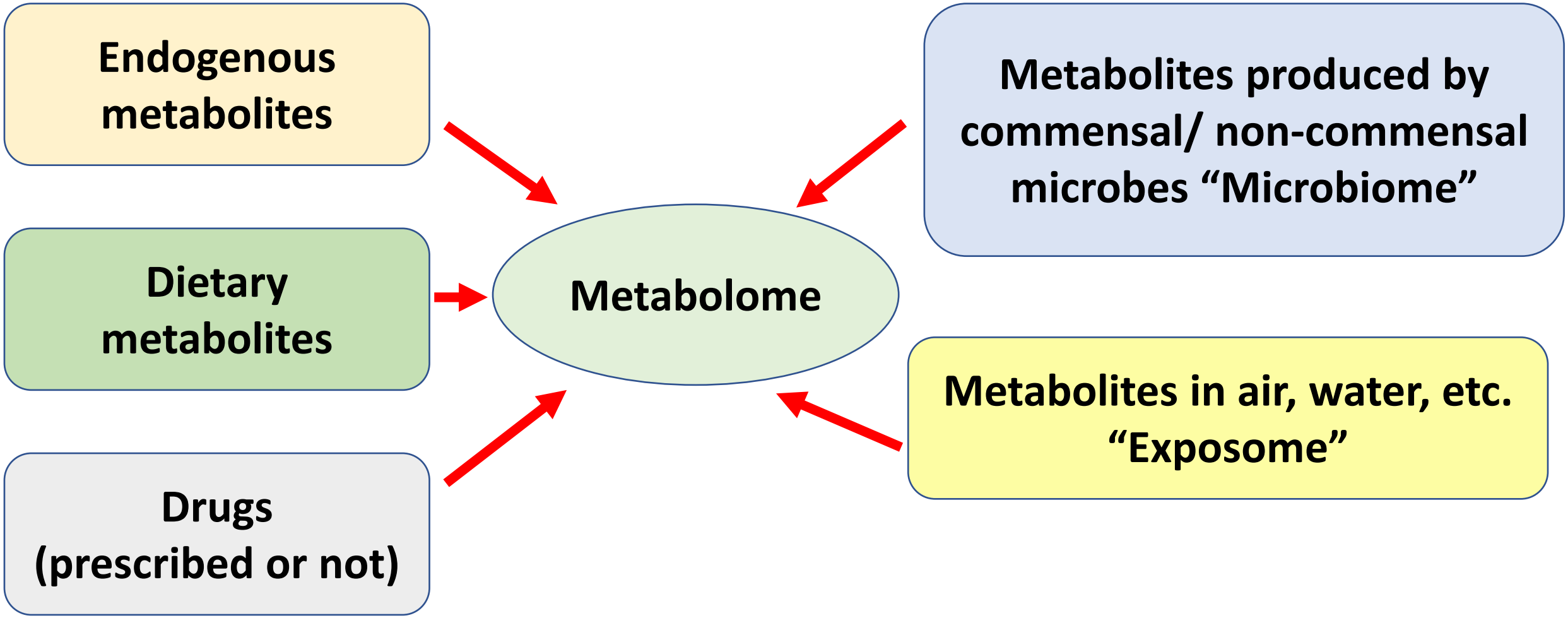
Metabolomics Workbench: https://www.metabolomicsworkbench.org

Contains the National Metabolomics Data Repository (NMDR)

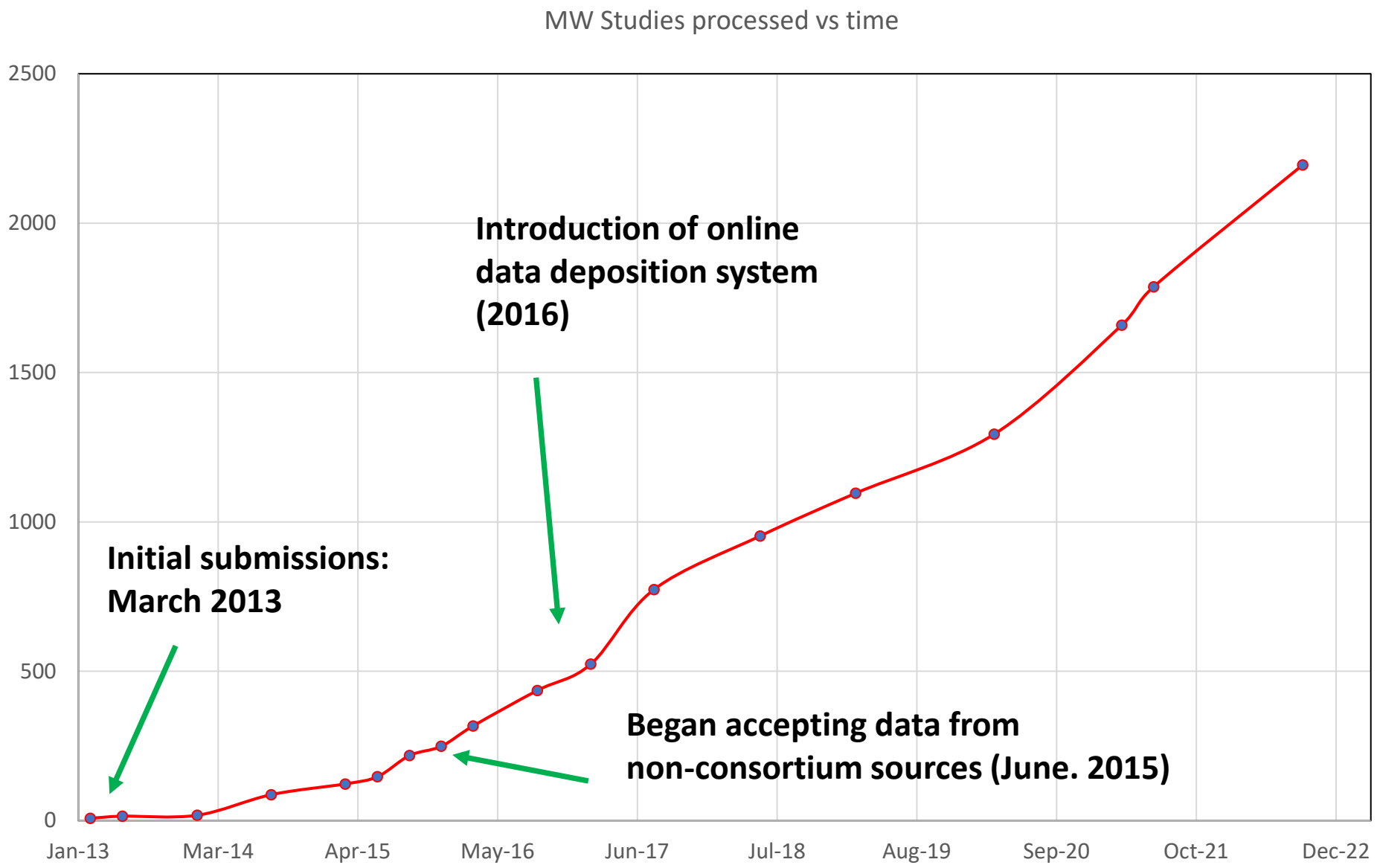
Metabolomics Workbench website: what does it contain?

- National Metabolomics Data Repository (NMDR)
  - MS and NMR metabolomics studies
  - Metadata, targeted/untargeted measurements, raw data
- Metabolomics Workbench Metabolite database
- RefMet standardized metabolite nomenclature resource
- Online suite of statistical analysis tools
  - For NMDR studies and ad-hoc user–supplied datasets
- MetStat summary reporting tool
- Human gene/protein database of metabolism-related genes
- Protocols for metabolomics experiments
- REST service
- MS search tools
- Other metabolomics software (MW group and collaborators)

The scope of Metabolomics



NMDR currently contains ~2200 studies from over 350 different institutions

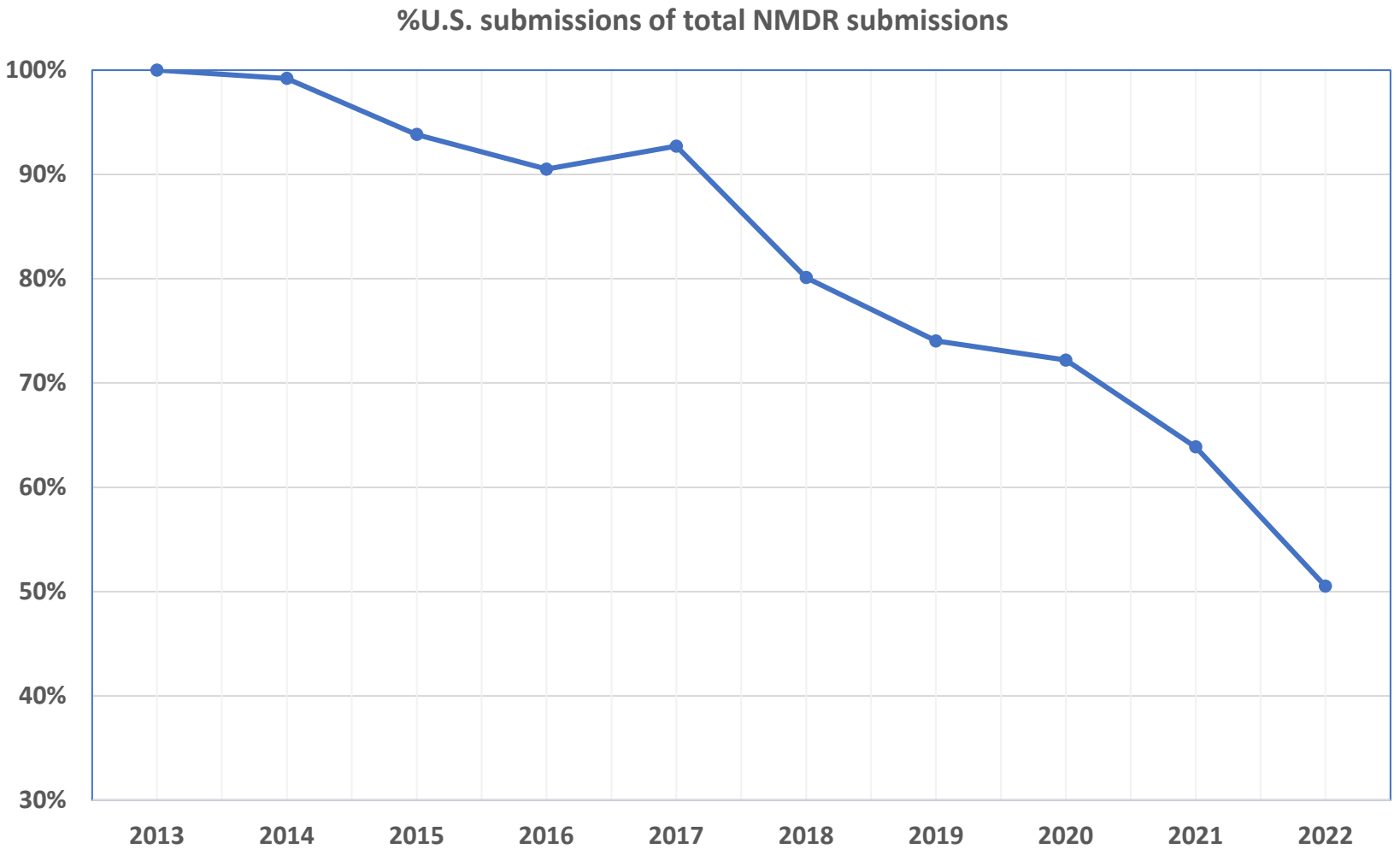


NMDR studies: Submissions by country (as of May 2022)

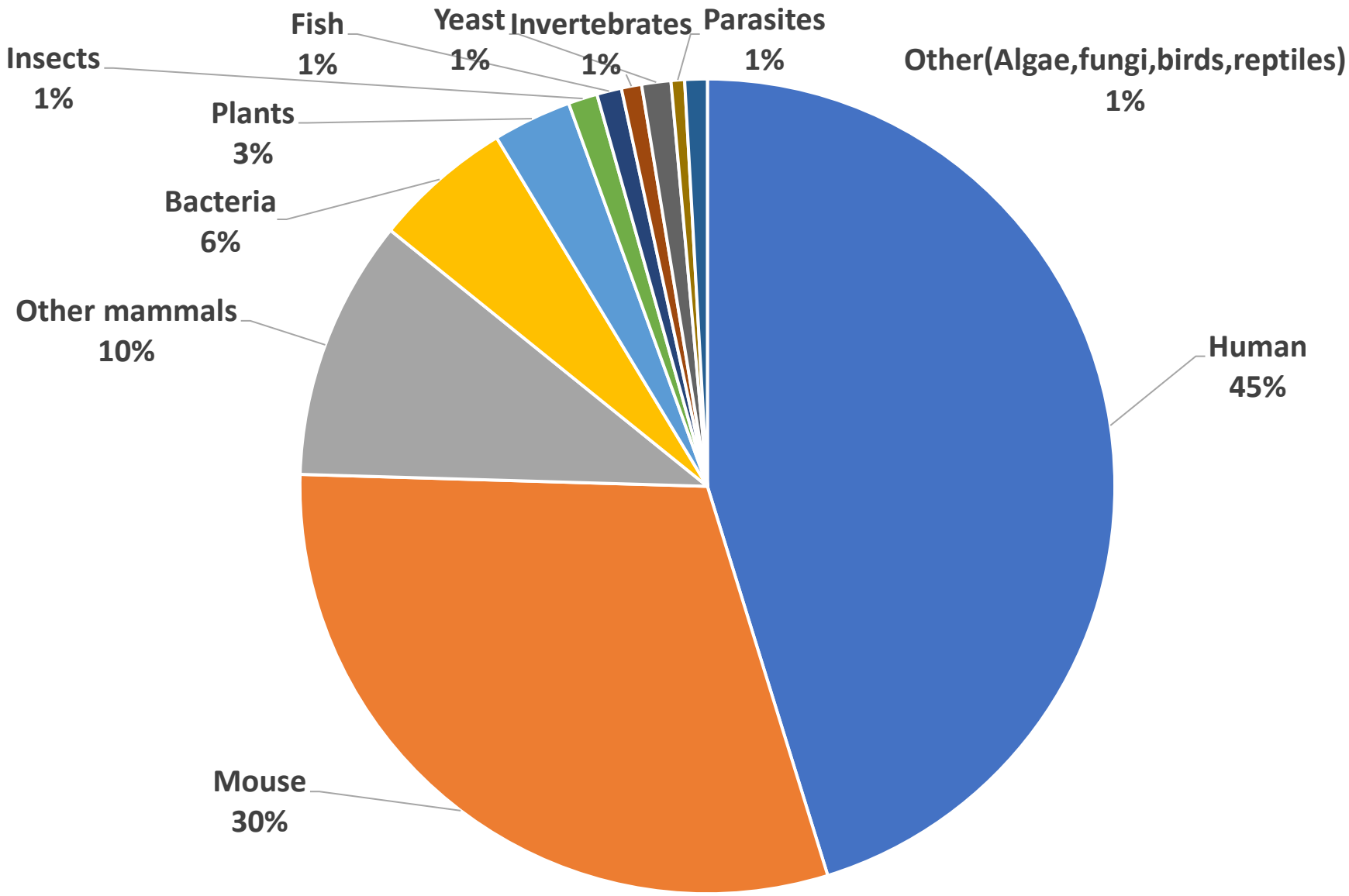
Country	Studies		Country	Studies
USA	1650		Sweden	5
China	87		Israel	4
Australia	43		Puerto Rico	4
Japan	41		Abu Dhabi	3
Canada	26		Luxembourg	3
Spain	26		Malaysia	3
Germany	25		Russia	3
India	17		Switzerland	3
UK	16		Belgium	2
Finland	15		Greece	2
France	15		Nigeria	2
South Africa	15		Oman	2
South Korea	15		Qatar	2
Brazil	13		Colombia	1
Holland	11		Indonesia	1
Italy	9		Pakistan	1
Portugal	6		Thailand	1
Singapore	6		Hong Kong	1
Austria	5		UAE	1
Denmark	5		Vietnam	1

40 countries total

NMDR Submissions over time: Percentage of submissions by year from the U.S.

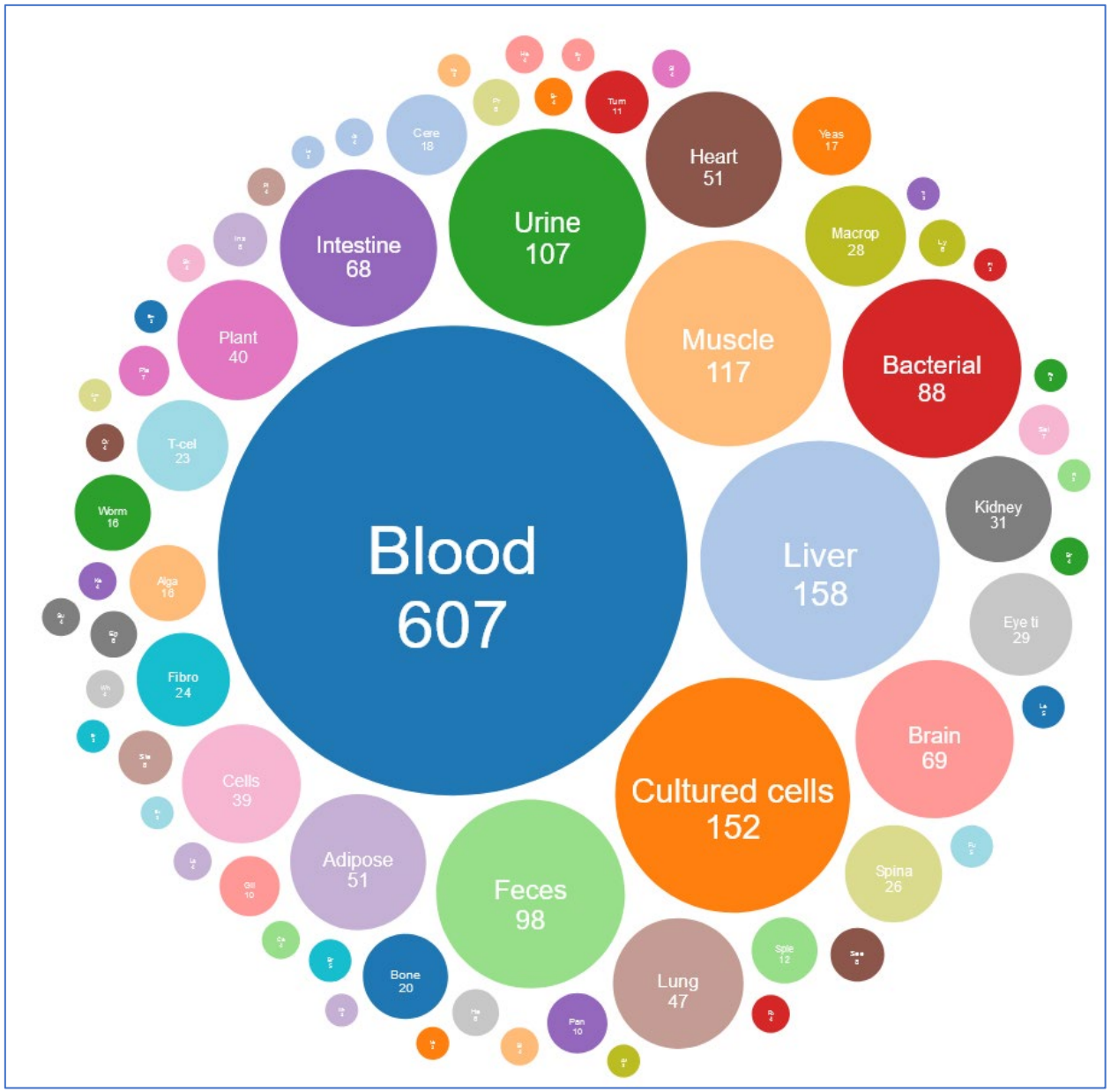


Major Taxonomic categories



155 different species represented in NMDR studies

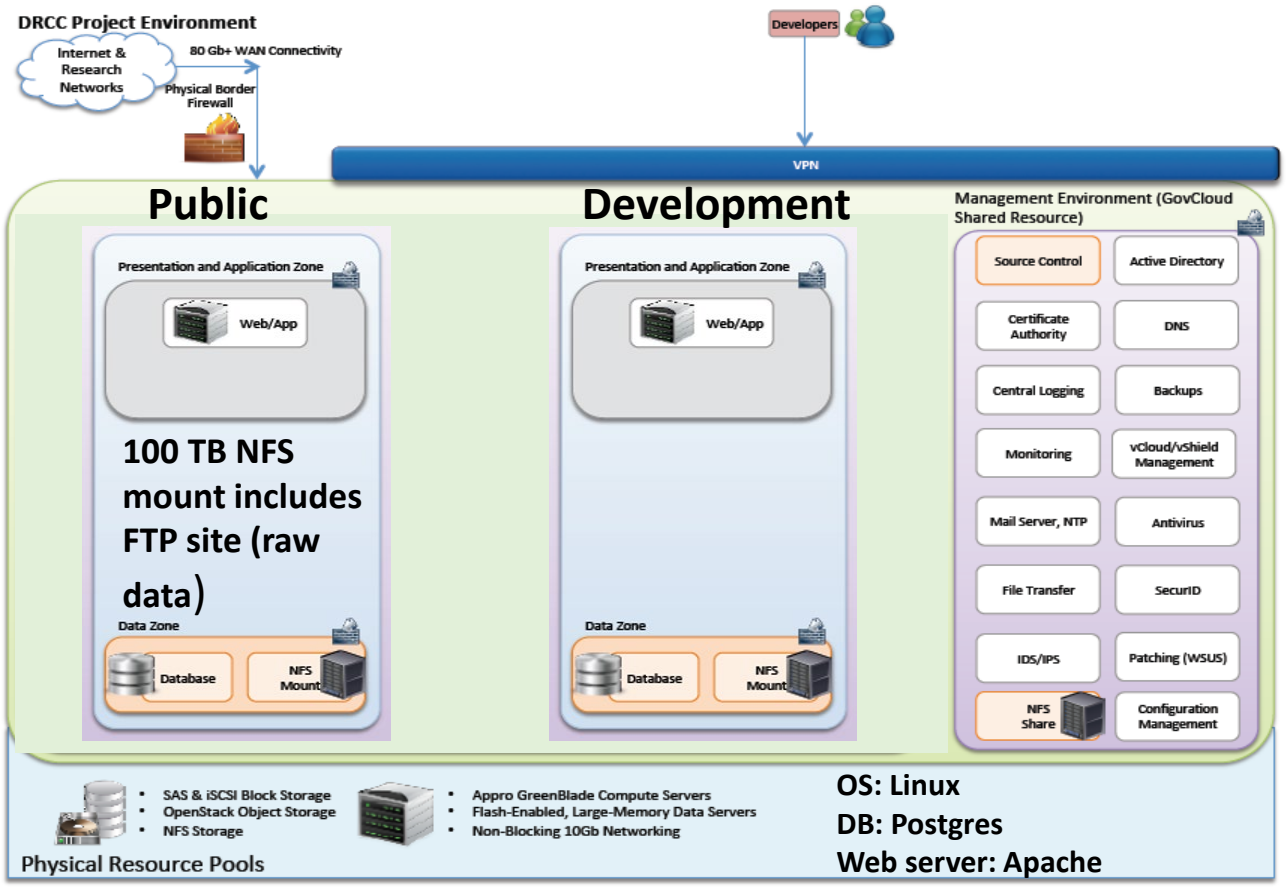
Sample source in NMDR studies (164 different types)



Sample source data (All studies)

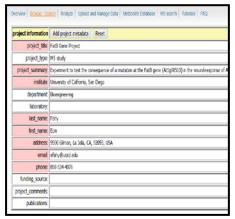
Sample Source	Studies
Blood	607
Liver	158
Cultured cells	152
Muscle	117
Urine	107
Feces	98
Bacterial cells	88
Brain	69
Intestine	68
Adipose tissue	51
Heart	51
Lung	47
Plant	40
Cells	39
Kidney	31
Eye tissue	29
Macrophages	28
Spinal cord	26
Fibroblast cells	24

Overview of NMDR cloud computing infrastructure
(located at the San Diego Supercomputer Center)



Overview of NMDR Inputs and Outputs

Online data submission



Metadata
Targeted data measurements
Protocols/Methods files
Untargeted data measurement files

Raw data (MS/NMR binary files) + other pertinent files

FTP

NMDR Data Repository

Browsing/searching/statistical analysis via web browser

Targeted data (named metabolites)

Untargeted data (Features, NMR binned increments)

Download targeted measurements
Download untargeted measurements

Download Raw Data

Download mwTab file (Metadata/data)

Formats:
Plain text
JSON

REST service

Metabolomics Data Repository: Overall Strategy

Experimental data

Online study submission system

Named metabolite data/ smaller datasets (paste into web forms)

Relational Database (Data/Metadata)

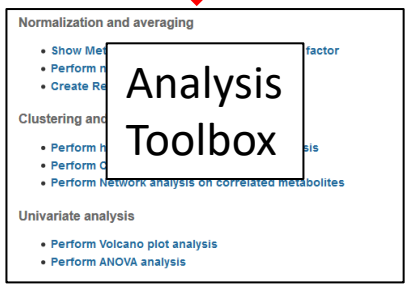
Untargeted data/ larger datasets (upload as files)

Metadata

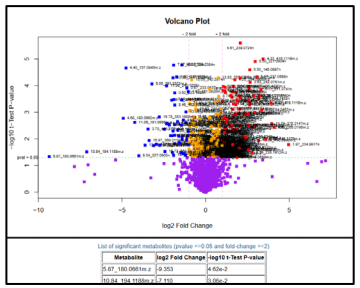
"Big data" file system: Mwtab files, Results files

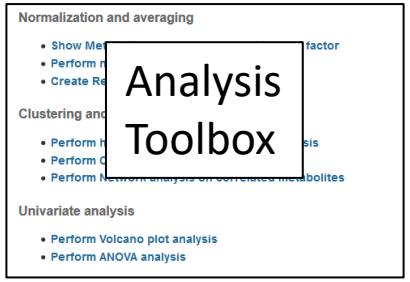
Transpose
Fix zero/null data
Average technical reps.
Apply filters

Processed text files(smaller) Save to file system for data analysis



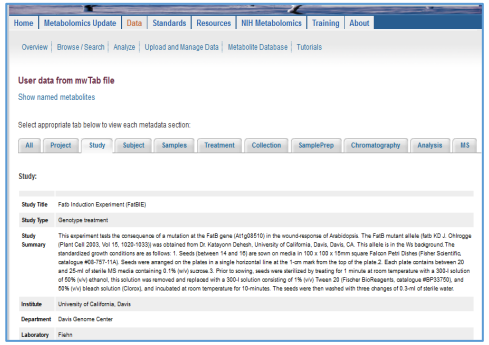
Data analysis



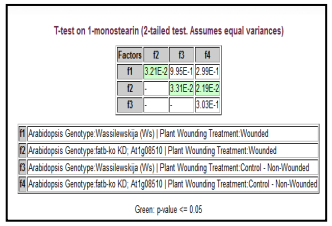


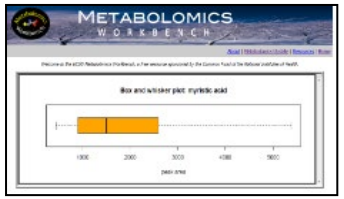
Online submission overview

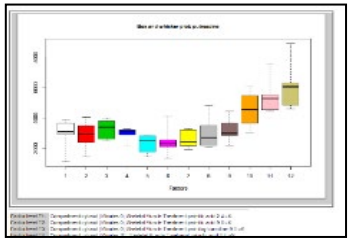
View metadata

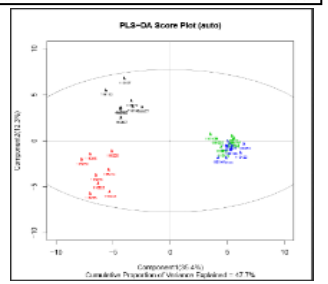


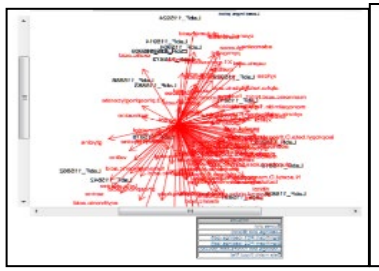
View data. Perform analyses

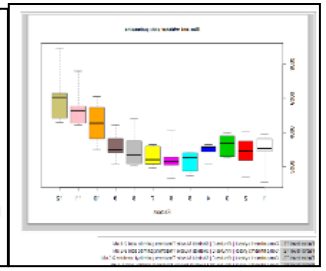












Online data submission

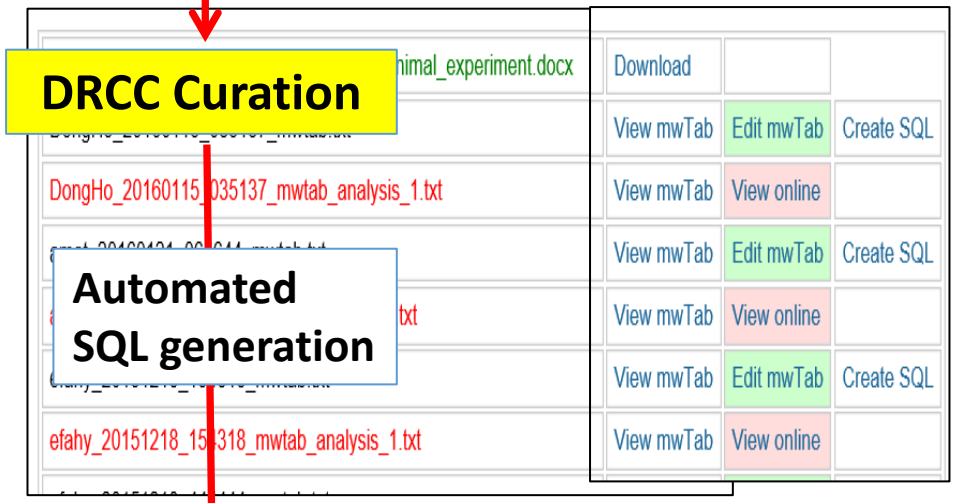
Metadata

Results

Protocol files

mwTab file

DRCC Curation



Automated SQL generation

Database

The mwTab format: A “common currency” for metadata/data sharing and storage

SECTIONS:

Metadata

Project
Study
Experimental variables (factors)
Subject
Collection
Treatment
Sample preparation
Chromatography
Analysis
MS
NMR

Data

Named metabolite measurements (table)
Named metabolites and annotations
File names for untargeted datasets

Additional

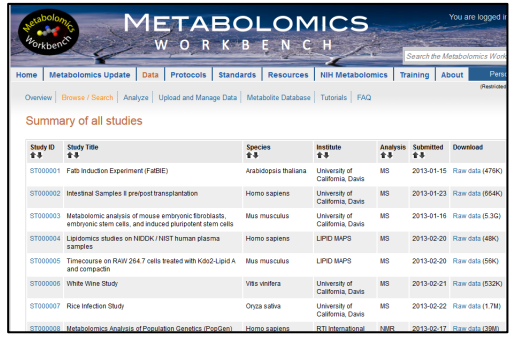
Comments preceded by a #

```
#METABOLOMICS WORKBENCH Nagireddy_Putluri_20211115_090410 DATATRACK_ID:2929 STUDY_ID:ST002005 ANALYSIS_ID:AN003268 PROJECT_ID:PR001271
VERSION                 1
CREATED_ON              November 29, 2021, 7:26 pm
#PROJECT
PR:PROJECT_TITLE                        Alterations of lipids in tumor tissues from African American and European
PR:PROJECT_TITLE                        American patient with bladder cancer
PR:PROJECT_SUMMARY                      Cancer affects all individuals in the United States, unfortunately due to
PR:PROJECT_SUMMARY                      socioeconomics, and environmental disadvantages, certain group of populations
PR:PROJECT_SUMMARY                      especially African American (AA) community bear a high burden of cancer than the
PR:PROJECT_SUMMARY                      other communities. Based on different social epidemiological study reported that
PR:PROJECT_SUMMARY                      higher incidence and mortality rate of bladder cancer in AA community. To
PR:PROJECT_SUMMARY                      understand and reveal the biological mechanism in terms of lipidomics,
PR:PROJECT_SUMMARY                      lipidomics profile were performed in 98 bladder cancer (African American and
PR:PROJECT_SUMMARY                      European America) tissues including benign.
PR:INSTITUTE                            Baylor College of Medicine
PR:LAST_NAME                            Putluri
PR:FIRST_NAME                           Nagireddy
PR:ADDRESS                              One Baylor Plaza, Houston, Texas 77030
PR:EMAIL                                putluri@bcm.edu
PR:PHONE                                (713) 798-3139
#STUDY
ST:STUDY_TITLE                          Alterations of lipids in tumor tissues from African American and European
ST:STUDY_TITLE                          American patient with bladder cancer
ST:STUDY_SUMMARY                        Cancer affects all individuals in the United States, unfortunately due to
ST:STUDY_SUMMARY                        socioeconomics, and environmental disadvantages, certain group of populations
ST:STUDY_SUMMARY                        especially African American (AA) community bear a high burden of cancer than the
ST:STUDY_SUMMARY                        other communities. Based on different social epidemiological study reported that
ST:STUDY_SUMMARY                        higher incidence and mortality rate of bladder cancer in AA community. To
ST:STUDY_SUMMARY                        understand and reveal the biological mechanism in terms of lipidomics,
ST:STUDY_SUMMARY                        lipidomics profile were performed in 98 bladder cancer (African American and
ST:STUDY_SUMMARY                        European America) tissues including benign.
ST:INSTITUTE                            Baylor College of Medicine
ST:DEPARTMENT                           Molecular and Cellular Biology
ST:LAST_NAME                            Putluri
ST:FIRST_NAME                           Nagireddy
ST:ADDRESS                              One Baylor Plaza, Houston, Texas 77030
ST:EMAIL                                putluri@bcm.edu
ST:PHONE                                (713) 798-3139
#SUBJECT
SU:SUBJECT_TYPE                         Human
SU:SUBJECT_SPECIES                      Homo sapiens
SU:TAXONOMY_ID                          9606
#FACTORS
#SUBJECT_SAMPLE_FACTORS:                SUBJECT(optional)[tab]SAMPLE[tab]FACTORS(NAME:VALUE pairs separated by |)[tab]Raw file names an
SUBJECT_SAMPLE_FACTORS                  -       03-22-2021-Pos-34734 BENIGN-30  Group:Benign
SUBJECT_SAMPLE_FACTORS                  -       03-22-2021-Pos-34880 BENIGN-32  Group:Benign
SUBJECT_SAMPLE_FACTORS                  -       03-22-2021-Pos-35088 BENIGN-36  Group:Benign
SUBJECT_SAMPLE_FACTORS                  -       03-22-2021-Pos-35603 BENIGN-38  Group:Benign
SUBJECT_SAMPLE_FACTORS                  -       03-22-2021-Pos-35599 BENIGN-40  Group:Benign
SUBJECT_SAMPLE_FACTORS                  -       03-22-2021-Pos-35774 BENIGN-42  Group:Benign
```

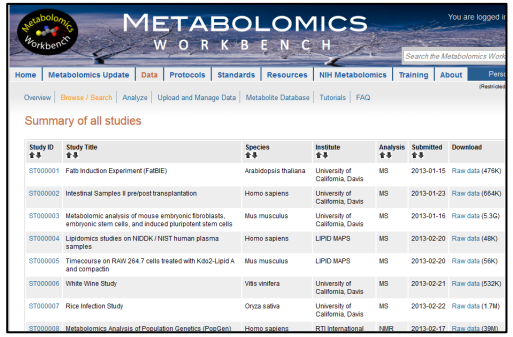
MwTab specification: https://www.metabolomicsworkbench.org/data/mwTab_specification.pdf

NMDR online portals

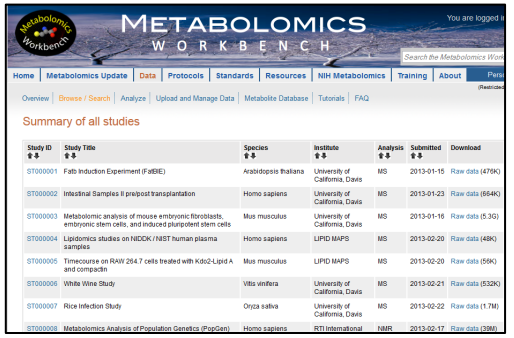
Public website

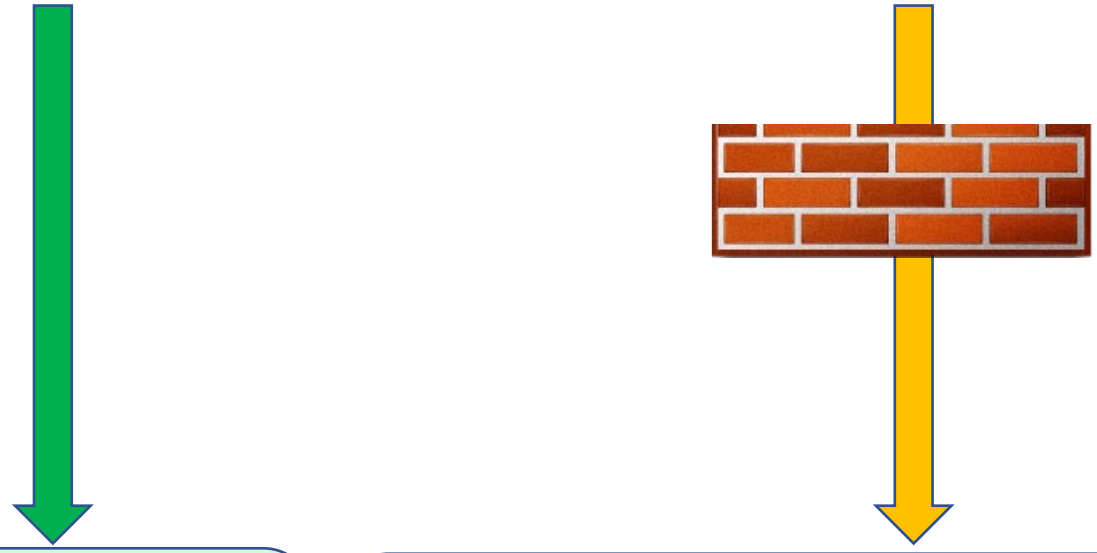


Data submission/review portal



Development websites





Open access

(non-embargoed studies)

Access controlled

Submit/View data/metadata submitted by your institution (or other institutions for which you have permission)

NMDR only

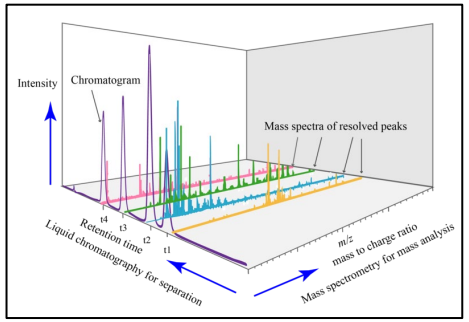
(testing/development)

Metabolomics study workflow

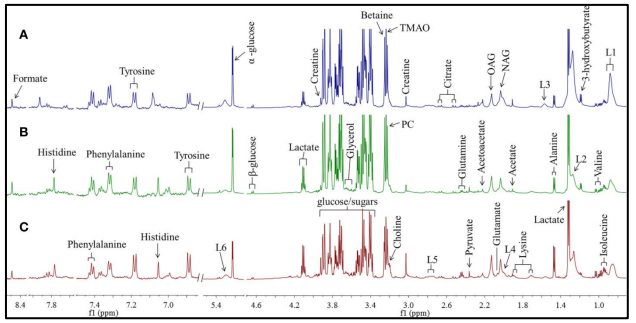
Study design

Sample prep

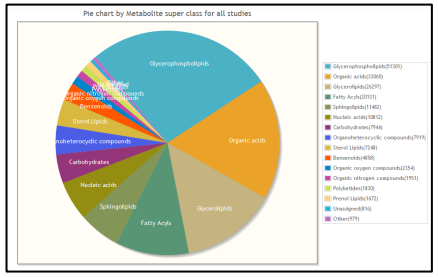
Data processing/databasing

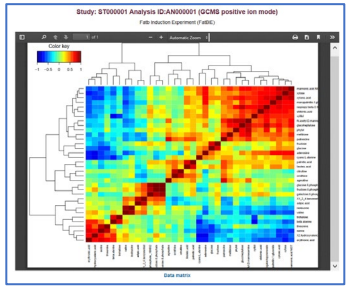


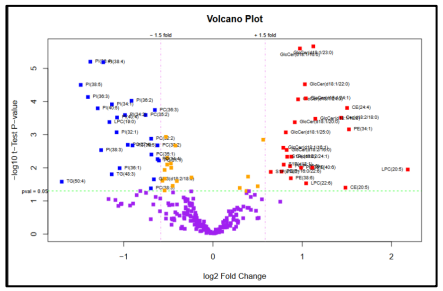
MS

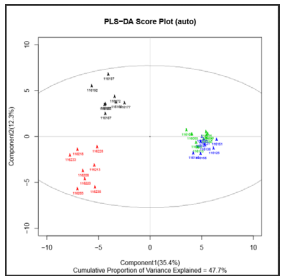


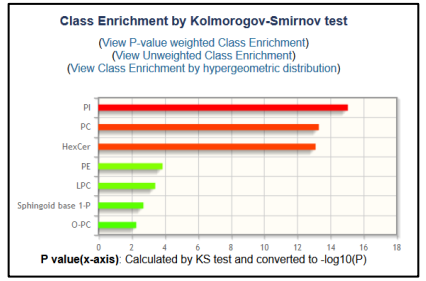
NMR

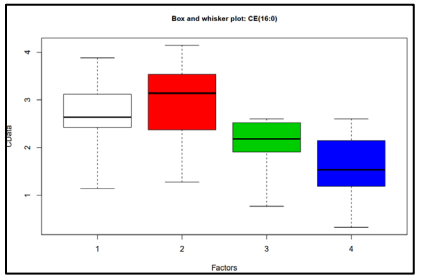






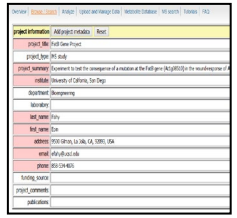






Data analysis

Online data/metadata submission flowchart



Online GUI's

Project → Study → Subject → Study design

Collection → Treatment → Sample prep.

Sample prep. → Analysis type?

Analysis type? → NMR

Analysis type? → MS

NMR

mwTab file

Load NMR results/metadata

MS

# of chromatography methods?

Chromatography

# of MS methods?

# of analyses =#CH * #MS

An_1 An_2 An_3 ..... An_n

Load results/metadata for each analysis

National Metabolomics Data Repository Online Data Submission Tutorial

Before you start:

- Have a summary of the study ready (a paragraph describing the goal and design of the experiment for the benefit of the general research community- a publication abstract or equivalent would be ideal).

- Have a study design table ready with sample names and experimental variables in separate columns. Subject information and other measurements may also included.

- Make sure that sample names in submitted results tables exactly match those in the study design table. Otherwise you won't be able to proceed with the submission.

- Collect all relevant protocols and raw data for upload to the WorkBench. Protocol/methods files may be uploaded at appropriate points during the online metadata submission process whereas (large) raw data is uploaded during the final registration step.

Online Data Submission

https://www.metabolomicsworkbench.org/data/DRCCDataDeposit.php

Register/login

Upload/manage studies

Requirements for depositing data via the Metabolomics Workbench:

*****Please read the **NMDR study submission tutorial** first!*****

1. **Register** (you will then be authorized to submit studies)
2. **Log in**.
3. View the list of exemplary studies (below) for examples of best practices for study submissions.
4. The use of the common metabolite names in the **RefMet** database is *strongly encouraged* in order to be able to compare and contrast metabolite data across different experiments and studies. For your convenience an **online tool** is available to map your current metabolite identifications (where possible) to the corresponding RefMet names.
5. Use the **'New Data Upload'** tab to (a) register your study, (b) submit metadata and processed data and (c) upload raw data/supplementary material. Please indicate the date when the study may be made available to the public.
6. **E-mail us for additional assistance** (help@metabolomicsworkbench.org), if needed.

(a): Complete the registration form

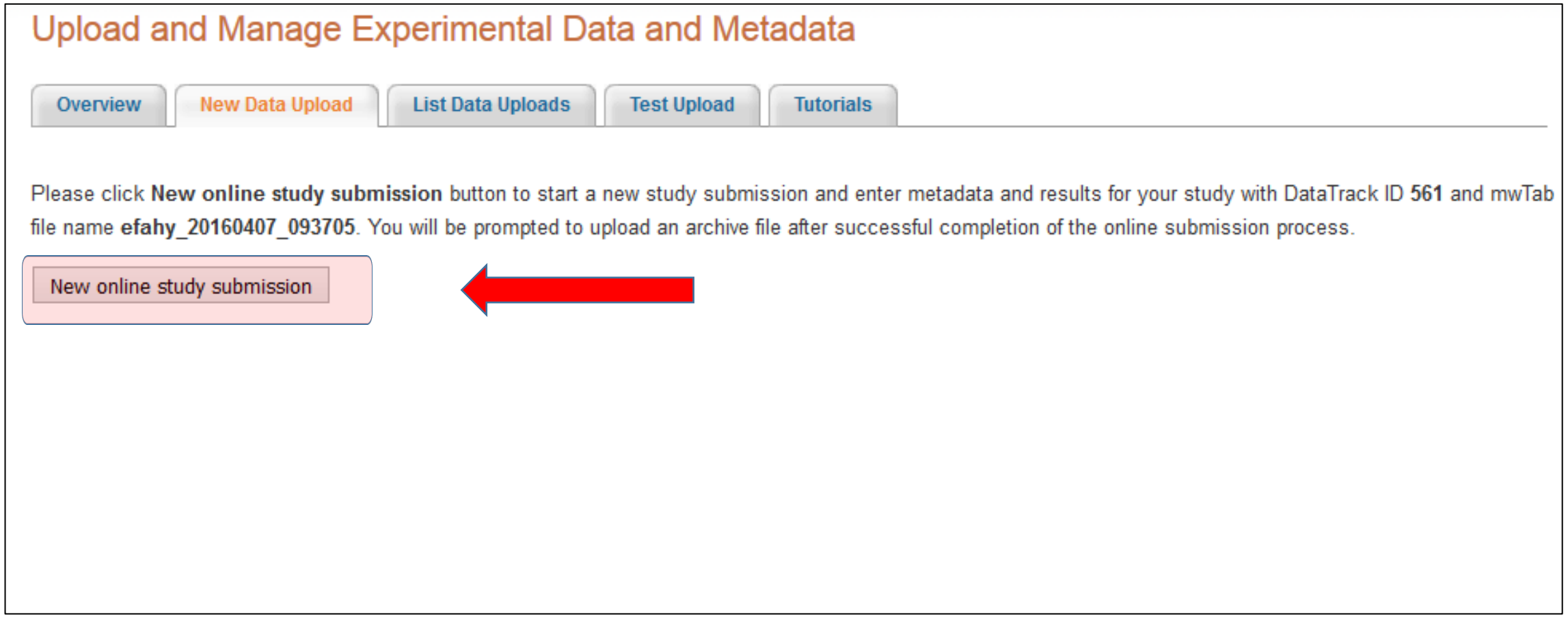
Use separate submissions if your study contains both MS and NMR data

Specify the embargo date if applicable

Please tell us about the data you plan to upload. (* = required)

* mwTab file name	efahy_20210210_135208_mwtab.txt	(Automatically assigned name)
* Name of archive file to be uploaded	EF-_45.zip	(e.g. MyData.zip, MyData.7z or MyData.gz)
* Data type being submitted	MS	(Use separate submissions for studies containing both MS and NMR data)
* Protocol methods filename(s)	PR_SP45.pdf PR_TR45.pdf	
* MS/NMR instrument manufacturer	ABI-SCIEX	
* MS/NMR instrument model	4000-QTRAP	
* Binary data format	.wiff	(e.g. .WIFF (ABI/Sciex), .RAW (Thermo) or .d (Agilent))
* Multi-part study	No	(For multi-part studies, add additional information such as "Study part m of n" in comments field)
* Embargo	Yes	(e.g. If Yes, then please specify date below)
Embargo until	2021-06-12	(e.g. 1 year, 6 months, or YYYY-MM-DD)
Open source text formats	.mzML	

(b): Begin the online submission of metadata and results



(b): Begin the online submission of metadata and results

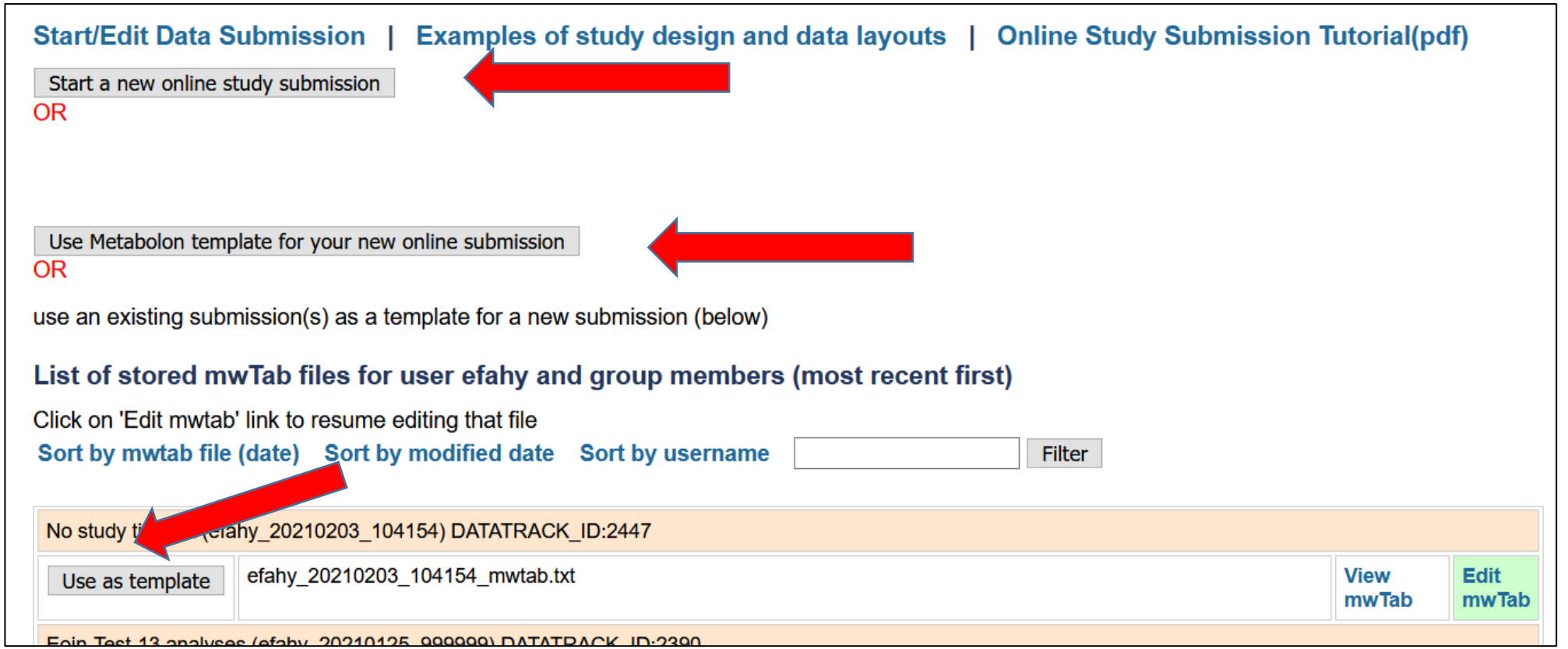
Start a new study from scratch (most common option, especially for new users)

or

use the Metabolon template if the new submission is composed of Metabolon analyses

or

use an existing study as a template for a new submission



Project information

Items in pink are required fields

Personal information such as name, address, email is autopopulated in the form based on your login credentials (but you may edit these fields if not correct or appropriate)

This is your unique Submission identifier (contains your login name and date/time)

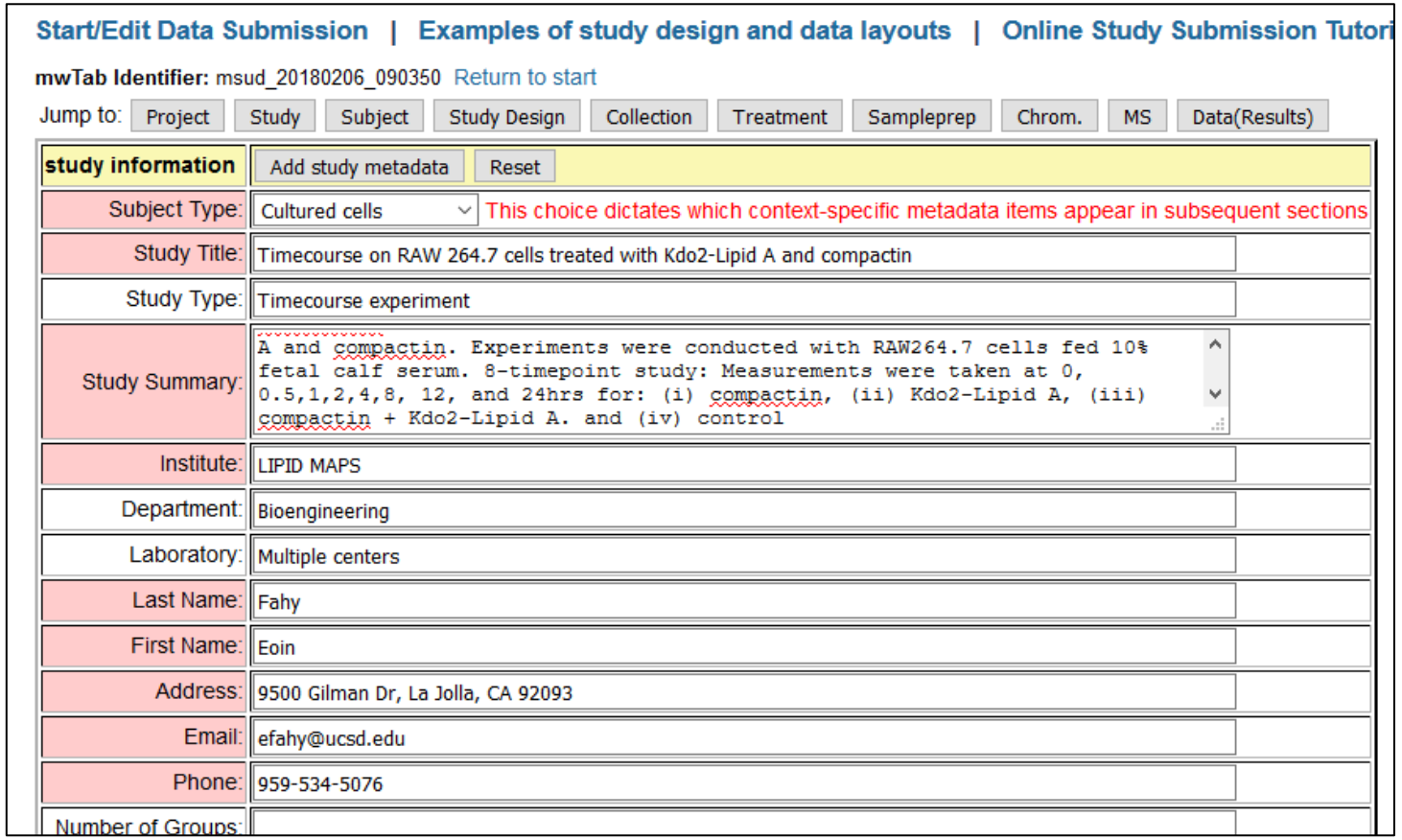
Start/Edit Data Submission | Examples of study design and data layouts | Upload and Manage Data | Tutorial

mwTab identifier: efahy_20151117_182353

project information	Add project metadata	Reset
Project Title:	LIPID MAPS Lipidomics studies	
Project Type:	MS quantitative analysis	
Project Summary:	Multi-center quantitative lipidomics studies on samples from human and murine sources (LIPIDMAPS)	
Institute:	University of California, San Diego	
Department:	Bioengineering	
Laboratory:	Multiple centers	
Last Name:	Fahy	
First Name:	Eoin	
Address:	9500 Gilman, La Jolla, CA, 92093, USA	
Email:	efahy@ucsd.edu	
Phone:	858-534-4076	
Funding Source:	NIGMS	

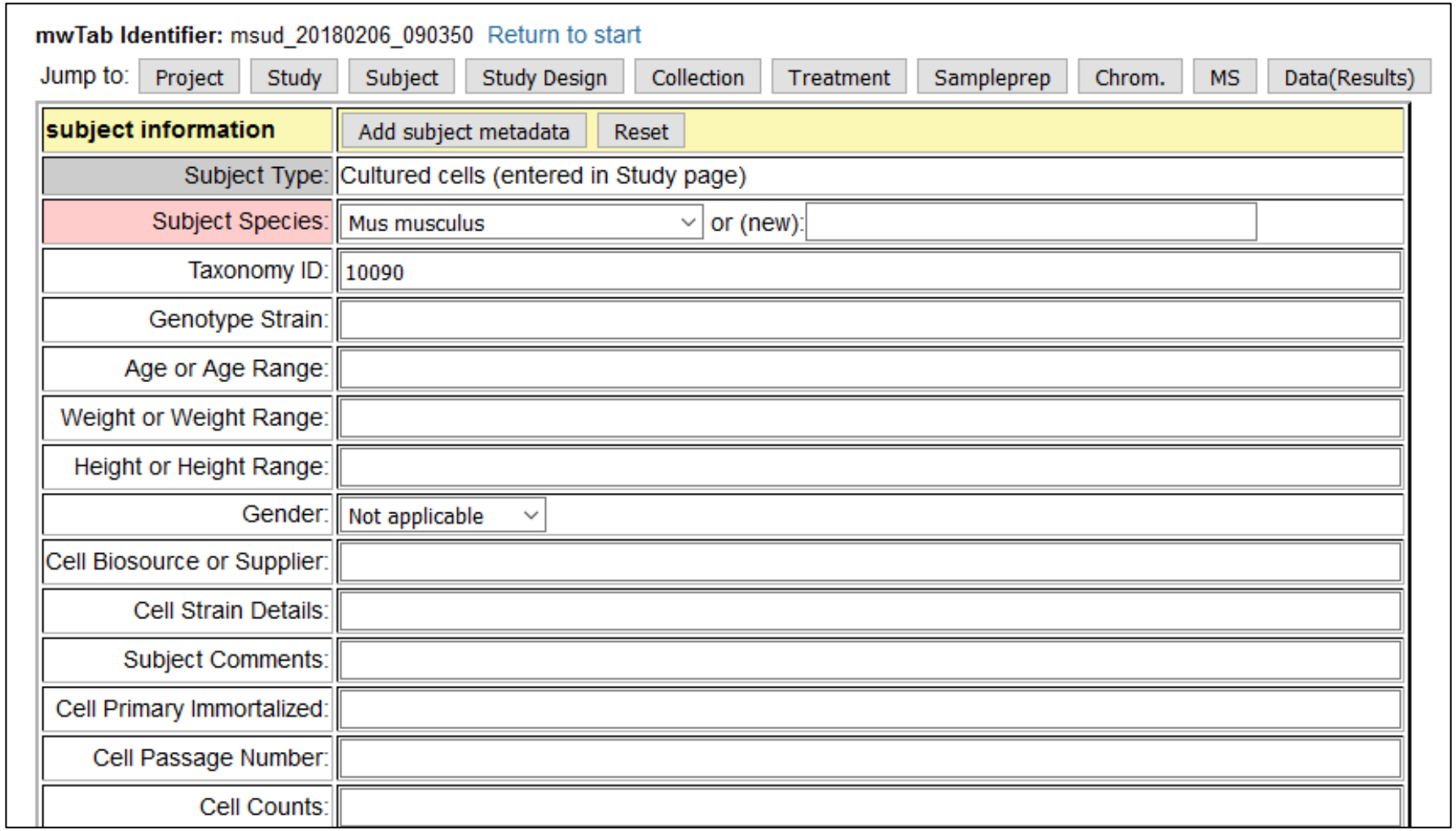
Study information

Subject type is mandatory and creates context-specific metadata items in subsequent sections
Study title should be unique (if you're submitting multiple studies)
Study summary is very important in order to describe the objectives of the experiment to the general public.
Ideally it should be a paragraph similar to an abstract in a publication
Personal information such as name, address, email is autopopulated in the form based on your login credentials (but you may edit these fields if not correct or appropriate)



Subject information

Choose subject species from pulldown menu or enter a new species (Latin name)



mwTab Identifier: msud_20180206_090350 Return to start

Jump to: Project | Study | Subject | Study Design | Collection | Treatment | Sampleprep | Chrom. | MS | Data(Results)

subject information	Add subject metadata	Reset
Subject Type:	Cultured cells (entered in Study page)	
Subject Species:	Mus musculus	or (new):
Taxonomy ID:	10090	
Genotype Strain:		
Age or Age Range:		
Weight or Weight Range:		
Height or Height Range:		
Gender:	Not applicable	
Cell Biosource or Supplier:		
Cell Strain Details:		
Subject Comments:		
Cell Primary Immortalized:		
Cell Passage Number:		
Cell Counts:		

Study design information

This section contains essential study design information for the study which must include sample identifiers and at least one experimental variable(factor) in tabular format. An additional "subject_id" column relating the samples to a particular source (patient, animal, cell etc.) may also be included. Additional information unique to each sample (e.g. height, weight, BMI, age, assay measurement, etc.) may also be included but should NOT be designated as factors (Designate these as "Other" in the next step)

Include a column with raw data file names

Subject_ID	Sample_ID	Genotype	Treatment	Batch	RAW_FILE_NAME
CA11	CA11W0	Wild-type	Control	1a	SC_20190410_CA11W0.mzML
CA12	CA12W0	Wild-type	Control	1a	SC_20190410_CA12W0.mzML
CA13	CA13W0	Wild-type	Control	1a	SC_20190410_CA13W0.mzML
CA11	CA11W50	Wild-type	50uM	1a	SC_20190410_CA11W50.mzML
CA12	CA12W50	Wild-type	50uM	1a	SC_20190410_CA12W50.mzML
CA13	CA13W50	Wild-type	50uM	1a	SC_20190410_CA13W50.mzML
MX01	MX01M0	Mutant	Control	1a	SC_20190410_MX01M0.mzML
MX02	MX02M0	Mutant	Control	1a	SC_20190410_MX02M0.mzML
MX03	MX03M0	Mutant	Control	1a	SC_20190410_MX03M0.mzML
MX01	MX01M50	Mutant	50uM	1a	SC_20190410_MX01M50.mzML
MX02	MX02M50	Mutant	50uM	1a	SC_20190410_MX02M50.mzML
MX03	MX03M50	Mutant	50uM	1a	SC_20190410_MX03M50.mzML

Start/Edit Data Submission | Examples of study design and data layouts | Online Study Submission Tutor

mwTab Identifier: efahy_20210727_112136 Return to start

IMPORTANT!!

Make sure that sample names in submitted results table(s) or file(s) exactly match those in the study design table.
Otherwise you won't be able to complete the submission.
(One needs to be able to relate experimental conditions in the study-design section via sample names in ALL submitted datasets)

Input **Study Design** information (tab-delimited). Sample names, experimental factor(s) and raw data file names (if submitting raw data) are required.
Subject name and additional sample data are optional.
First row must contain headings

Subject_ID	Sample_ID	Genotype	Treatment	Batch	RAW_FILE_NAME
CA11	CA11W0	Wild-type	Control	1a	SC_20190410_CA11W0.mzML
CA12	CA12W0	Wild-type	Control	1a	SC_20190410_CA12W0.mzML
CA13	CA13W0	Wild-type	Control	1a	SC_20190410_
CA11	CA11W50	Wild-type	50uM	1a	SC_20190410_
CA12	CA12W50	Wild-type	50uM	1a	SC_20190410_
CA13	CA13W50	Wild-type	50uM	1a	SC_20190410_
MX01	MX01M0	Mutant	Control	1a	SC_20190410_
MX02	MX02M0	Mutant	Control	1a	SC_20190410_MX02M0.mzML
MX03	MX03M0	Mutant	Control	1a	SC_20190410_MX03M0.mzML
MX01	MX01M50	Mutant	50uM	1a	SC_20190410_MX01M50.mzML

Copy/paste as tab-delimited data from Excel or text file (View the "See examples.." link for more help)

View/check study design | See examples of study design layout

Then click on "View/check study design" to view in tabular format

Study design information

Instructions:
Sample names/identifiers in the required **'Sample_ID'** column should be unique and should exactly match those names used in the processed results.
The required **'Raw file name'** column must be completed when submitting raw data. The sample name to raw file name mapping is essential in order to enable re-analysis of raw data.
The optional **'Subject_ID'** column may be used to designate the submitter's source identifier for a given sample (e.g. subject/patient/animal identifer).
The required **'Factor'** column(s) are used to assign experimental variables (factors) to sample groups (e.g. treatment condition, time, genotype, phenotype, etc.).
The optional **'Other'** column(s) may be used to include additional data such as BMI, age, glucose measurements, etc. that are unique to each sample. These types of measurements should NOT be designated as factors.

Assign every column(below) as 'Subject ID'(optional), 'Sample ID'(required:1 and only 1), 'Factor'(required:at least 1) or 'Other'(optional additional sample data). Columns assigned 'Ignore' will be ignored.

Process study design data **Does submission contain raw data?:**

Subject_ID	Sample_ID	Genotype	Treatment	Batch	RAW_FILE_NAME
CA11	CA11W0	Wild-type	Control	1a	SC_20190410_CA11W0.mzML
CA12	CA12W0	Wild-type	Control	1a	SC_20190410_CA12W0.mzML
CA13	CA13W0	Wild-type	Control	1a	SC_20190410_CA13W0.mzML
CA11	CA11W50	Wild-type	50uM	1a	SC_20190410_CA11W50.mzML
CA12	CA12W50	Wild-type	50uM		
CA13	CA13W50	Wild-type	50uM		

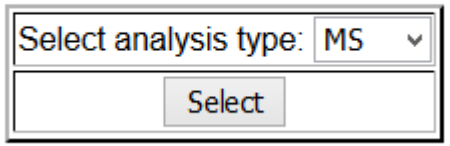
Assign each column as "Subject_ID", "Sample_ID", "Factor", "Raw file name", "Other" or "Ignore"

Process study design data **Does submission contain raw data?:** Yes

Subject_ID	Sample_ID	Factor	Factor	Other	Raw file name
Subject_ID	Sample_ID	Genotype	Treatment	Batch	RAW_FILE_NAME
CA11	CA11W0	Wild-type	Control	1a	SC_20190410_CA11W0.mzML
CA12	CA12W0	Wild-type	Control	1a	SC_20190410_CA12W0.mzML
CA13	CA13W0	Wild-type	Control	1a	SC_20190410_CA13W0.mzML
CA11	CA11W50	Wild-type	50uM	1a	SC_20190410_CA11W50.mzML
CA12	CA12W50	Wild-type	50uM	1a	SC_20190410_CA12W50.mzML

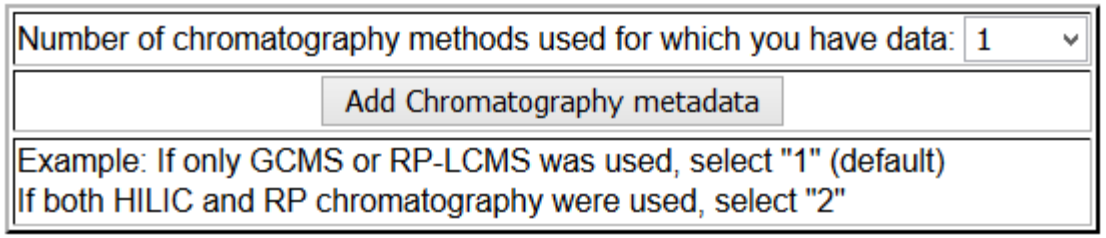
After editing/assignment, proceed by clicking on "Process study design data"

Decision point: MS or NMR experiment?



If MS is chosen, the user is prompted to enter chromatography information

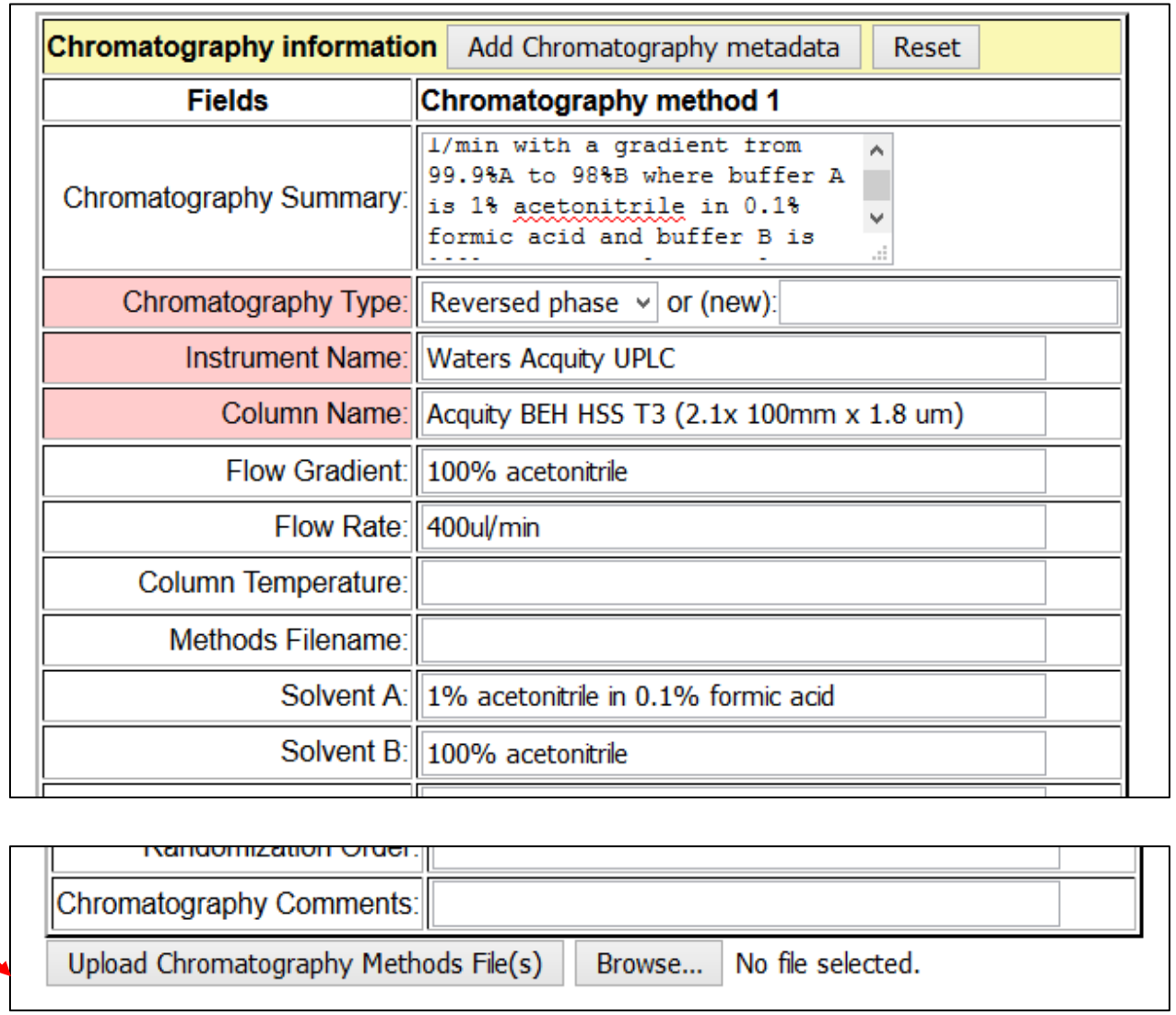
Choose number of chromatography methods for which you have data (default=1)



Chromatography information

Metadata related to chromatography (LC/GC) protocols

User may upload a methods/protocol file relating to chromatography



Chromatography information | Add Chromatography metadata | Reset

Fields	Chromatography method 1
Chromatography Summary:	1/min with a gradient from 99.9%A to 98%B where buffer A is 1% acetonitrile in 0.1% formic acid and buffer B is
Chromatography Type:	Reversed phase or (new):
Instrument Name:	Waters Acquity UPLC
Column Name:	Acquity BEH HSS T3 (2.1x 100mm x 1.8 um)
Flow Gradient:	100% acetonitrile
Flow Rate:	400ul/min
Column Temperature:	
Methods Filename:	
Solvent A:	1% acetonitrile in 0.1% formic acid
Solvent B:	100% acetonitrile

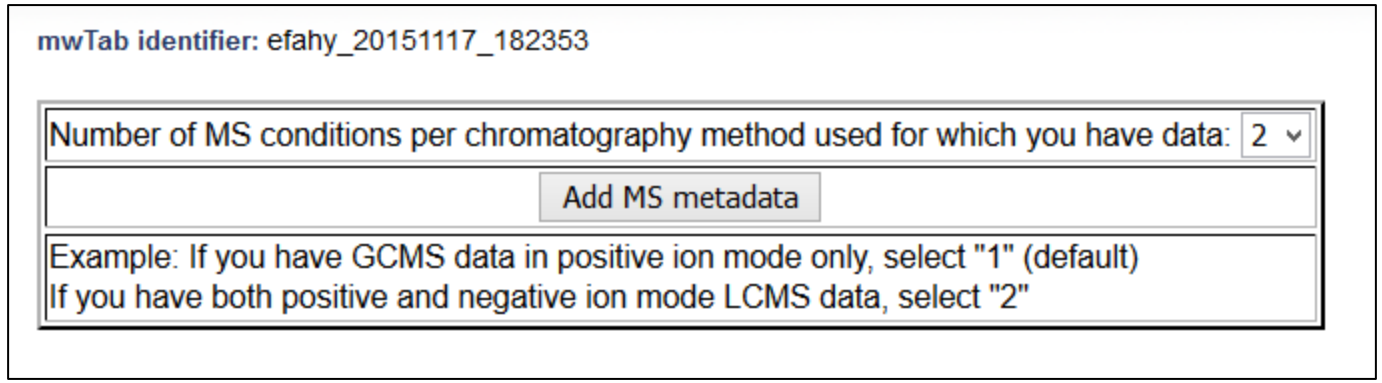
Randomization Order:

Chromatography Comments:	

Upload Chromatography Methods File(s) | Browse... | No file selected.

Number of MS conditions per chromatography method

In the case of LCMS this is typically 2 (Positive and negative ion mode)

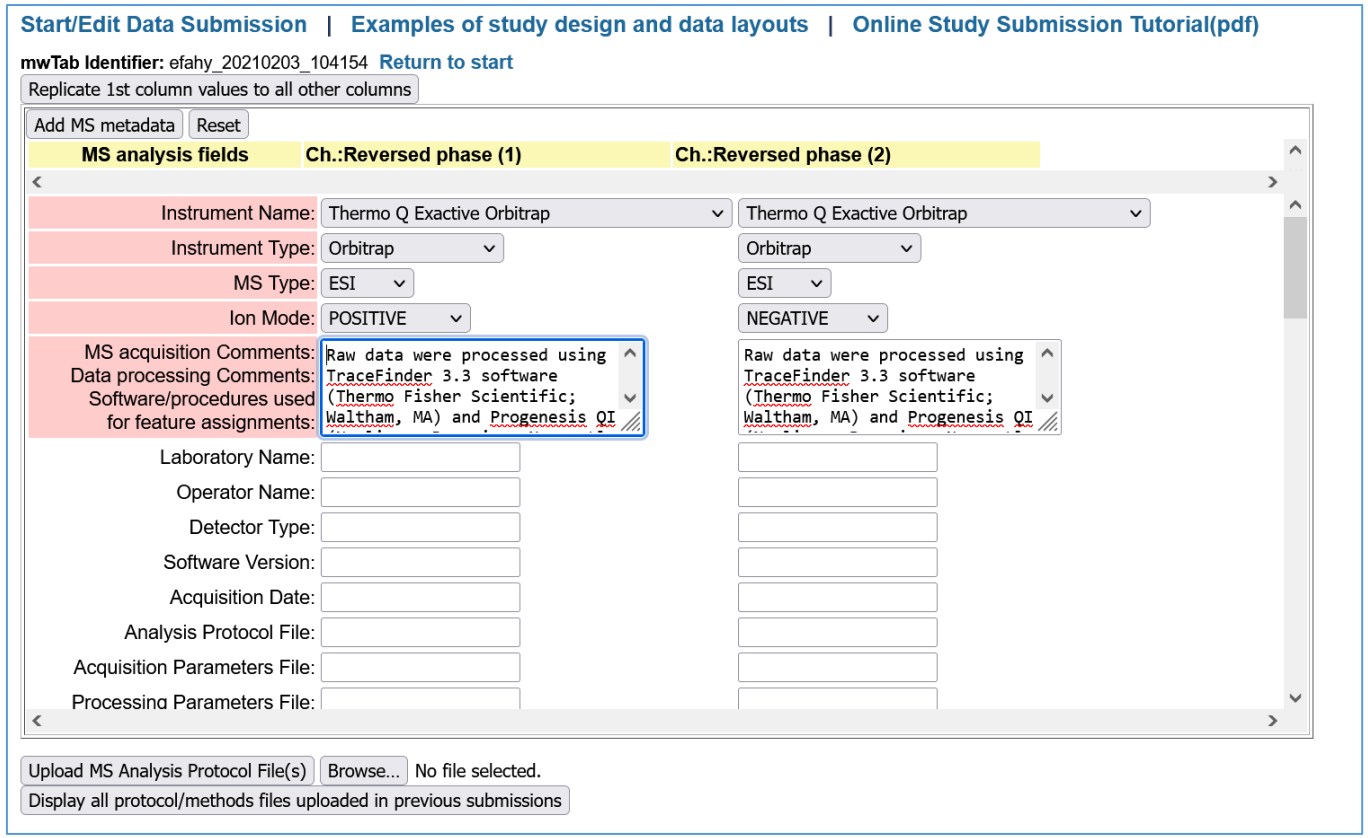


MS information

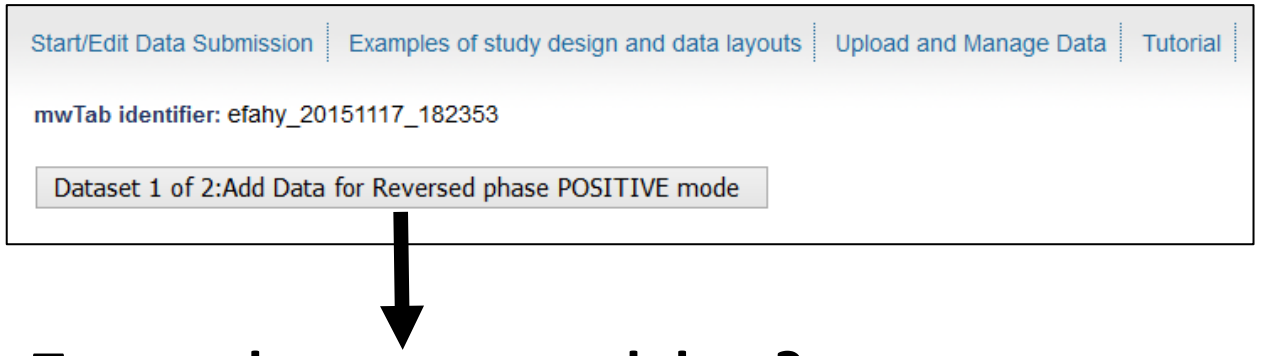
Metadata related to MS methods

The number of data columns will equal the number of chromatography conditions multiplied by the number of MS conditions. For example, if reversed-phase and HILIC chromatography were specified in conjunction with 2 MS modes (+ and – mode detection), then 2x2=4 columns are displayed

Hint: Fill out the parameters in the column on the left only, click the "Replicate.." button to copy the content to the other columns, then adjust any unique values as appropriate



Enter processed data for each chromatography/MS combination that you have specified



Decision point: Targeted or untargeted data?

Option1: Measurements for **named** metabolites from **targeted** experiments, e.g. GC-MS analyses or LC-MS assays with known standards.

Option2: Measurements from **untargeted** experiments e.g. high-resolution LC-MS analyses. Detected features are typically m/z-retention time values

OPTION 1: Targeted assays containing identified (named) metabolites

Input Data in tab-delimited format in the text area below.
First column must contain metabolite names.
Subsequent columns must contain sample data with identical sample names as in Study Design submission.
First row must contain sample names.

Tabular results (typically tens or hundreds of named metabolites) are pasted into this textarea

Units of measurement (required): xxx

View/check metabolite data | See examples of metabolite data layout | Delete existing metabolite data (this analysis only)

OPTION 2: Untargeted assays not containing identified (named) metabolites

(e.g. datasets with m/z,retention time features from LC-MS experiments, NMR binned data)

A file of tabular results (typically thousands of unidentified features) is uploaded here

Add/replace results as a tab-delimited text file:
Ideally, feature names should be formatted as 'm/z underscore retention time', e.g. 645.5327_
IMPORTANT!:If unidentified featues are listed by neutral mass rather than m/z ratio, this must be specified in the menu below
This will enable analysis of the dataset by a larger number of tools on the Metabolomics Workbench

Units of measurement (required):	Feature names contain m/z values*? (required):	Feature names contain retention time values? (required):	Time units:

* **By "m/z values" we are referring to mass-to-charge ratios and NOT neutral masses.**

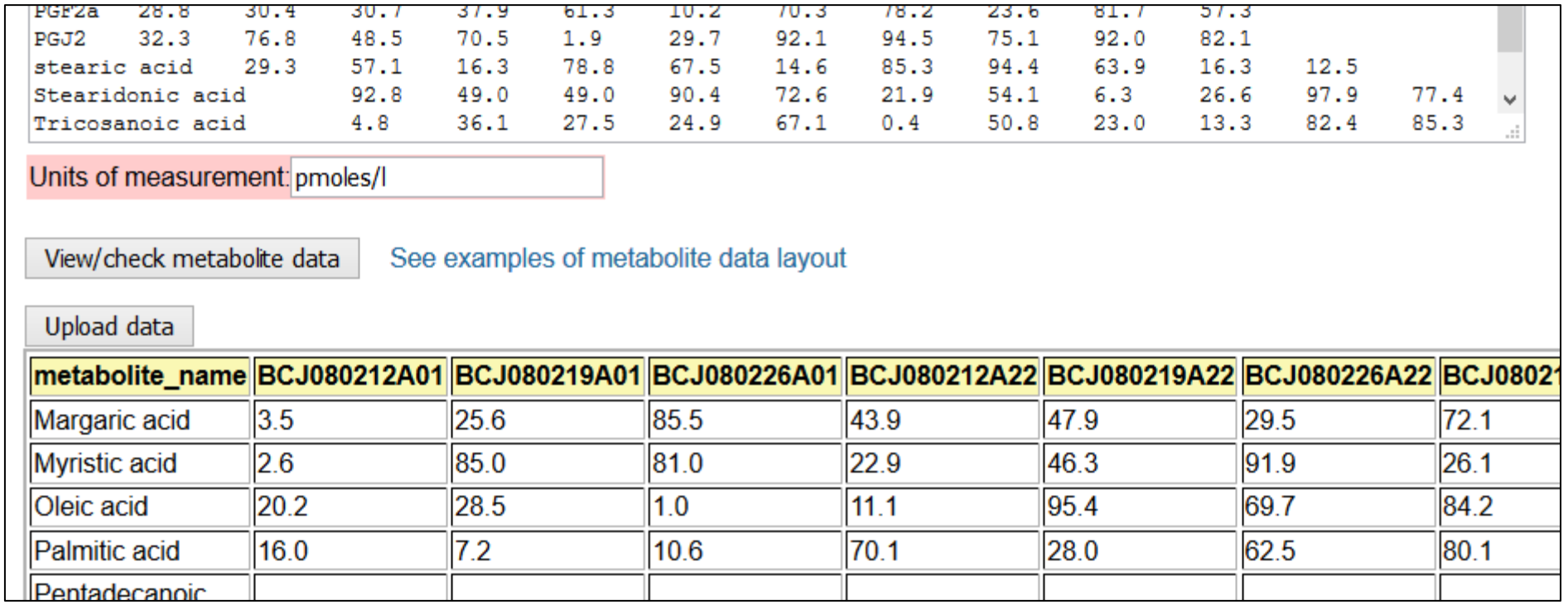
Upload tab-delimited datafile | Browse... | No file selected.

The first line in the submitted file should contain sample names exactly matching those that you submitted in the 'Study Design' section.

Option1:
Targeted data

Processed data upload: Review in tabular form, then Upload data

Note: sample names must match those submitted in the "study design" section, otherwise a warning will be generated and this must be resolved before proceeding



PGF2a	28.8	30.4	30.7	37.9	61.3	10.2	70.3	78.2	23.6	81.7	57.3	
PGJ2	32.3	76.8	48.5	70.5	1.9	29.7	92.1	94.5	75.1	92.0	82.1	
stearic acid		29.3	57.1	16.3	78.8	67.5	14.6	85.3	94.4	63.9	16.3	12.5
Stearidonic acid			92.8	49.0	49.0	90.4	72.6	21.9	54.1	6.3	26.6	97.9
Tricosanoic acid			4.8	36.1	27.5	24.9	67.1	0.4	50.8	23.0	13.3	82.4

Units of measurement: pmoles/l

View/check metabolite data See examples of metabolite data layout

Upload data

metabolite_name	BCJ080212A01	BCJ080219A01	BCJ080226A01	BCJ080212A22	BCJ080219A22	BCJ080226A22	BCJ0802
Margaric acid	3.5	25.6	85.5	43.9	47.9	29.5	72.1
Myristic acid	2.6	85.0	81.0	22.9	46.3	91.9	26.1
Oleic acid	20.2	28.5	1.0	11.1	95.4	69.7	84.2
Palmitic acid	16.0	7.2	10.6	70.1	28.0	62.5	80.1
Pentadecanoic							

Option1:
Targeted data

Metabolite metadata upload

Copy/paste metabolite annotations in tabular format (PubChem CID, KEGG ID, InCHi Key, LC/GC retention time/index, etc.) Metabolite names MUST match those submitted in the previous data section. If you don't have any metabolite annotations, just submit the column of metabolite names.

mwTab identifier: efahy_20151117_182353

Metabolite metadata in tab-delimited format. First column must contain metabolite names.
Subsequent columns should contain KEGG,PubChem identifiers, retention index,quantitated m/z, etc.
First row must contain headings.

```
Metabolite Name Pubchem Id      Kegg Id
Margaric acid   10465   -
Myristic acid   11005   C06424
Oleic acid      445639  C00712
Palmitic acid   985     C00249
Pentadecanoic acid      13849   C16537
PGD2    448457  C00696
PGE2    5283116 C00584
PGF2a   5280363 -
PGJ2    5311211 C05957
stearic acid    5281    C01530
```

View/check metabolite metadata See examples of metabolite metadata layout

```
Stearidonic acid        5282837 C16300
Tricosanoic acid        17085   -
```

View/check metabolite data See examples of metabolite data layout

Upload metabolite metadata

metabolite_name	Pubchem Id	Kegg Id
Margaric acid	10465	-
Myristic acid	11005	C06424
Oleic acid	445639	C00712
Palmitic acid	985	C00249
Pentadecanoic acid	13849	C16537
PGD2	448457	C00696
PGE2	5283116	C00584
PGF2a	5280363	-
PGJ2	5311211	C05957

After checking the table of metabolite annotations, click "Upload metabolite metadata"

Option2:
Untargeted data

Measurements from untargeted experiments e.g. high-resolution LC-MS analyses are uploaded as a tab-delimited text file containing a table of unidentified features (typically m/z-retention time values) and associated measurements.

OPTION 2: Untargeted assays not containing identified (named) metabolites

(e.g. datasets with m/z,retention time features from LC-MS experiments, NMR binned data)

Add/replace results as a tab-delimited text file:
Ideally, feature names should be formatted as 'm/z underscore retention time', e.g. 645.5327_24.91
IMPORTANT!:If unidentified featues are listed by neutral mass rather than m/z ratio, this must be specified in the menu below
This will enable analysis of the dataset by a larger number of tools on the Metabolomics Workbench

Units of measurement (required):	Feature names contain m/z values*? (required):	Feature names contain retention time values? (required):	
Peak area	Yes	Yes	Time units: Minutes

*** By "m/z values" we are referring to mass-to-charge ratios and NOT neutral masses.**

Upload tab-delimited datafile | Browse... | jwalejko_20181204_201054_mwtab.txt

The first line in the submitted file should contain sample names exactly matching those that you submitted in the 'Study Design' section.

C:\Users\eoinf\Downloads\untargeted_data_table.txt

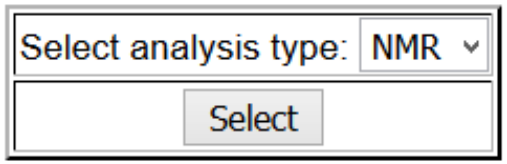
	Feature(m/z_RT)	samp1	samp2	samp3	samp4	sam
2	100.02005_15.5	8875.5	9273.9	1559.0	1160.0	894
3	100.07742_65.4	2744.3	2152.3	6895.3	9465.8	212
4	101.06952_73.9	6646.6	3736.5	1458.4	9832.6	653
5	102.08992_29.2	4164.2	2195.9	8447.9	1920.1	274
6	102.08983_25.0	8187.6	8647.8	4984.4	9747.3	741
7	103.05251_42.6	2432.0	2431.9	4988.6	3383.4	820
8	103.78777_17.7	5714.7	3217.8	4914.0	8954.6	414
9	104.05150_20.6	9814.3	8541.1	6641.6	2744.3	215
10	104.06962_16.9	1481.1	1368.9	2780.0	2206.6	513
11	104.10595_11.6	5430.2	6389.2	8495.9	9654.2	848
12	104.10562_72.7	2614.9	2431.9	2140.9	9045.2	155
13	104.99081_88.7	6193.2	5506.5	7210.6	5457.4	991
14	106.04841_24.7	5995.0	8896.7	4185.6	2675.6	556
15	106.08454_13.2	2862.1	9659.3	2016.6	1539.5	527
16	108.01019_20.6	5768.7	4539.3	4992.9	1156.6	166
17	109.09961_16.9	4128.3	5113.5	6015.4	8823.3	348
18	110.05838_71.2	9221.6	1079.8	7146.5	8210.4	155
19	110.06358_79.4	5995.0	8896.7	1570.0	2258.1	991
20	110.10667_56.9	602.8	1942.7	4983.4	1102.9	556

Select results file from your file system. Sample names should exactly match those submitted in the "Study Design" section of the metadata submission

Example of a file with untargeted MS data. Note the 1st column contains m/z_retention time features. Subsequent columns contain measurements for each sample.

Decision point: MS or NMR experiment?

NMR option



mwTab identifier: efahy_20151112_141949

nmr information	Add nmr metadata / Reset
Instrument Name:	Bruker Avance III
Instrument Type:	FT-NMR
NMR Experiment Type:	1D-1H
NMR Comments:	
Field Frequency Lock:	Deuterium
Standard Concentration:	0.5 mM
Spectrometer Frequency:	950 MHz
NMR Probe:	cryo, inverse
NMR Solvent:	D2O
NMR Tube Size:	5mm x 7 in
Shimming Method:	Topshim

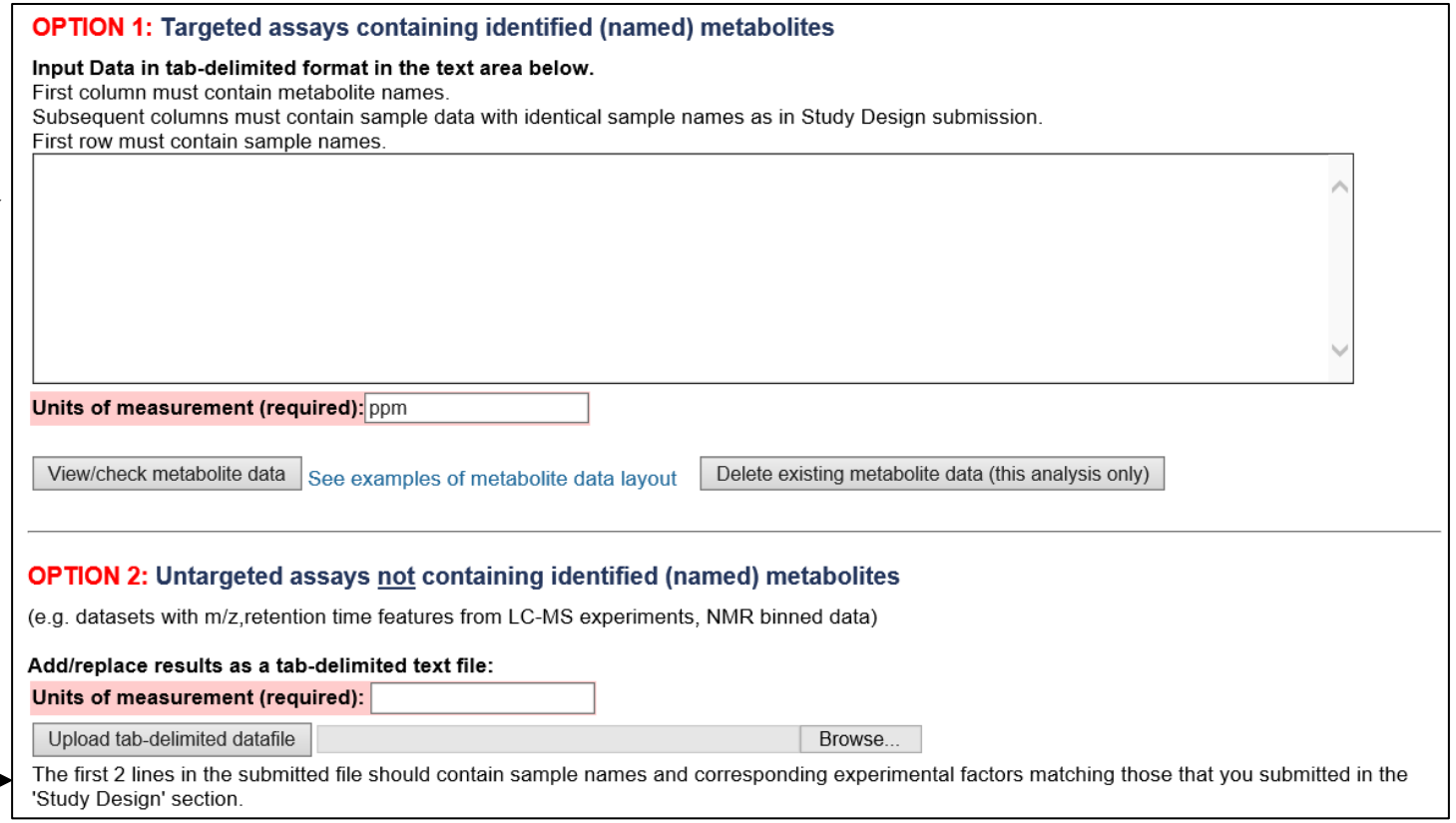
NMR experiment option

Add NMR results data

Decision point: Targeted or untargeted data?

Option1: Measurements for **named** metabolites from **targeted** NMR analyses.

Option2: Measurements from **untargeted** experiments e.g. binned NMR analyses. Detected features are typically binned chemical shift ranges.

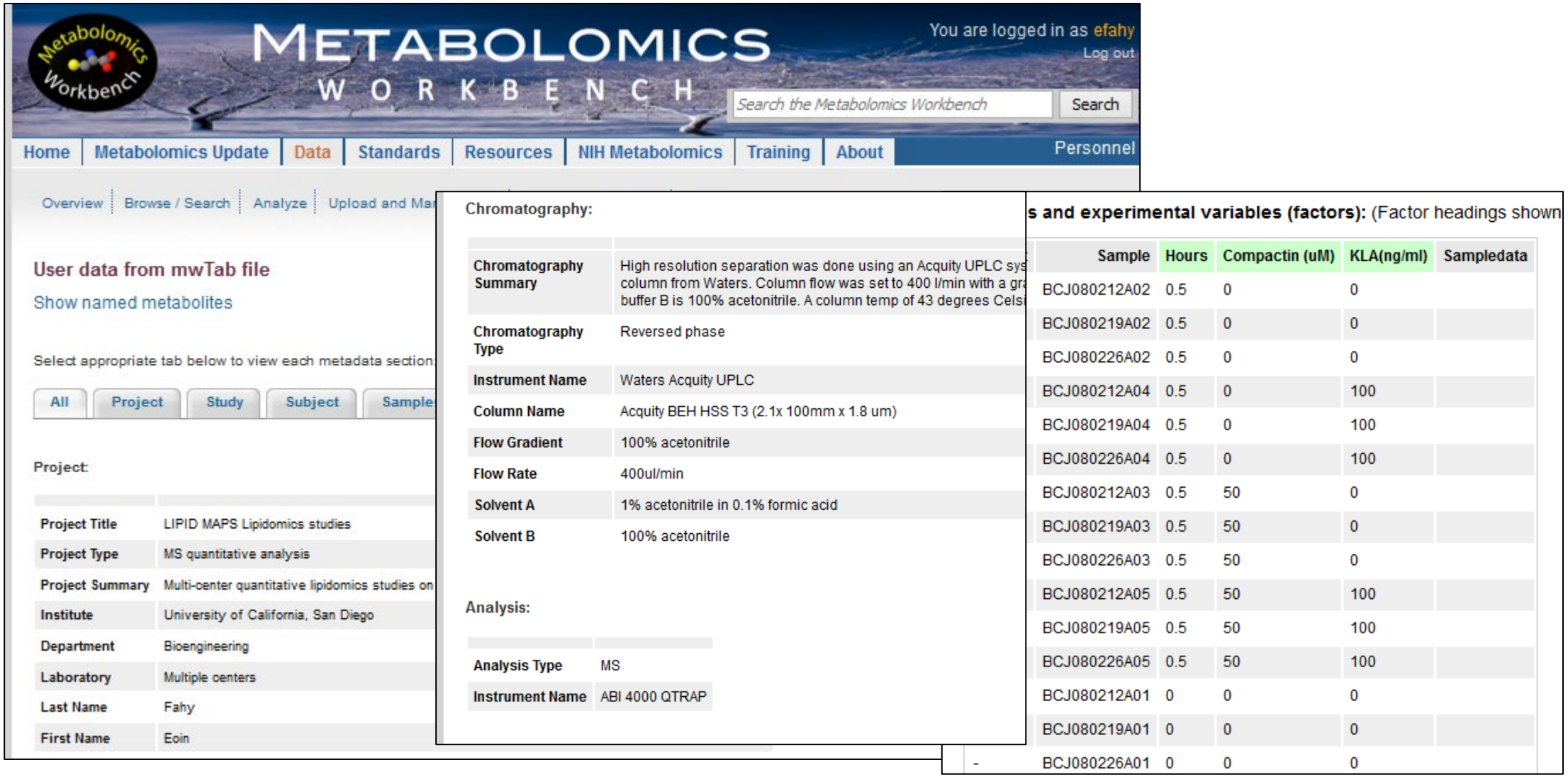


View/download the completed mwTab files

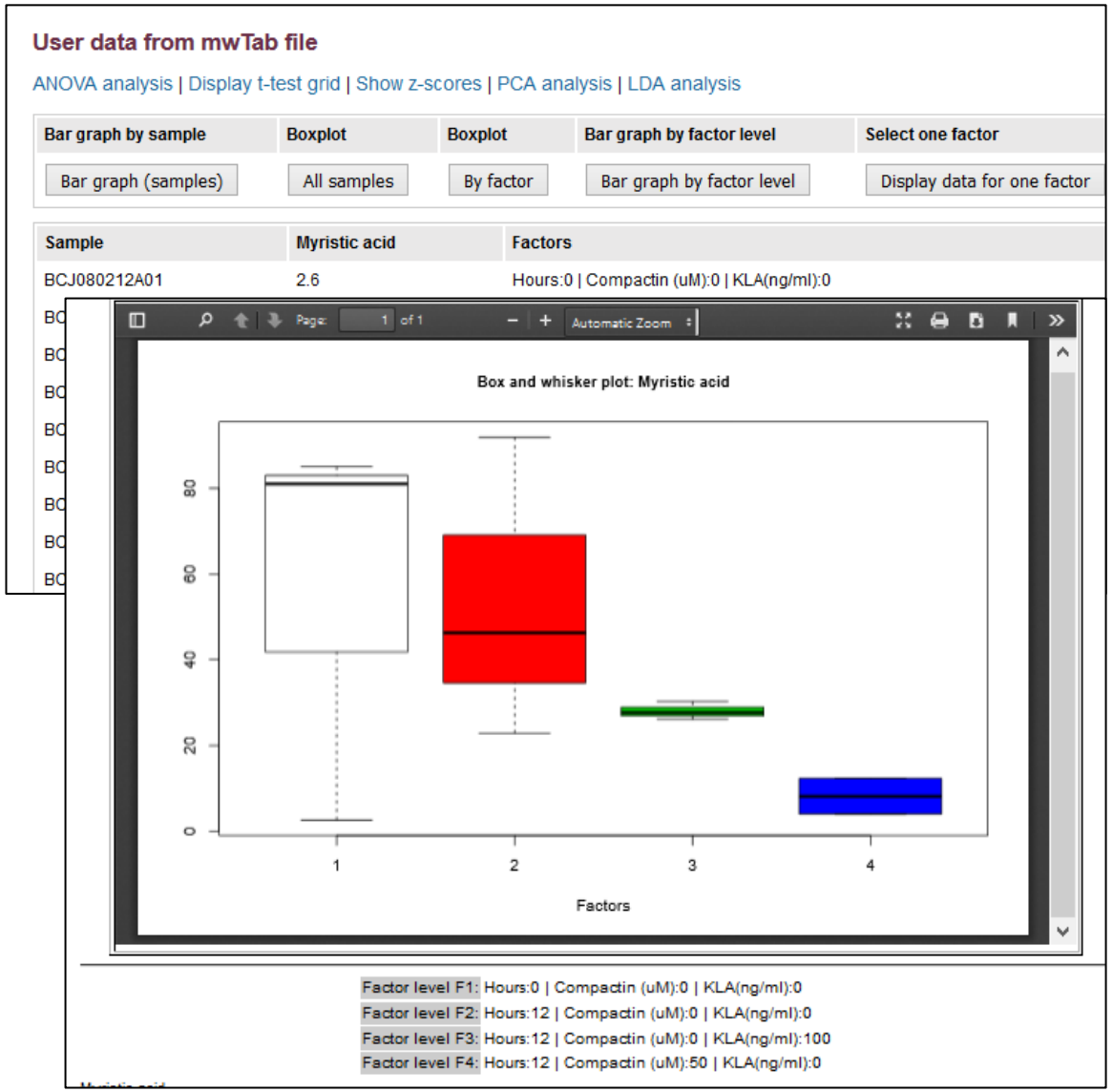
These are saved in the user's login area

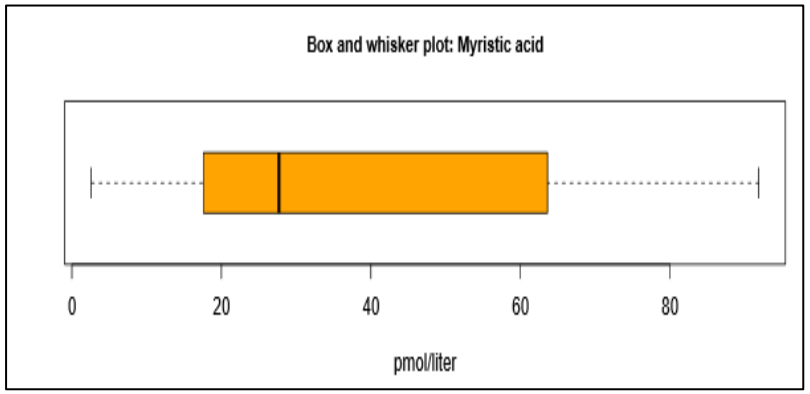
```
#METABOLOMICS WORKBENCH efahy_20151117_182353
VERSION                 1
CREATED_ON              November 17, 2015, 6:23 pm
#PROJECT
PR:PROJECT_TITLE                        LIPID MAPS Lipidomics studies
PR:PROJECT_TYPE                         MS quantitative analysis
PR:PROJECT_SUMMARY                      Multi-center quantitative lipidomics s
PR:PROJECT_SUMMARY                      sources (LIPIDMAPS)
PR:INSTITUTE                            University of California, San Diego
PR:DEPARTMENT                           Bioengineering
PR:LABORATORY                           Multiple centers
PR:LAST_NAME                            Fahy
PR:FIRST_NAME                           Eoin
PR:ADDRESS                              9500 Gilman, La Jolla, CA, 92093, USA
PR:EMAIL                                efahy@ucsd.edu
PR:PHONE                                858-534-4076
PR:FUNDING_SOURCE                       NIGMS
#STUDY
ST:STUDY_TITLE                          Timecourse on RAW 264.7 cells treated
ST:STUDY_TYPE                           Timecourse experiment
ST:STUDY_SUMMARY                        Lipidomics studies on macrophages - RA
ST:STUDY_SUMMARY                        and compactin. Experiments were conduc
ST:STUDY_SUMMARY                        serum. 8-timepoint study: Measurements
ST:STUDY_SUMMARY                        24hrs for: (i) compactin, (ii) Kdo2-Li
ST:STUDY_SUMMARY                        (iv) control
ST:INSTITUTE                            University of California, San Diego
ST:DEPARTMENT                           Bioengineering
ST:LABORATORY                           Multiple centers
ST:LAST_NAME                            Fahy
ST:FIRST_NAME                           Eoin
```

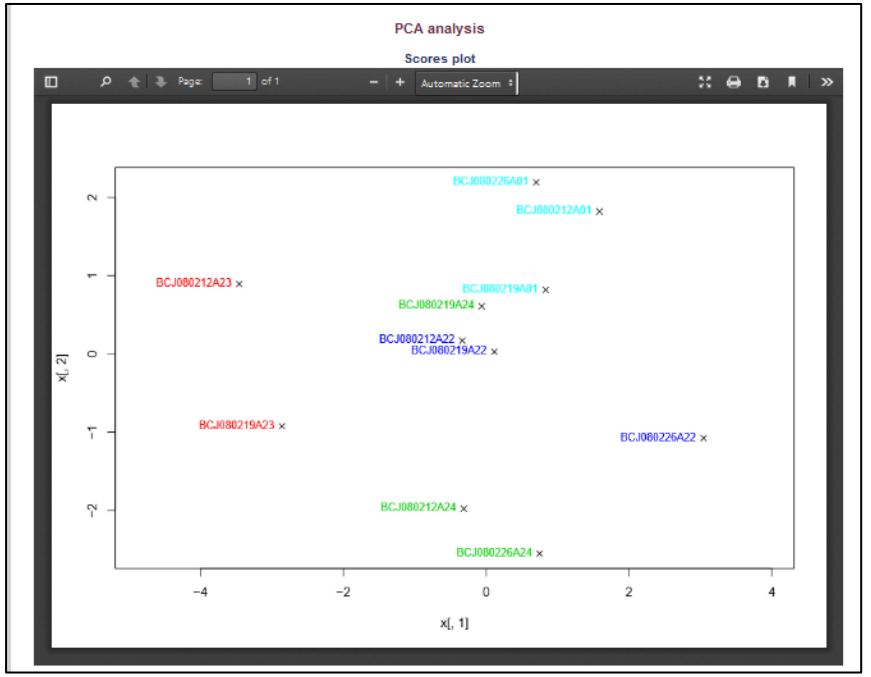
The “View Online “ link allows users to view and analyze the study to review the data/metadata. This viewer simulates how the study will appear on the Metabolomics WorkBench after NMDR curation and database upload



The “View Online “ link allows users to perform analysis on their datasets via the mwTab format prior to NMDR registration and database upload

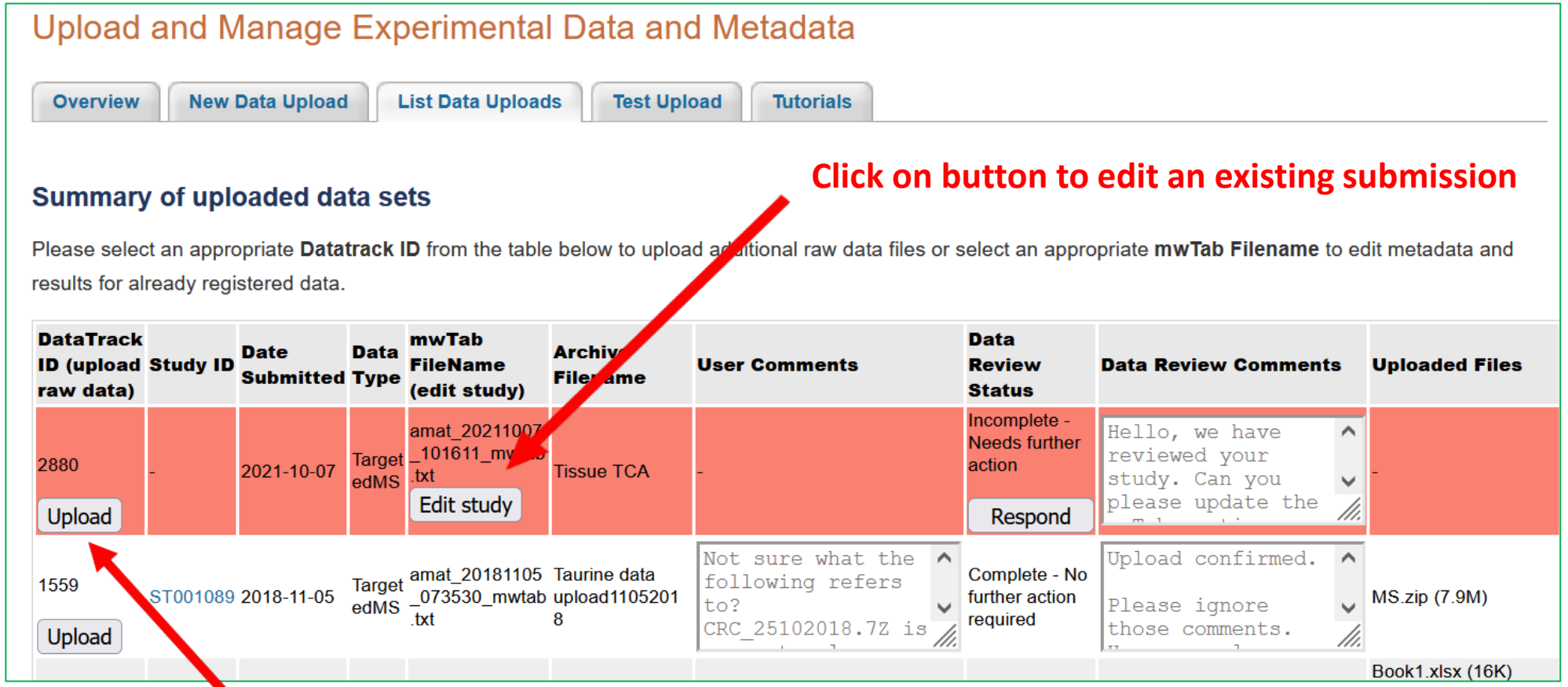






Edit your Data Submission (DataTrack_ID)

Resume submission or edit an existing submission from the “List Data Uploads” section at https://www.metabolomicsworkbench.org/data/DRCCDataDeposit.php

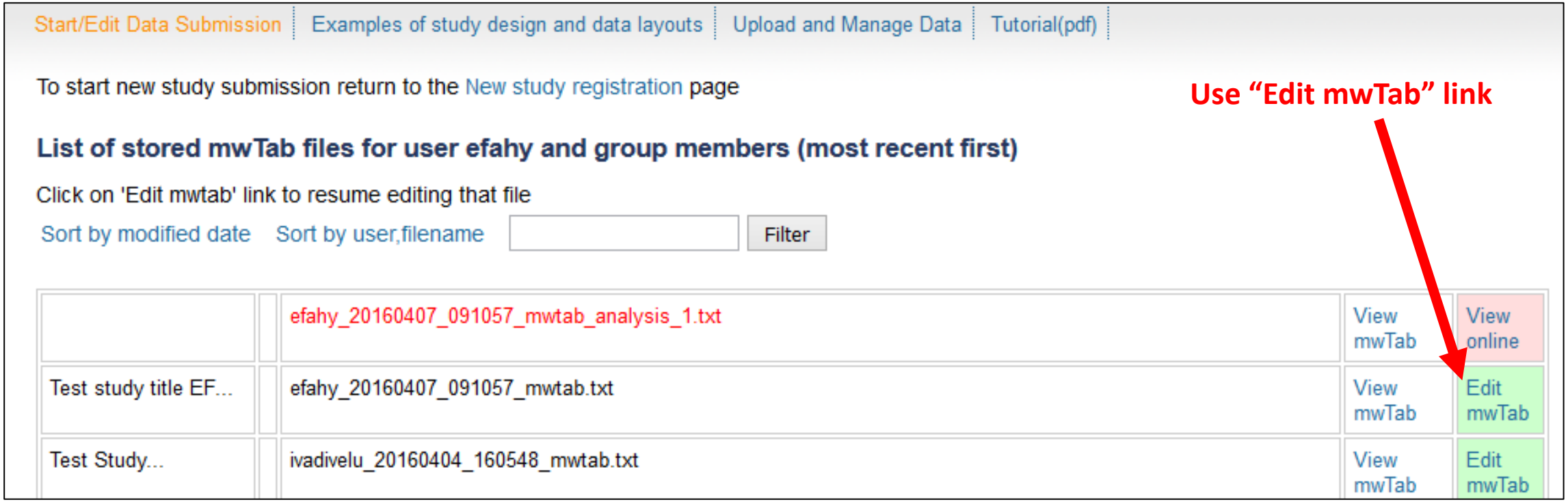


Click on button to edit an existing submission

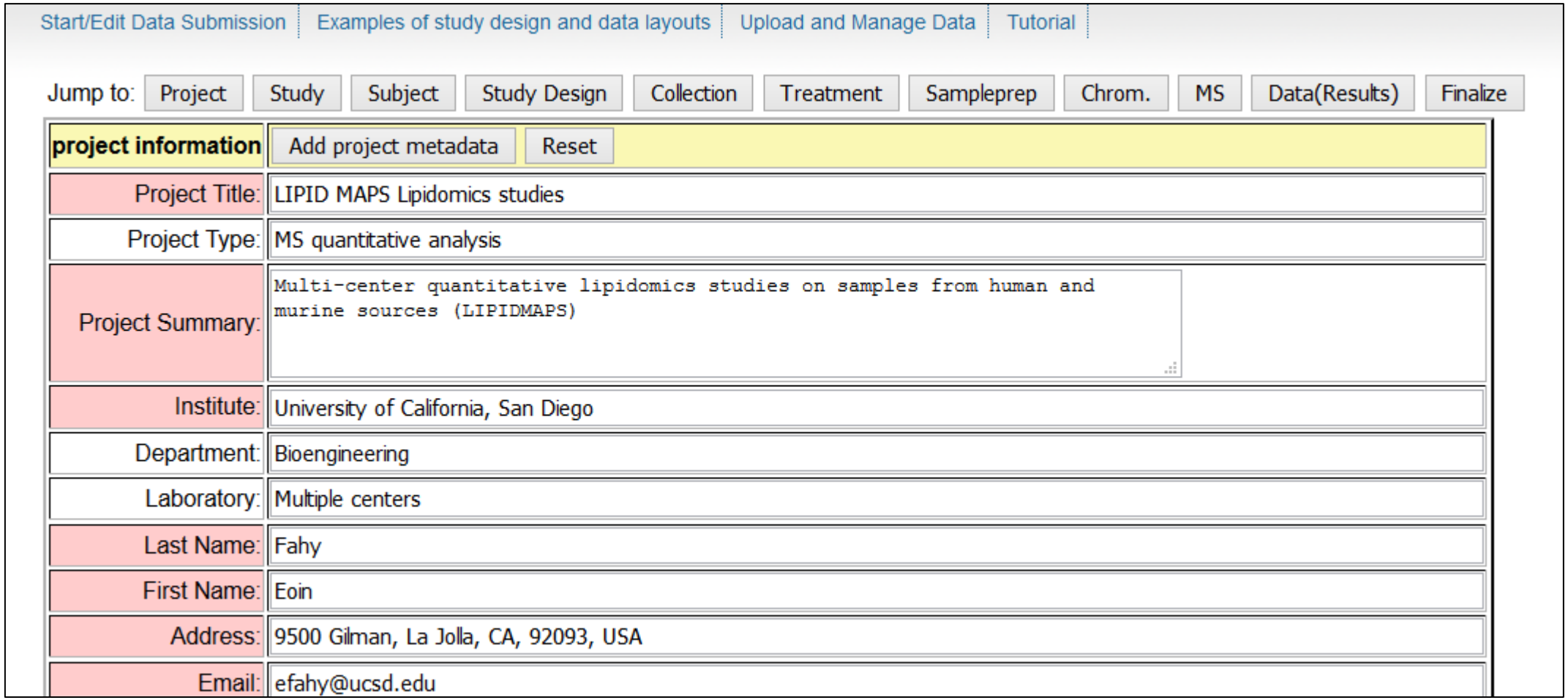
Upload raw data for a submission by clicking on the Upload button

Edit your Data Submission

Resume submission of a new study or edit an existing study from the online GUI at http://www.metabolomicsworkbench.org/data/ds_main.php



Study editing interface: Jump to section of interest



Upload your raw and supplementary data via a standalone FTP client
Your raw data should be submitted as a compressed file (.zip, .7Z, .gz, etc)
IMPORTANT! Please upload raw data in open-source format (e.g. mzML, mzXML, CDF)
if at all possible to enable re-use and re-analysis by other researchers
Please do not upload individual raw files- combine them in a single compressed archive (.zip,.7z)

Upload additional files for already registered data with data track ID 3109

Please review the following information before you continue to upload data to remote directory **77/DataTrackID3109**:

- **Raw data upload**:
  IMPORTANT! Please upload raw data in open-source format (mzML,mzXML,CDF) if at all possible to enable re-use and re-analysis.
  Please do not upload individual raw files- combine them in a single compressed archive (.zip,.7z) first.
  Compressed (zip, 7z) data files are selected and uploaded to the NMDR FTP server through a FTP client. A variety of free and commercial standalone file transfer clients exist to upload large data files directly to the FTP servers: **FileZilla** , **WinSCP** , etc. The usage of **FileZilla** is recommended for uploading data to the NMDR.
- Use the following credentials to upload data to the NMDR:
  - **Server Name:** www.metabolomicsworkbench.org
  - **User Name:** drccupload
  - **Password:** [redacted]
- After connecting to the NMDR FTP server, please change remote directory to **77/DataTrackID3109** before uploading the compressed (zip, 7z) data file.

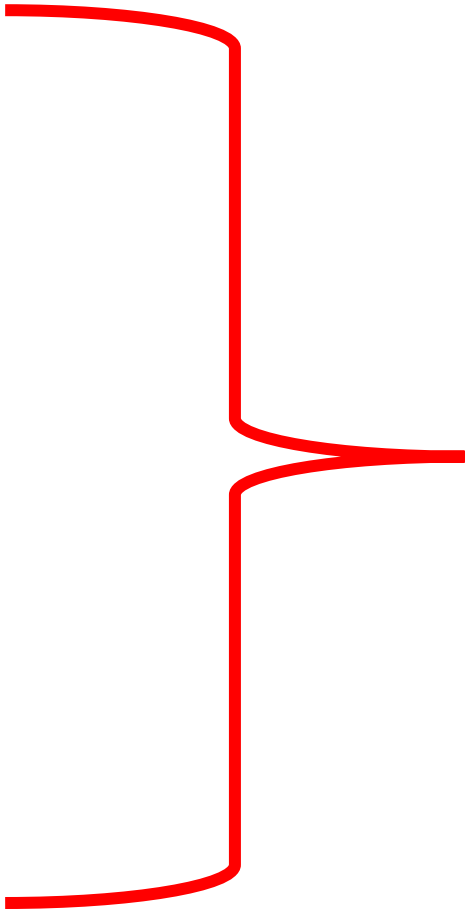
Password will be visible when you navigate to the appropriate datatrack_id in your data upload list

Upon completion of registration, your dataset is entered in the NMDR processing queue where it will be curated and uploaded on the Metabolomics WorkBench public website (depending on embargo conditions)

Metabolite nomenclature harmonization is an important consideration

NMDR: DIFFERENT SUBMITTED NAMES for the same metabolite

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



LPC 16:0

(RefMet name)

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

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

Why do we need it?

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

How is it implemented?

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

RefMet standardized metabolite nomenclature

Home | Data Repository | Databases | Protocols | Tools | Training / Events | About

Overview | Metabolite Database | ternal Metabolc

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

RefMet: A Refere

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

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

RefMet: A Reference set of Metabolite names

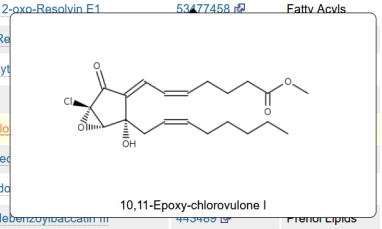
(A total of 154667 compounds or isobaric mixtures as of 04/23/21)

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

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

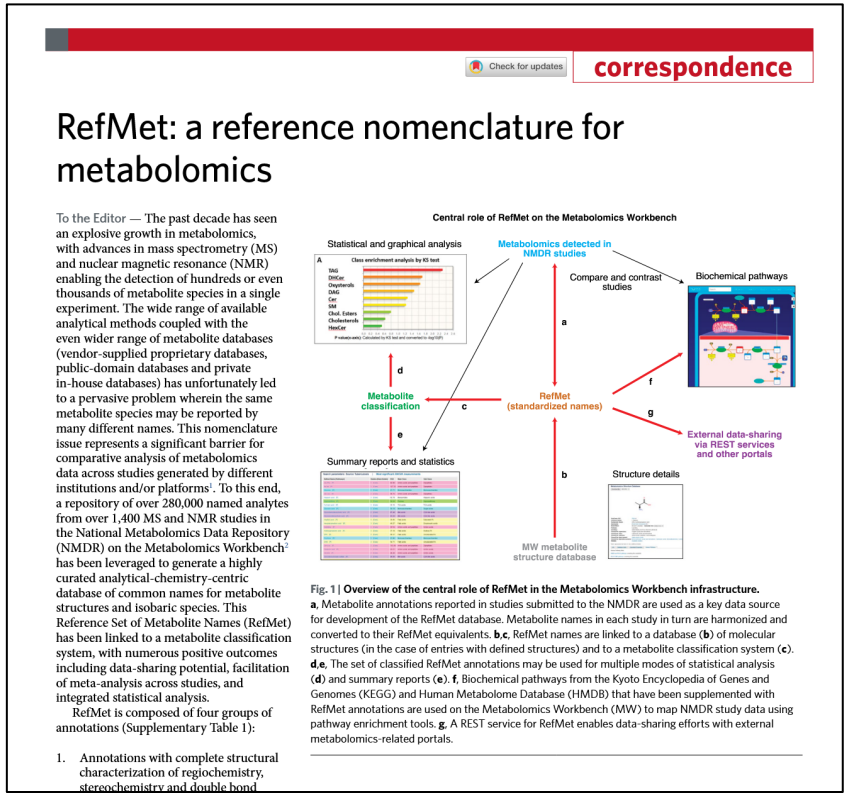
Name: Contains Super class(?): Main class(?): Sub class(?): Reset

Metabolite name | *MONA MS spectra*	PubChem CID	Super class	Main class	Sub class	Formula	Exact mass
10,11-DiHDPE	16061145	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{34}O_4$	362.2457
10,11-Dihydro-12-oxo-Resolvin E1	53477458	Fatty Acyls	Eicosanoids	HETE	$C_{20}H_{30}O_5$	350.2093
10,11-Dihydro-Re			Eicosanoids	HETE	$C_{20}H_{32}O_5$	352.2250
10,11-Dimethoxyt			Harmala alkaloids	Harmala alkaloids	$C_{29}H_{37}N_3O_2$	459.2886
10(11)-EpDPE			Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10,11-Epoxy-chlo			Eicosanoids	Clavulones	$C_{21}H_{29}ClO_5$	396.1704
10,12,15-Octadec			Fatty acids	Unsaturated FA	$C_{18}H_{30}O_2$	278.2246
10,22-Dimethyldo			Hydrocarbons	Hydrocarbons	$C_{34}H_{70}$	478.5478
10-Deacetyl-2-debenzoylbaccatin III	443459	Prenol Lipids	Isoprenoids	Taxanes	$C_{22}H_{32}O_9$	440.2046
10-Deoxymethymycin	5282032	Polyketides	Macrolides and analogues	Macrolides	$C_{25}H_{43}NO_6$	453.3090
10-Deoxymethynolide	5282031	Polyketides	Macrolides and analogues	Macrolides	$C_{17}H_{28}O_4$	296.1988
10-HDoHE | *MS spectra*	11537494	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10-Hendecenoic acid	5634	Fatty Acyls	Fatty acids	Unsaturated FA	$C_{11}H_{20}O_2$	184.1463
10-HpODE	5282857	Fatty Acyls	Octadecanoids	HpODEs	$C_{18}H_{32}O_4$	312.2301
10-HpOME	13801082	Fatty Acyls	Octadecanoids	HpOMEs	$C_{18}H_{34}O_4$	314.2457



10,11-Epoxy-chlorovulone I

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



Check for updates **correspondence**

RefMet: a reference nomenclature for metabolomics

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

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

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

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

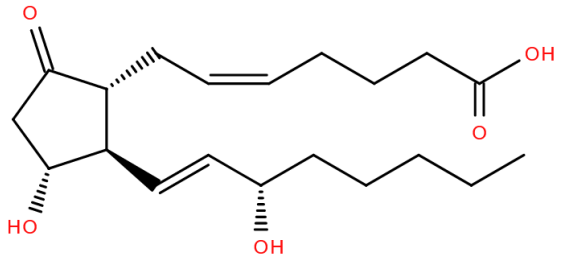
Fahy, E., Subramaniam, S. RefMet: a reference nomenclature for metabolomics. *Nature Methods* **17**, 1173–1174 (2020).

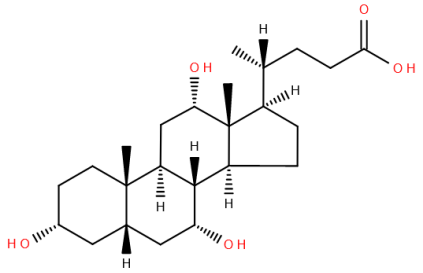
RefMet annotation levels

Level 1: Complete structure level

Comments Exact structure (including stereochemistry and bond geometry)

Examples: PGE2, 12S-HETE, Cholic acid

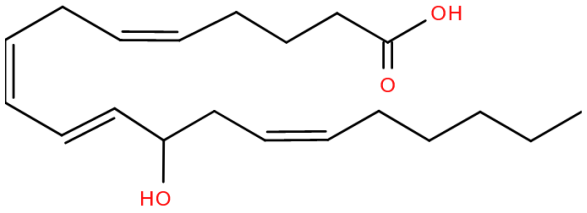


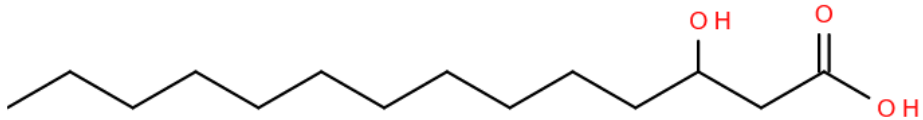


Level 2: Regiochemistry level

Comments Known regiochemistry (excluding stereochemistry and bond geometry)

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





Level 3: Molecular Species level

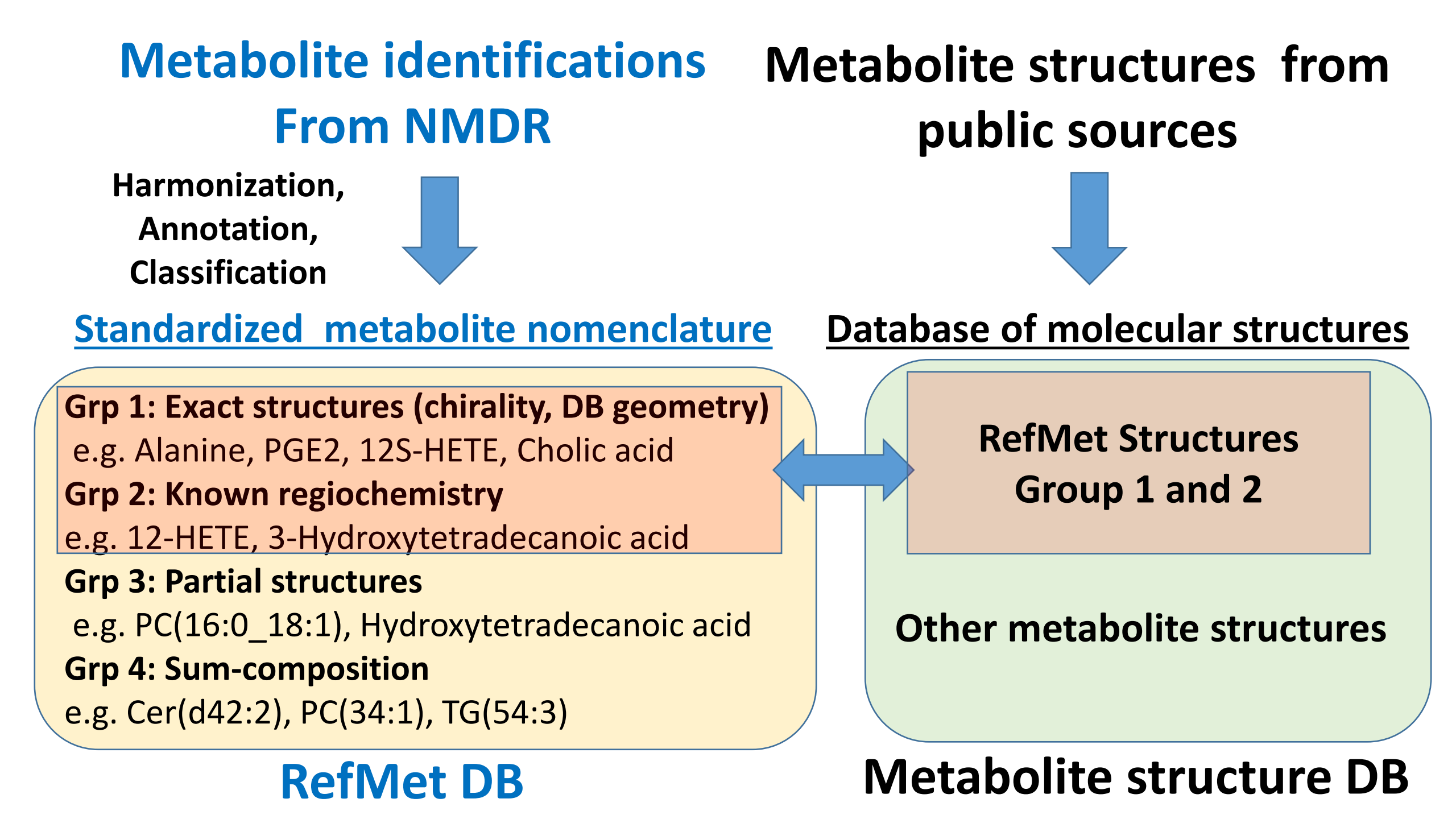
Comments Information on structural features, but complete regiochemistry unknown

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

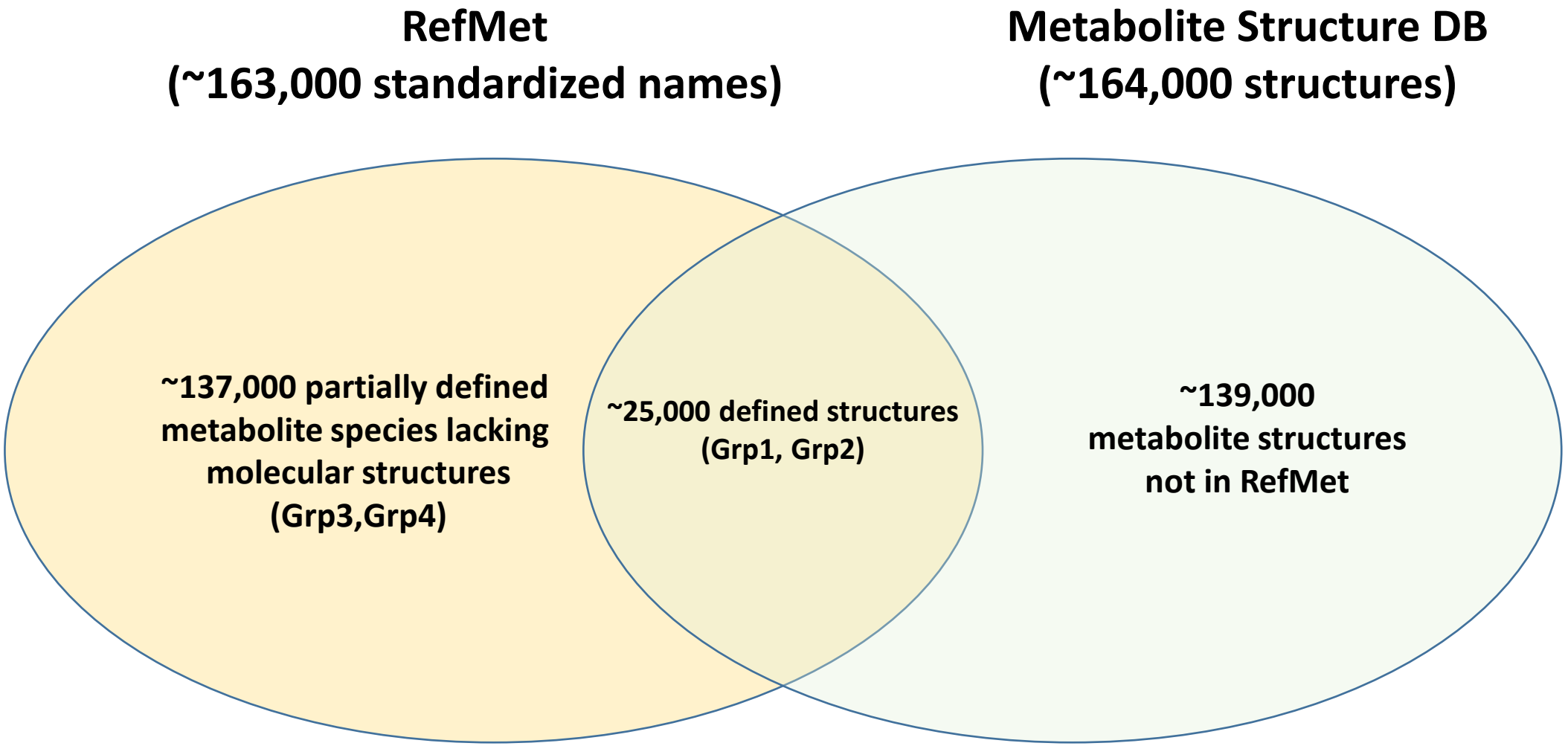
Level 4: Species level

Comments Metabolite class, number of chain carbons and unsaturations known

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


Metabolite identifications
From NMDR
Metabolite structures from public sources
Harmonization,
Annotation,
Classification
Standardized metabolite nomenclature
Database of molecular structures
Grp 1: Exact structures (chirality, DB geometry)
e.g. Alanine, PGE2, 12S-HETE, Cholic acid
Grp 2: Known regiochemistry
e.g. 12-HETE, 3-Hydroxytetradecanoic acid
Grp 3: Partial structures
e.g. PC(16:0_18:1), Hydroxytetradecanoic acid
Grp 4: Sum-composition
e.g. Cer(d42:2), PC(34:1), TG(54:3)
RefMet Structures
Group 1 and 2
Other metabolite structures
RefMet DB
Metabolite structure DB

Relationship between RefMet and Metabolite Structure DB



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

9Z-palmitoleic acid Cis-9-palmitoleic acid cis-9-Palmitoleic acid cis-9-Palmitoleic acid TOTAL FFA(16:1n-7) palmitoleic acid PALMITOLEIC ACID palmitoleic acid	Palmitoleic acid
AC(8:0) Acylcarnitine C8:0 Acylcarnitine(C8:0) C8, Octanoylcarnitine C8:0 acylcarnitine Octanoylcarnitine OCTANOYLCARNITINE Octanoyl-L-carnitine	CAR 8:0
alpha-glucose beta-glucose D-Glucose glucose	Glucose
PC(p-38:2) or PC(o-38:3) PC(p-38:3) or PC(o-38:4) A PC(p-38:3)/PC(o-38:4)	PC P-38:3 or PC O-38:4
C24 Ceramide C24-Cer Cer(d18:1/24:0)	Cer 18:1;O2/24:0
GPEtn 16:0_18:2 PE(16:0_18:2)	PE 16:0_18:2

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

RefMet: A Reference list of Metabolite names

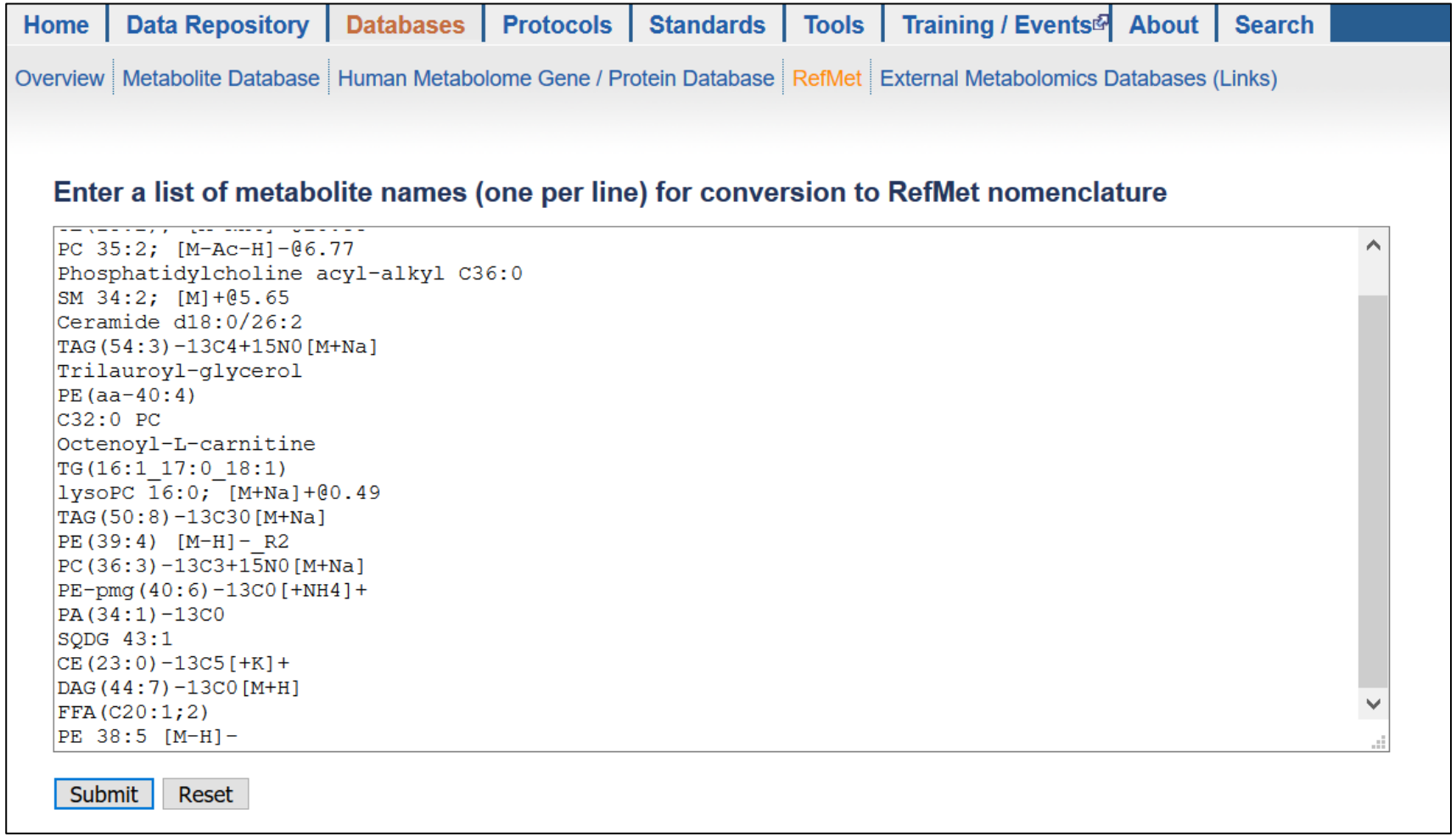
The main objective of RefMet is to provide a standardized reference nomenclature for both discrete metabolite structures and metabolite species identified by spectroscopic techniques in metabolomics experiments. **This is an essential prerequisite for the ability to compare and contrast metabolite data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

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

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

Convert a list of metabolite names to RefMet nomenclature

- Browse/Search/Download Refmet
- Convert(map) a list of metabolite names to RefMet nomenclature
- Help on RefMet
- Lipid Notation in RefMet and lipid m/z calculation tools



Metabolite name-to-RefMet conversion results

Return to RefMet conversion form

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

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

RefMet Search Page

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

- Browse/Search/Download Refmet
- Convert(map) a list of metabolite names to RefMet nomenc
- Help on RefMet
- Lipid Notation in RefMet and lipid m/z calculation tools

RefMet: A Reference set of Metabolite names

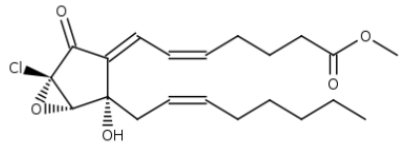
(A total of 154667 compounds or isobaric mixtures as of 04/23/21)

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

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

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

Metabolite name | *MONA MS spectra*	PubChem CID	Super class	Main class	Sub class	Formula	Exact mass
10,11-DiHDPE	16061145	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{34}O_4$	362.2457
10,11-Dihydro-12-oxo-Resolvin E1	53477458	Fatty Acyls	Eicosanoids	HETE	$C_{20}H_{30}O_5$	350.2093
10,11-Dihydro-Re			Eicosanoids	HETE	$C_{20}H_{32}O_5$	352.2250
10,11-Dimethoxyt			Harmala alkaloids	Harmala alkaloids	$C_{29}H_{37}N_3O_2$	459.2886
10(11)-EpDPE			Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10,11-Epoxy-chlo			Eicosanoids	Clavulones	$C_{21}H_{29}ClO_5$	396.1704
10,12,15-Octadec			Fatty acids	Unsaturated FA	$C_{18}H_{30}O_2$	278.2246
10,22-Dimethyldo			Hydrocarbons	Hydrocarbons	$C_{34}H_{70}$	478.5478
10-Deacetyl-2-debenzoylbaccatin III	445489	Prenol Lipids	Isoprenoids	Taxanes	$C_{22}H_{32}O_9$	440.2046
10-Deoxymethymycin	5282032	Polyketides	Macrolides and analogues	Macrolides	$C_{25}H_{43}NO_6$	453.3090
10-Deoxymethynolide	5282031	Polyketides	Macrolides and analogues	Macrolides	$C_{17}H_{28}O_4$	296.1988
10-HDoHE | *MS spectra*	11537494	Fatty Acyls	Docosanoids	Docosanoids	$C_{22}H_{32}O_3$	344.2351
10-Hendecenoic acid	5634	Fatty Acyls	Fatty acids	Unsaturated FA	$C_{11}H_{20}O_2$	184.1463
10-HpODE	5282857	Fatty Acyls	Octadecanoids	HpODEs	$C_{18}H_{32}O_4$	312.2301
10-HpOME	13801082	Fatty Acyls	Octadecanoids	HpOMEs	$C_{18}H_{34}O_4$	314.2457



10,11-Epoxy-chlorovulone I

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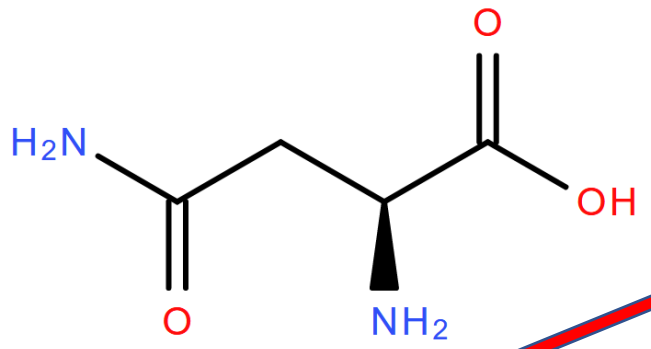
RefMet detail page for Asparagine

RefMet Compound Details



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

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

Calculate m/z for a MS adduct of asparagine

View other metabolites with this formula

View enantiomers/diastereomers (if any)

View biochemical reactions involving asparagine

Table of KEGG reactions in human pathways involving Asparagine

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

Table of KEGG human pathways containing Asparagine

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

RefMet/Metabolite databases have links to MONA MS spectra

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

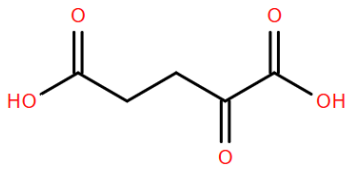
RefMet database

InChIKey: Mol. Formula

Name: Contains oxoglutaric acid Super class(2)

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

Metabolite database



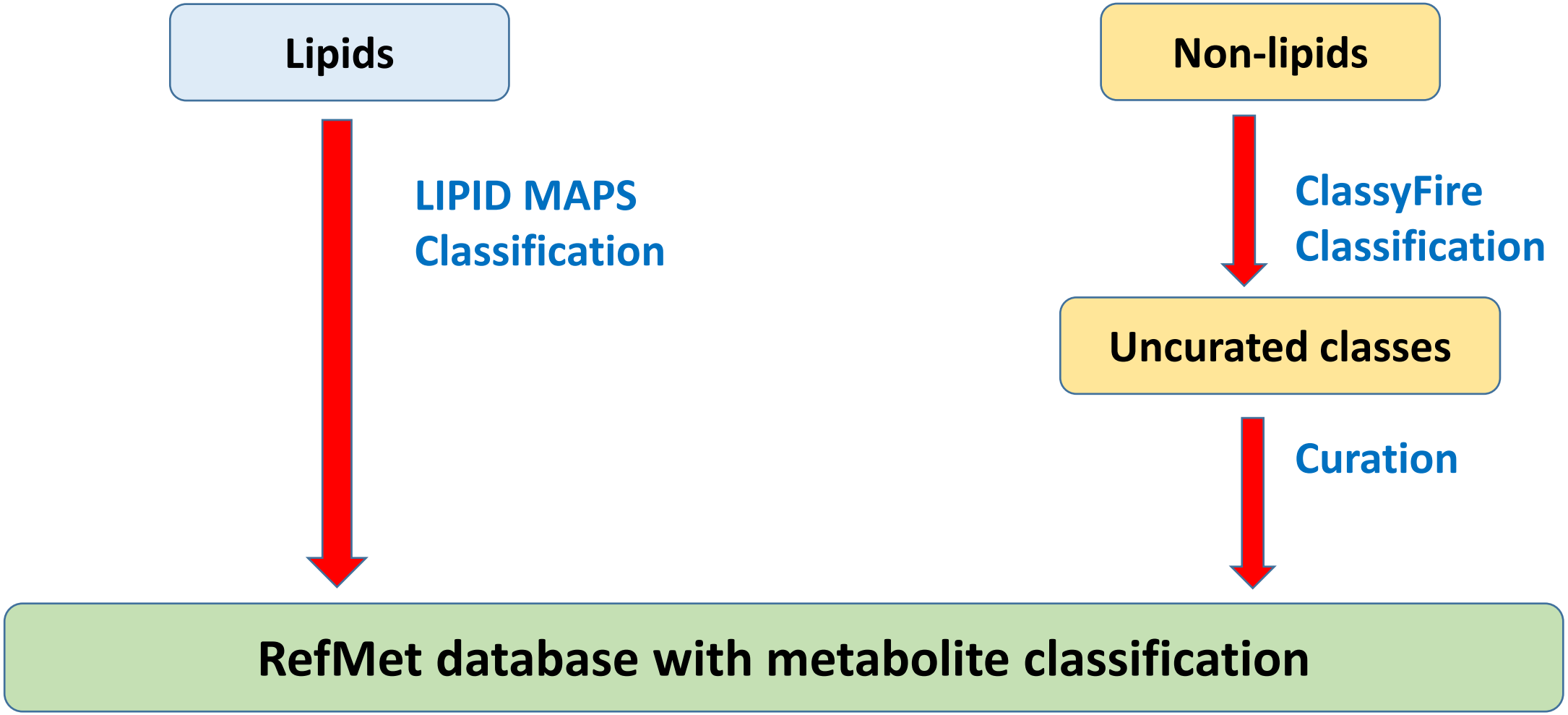
MW REGNO:	37135
PubChem CID:	51
Common Name:	Oxoglutaric acid
Systematic Name:	2-oxopentanedioic acid
Synonyms:	alpha-ketoglutaric acid; alpha-ketoglutarate; Oxoglutarate [PubChem Synonyms]
Exact Mass:	146.0215 (neutral) Calculate m/z: (Select m/z)
Formula:	$C_5H_6O_5$
InChIKey:	KPGXRSRHYNQIFN-UHFFFAOYSA-N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

MONA MS database records for REGNO 37135

Massbank ID	Metabolite	Instrument	Inst. type	MS type	Collision energy	Ion type	Ion mode	MS level
FiehnLib000378	Oxoglutaric acid	Leco Pegasus IV	-	EI	-	-	Positive	MS1
KZ000080	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	MS1
OUF00113	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	MS1
PR010210	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	MS1
HMDB00208_1231	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	-
HMDB00208_1263	Oxoglutaric acid	Pegasus III TOF-MS system, Lec...	-	EI	-	-	Positive	-
KO001528	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	10 V	[M-H]-	Negative	MS2
KO001529	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	20 V	[M-H]-	Negative	MS2
KO001530	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	30 V	[M-H]-	Negative	MS2
KO001531	Oxoglutaric acid	API3000, Applied Biosystems	LC-ESI-QQ	ESI	40 V	[M-H]-	Negative	MS2
KNA00530	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS1
KNA00700	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS1
KNA00531	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
KNA00533	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
KNA00701	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
KNA00702	Oxoglutaric acid	LTQ Orbitrap XL, Thermo Scient...	LC-ESI-ITFT	ESI	35eV	-	Negative	MS2
PS037807	Oxoglutaric acid	TQD, Waters	-	ESI	10	-	-	-
HMDB00208_337	Oxoglutaric acid	TQD, Waters	Quattro_QQQ	ESI	10eV	-	Negative	-
HMDB00208_338	Oxoglutaric acid	TQD, Waters	Quattro_QQQ	ESI	25eV	-	Negative	-
HMDB00208_339	Oxoglutaric acid	TQD, Waters	Quattro_QQQ	ESI	40eV	-	Negative	-
HMDB00208_998	Oxoglutaric acid	TQD, Waters	-	-	-	-	-	-

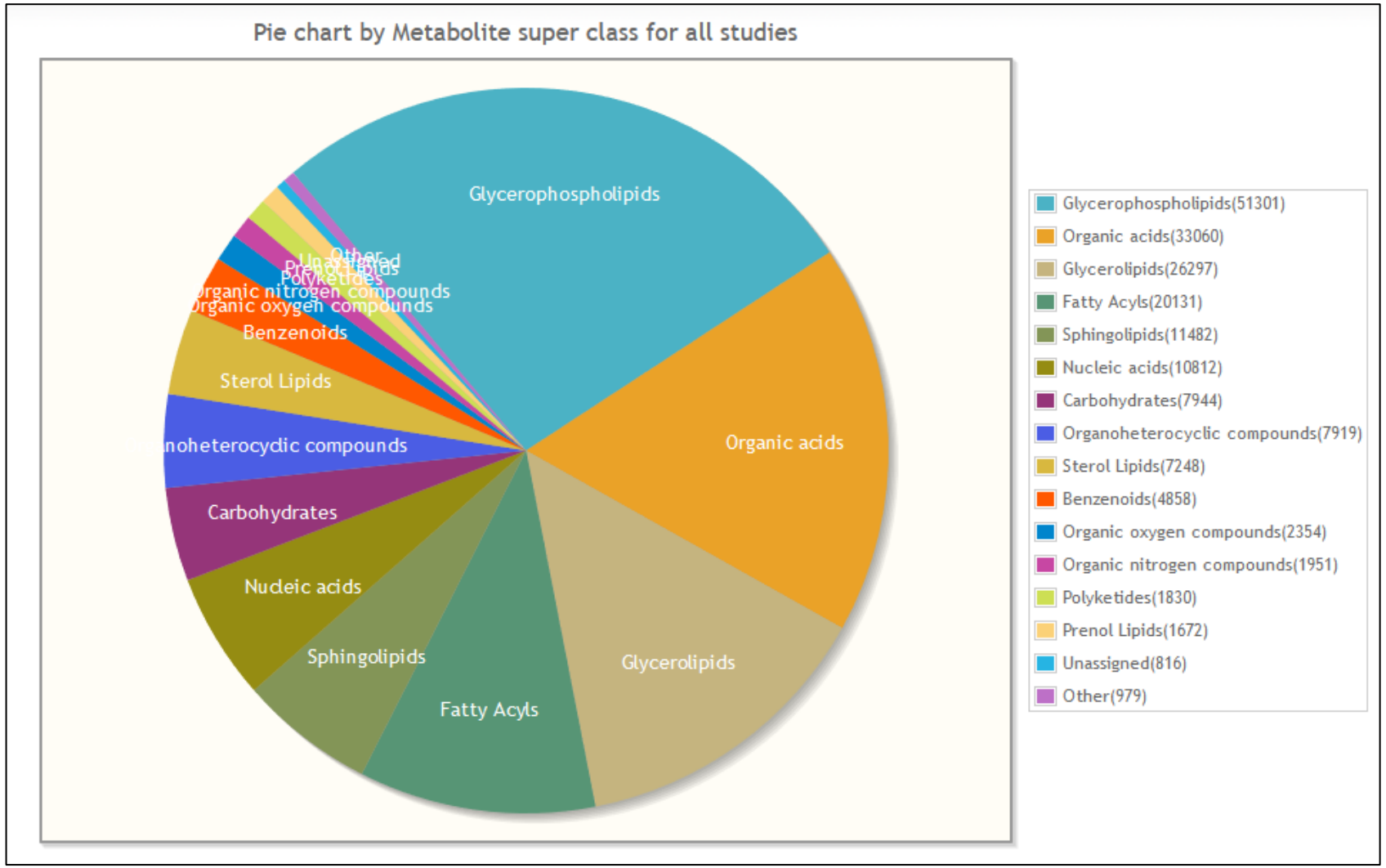
Listing of MONA spectra for metabolite

RefMet Metabolite Classification



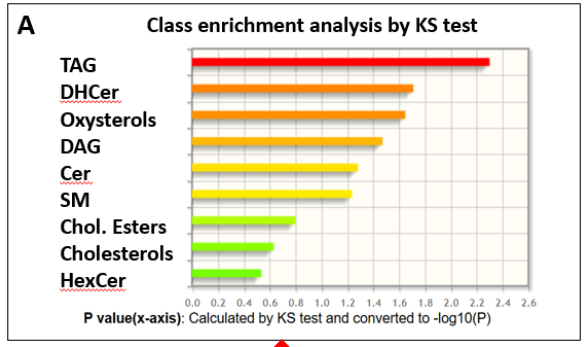
RefMet classification at superclass, main class and sub class levels available for each study in Analysis Toolbox

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



Central role of RefMet on the Metabolomics Workbench

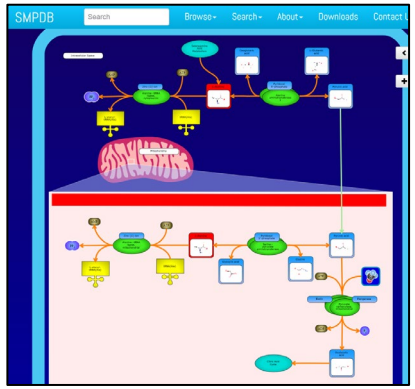
Statistical/graphical analysis



Metabolites detected in NMDR studies

Compare/contrast studies

Biochemical pathways



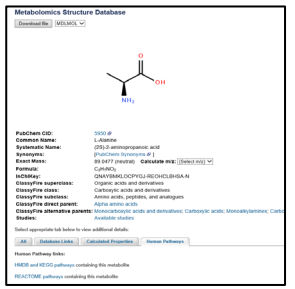
Metabolite classification

RefMet (standardized names)

Summary reports/statistics

MW metabolite structure database

Structure details



External datasharing via REST services and other portals

RefMet: What are the positive outcomes?

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

Ability to perform comparative analysis across metabolomics studies.

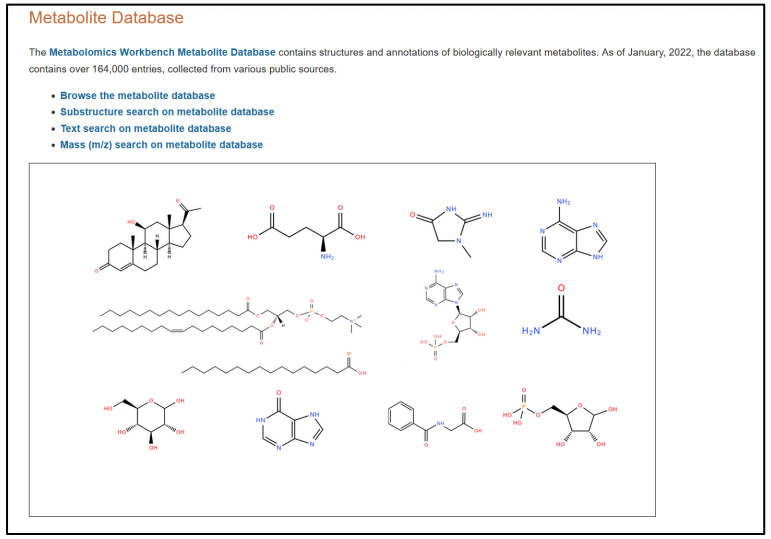
Exact structures are linked to metabolite structure database.

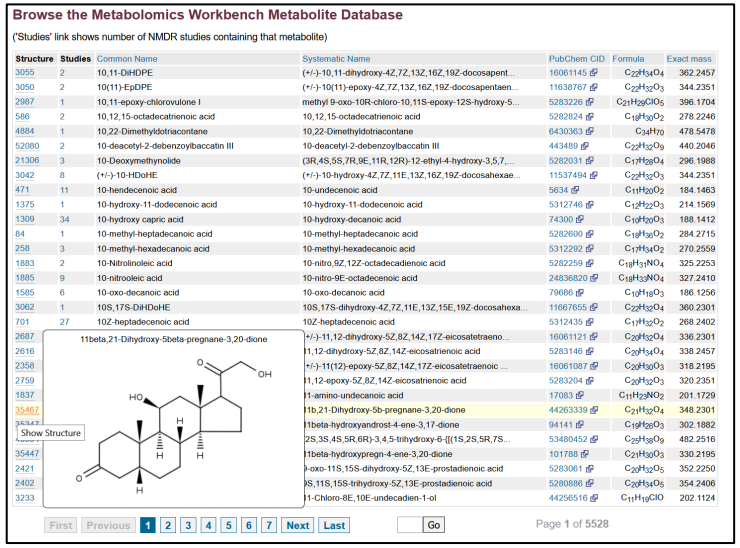
Comprehensive chemical classification provides numerous advantages for data visualization/statistical analysis.

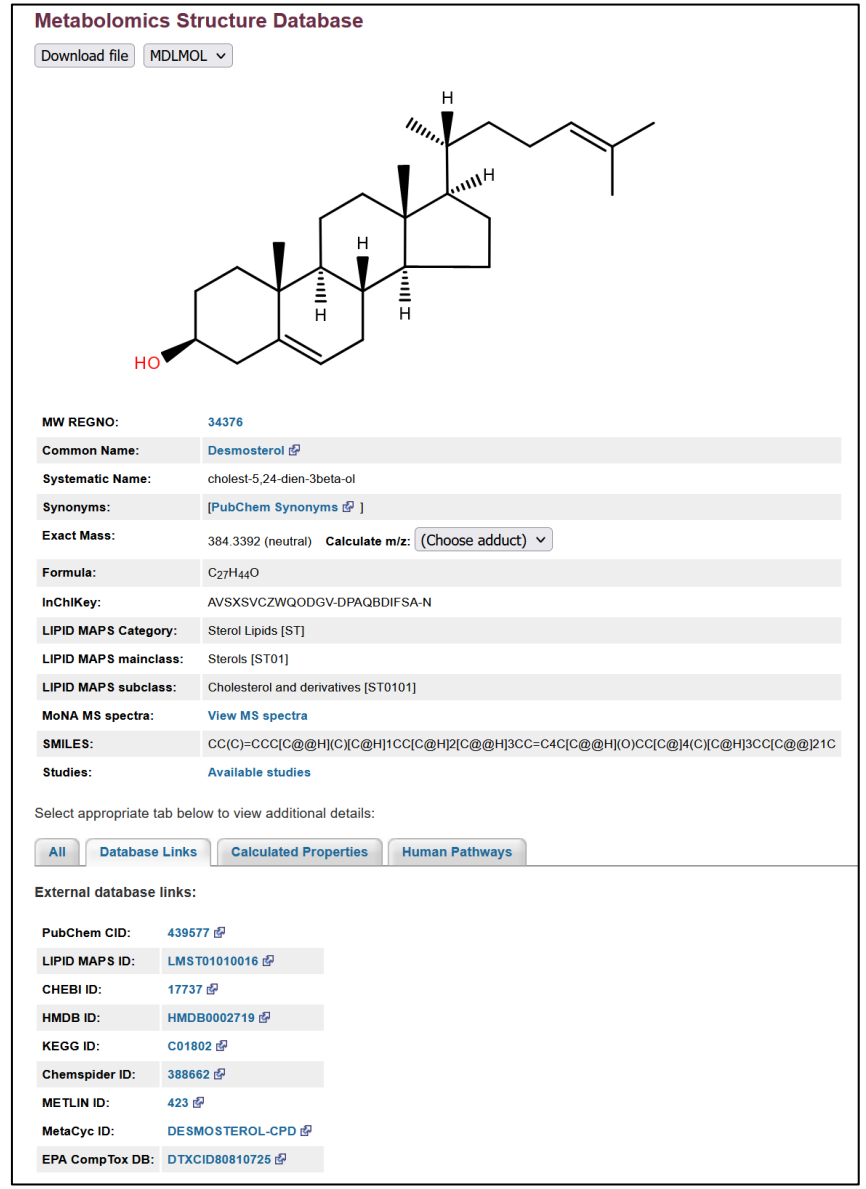
Integration with biochemical pathway tools enables mapping of RefMet names via systems biology approaches.

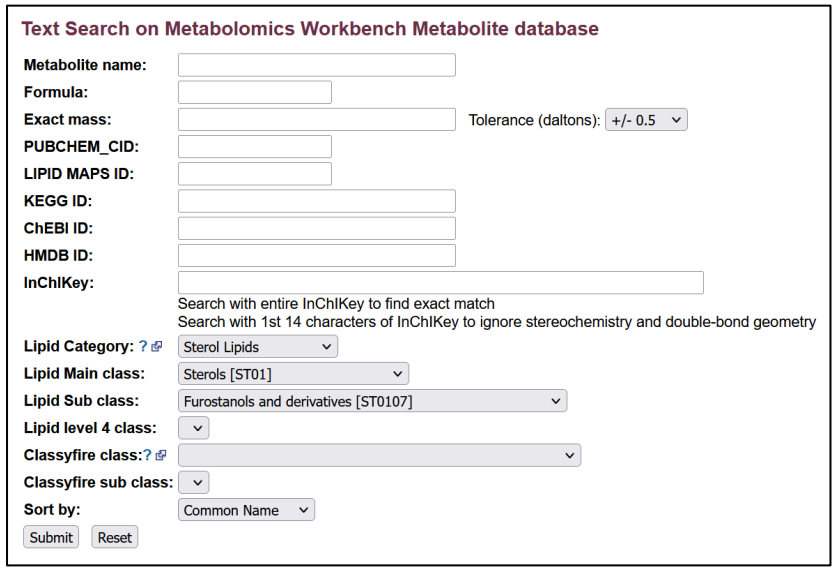
Metabolomics Workbench Metabolite structure database

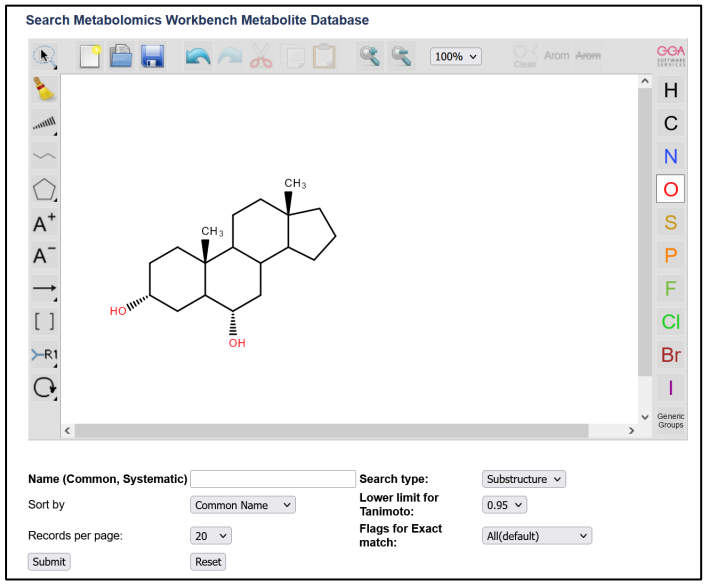
~164,000 metabolite structures and annotations Linked to NMDR studies via RefMet











Browse the Metabolomics Workbench Metabolite structure database

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

Click on “Studies” link to access studies reporting that metabolite

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

List of Studies (Metabolite:10-Hydroxydecanoic acid)

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

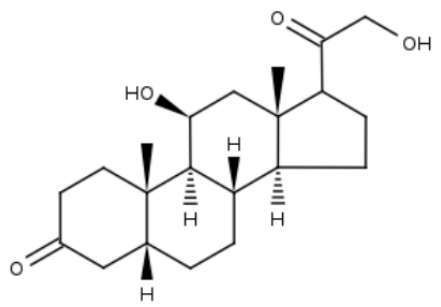
Click on “Structure” link to access metabolite detail page

Browse the Metabolomics Workbench Metabolite Database

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

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

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



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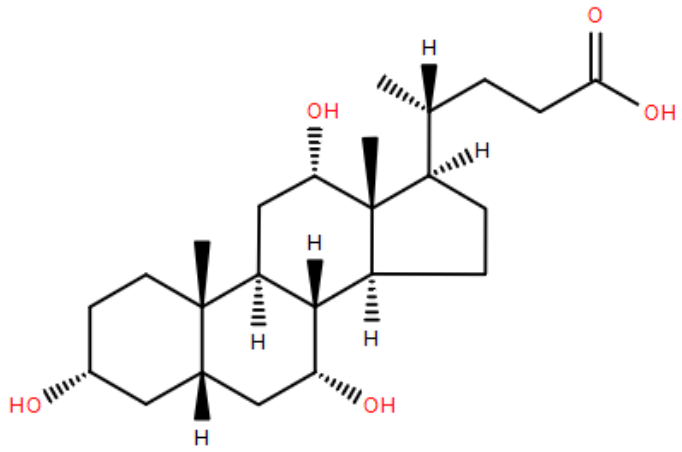
Metabolite Database : Molecule Detail View

Metabolomics Structure Database

Download file | MDLMOL



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

All | Database Links | Calculated Properties | Human Pathways

External database links:

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

All | Database Links | Calculated Properties | Human Pathways

Human Pathway links:

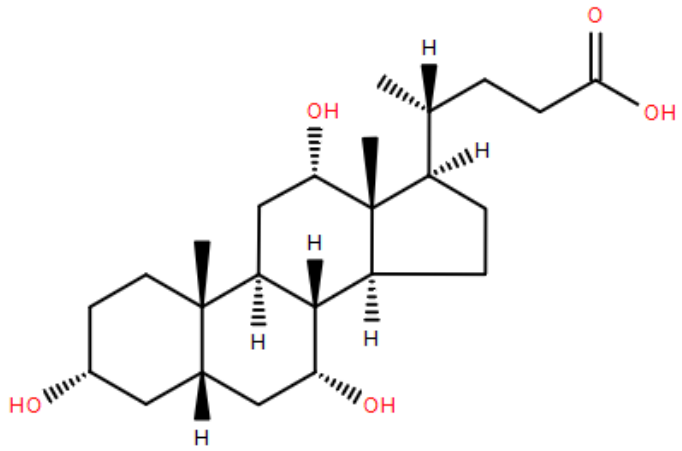
HMDB and KEGG pathways containing this metabolite

REACTOME pathways containing this metabolite

Metabolite Database : View MoNA MS spectra

Metabolomics Structure Database

Download file | MDLMOL



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

MoNA MS database records for Cholic acid

Massbank ID	Instrument	Inst. type	MS type	Collision energy	Ion type	Ion mode	MS level
NU000191	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000192	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000193	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000194	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
NU000195	JMS-T100LP, JEOL Ltd.	LC-ESI-TOF	ESI	-	[M-H]-	negative	MS1
UF415353	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	35 (nominal)	[M-H]-	negative	MS2
UF422953	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	35 (nominal)	[M-H]-	negative	MS2
UF41[illegible]	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF41535[illegible]	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF422951	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF422954	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	55 (nominal)	[M-H]-	negative	MS2
UF415352	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	80 (nominal)	[M-H]-	negative	MS2
UF422952	LTQ Orbitrap XL Thermo Scienti...	LC-ESI-ITFT	ESI	80 (nominal)	[M-H]-	negative	MS2
MT000010	[illegible]TQ XL, Thermo Finnigan	LC-ESI-IT	ESI	40	[M-H]-	negative	MS2
PT206683	[illegible]f Premier, Waters	LC-Q-TOF/MS	ESI	30 V	[M-H]-	negative	MS2
PT206680	[illegible]remier, Waters	LC-Q-TOF/MS	ESI	Ramp 5-45 V	[M-H]-	negative	MS2
PS066807	TQD, [illegible]	Flow-injection QqQ/MS	ESI	10	[M-H]-	negative	MS2
PS066808	TQD, Wa[illegible]	Flow-injection QqQ/MS	ESI	20	[M-H]-	negative	MS2
PS066809	TQD, Waters	Flow-injection QqQ/MS	ESI	30	[M-H]-	negative	MS2
PS066810	TQD, Waters	Flow-injection QqQ/MS	ESI	40	[M-H]-	negative	MS2
PS066811	TQD, Waters	Flow-injection QqQ/MS	ESI	50	[M-H]-	negative	MS2
PS066801	TQD, Waters	Flow-injection QqQ/MS	ESI	10	[M+H]+	positive	MS2
PS066802	TQD, Waters	Flow-injection QqQ/MS	ESI	20	[M+H]+	positive	MS2
PS066803	TQD, Waters	[illegible]w-injection QqQ/MS	ESI	30	[M+H]+	positive	MS2
PS066804	TQD, Waters	[illegible]ection QqQ/MS	ESI	40	[M+H]+	positive	MS2
PR100738	UPLC Q-Tof Premier, Waters	LC-[illegible]TOF	ESI	30 V	[M-H]-	negative	MS2
PR100737	UPLC Q-Tof Premier, Wate[illegible]						
BML00989	Agilent 1200 RRLC; Agilent						
BML00997	Agilent 1200 RRLC; Agilent						
BML01005	Agilent 1200 RRLC; Agilent						
BML80931	Agilent 1200 RRLC; Agilent						
BML80933	Agilent 1200 RRLC; Agilent						
BML00963	Agilent 1200 RRLC; Agilent						
BML00972	Agilent 1200 RRLC; Agilent						
BML80930	Agilent 1200 RRLC; Agilent						
VF-NPL-QTOF003408	Agilent 6530 Q-TOF						
VF-NPL-QTOF[illegible]	Agilent 6530 Q-TOF						
VF-NPL-QTO[illegible]	Agilent 6530 Q-TOF						
VF-NPL-[illegible]	Agilent 6530 Q-TOF						

Spectrum UF415353 for Cholic acid

CLEAN

Rating: ★★★★★

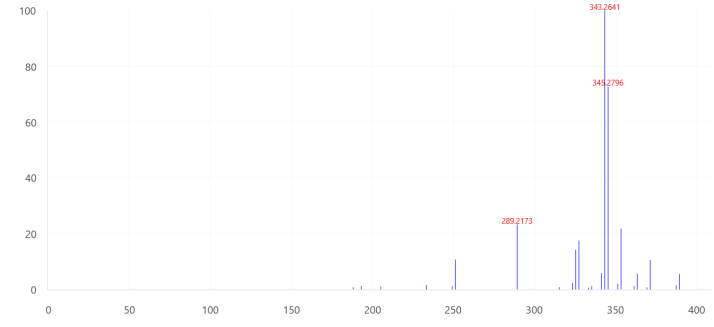
Originally submitted to the MassBank High Quality Mass Spectral Database

MassBank | LC-MS

SPLASH: splash10-0007-0019000000-285d3d0d87f5471b419a

Submitter: Tobias Schulze

Mass Spectrum



Ion Table / Peak Table

Text search on the Metabolomics Workbench Metabolite structure database

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

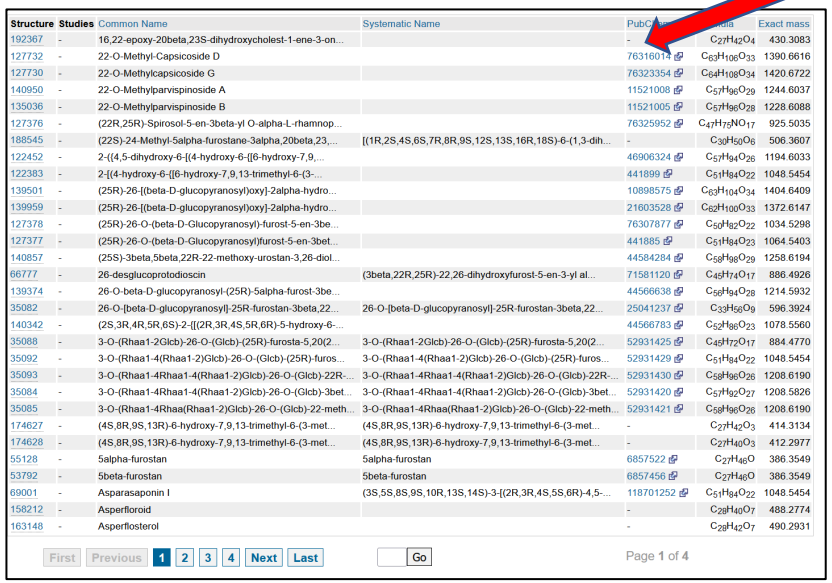
Text Search on Metabolomics Workbench Metabolite database

Metabolite name:
Formula:
Exact mass: Tolerance (daltons): +/- 0.5
PUBCHEM_CID:
LIPID MAPS ID:
KEGG ID:
ChEBI ID:
HMDB ID:
InChIKey:

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

Lipid Category: ? Sterol Lipids
Lipid Main class: Sterols [ST01]
Lipid Sub class: Furostanols and derivatives [ST0107]
Lipid level 4 class:
Classyfire class:?
Classyfire sub class:
Sort by: Common Name

Submit Reset



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

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Lipid classification example

Text search on the Metabolomics Workbench Metabolite structure database

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

Text Search on Metabolomics Workbench Metabolite database

Metabolite name:
Formula:
Exact mass: Tolerance (daltons): +/- 0.5
PUBCHEM_CID:
LIPID MAPS ID:
KEGG ID:
ChEBI ID:
HMDB ID:
InChIKey: BHQCQFFYRZLCQQ

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

Lipid Category: ?
Lipid Main class:
Lipid Sub class:
Lipid level 4 class:
Classyfire class:?
Classyfire sub class:
Sort by: Common Name

Submit Reset

Database search results for " BHQCQFFYRZLCQQ "

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

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

Text search on the Metabolomics Workbench Metabolite structure database

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

Text Search on Metabolomics Workbench Metabolite database

Metabolite name: cholic

Formula:

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

PUBCHEM_CID:

LIPID MAPS ID:

KEGG ID:

ChEBI ID:

HMDB ID:

InChIKey:

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

Lipid Category: ?

Lipid Main class:

Lipid Sub class:

Lipid level 4 class:

Classyfire class:?

Classyfire sub class:

Sort by: Common Name

Submit Reset

Database search results for " CHOLIC "

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

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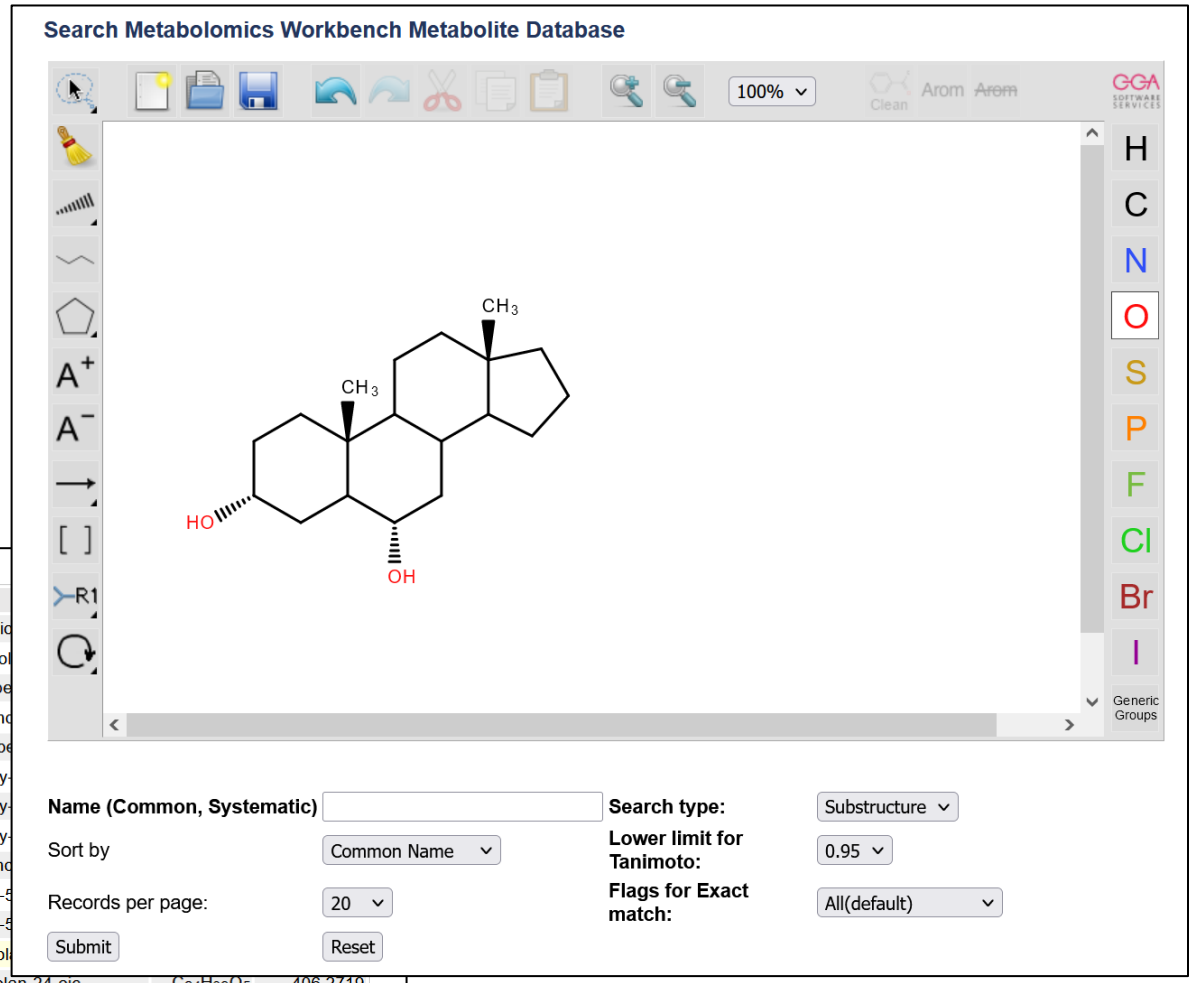
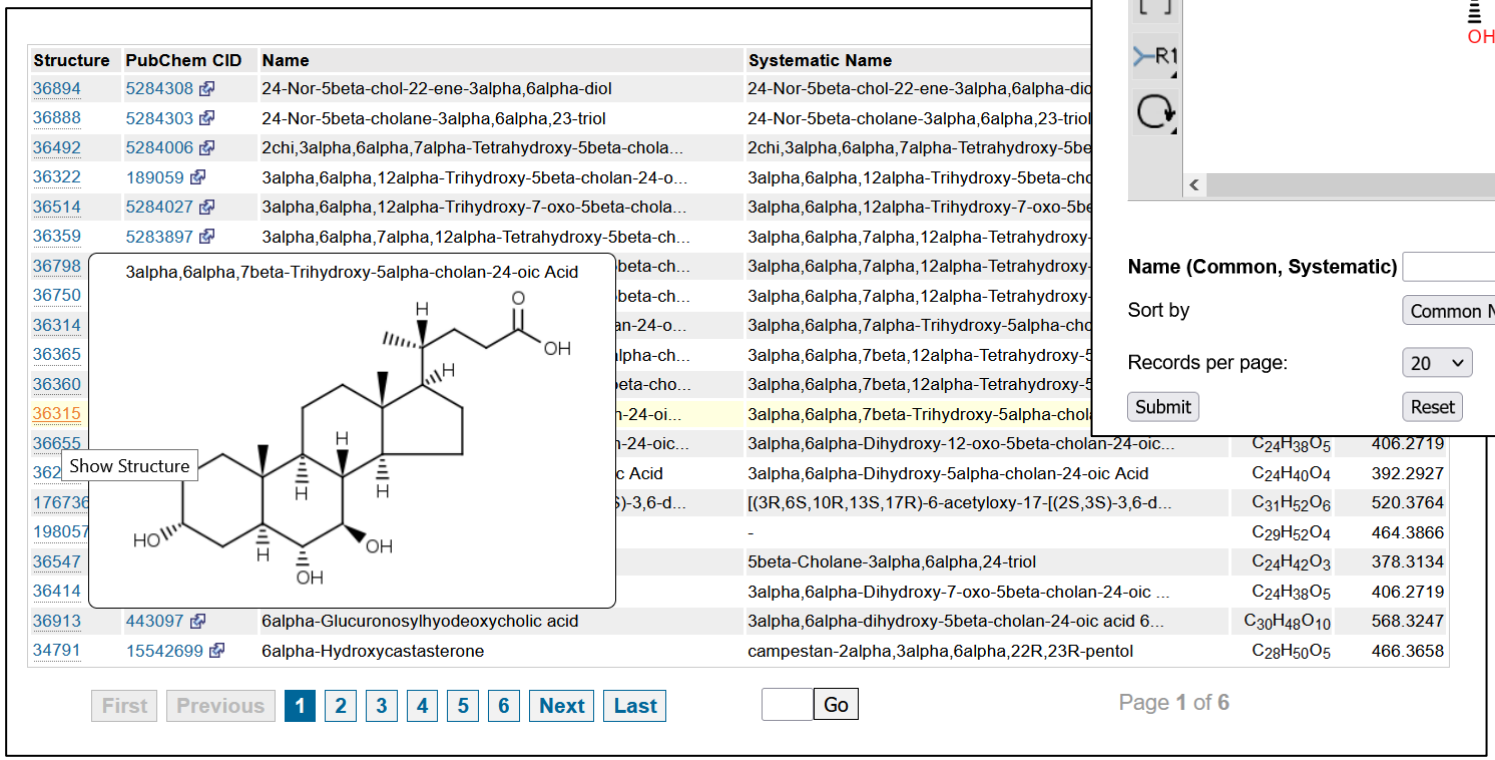
Metabolite name example

Structure search on Metabolomics Workbench Metabolite structure database

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





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

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

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

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

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

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

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

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

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

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

Ion adducts (choose at least one with appropriate polarity)

Positive mode:

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

Negative mode:

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

Neutral:

☐ Neutral

Lipid even chains only ☐

Sort by Delta

Submit Reset

List of precursor ions :

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

Or upload a peaklist file

Browse... No file selected.

Metabolomics Workbench Data Portal: Studies

Default sorting order is by most recently released study

Browse and Search Studies

- **Browse**
  - Summary of all studies
  - Summary of all projects (groups of studies)
  - Bubble plots of studies by disease, sample source, species, pathway and metabolite class
  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)
- **Search**
  - Experimental Projects / Studies
  - MetStat: Perform meta-analysis on named metabolites across all studies:
    Refine by analysis type, species, sample source, disease association, metabolite classification and biochemi
  - Select Studies by species, sample source or disease association
  - Search data/metadata in experimental projects/studies
  - Search Untargeted MS data by m/z, retention time, instrumentation
  - REST service
  - Use the Metabolomics Workbench REST service to retrieve different types of data

Summary of all studies

Click the Study ID to access detailed study information; download the mwTab (metadata and processed data) text file; and access the Statistics Toolbox for that study. Please refer to our **Data:FAQ** and **About:How to Cite** pages for information regarding how to cite the Metabolomics Workbench and datasets that you have uploaded or downloaded.

Showing page 1 of 35 **Results:** 1 2 3 4 5 Next Last Showing results 1 to 50 of 1726 (#: Contains untargeted data) Results per page: 50

Study ID	Study Title	Species	Institute	Analysis	Released	Version	Samples	Download (* : Contains raw data)
ST002058	Muscle/Lung/Tumor metabolomics	Mus musculus	University of Colorado Anschutz Medical Campus	LC-MS	2022-02-14	1	32	Uploaded data (267.1M)* (Data format:mzXML)
ST002059	4T1 and SkM cells	Homo sapiens	University of Colorado Anschutz Medical Campus	LC-MS	2022-02-14	1	12	Uploaded data (65.5M)* (Data format:mzXML)
ST002067	Time-Resolved Metabolomics of a Mouse Model of Ovarian High-Grade Serous Carcinoma (LC-MS)	Mus musculus	Georgia Institute of Technology	LC-MS*	2022-02-14	1	356	Uploaded data (143.9G)* (Data format:raw(Thermo))
ST002068	Mutant CHCHD10 causes an extensive metabolic rewiring that precedes OXPHOS dysfunction in a murine model of mitochondrial cardiomyopathy	Mus musculus	Weill Cornell Medicine	LC-MS	2022-02-14	1	32	Uploaded data (609M)* (Data format:mzXML)
ST002070	Lipidomic Comparison of 2D and 3D Colon Cancer Cell Culture Models	Homo sapiens	The Ohio State University	LC-MS	2022-02-14	1	59	Uploaded data (17.1G)* (Data format:d)
ST002071	Metabolic profiling of mouse CD27+ and CD27- gammadelta T cells	Mus musculus	University of Louisville	LC-MS	2022-02-14	1	11	Uploaded data (1.2G)* (Data format:raw(Thermo))
ST002044	An observational study of cardiovascular patients in India	Homo sapiens	Translational Health Science And Technology Institute (THSTI)	LC-MS*	2022-02-08	1	286	Uploaded data (10.8G)* (Data format:mzML)
ST001950	Lipidome Alterations Following Mild Traumatic Brain Injury.	Rattus norvegicus	Georgia Institute of Technology	LC-MS	2022-02-07	1	114	Uploaded data (24.7G)* (Data format:mzML)
ST002060	Pollen metabolomics using Arabidopsis thaliana: Comparison of pollen at mature, hydration and germination stage	Arabidopsis thaliana	University of Illinois, Urbana-Champaign	LC-MS*	2022-02-07	1	72	Uploaded data (1.2G)* (Data format:mzML)
ST002061	Glutamine flux in macrophages treated with stable-isotope labeled analog 4 mM (U-13C5) glutamine	Mus musculus	Shanghai Jiao Tong University affiliated Renji Hospital	LC-MS	2022-02-07	1	16	Uploaded data (251.3M)* (Data format:mzXML)
ST001926	Modular evolution of the Drosophila metabolome	Drosophila melanogaster	University of Washington	LC-MS*	2022-02-02	1	261	Uploaded data (5.2G)* (Data format:mzXML)
ST002019	TIPs Metabolomics (blood)	Homo sapiens	Vanderbilt University Medical Center	MS	2022-02-02	1	70	Not available
ST002064	Metabolic impact of anticancer drugs Pd2Spermine and Cisplatin on the polar extracts of brain from healthy mice (part 1)	Mus musculus	University of Aveiro	NMR*	2022-02-02	1	44	Not available
ST002065	Metabolic impact of anticancer drugs Pd2Spermine and Cisplatin on the nonpolar extracts of brain from healthy mice (part 2)	Mus musculus	University of Aveiro	NMR*	2022-02-02	1	44	Not available
ST002056	Integrated Multilayer Omics Reveals the Genomic, Proteomic and Metabolic Influences of the Histidyl Dipeptides on Heart	Mus musculus	University of Louisville	GC-MS	2022-01-31	1	8	Not available
ST002062	Endophytic bacteria are key players in the modulation of the secondary metabolome of Lithospermum officinale L.	Lithospermum officinale	Aristotle University of Thessaloniki	LC-MS*	2022-01-31	1	45	Uploaded data (1.6G)* (Data format:raw(Thermo))
ST001680	Metabolome of NAFLD in high fat diet mouse model	Mus musculus	Weill Cornell Medicine	LC-MS	2022-01-27	1	96	Uploaded data (40.3G)* (Data format:d)
ST001713	Effects of different planting densities on the metabolism of Panax notoginseng	Panax notoginseng	Yunnan Agricultural University	GC-MS*	2022-01-25	1	20	Uploaded data (469.4M)* (Data format:d)
ST002057	Distinct Human Hepatocyte Lipidomics Profiles for Nonalcoholic Steatohepatitis and In Vitro-Induced Steatosis	Homo sapiens	Monash Institute of Pharmaceutical Sciences	LC-MS	2022-01-25	1	103	Uploaded data (18.5G)* (Data format:raw(Thermo))

Metabolomics Workbench Data Portal:Projects

Studies may be grouped into projects (studies with same theme/objective)

Browse and Search Studies

- **Browse**
  - Summary of all studies
  - Summary of all projects (groups of studies)
  - Bubble plots of studies by disease, sample source, species, pathway and metabolite class
  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)

Summary of all projects

Showing page 3 of 25 **Results:** Previous 1 2 **3** 4 5 Next Last Showing results 101 to 150 of 1224 (#: Contains untargeted data) Results per page: 50

Project ID	Project Title	Institute(Experimental)	Institute(Analysis)	Number Of Studies
PR001299	Reduced ER-mitochondria connectivity promotes neuroblastoma multidrug resistance	Columbia University - Medical Center	Columbia University	1
PR001297	In vitro maturation of Toxoplasma gondii bradyzoites in human myotubes and their metabolomic characterization	Robert Koch-Institut	Robert Koch-Institut	1
PR001297	In vitro maturation of Toxoplasma gondii bradyzoites in human myotubes and their metabolomic characterization	Robert Koch-Institut	Robert Koch-Institute	1
PR001294	Lyso-lipid induced oligodendrocytes maturation underlie restoration of optic nerve function	University of Miami	University of Miami	1
PR001292	massNet: integrated processing and classification of spatially resolved mass spectrometry data using deep learning for rapid tumor delineation	Brigham and Women's Hospital	Brigham and Women's Hospital	1
PR001291	An observational study of cardiovascular patients in India	Translational Health Science And Technology Institute (THSTI)	Translational Health Science And Technology Institute (THSTI)	1
PR001290	Maternal Hypoxemia and Oxidative Stress	LOMA LINDA UNIVERSITY	Loma Linda University School of Medicine	1
PR001288	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs	University of Colorado Anschutz Medical Campus	University of Colorado Anschutz Medical Campus	11
PR001284	A Sentinel Serum Quality Management Program for NMR Metabolomics	University of Michigan	University of Michigan	1

Summary of all studies in project PR001288

Study ID	Study Title	Species	Institute	Analysis (* : Contains Untargted data)	Release Date	Version	Samples	Download (* : Contains raw data)
ST002031	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Whole blood)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (4.1G)*
ST002032	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Blood plasma)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (4.2G)*
ST002033	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Prestool)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	57	Uploaded data (4.4G)*
ST002034	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Poststool)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (4.6G)*
ST002035	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Heart)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (3.9G)*
ST002036	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Kidney)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (4G)*
ST002037	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Liver)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (4.9G)*
ST002038	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Duodenum)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (4.9G)*
ST002039	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Brain)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (3.9G)*
ST002040	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Colon)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	57	Uploaded data (3.9G)*
ST002041	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs (Spleen)	Mus musculus	University of Colorado Anschutz Medical Campus	MS	2022-01-21	1	58	Uploaded data (3.9G)*

NMDR:Study-level view contains multiple metadata sections

Summary of study ST001140

This data is available at the NIH Common Fund's National Metabolomics Data Repository (NMDR) website, the Metabolomics Workbench, https://www.metabolomicsworkbench.org, where it has been assigned Project ID PR000761. The data can be accessed directly via it's Project DOI: 10.21228/M89Q32
This work is supported by NIH grant, U2C- DK119886. See: https://www.metabolomicsworkbench.org/about/howtocite.php

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download mwTab file (text) | Download mwTab file(JSON) | Download data (Contains raw data)

Study ID	ST001140
Study Title	Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure
Study Summary	Glucocorticoids (GCs) are widely used in veterinary and human medicine. Chromic endogenous or iatrogenic GC overexposure impairs metabolic function and can result in diverse side-effects, including Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess (induced by prednisolone and tetracosactide, respectively) on the plasma lipidome of Beale dogs. Both, long- and short-term GC resulted in significant changes of the plasma lipidome.
Institute	National University of Singapore;University of Zurich
Department	Singapore Lipidomics Incubator (SLING);Vetsuisse Faculty, University of Zurich
Laboratory	Singapore Lipidomics Incubator (SLING), National University of Singapore

Select appropriate tab below to view additional metadata details:

All | Project | Subject | Study Design | Collection | Treatment | Sample Preparation | Chromatography | Analysis | MS

← View Metadata

Example: Analysis section

Combined analysis:

Analysis ID	AN001870	AN001871	AN001872	AN001873
Analysis type	MS	MS	MS	MS
Chromatography type	Reversed phase	Reversed phase	HILIC	Normal phase
Chromatography system	Agilent 1290 Infinity	Agilent 1290 Infinity	Agilent 1290 Infinity	Agilent 1100
Column	Agilent Zorbax RRHD Eclipse Plus C18 (50 x 2.1 mm, 1.8 µm, 95 Å)	Agilent Zorbax RRHD Eclipse Plus C18 (50 x 2.1 mm, 1.8 µm, 95 Å)	Waters Acquity BEH HILIC (100 x 2.1mm,1.7 µm, 130 Å)	Agilent Zorbax Eclipse XDB-C18 Silica (150 x 3mm, 1.8 µm, 80 Å)
MS Type	ESI	ESI	ESI	ESI
MS instrument type	Triple quadrupole	Triple quadrupole	Triple quadrupole	Triple quadrupole
MS instrument name	Agilent 6460 QQQ	Agilent 6495 QQQ	Agilent 6490 QQQ	ABI Sciex 4000 QTrap
Ion Mode	POSITIVE	POSITIVE	POSITIVE	POSITIVE
Units	µmol/L	µmol/L	µmol/L	µmol/L

Study-level view : Show named metabolites and measurements

Summary of study ST001140

This data is available at the NIH Common Fund's National Metabolomics Data Repository (NMDR) website, the Metabolomics Workbench, https://www.metabolomicsworkbench.org, where it has been assigned Project ID PR000761. The data can be accessed directly via it's Project DOI: 10.21228/M89Q32
This work is supported by NIH grant, U2C- DK119886. See: https://www.metabolomicsworkbench.org/about/howtocite.php

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download mwTab file (text) | Download mwTab file(JSON) | Download data (Contains raw data)

Study ID	ST001140
Study Title	Changes in the Canine Plasma Lipidome after Short- and Long-Term Exposure Glucocorticoid Exposure
Study	Glucocorticoids (GCs) are widely used in veterinary and human medicine. Chromic endogenous or iatrogenic GC overexposure impairs metabolic function and can Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess actide, respectively) on the plasma lipidome of Beale dogs. Both, long- and short-term GC resulted in significant changes of
	rsity of Zurich
	G);Vetsuisse Faculty, University of Zurich

Return to study ST001140 main page

Analysis: Phospholipids, Chol. esters and Diacylglycerols

Show values for a selected metabolite or ratios for 2 selected metabolites

Select	Metabolite Name	RefMet Name/Standardized Name*
☑	CE(16:0)	CE 16:0
☐	CE(16:1)	CE 16:1
☐	CE(17:0)	CE 17:0
☐	CE(17:1)	CE 17:1
☐	CE(18:0)	CE 18:0
☐	CE(18:1)	CE 18:1
☐	CE(18:2)	CE 18:2
☐	CE(18:3)	CE 18:3
☐	CE(20:1)	CE 20:1
☐	CE(20:2)	CE 20:2
☐	CE(20:3)	CE 20:3
☐	CE(20:4)	CE 20:4
☐	CE(20:5)	CE 20:5
☐	CE(22:4)	CE 22:4
☐	CE(22:5)	CE 22:5
☐	CE(22:6)	CE 22:6
☐	CE(24:4)	CE 24:4
☐	DG(16:0_20:4)	DG 16:0_20:4

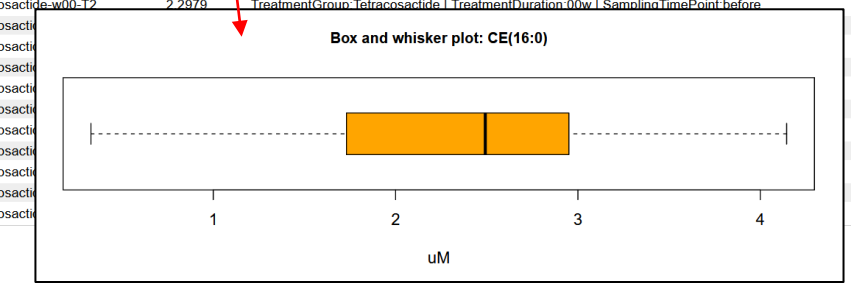
Select a metabolite (checkbox)

CE(16:0) values for ST001140 (Units: uM)

Run ANOVA on this analyte | Run t-test on this analyte| Calculate z-scores for this analyte

Bar graph by sample: Bar graph (samples) | Boxplot: All samples | Boxplot: By factor | Bar graph of values for each factor level: Display bar graph for each factor level | View data for a sele… Factor:

Sample	CE(16:0)	Factors	
Prednisolone-d0-P1	2.3688	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	
Prednisolone-d0-P2	1.1431	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	
Prednisolone-d0-P3	3.8792	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	uM
Prednisolone-d0-P4	2.5141	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	uM
Prednisolone-d0-P5	2.4696	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	uM
Prednisolone-d0-P6	2.7607	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	
Prednisolone-d0-P7	3.0938	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	
Prednisolone-d0-P8	3.1449	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	
Prednisolone-d4-P1	3.5690	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P2	2.2201	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P3	1.2771	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P4	2.5287	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P5	3.5024	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P6	4.1451	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P7	2.8065	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Prednisolone-d4-P8	3.4714	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	
Tetracosactide-w00-T1	2.0652	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before	
Tetracosactide-w00-T2	2.2979	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before	
Tetracosacti…			



ANOVA results for CE(16:0) in Study ST001140

ANALYTE	TreatmentGroup
CE(16:0)	2.621E-3

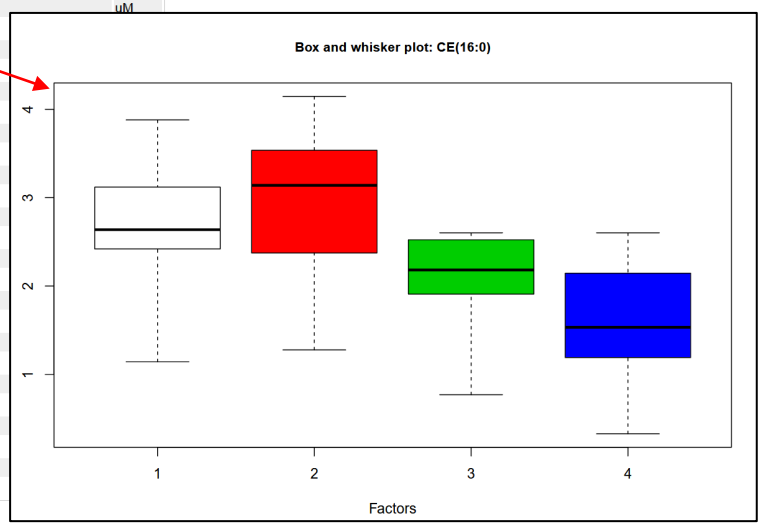
(Green: p value<=0.05)

T-test on CE(16:0) (2-tailed test. Assumes equal variances)

Factors	f2	f3	f4
f1	5.41E-1	1.34E-1	2.22E-2
f2	-	6.31E-2	1.19E-2
f3	-	-	2.89E-1

f1	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before
f2	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after
f3	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before
f4	TreatmentGroup:Tetracosactide | TreatmentDuration:25w | SamplingTimePoint:after

Green: p-value <= 0.05



NMDR:Study-level view/download options

Summary of study ST001140

This data is available at the NIH Common Fund's National Metabolomics Data Repository (NMDR) website, the Metabolomics Workbench, https://www.metabolomicsworkbench.org, where it has been assigned Project ID PR000761. The data can be accessed directly via it's Project DOI: 10.21228/M89Q32
This work is supported by NIH grant, U2C- DK119886. See: https://www.metabolomicsworkbench.org/about/howtocite.php

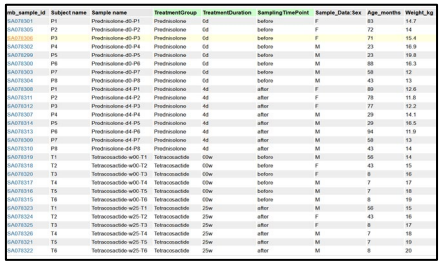
Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download mwTab file (text) | Download mwTab file(JSON) | Download data (Contains raw data)

Study ID	ST001140
Study Title	Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure
Study Summary	Glucocorticoids (GCs) are widely used in veterinary and human medicine. Chronic endogenous or iatrogenic GC overexposure impairs metabolic function and can result in diverse side-effects, including Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess (induced by prednisolone and tetracosactide, respectively) on the plasma lipidome of beale dogs. Both, long- and short-term GC resulted in significant changes of the plasma lipidome.
Institute	National University of Singapore;University of Zurich
Department	Singapore Lipidomics Incubator (SLING);Vetsuisse Faculty, University of Zurich
Laboratory	Singapore Lipidomics Incubator (SLING), National University of Singapore

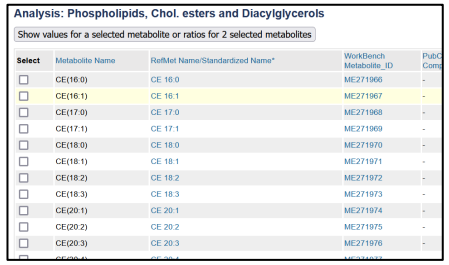
Select appropriate tab below to view additional metadata details:

All | Project | Subject | Study Design | Collection | Treatment | Sample Preparation | Chromatography | Analysis | MS

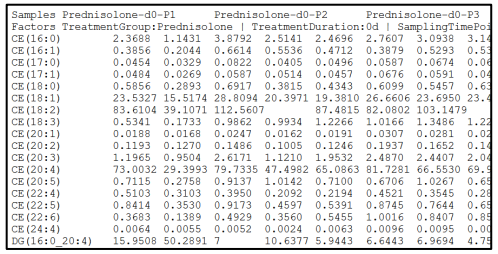
← View Metadata



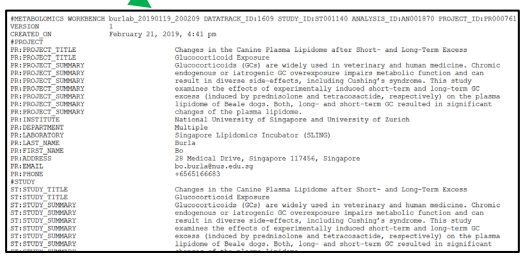
Samples/study design



Named metabolites



Download dataset



Download mwTab (text)

Download mwTab (json)

NMDR: raw data view/download

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download mwTab file (text) | Download mwTab file(JSON) | Download data (Contains raw data)

Download data

You have selected to download data for study **ST001738**. The following data file(s) are available for download:

- View archive contents
- Download individual raw files
- ST001738_File_Naming_AdipoAtlas.xlsx (16.4K)
- ST001738_ccms_peak_identification.zip (4.6G)
- ST001738_ccms_peak_quantification.zip (2.1G)

} Download compressed raw files

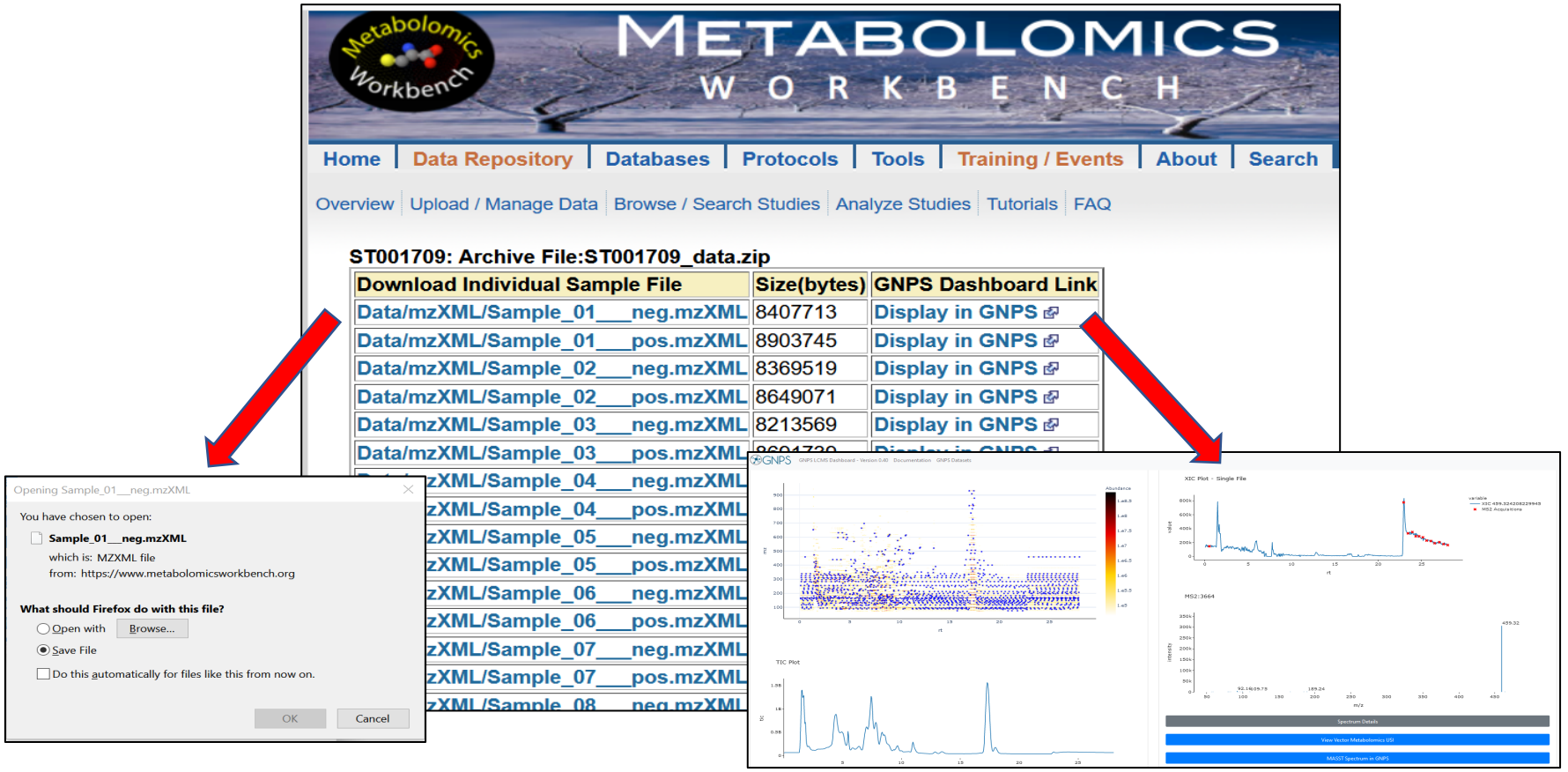
ST001738: Archive File:ST001738_ccms_peak_identification.zip

```
Archive:  .test/Studies/ST001738_ccms_peak_identification.zip
  Length      Date    Time    Name
---------  ---------- -----   ----
135568928  04-12-2021 16:42   Polar_Fusion_NEG_SAT_ob_1.mzML
134904804  04-12-2021 16:42   Polar_Fusion_NEG_SAT_ob_2.mzML
134393660  04-12-2021 16:43   Polar_Fusion_NEG_SAT_ob_3.mzML
134892339  04-12-2021 16:43   Polar_Fusion_NEG_SAT_ob_4.mzML
135015899  04-12-2021 16:43   Polar_Fusion_NEG_SAT_ob_5.mzML
134443440  04-12-2021 16:43   Polar_Fusion_NEG_SAT_ob_6.mzML
135875506  04-12-2021 16:43   Polar_Fusion_NEG_VAT_ob_1.mzML
134398714  04-12-2021 16:43   Polar_Fusion_NEG_VAT_ob_2.mzML
134824391  04-12-2021 16:44   Polar_Fusion_NEG_VAT_ob_3.mzML
135063431  04-12-2021 16:44   Polar_Fusion_NEG_VAT_ob_4.mzML
134428351  04-12-2021 16:44   Polar_Fusion_NEG_VAT_ob_5.mzML
134646218  04-12-2021 16:44   Polar_Fusion_NEG_VAT_ob_6.mzML
150138692  04-12-2021 16:44   Polar_Fusion_POS_SAT_ob_1.mzML
153953775  04-12-2021 16:45   Polar_Fusion_POS_SAT_ob_2.mzML
150902785  04-12-2021 16:45   Polar_Fusion_POS_SAT_ob_3.mzML
150986956  04-12-2021 16:45   Polar_Fusion_POS_SAT_ob_4.mzML
149881393  04-12-2021 16:45   Polar_Fusion_POS_SAT_ob_5.mzML
149650855  04-12-2021 16:46   Polar_Fusion_POS_SAT_ob_6.mzML
152479314  04-12-2021 16:46   Polar_Fusion_POS_VAT_ob_1.mzML
149743624  04-12-2021 16:46   Polar_Fusion_POS_VAT_ob_2.mzML
```

ST001738: Archive File:ST001738_ccms_peak_identification.zip

Download Individual Sample File	Size(bytes)	GNPS Dashboard Link
Polar_Fusion_NEG_SAT_ob_1.mzML	135568928	Display in GNPS
Polar_Fusion_NEG_SAT_ob_2.mzML	134904804	Display in GNPS
Polar_Fusion_NEG_SAT_ob_3.mzML	134393660	Display in GNPS
Polar_Fusion_NEG_SAT_ob_4.mzML	134892339	Display in GNPS
Polar_Fusion_NEG_SAT_ob_5.mzML	135015899	Display in GNPS
Polar_Fusion_NEG_SAT_ob_6.mzML	134443440	Display in GNPS
Polar_Fusion_NEG_VAT_ob_1.mzML	135875506	Display in GNPS
Polar_Fusion_NEG_VAT_ob_2.mzML	134398714	Display in GNPS
Polar_Fusion_NEG_VAT_ob_3.mzML	134824391	Display in GNPS
Polar_Fusion_NEG_VAT_ob_4.mzML	135063431	Display in GNPS
Polar_Fusion_NEG_VAT_ob_5.mzML	134428351	Display in GNPS
Polar_Fusion_NEG_VAT_ob_6.mzML	134646218	Display in GNPS
Polar_Fusion_POS_SAT_ob_1.mzML	150138692	Display in GNPS
Polar_Fusion_POS_SAT_ob_2.mzML	153953775	Display in GNPS

Collaboration with Global Natural Product Social Molecular Networking (GNPS)



View spectral details of MS raw data files deposited in NMDR via the GNPS dashboard

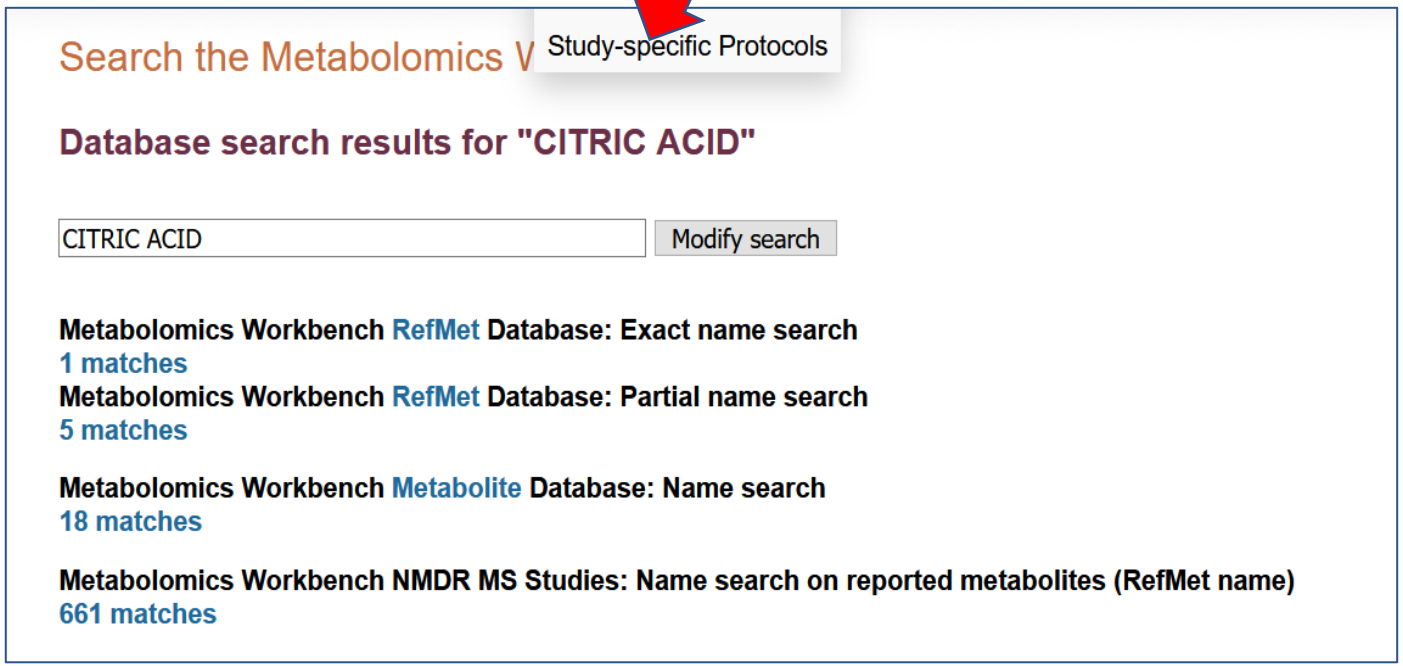
GNPS Dashboard: Collaborative Analysis of Mass Spectrometry Data in the Web Browser

D. Petras et al, Nature Methods (2021) https://doi.org/10.1038/s41592-021-01339-5

Metabolomics Workbench Quick search

What is searched?

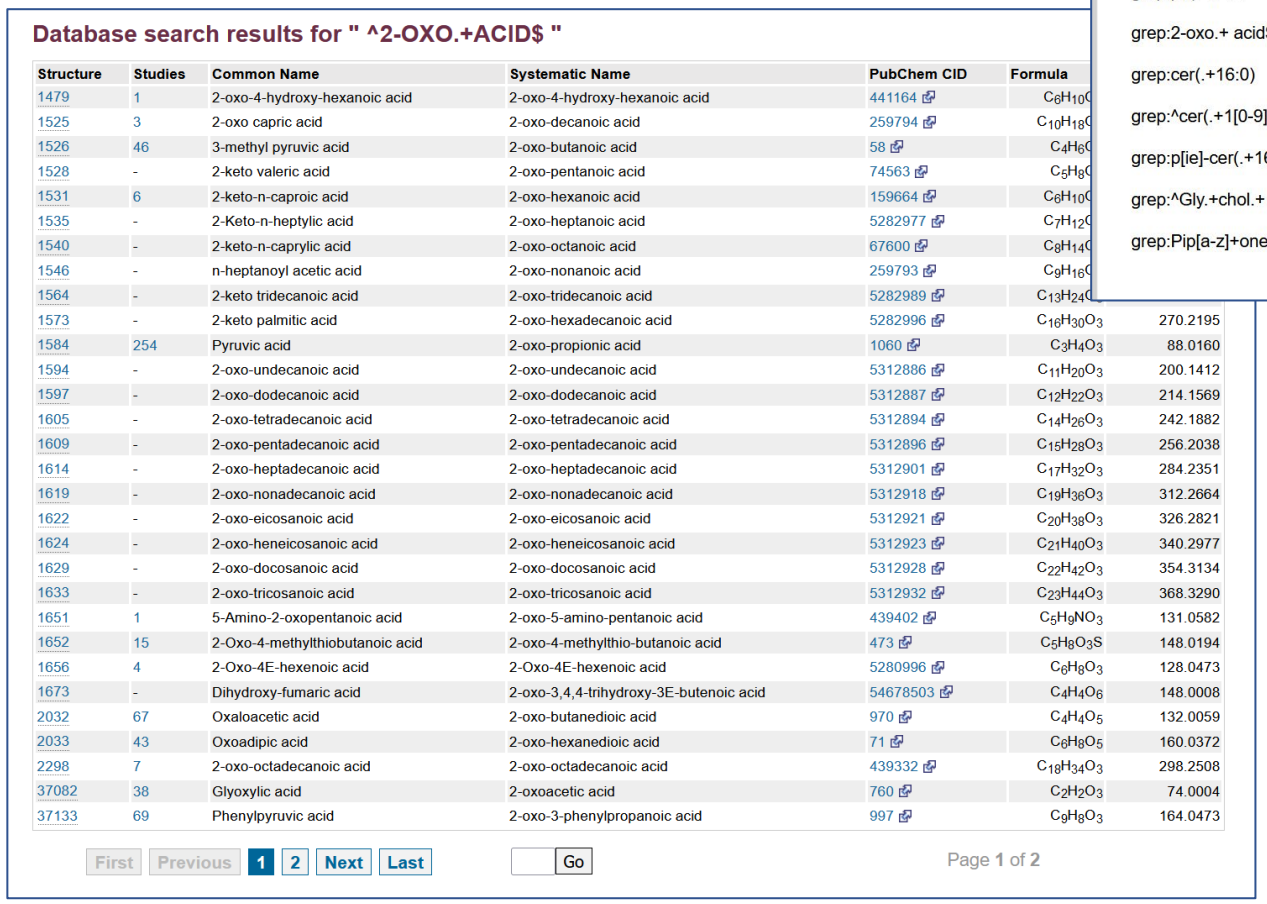
- Metabolite name
- Metabolite InChIKey
- PubChem Compound ID
- Molecular formula
- Metabolite mass (+/- 0.5 daltons)
- Metabolite class
- Study title
- NMDR Study ID
- NMDR Project ID
- NMDR studies containing that metabolite



Regular expression search

What is searched?

- **Metabolite common names and systematic names in MW metabolite database**



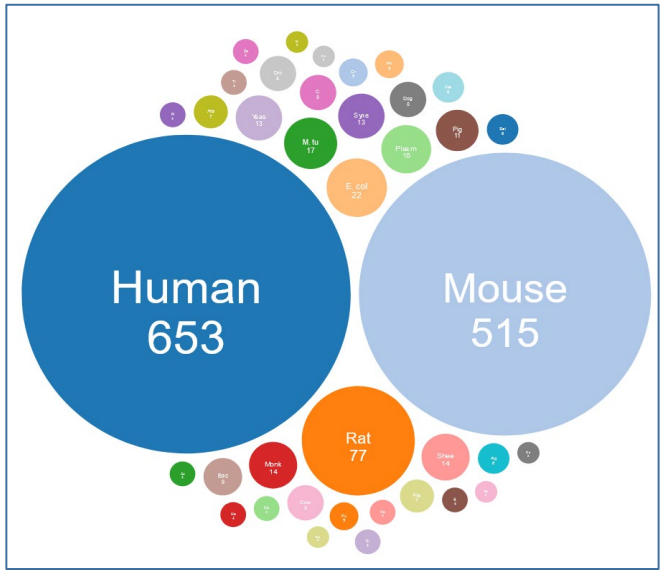
Database search results for " ^2-OXO.+ACID$ "

Structure	Studies	Common Name	Systematic Name	PubChem CID	Formula	
1479	1	2-oxo-4-hydroxy-hexanoic acid	2-oxo-4-hydroxy-hexanoic acid	441164	$C_6H_{10}O$	
1525	3	2-oxo capric acid	2-oxo-decanoic acid	259794	$C_{10}H_{18}O$	
1526	46	3-methyl pyruvic acid	2-oxo-butanoic acid	58	C_4H_6O	
1528	-	2-keto valeric acid	2-oxo-pentanoic acid	74563	C_5H_8O	
1531	6	2-keto-n-caproic acid	2-oxo-hexanoic acid	159664	$C_6H_{10}O$	
1535	-	2-Keto-n-heptylic acid	2-oxo-heptanoic acid	5282977	$C_7H_{12}O$	
1540	-	2-keto-n-caprylic acid	2-oxo-octanoic acid	67600	$C_8H_{14}O$	
1546	-	n-heptanoyl acetic acid	2-oxo-nonanoic acid	259793	$C_9H_{16}O$	
1564	-	2-keto tridecanoic acid	2-oxo-tridecanoic acid	5282989	$C_{13}H_{24}O$	
1573	-	2-keto palmitic acid	2-oxo-hexadecanoic acid	5282996	$C_{16}H_{30}O_3$	270.2195
1584	254	Pyruvic acid	2-oxo-propionic acid	1060	$C_3H_4O_3$	88.0160
1594	-	2-oxo-undecanoic acid	2-oxo-undecanoic acid	5312886	$C_{11}H_{20}O_3$	200.1412
1597	-	2-oxo-dodecanoic acid	2-oxo-dodecanoic acid	5312887	$C_{12}H_{22}O_3$	214.1569
1605	-	2-oxo-tetradecanoic acid	2-oxo-tetradecanoic acid	5312894	$C_{14}H_{26}O_3$	242.1882
1609	-	2-oxo-pentadecanoic acid	2-oxo-pentadecanoic acid	5312896	$C_{15}H_{28}O_3$	256.2038
1614	-	2-oxo-heptadecanoic acid	2-oxo-heptadecanoic acid	5312901	$C_{17}H_{32}O_3$	284.2351
1619	-	2-oxo-nonadecanoic acid	2-oxo-nonadecanoic acid	5312918	$C_{19}H_{36}O_3$	312.2664
1622	-	2-oxo-eicosanoic acid	2-oxo-eicosanoic acid	5312921	$C_{20}H_{38}O_3$	326.2821
1624	-	2-oxo-heneicosanoic acid	2-oxo-heneicosanoic acid	5312923	$C_{21}H_{40}O_3$	340.2977
1629	-	2-oxo-docosanoic acid	2-oxo-docosanoic acid	5312928	$C_{22}H_{42}O_3$	354.3134
1633	-	2-oxo-tricosanoic acid	2-oxo-tricosanoic acid	5312932	$C_{23}H_{44}O_3$	368.3290
1651	1	5-Amino-2-oxopentanoic acid	2-oxo-5-amino-pentanoic acid	439402	$C_5H_9NO_3$	131.0582
1652	15	2-Oxo-4-methylthiobutanoic acid	2-oxo-4-methylthio-butanoic acid	473	$C_5H_8O_3S$	148.0194
1656	4	2-Oxo-4E-hexenoic acid	2-Oxo-4E-hexenoic acid	5280996	$C_6H_8O_3$	128.0473
1673	-	Dihydroxy-fumaric acid	2-oxo-3,4,4-trihydroxy-3E-butenoic acid	54678503	$C_4H_4O_6$	148.0008
2032	67	Oxaloacetic acid	2-oxo-butanedioic acid	970	$C_4H_4O_5$	132.0059
2033	43	Oxoadipic acid	2-oxo-hexanedioic acid	71	$C_6H_8O_5$	160.0372
2298	7	2-oxo-octadecanoic acid	2-oxo-octadecanoic acid	439332	$C_{18}H_{34}O_3$	298.2508
37082	38	Glyoxylic acid	2-oxoacetic acid	760	$C_2H_2O_3$	74.0004
37133	69	Phenylpyruvic acid	2-oxo-3-phenylpropanoic acid	997	$C_9H_8O_3$	164.0473

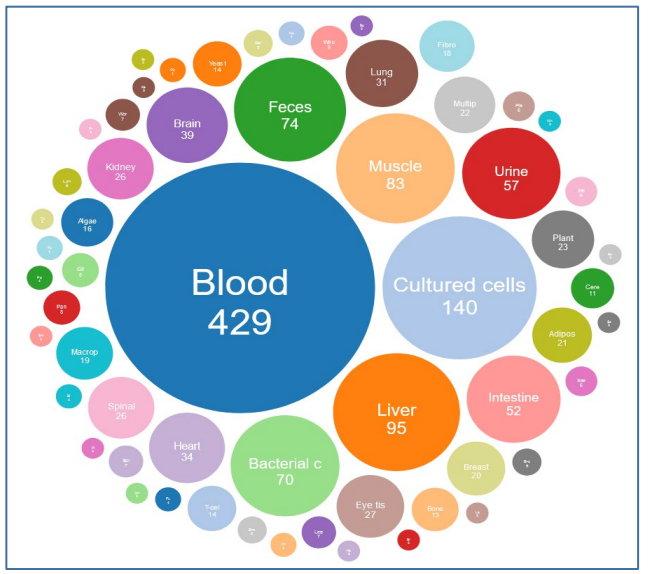
First Previous 1 2 Next Last Go Page 1 of 2

MW Usability: Bubble chart access to key NMDR study search parameters (Species, disease, sample source, metabolic pathways, metabolite classes)

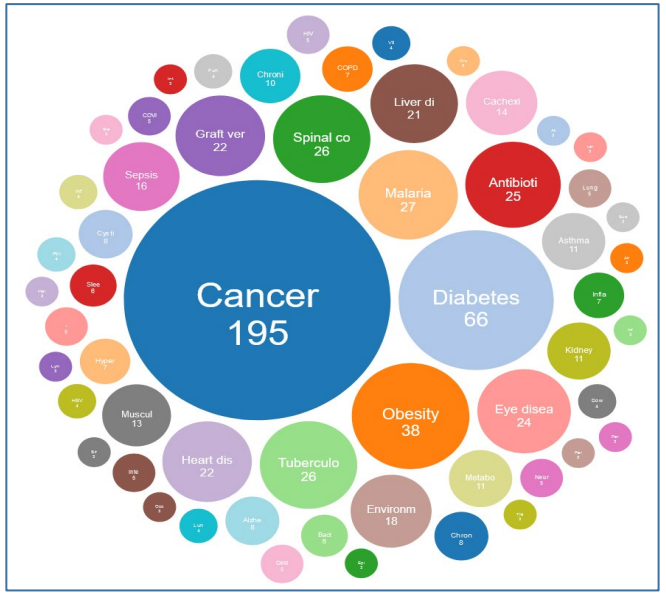
Species



Sample source



Disease



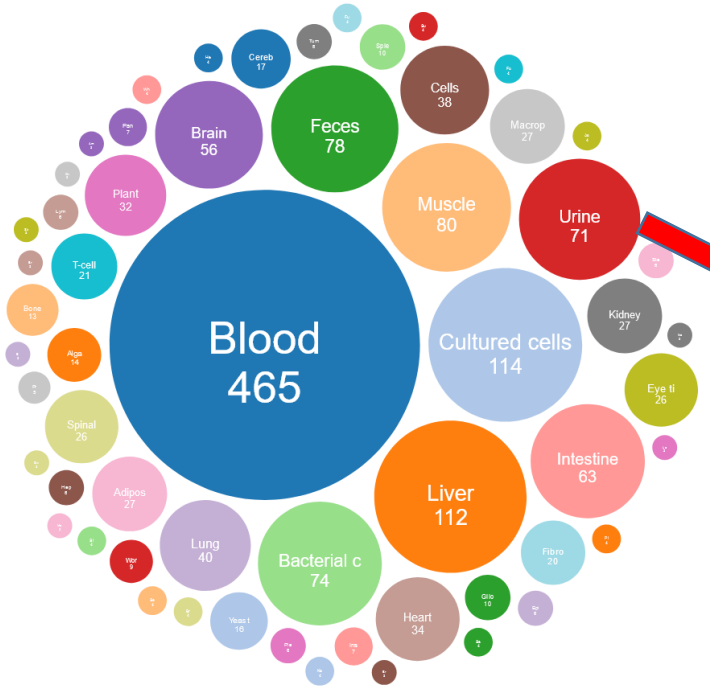
Metabolite class

MW Usability: Bubble chart access to key NMDR study search parameters (Species, disease, sample source, metabolic pathways, metabolite classes)

Select Sample source link

Sample Source | Species class | Species | Disease | Human pathways | Metabolite class

Sample source: Minimum studies: 3 | Chart size: Medium | Color scheme: Medium



Sample source data (All studies)

Sample Source	Studies
Blood	465
Cultured cells	114
Liver	112
Muscle	80
Feces	78
Bacterial cells	74
Urine	71
Intestine	63
Brain	56
Lung	40

Browse and Search Studies

- **Browse**
  - Summary of all studies
  - Summary of all projects (groups of studies)
  - Bubble plots of studies by disease, sample source, species, pathway and metabolite class
  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)

Click on "Urine" bubble

Click on "Urine" link

Studies involving sample source:Urine

Study ID	Study Title	Species	Institute
ST000020	Biomarker Discovery in Knee Osteoarthritis (I)	Human	University of North Carolina
ST000022	Biomarker Discovery in Knee Osteoarthritis (II)	Human	University of North Carolina
ST000028	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Urine)	Mouse	University of North Carolina
ST000037	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Urine)	Mouse	University of North Carolina
ST000050	Preterm Neonatal Urinary Renal Developmental and acute kidney injury Metabolomic Profiling	Human	University of North Carolina
ST000092	A statistical analysis of the effects of urease pre-treatment on the measurement of the urinary metabolome by gas chromatographymass spectrometry	Human	Pacific Northwest National Laboratory
ST000236	Quick Comparison of Urine Metabolites in Human and SD Rats of Different Sex by Untargeted UPLC-TOFMS and In-house Software Platform	Human	Beijing Institute of Radiation Medicine
ST000236	Quick Comparison of Urine Metabolites in Human and SD Rats of Different Sex by Untargeted UPLC-TOFMS and In-house Software Platform	Rat	Beijing Institute of Radiation Medicine
ST000256	Signal Intensities Derived from Different NMR Probes and Parameters Contribute to Variations in Quantification of Metabolites	Human	University of Michigan
ST000291	LC-MS Based Approaches to Investigate Metabolomic Differences in the Urine of Young Women after Drinking Cranberry Juice or Apple Juice	Human	University of Florida
ST000329	Minimal change disease and focal segmental sclerosis in urine	Human	University of California, Davis
ST000381	Urinary Metabolites in IC/PBS Diagnosis (part I)	Human	University of California, Davis
ST000382	Urinary Metabolites in IC/PBS Diagnosis (part II)	Human	University of California, Davis
ST000398	Metabolic profiling of maternal urine can aid clinical management of Gestational Diabetes Mellitus (GDM)	Human	University of Aveiro
ST000444	Preconcentration of organic solutes in urine by bubble bursting	Human	V.I. Kulakov Research Center for Obstetrics, Gynecology and Perinatology
ST000559	Urine metabolomic profiling of diabetic nephropathy in the steptozotocin induced type-1 diabetes mouse model.	Mouse	RTI International
ST000573	Exploratory research on first and second trimester urinary metabolic profiles and fetal growth restriction	Human	Mayo Clinic
ST000603	Urinary Volatile Compound, Associated with Chronic Inflammation In Interstitial Cystitis	Human	University of California, Davis
ST000611	Relative level of inosine/adenosine and sarcosine	Human	Baylor College of Medicine
ST000615	GC/MS measurement of sarcosine in urine samples	Human	Baylor College of Medicine
ST000628	TCA Cycle Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from 20 Participants of the DASH2 Clinical Trial (part I)	Human	Mayo Clinic
ST000629	Amino Acid Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from 20 Participants of the DASH2 Clinical Trial (part II)	Human	Mayo Clinic
ST000630	Neuromodulator Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from 20 Participants of the DASH2 Clinical Trial (part III)	Human	Mayo Clinic
ST000631	TCA Cycle Metabolites of Dietary Salt Effects on Blood Pressure in Rat Urine (part IV)	Rat	Mayo Clinic
ST000632	Amino Acid Metabolites of Dietary Salt Effects on Blood Pressure in Rat Urine (part V)	Rat	Mayo Clinic
ST000633	Neuromodulator Metabolites of Dietary Salt Effects on Blood Pressure in Rat Urine (part VI)	Rat	Mayo Clinic
ST000634	TCA Cycle Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from DASH2 Clinical Trial (part VII)	Human	Mayo Clinic
ST000635	Amino Acid Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from DASH2 Clinical Trial (part VIII)	Human	Mayo Clinic
ST000636	Neuromodulator Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from DASH2 Clinical Trial (part IX)	Human	Mayo Clinic
ST000786	N-acetylisoputreanine-g-lactam Identification	Human	Colorado State University
ST000891	NMR comparison of urine samples by 1D NOESY presat and PURGE	Human	University of Georgia
ST000907	Murine vitamin A deficiency results in a hypermetabolic state and alterations in bacterial community structure and metabolism (Urine)	Mouse	Pennsylvania State University
ST000917	Biomarkers of NAFLD progression: a lipidomics approach to an epidemic. Part 3:Urine	Human	LIPID MAPS
ST000922	Crab Urine Study	Crab	Georgia Institute of Technology
ST000934	Metabolome profiles in urogenital schistosomiasis and associated pathologies	Human	University of Ibadan, Nigeria
ST000973	Metabolome profiles in urogenital schistosomiasis and associated pathologies (part II)	Human	University of Ibadan, Nigeria
ST001039	Denver Asthma Panel Study-CHEAR Ancillary Study (part II)	Human	Emory University
ST001047	1H-NMR urinary metabolomic profiling for diagnosis of gastric cancer.	Human	University of Alberta
ST001048	Pediatric Inner-City Environmental Exposures at School and Home and Asthma Study	Human	Icahn School of Medicine at Mount Sinai
ST001069	Evaluation of Seryl-leucine core 1 O-glycosylated peptide (SLC1G) in TB patient urine	Human	Colorado State University

List of all studies with urine as a sample source

Text search on NMDR studies/projects

Data/metadata in experimental projects/studies

Search specific data fields

Subject type: Human
Species: Homo sapiens
Project or study title: NAFLD
Institution: University of California, Davis
Year submitted: 2021
Analysis type: MS

Additional MS parameters:

MS type:
MS ion mode:
MS instrument type:
MS instrument name:

Display by: Study

Search Reset

Browse and Search Studies

- **Browse**
  - Summary of all studies
  - Summary of all projects (groups of studies)
  - Bubble plots of studies by disease, sample source, species, pathway and metabolite class
  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)
- **Search**
  - Experimental Projects / Studies
  - MetStat: Perform meta-analysis on named metabolites across all studies:
    Refine by analysis type, species, sample source, disease association, metabolite classification and biochemical pathway
  - Select Studies by species, sample source or disease association
  - Search data/metadata in experimental projects/studies
  - Search Untargeted MS data by m/z, retention time, instrumentation
  - REST service
  - Use the Metabolomics Workbench REST service to retrieve different types of data

Showing results 1 to 4 of 4 (#: Contains untargeted data) Results per page: 50

Study ID	Study Title	Species	Institute	Analysis	Released	Version	Samples	Download (* : Contains raw data)
ST001845	Identification of unique metabolite networks between Latino and Caucasian patients with nonalcoholic fatty liver disease (NAFLD) (part V)	Homo sapiens	University of California, Davis	MS	2021-07-05	1	21	Uploaded data (7.1M)* (Data format:wiff)
ST001844	Identification of unique metabolite networks between Latino and Caucasian patients with nonalcoholic fatty liver disease (NAFLD) (part III)	Homo sapiens	University of California, Davis	MS	2021-07-05	1	61	Uploaded data (9.4M)* (Data format:wiff)
ST001843	Identification of unique metabolite networks between Latino and Caucasian patients with nonalcoholic fatty liver disease (NAFLD) (part II)	Homo sapiens	University of California, Davis	MS	2021-07-05	1	60	Uploaded data (17.1G)* (Data format:d)
ST001842	Identification of unique metabolite networks between Latino and Caucasian patients with nonalcoholic fatty liver disease (NAFLD) (part I)	Homo sapiens	University of California, Davis	MS	2021-07-05	1	60	Uploaded data (614.4M)* (Data format:cdf)

Text search on NMDR metadata (all sections)

Data/metadata in experimental projects/studies

Search specific data fields

Subject type:
Species:
Project or study title:
Institution:
Year submitted:
Analysis type:

Display by: Study

Search Reset

Search all experimental metadata fields

Text query NAFLD

Search Reset

Browse and Search Studies

- **Browse**
  - Summary of all studies
  - Summary of all projects (groups of studies)
  - Bubble plots of studies by disease, sample source, species, pathway and metabolite class
  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)
- **Search**
  - **Experimental Projects / Studies**
  - MetStat: Perform meta-analysis on named metabolites across all studies:
    Refine by analysis type, species, sample source, disease association, metabolite classification and biochemical pathway
  - Select Studies by species, sample source or disease association
  - Search data/metadata in experimental projects/studies
  - Search Untargeted MS data by m/z, retention time, instrumentation
  - **REST service**
  - Use the Metabolomics Workbench REST service to retrieve different types of data

ST000917	ST:STUDY_TITLE	Biomarkers of NAFLD progression: a lipidomics approach to an epidemic. Part
ST000977	CO:COLLECTION_SUMMARY	2 weeks prior to operation day (bariatric surgery) for the NAFLD group and among
ST000977	PR:PROJECT_SUMMARY	of metabolic syndrome. NAFLD is a very heterogeneous disease, as it presents in
ST000977	PR:PROJECT_TITLE	patients with nonalcoholic fatty liver disease (NAFLD)
ST000977	ST:STUDY_SUMMARY	Nonalcoholic fatty liver disease (NAFLD) is a spectrum of liver pathology
ST000977	ST:STUDY_TITLE	patients with nonalcoholic fatty liver disease (NAFLD)
ST000977	TR:TREATMENT_SUMMARY	fatty liver disease (NAFLD)
ST001680	PR:PROJECT_SUMMARY	metabolites changed in high fat fed NAFLD mouse model. We suggest that AC261066
ST001680	PR:PROJECT_TITLE	Metabolome of NAFLD in high fat diet mouse model
ST001680	ST:STUDY_SUMMARY	metabolites changed in high fat fed NAFLD mouse model. We suggest that AC261066
ST001680	ST:STUDY_TITLE	Metabolome of NAFLD in high fat diet mouse model
ST001710	PR:PROJECT_SUMMARY	Background and Aims: Nonalcoholic fatty liver disease (NAFLD) is a progressive
ST001710	ST:STUDY_TITLE	Metabolic signatures of NAFLD - Lipidomics data (part 1 of 3)
ST001711	PR:PROJECT_SUMMARY	Background and Aims: Nonalcoholic fatty liver disease (NAFLD) is a progressive
ST001711	ST:STUDY_TITLE	Metabolic signatures of NAFLD - Polar metabolomics data (part II)
ST001842	CO:COLLECTION_SUMMARY	2 weeks prior to operation day (bariatric surgery) for the NAFLD group and among
ST001842	PR:PROJECT_SUMMARY	Nonalcoholic fatty liver disease (NAFLD) is a spectrum of liver pathology
ST001842	PR:PROJECT_TITLE	patients with nonalcoholic fatty liver disease (NAFLD)
ST001842	ST:STUDY_SUMMARY	of metabolic syndrome. NAFLD is a very heterogeneous disease, as it presents in
ST001842	ST:STUDY_TITLE	patients with nonalcoholic fatty liver disease (NAFLD) (part II)
ST001842	TR:TREATMENT_SUMMARY	fatty liver disease (NAFLD)
ST001843	CO:COLLECTION_SUMMARY	2 weeks prior to operation day (bariatric surgery) for the NAFLD group and among
ST001843	PR:PROJECT_SUMMARY	Nonalcoholic fatty liver disease (NAFLD) is a spectrum of liver pathology

Search untargeted MS data IN NMDR (m/z, retention time “features”)

Browse and Search Studies

- **Browse**
  - Summary of all studies
  - Summary of all projects (groups of studies)
  - Bubble plots of studies by disease, sample source, species, pathway and metabolite class
  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)
- **Search**
  - Experimental Projects / Studies
  - MetStat: Perform meta-analysis on named metabolites across all studies:
    Refine by analysis type, species, sample source, disease association, metabolite classificat
  - Select Studies by species, sample source or disease association
  - Search data/metadata in experimental projects/studies
  - Search Untargeted MS data by m/z, retention time, instrumentation
  - REST service
  - Use the Metabolomics Workbench REST service to retrieve different types of data

Search untargeted MS data on the Metabolomics Workbench

This portal searches over 3.4 million m/z features from over 675 NMDR studies and over 1150 LC-MS analyses.

m/z:	657.48
Tolerance (m/z):	0.01
Retention time:	
Tolerance(min or sec):	0.2
Ion mode:	Positive
Chromatography type:	
MS instrument name:	
MS instrument type:	
Limit search to studies by disease association, sample source and/or species	
Disease:	
Sample source:	
Species:	
Sort by:	mz
Search / Reset	

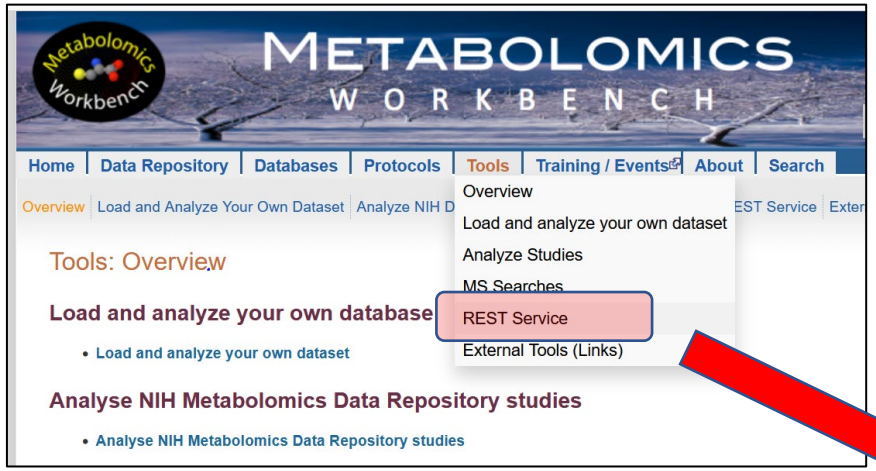
- Features that have been identified will appear in the "Name" column in the results table.
- Optionally specify a retention time value and tolerance window to restrict the search.
- Leave both m/z and retention time fields blank to search for studies using a selected MS/chromatography parameter.

Metadata details for analysis AN001609	
Study ID	ST000983
Analysis ID	AN001609
Study Title	Validating Quantitative Untargeted Lipidomics Across Nine Liquid Chromatography-High-Resolution Mass Spectrometry Platforms (Part I)
Institute	University of California, Davis
Species	Homo sapiens
Ion_mode	POSITIVE
MS type	ESI
MS Instrument Name	Agilent 6530 QTOF
MS Instrument Type	QTOF
Chromatography Instrument Name	Agilent 6530
Chromatography Type	Reversed phase
Chromatography Column	Waters Acquity CSH C18 (100 x 2.1mm, 1.7um)
Solvent A	60:40 Acetonitrile:Water +10mM Ammonium Formate +10mM Formic Acid
Solvent B	9:1 Isopropanol:Acetonitrile +10mM Ammonium Formate +10mM Formic Acid

Results for untargeted MS search on m/z:657.485 (+/-0.01) POSITIVE mode

Details	Name	m/z	RT	RT_Units	Study	Ion_mode	MS_Instrument	MS_Inst_Type	Chromatography
AN001527		657.4762	1.03	Minutes	ST000932	POSITIVE	Agilent 6220 TOF	TOF	Normal phase
AN001064		657.4765	23.5	Minutes	ST000689	POSITIVE	Agilent 6530 QTOF	QTOF	Reversed phase
AN001532		657.4779	1.02	Minutes	ST000935	POSITIVE	Agilent 6220 TOF	TOF	Normal phase
AN002964		657.4785	22.27	Minutes	ST001828	POSITIVE	Agilent 6445 Q-TOF	QTOF	Reversed phase
AN000806		657.4801	16.34	Minutes	ST000528	POSITIVE	Thermo Orbitrap	Orbitrap	Reversed phase
AN003044		657.48059	2.92	Minutes	ST001882	POSITIVE	Thermo Q Exactive HF hybrid Orbitrap	Orbitrap	Reversed phase
AN000806		657.4806	21.25	Minutes	ST000528	POSITIVE	Thermo Orbitrap	Orbitrap	Reversed phase
AN003049		657.48176	2.16	Minutes	ST001885	POSITIVE	Thermo Orbitrap ID-X tribrid	Orbitrap/ion trap	Reversed phase
AN003049		657.48183	2.48	Minutes	ST001885	POSITIVE	Thermo Orbitrap ID-X tribrid	Orbitrap/ion trap	Reversed phase
AN000627		657.4820	4.4	Minutes	ST000391	POSITIVE	Agilent 6530A QTOF	QTOF	HILIC
AN000741		657.4824	16.31	Minutes	ST000476	POSITIVE	Orbitrap	Orbitrap	Reversed phase
AN000808		657.4836	16.2	Minutes	ST000530	POSITIVE	Thermo Orbitrap	Orbitrap	Reversed phase
AN001776		657.4841	51.5	Seconds	ST001091	POSITIVE	Thermo Fusion Tribrid Orbitrap	Orbitrap/ion trap	HILIC
AN000953		657.4848	46.54	Minutes	ST000621	POSITIVE	Waters Synapt G2 S QTOF	QTOF	Reversed phase
AN000627		657.4850	2.4	Minutes	ST000391	POSITIVE	Agilent 6530A QTOF	QTOF	HILIC
AN001516		657.4850	9.08	Minutes	ST000923	POSITIVE	Thermo Q Exactive Plus Orbitrap	Orbitrap	Reversed phase
AN001436		657.4853	8.87	Minutes	ST000880	POSITIVE	Thermo Q Exactive Plus Orbitrap	Orbitrap	Reversed phase
AN000347		657.4853	20.14	Minutes	ST000232	POSITIVE	Thermo Q Exactive Orbitrap	Orbitrap	Reversed phase
AN001609	DG (36:3) [M+K]+	657.4854	6.59	Minutes	ST000983	POSITIVE	Agilent 6530 QTOF	QTOF	Reversed phase
AN001610	DG (36:3) [M+K]+	657.4854	6.59	Minutes	ST000984	POSITIVE	Agilent 6530 QTOF	QTOF	Reversed phase
AN001611	DG (36:3) [M+K]+	657.4854	6.59	Minutes	ST000985	POSITIVE	Agilent 6550 QTOF	QTOF	Reversed phase
AN001612	DG (36:3) [M+K]+	657.4854	6.59	Minutes	ST000986	POSITIVE	Agilent 6560 Ion Mobility	QTOF	Reversed phase
AN001613	DG (36:3) [M+K]+	657.4854	6.59	Minutes	ST000987	POSITIVE	Leco Citius LC-HRT	QTOF	Reversed phase

MW REST service access on the Metabolomics Workbench



Home | Data Repository | Databases | Protocols | Tools | Training / Events | About | Search

Overview | Load and Analyze Your Own Dataset | Analyze NIH Data Repository Studies | MS Searches | REST Service | External Tools (Links)

Metabolomics WorkBench REST service

MW REST API (v1.0, 5/7/2019) Download API (pdf)

*Note: A number of new REST queries have been added that are not described in this API version (see new examples below)

The Metabolomics WorkBench REST service enables access to a variety of data (including metabolite structures, study metadata and experimental results) using HTTP requests. These requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP request and interact with datasets such as this REST service.

The REST URL consists of three main parts, separated by forward slashes, after the common prefix specifying the invariant base URL: (https://www.metabolomicsworkbench.org/rest/)

a. The **context** specification dictates which type of resource to access and is chosen from one of the following:
<study | compound | refmet | gene | protein | moverz | exactmass>

b. The **input** specification is composed of 2 required parameters separated by forward slashes. The first parameter is the *input item* which depends on the context. The 2nd parameter is an appropriate *input value* for the chosen item. Examples of an input specification are:

```
/compound/pubchem_cid/311/
/compound/formula/C20H34O/
/study/study_id/ST000001/
/study/study_title/diabetes/
/refmet/name/Cholesterol/
/refmet/match/LysoPC16:0/
/gene/gene_symbol/acaca/
/protein/uniprot_id/Q13085/
```

Exceptions to this input specification occur when the 'moverz' context (MS search) is selected. In this case the input value must consist of 3 parts separated by forward slashes: *<m/z value>/<adduct>/<tolerance(Daltons)>*, e.g. '635.52/M+H/0.2'. In the case of the 'exactmass' context the input value must consist of 2 parts separated by forward slashes: *<lipid bulk abbreviation>/<adduct>*, e.g. 'PC(34:1)/M+H' and the input and output items are ignored.

c. The **output** specification is composed of a required *output item* parameter and an optional *output format* parameter. The list of possible output items depends on the value chosen for the context. In the case of the "compound" context one or more (separated by commas) of 'regno', 'formula','exactmass', 'inchi_key', 'name', 'sys_name', 'smiles', 'lm_id', 'pubchem_cid', 'hmdb_id', 'kegg_id', 'chebi_id', 'metacyc_id' may be specified. More conveniently, an output type of 'all' may be specified to retrieve all compound-related fields. Also an output type of 'classification' retrieves the LIPID MAPS/ClassyFire classification hierarchy. In the case of the "study" context, allowed output types are 'summary', 'factors', 'analysis', 'metabolites' and 'data'. The default output format is JSON which is amenable to manipulation and parsing by various programming languages. Optionally a text ouput format may be specified, for example:

```
/compound/pubchem_cid/311/all/txt
```

Exceptions to this output specification occur when either 'molfile' (molfile is downloaded) or 'png' (png image is displayed in browser) is chosen as an output item in the "compound" context.

The interactive "REST url" creator below shows most of the currently available options for this service.

Base URL	/Context	/Input item	/Input value	/Output item	/Output format
https://www.metabolomicsworkbench.org/rest	/	/	/	/	/ text

Create REST URL | Reset | (What is REST?) (What is JSON?)

MW REST service API document

https://www.metabolomicsworkbench.org/tools/MWRestAPIv1.0.pdf

Metabolomics Workbench REST URL-based API Specification

Version: 1.0 Date: 5/7/2019

This document describes the Metabolomics Workbench REST API specifications, a web interface for accessing a variety of data such as metabolite structures, study metadata, experimental results etc. It details the syntax of the HTTP requests including both the names of the available requests and parameters. These HTTP requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP requests and interact with datasets through the REST API.

The URL Path

The REST URL consists of three main parts, separated by forward slashes, after the common prefix specifying the invariant base URL (https://www.metabolomicsworkbench.org/rest/):

https://www.metabolomicsworkbench.org/rest/<context>/<input specification>/<output specification>

Part 1: The **context** determines the type of data to be accessed from the Metabolomics Workbench, such as metadata or results related to the submitted studies, data from metabolites, genes/proteins and analytical chemistry databases as well as other services related to mass spectrometry and metabolite identification:

<context> = study | compound | refmet | gene | protein | moverz | exactmass

Part 2: The **input specification** consists of two required parameters describing the REST request:

<input specification> = <input item>/<input value>

Part 3: The **output specification** consists of two parameters describing the output generated by the REST request:

<output specification> = <output item>/[<output format>]

The first parameter is required in most cases. The second parameter is optional. The input and output

MW REST service overview

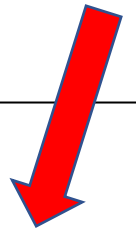
The MW REST service has 5 main contexts:

1. **Compound(metabolite) context (compound input)**
   Retrieve data on name, formula, mass, InChIKey, SMILES, molfile, classification, Pubchem ID etc. from the Metabolite structure database.
2. **NMDR Study context (study input)**
   Retrieve data on study summaries, study design, study metadata, experimental conditions, metabolite numbers, sample source, species, disease association , tables of measurements, etc from NMDR studies.
3. **RefMet context (refmet input)**
   Access RefMet standardized nomenclature and annotations, map metabolite names to RefMet names, download all RefMet names, chemical classification, etc.
4. **Gene/Protein context (gene or protein input)**
   Access DNA/RNA/protein identifiers, gene symbols, protein sequences, splice variants, homologs, etc, from the MW human Gene/Protein database of metabolism-related genes.
5. **Mass spectrometry context (moverz or exactmass input)**
   Perform precursor ion searches on RefMet database, Metabolite structure database and Lipid database by specifying m/z, adduct and mass tolerance. Calculate exact mass of a lipid molecular species ion.

MW REST service Query Builder

The online REST query builder has a menu-based format which covers most of the REST queries in the API

JSON or plain text



The interactive "REST url" creator below shows most of the currently available options for this service.

Base URL	/Context	/Input item	/Input value	/Output item	/Output format
https://www.metabolomicsworkbench.org/rest	/ compound	/ formula	/ C12H24O2	/ name	/ text

Create REST URL | Reset | (What is REST?) (What is JSON?)

Output (text)

```
formula C12H24O2
name    4,9-dimethyldecanoic acid

formula C12H24O2
name    2-Heptyl butyrate

formula C12H24O2
name    Hexyl hexanoate

formula C12H24O2
name    Ethyl decanoate

formula C12H24O2
name    Nonanal propyleneglycol acetal
```

Output (JSON)


```
{"Row1":{"formula":"C12H24O2","name":"4,9-dimethyldecanoic acid"},"R
{"formula":"C12H24O2","name":"Nonanal propyleneglycol acetal"},"Row6
{"formula":"C12H24O2","name":"2-methylbutyl heptanoate"},"Row10":{"f
{"formula":"C12H24O2","name":"3-methyl-undecanoic acid"},"Row14":{"f
{"formula":"C12H24O2","name":"3R-methyl-undecanoic acid"},"Row18":{"
{"formula":"C12H24O2","name":"(R)-Dihydrocitronellol acetate"},"Row2
{"formula":"C12H24O2","name":"2-(l-menthoxy)ethanol"}}
```

MW REST web page contains numerous examples for each context

Metabolomics WorkBench REST service

The Metabolomics WorkBench REST service enables access to a variety of data (including metabolite structures, study metadata and experimental results) using HTTP requests. These requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP request and interact with datasets such as this REST service.

Metabolite (structure) context

Study-specific (Metadata, data) context

Example request	Example URL
Compound context	
Fetch compound common name from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/name
Fetch all compound fields from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/all
Fetch all compound fields as text from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/all/txt
Fetch compound smiles from PubChem compound ID	https://www.metabolomicsworkbench.org/rest/compound/pubchem_cid/439577/smiles
Fetch compound common name and sytematic name from InChIKey	https://www.metabolomicsworkbench.org/rest/compound/inchi_key/JTWQQJDENGGSBJ-UHFFFAOYSA-N/name,sys_name
Fetch all compound fields from formula (multiple records)	https://www.metabolomicsworkbench.org/rest/compound/formula/C20H34O/all
Fetch compound classification hierarchy from PubChem compound ID	https://www.metabolomicsworkbench.org/rest/compound/pubchem_cid/5281365/classification
Download compound molfile from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/28606/molfile
Fetch png image of structure from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/png
Study context	
Show all publicly available studies (Project, Study, Analysis ID)	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/available
Fetch summary information for a study	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/summary
Fetch samples and experimental variables (factors) for a study	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/factors/
Fetch summary information for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/summary
Fetch analysis information for a study	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/analysis
Fetch metabolites and annotations detected in a study (one study at a time)	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000009/metabolites
Fetch named metabolite measurements for a study (one study at a time)	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/data
Fetch mwTab content for an analysis within a study in mwTab format	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/mwtab/txt
Fetch mwTab content for an analysis within a study in json format	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/mwtab
Fetch species information (as text) for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/species/txt
Fetch sample source information (as text) for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/source/txt
Fetch disease association (where applicable) for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/disease
Fetch list of studies with untargeted data in NMDR*New	https://www.metabolomicsworkbench.org/rest/study/study_id/x/untarg_studies/
Fetch untargeted data (where applicable) for an analysis within a study*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000113/untarg_data/
Fetch experimental factors for an untargeted data analysis within a study*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000113/untarg_factors/
Fetch list of studies with named metabolites in NMDR*New	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/named_metabolites/
Show number of named metbolites in a study*New	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/number_of_metabolites/
Fetch list of studies (as text) containing a RefMet name*New	https://www.metabolomicsworkbench.org/rest/study/refmet_name/Cholesterol/data/txt/
Fetch list of studies (as text) containing a KEGG_ID*New	https://www.metabolomicsworkbench.org/rest/study/kegg_id/C00002/data/txt/
Show metabolite name and RefMet name for a (NMDR) metabolite_id*New	https://www.metabolomicsworkbench.org/rest/study/metabolite_id/ME272191/available/
Fetch table of results (identified metabolites) for an analysis_id*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/datatable/
Download table of results (identified metabolites) for an analysis_id*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/datatable/file

In most cases, output may be specified as JSON or plain text format

MW REST web page contains numerous examples for each context

Metabolomics WorkBench REST service

The Metabolomics WorkBench REST service enables access to a variety of data (including metabolite structures, study metadata and experimental results) using HTTP requests. These requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP request and interact with datasets such as this REST service.

RefMet context

Gene/protein context

MS search context

RefMet context	
Fetch all RefMet fields from name	https://www.metabolomicsworkbench.org/rest/refmet/name/Cholesterol/all
Fetch all RefMet fields from formula	https://www.metabolomicsworkbench.org/rest/refmet/formula/C12H24O2/all
Standardize metabolite name to RefMet	https://www.metabolomicsworkbench.org/rest/refmet/match/citrate/name/
Fetch entire RefMet database (Name,exact mass,formula,InChIKey,PubChemID,classification)*New	https://www.metabolomicsworkbench.org/rest/refmet/all
Fetch all RefMet names*New	https://www.metabolomicsworkbench.org/rest/refmet/name
Fetch all RefMet names and chemical classification*New	https://www.metabolomicsworkbench.org/rest/refmet/classification
Gene/protein context	
Fetch all gene fields from gene symbol	https://www.metabolomicsworkbench.org/rest/gene/gene_symbol/acaca/all
Fetch gene name from Entrez gene id	https://www.metabolomicsworkbench.org/rest/gene/gene_id/31/gene_name
Fetch all protein fields from UniProt id	https://www.metabolomicsworkbench.org/rest/protein/uniprot_id/Q13085/all
Fetch all protein fields from Entrez gene id	https://www.metabolomicsworkbench.org/rest/protein/gene_id/19/all/
Fetch mRNA id from protein Refseq id	https://www.metabolomicsworkbench.org/rest/protein/refseq_id/NP_005493/mrna_id/
Mass spectrometry context	
Perform MS precursor ion search on Metabolomics Workbench database with m/z 635.52, ion-type* M+H and mass tolerance of 0.5 and output as text	https://www.metabolomicsworkbench.org/rest/moverz/MB/635.52/M+H/0.5/txt
Perform MS precursor ion search on LIPIDS virtual database with m/z 513.45, ion-type* M-2H (2-) and mass tolerance of 0.2 and output as text	https://www.metabolomicsworkbench.org/rest/moverz/LIPIDS/513.45/M-2H/0.2/txt
Perform MS precursor ion search on RefMet database with m/z 255.2, ion-type* M+H and mass tolerance of 0.2 and output as text	https://www.metabolomicsworkbench.org/rest/moverz/REFMET/255.2/M+H/0.2/txt
Calculate the exact mass (m/z) of the [M+H]+ ion of the lipid abbreviation# PC(34:1)	https://www.metabolomicsworkbench.org/rest/exactmass/PC(34:1)/M+H

MetStat Summary Statistics for experimental datasets in NMDR

Search/Summarize by **analysis type** (e.g. GCMS ,LCMS, NMR) and/or MS ion mode (+ or -)

Search/Summarize by **disease association** (cancer, diabetes, obesity, etc.)

Search/Summarize by **species** (human, mouse, rat, etc.)

Search/Summarize by **sample source** (blood, urine, feces, muscle, bacterial cells, etc.)

Summarize by metabolite **structural class**

What metabolites are **detected** within selected criteria (and which are most commonly detected)?

Which metabolites show **significant changes** across experimental conditions in selected data?

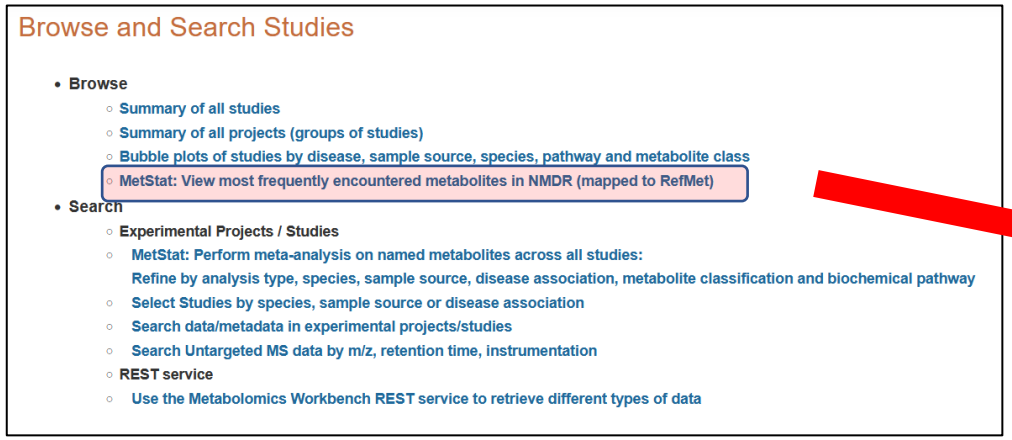
What (human) **biochemical pathways** are these metabolites involved in?

What is the average **variance across sample replicates** for a given metabolite?

What is the **ANOVA p-value** for a given metabolite under a given experimental condition?

MetStat: Summary Statistics for experimental datasets in NMDR

View most frequently encountered metabolites in NMDR studies across all conditions



MetStat: Summary table of metabolites most frequently reported in NMDR studies

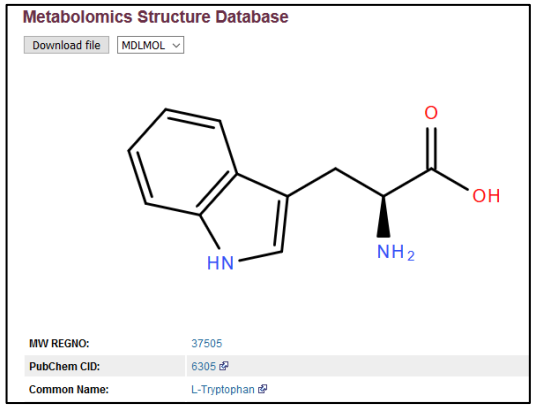
Perform detailed search (All metabolite names were mapped to RefMet nomenclature) Records to display: 200 Submit

Refmet Name	Studies	Super Class	Main Class	Sub Class
Glutamic acid	715	Organic acids	Amino acids and peptides	Amino acids
Phenylalanine	709	Organic acids	Amino acids and peptides	Amino acids
Glutamine	706	Organic acids	Amino acids and peptides	Amino acids
Tyrosine	703	Organic acids	Amino acids and peptides	Amino acids
Valine	683	Organic acids	Amino acids and peptides	Amino acids
Proline	669	Organic acids	Amino acids and peptides	Amino acids
Lysine	669	Organic acids	Amino acids and peptides	Amino acids
Aspartic acid	666	Organic acids	Amino acids and peptides	Amino acids
Tryptophan	650	Organic acids	Amino acids and peptides	Amino acids
Methionine	645	Organic acids	Amino acids and peptides	Amino acids
Alanine	632	Organic acids	Amino acids and peptides	Amino acids
Serine	622	Organic acids	Amino acids and peptides	Amino acids
Isoleucine	599	Organic acids	Amino acids and peptides	Amino acids
Histidine	598	Organic acids	Amino acids and peptides	Amino acids
Leucine	597	Organic acids	Amino acids and peptides	Amino acids
Succinic acid	596	Organic acids	TCA acids	TCA acids
Threonine	595	Organic acids	Amino acids and peptides	Amino acids
Malic acid	595	Organic acids	TCA acids	TCA acids
Lactic acid	593	Organic acids	Short-chain acids	Short-chain acids
Citric acid	587	Organic acids	TCA acids	TCA acids
Glycine	577	Organic acids	Amino acids and peptides	Amino acids
Ornithine	559	Organic acids	Amino acids and peptides	Amino acids
Asparagine	552	Organic acids	Amino acids and peptides	Amino acids
Taurine	527	Organic acids	Sulfonic acids	Sulfonic acids
Fumaric acid	522	Organic acids	TCA acids	TCA acids
Arginine	514	Organic acids	Amino acids and peptides	Amino acids
Hypoxanthine	495	Nucleic acids	Purines	Hypoxanthines
AMP	483	Nucleic acids	Purines	Purine rNMP
Palmitic acid	476	Fatty Acyls	Fatty acids	Saturated FA
Creatinine	466	Organoheterocyclic compounds	Azolines	Imidazolines
Pyroglutamic acid	462	Organoheterocyclic compounds	Pyrroline carboxylic acids	Pyrroline carboxylic acids
Citrulline	461	Organic acids	Amino acids and peptides	Amino acids
Stearic acid	461	Fatty Acyls	Fatty acids	Saturated FA
Glucose	459	Carbohydrates	Monosaccharides	Hexoses
Oxoglutaric acid	455	Organic acids	TCA acids	TCA acids
Inosine	446	Nucleic acids	Purines	Purine ribonucleosides
Pyruvic acid	440	Organic acids	Short-chain acids	Short-chain acids
Oleic acid	432	Fatty Acyls	Fatty acids	Unsaturated FA
Carnitine	430	Organic nitrogen compounds	Carnitines	Carnitines
Creatine	424	Organic acids	Amino acids and peptides	Amino acids
Pantothenic acid	412	Organic acids	Amino acids and peptides	Amino acids
Uric acid	407	Nucleic acids	Purines	Xanthines
Xanthine	406	Nucleic acids	Purines	Xanthines
Uridine	394	Nucleic acids	Pyrimidines	Pyrimidine ribonucleosides

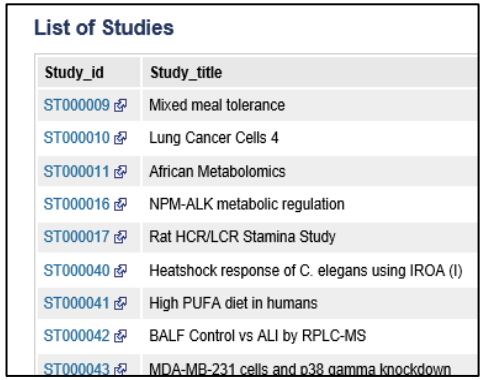
Links to MW structure database and list of studies containing each metabolite

Refmet Name	Studies	Super Class	Main Class	Sub Class
Glutamic acid	452	Organic acids	Amino acids and peptides	Amino acids
Tyrosine	441	Organic acids	Amino acids and peptides	Amino acids
Phenylalanine	437	Organic acids	Amino acids and peptides	Amino acids
Glutamine	435	Organic acids	Amino acids and peptides	Amino acids
Valine	428	Organic acids	Amino acids and peptides	Amino acids
Aspartic acid	423	Organic acids	Amino acids and peptides	Amino acids
Proline	413	Organic acids	Amino acids and peptides	Amino acids
Lysine	407	Organic acids	Amino acids and peptides	Amino acids
Malic acid	404	Organic acids	TCA acids	TCA acids
Tryptophan	395	Organic acids	Amino acids and peptides	Amino acids
Methionine	394	Organic acids	Amino acids and peptides	Amino acids
Isoleucine	392	Organic acids	Amino acids and peptides	Amino acids
Alanine	390	Organic acids	Amino acids and peptides	Amino acids

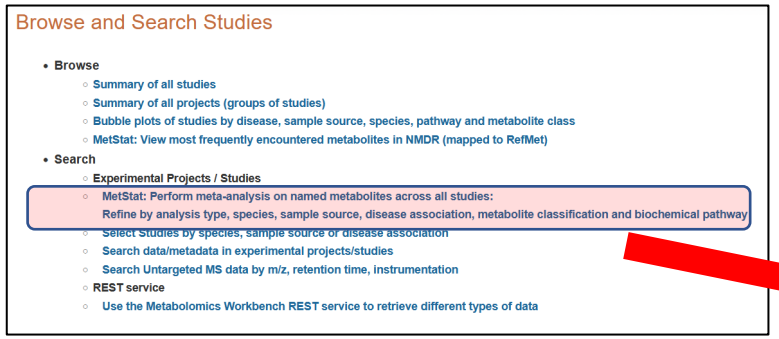
Structure (MW database)

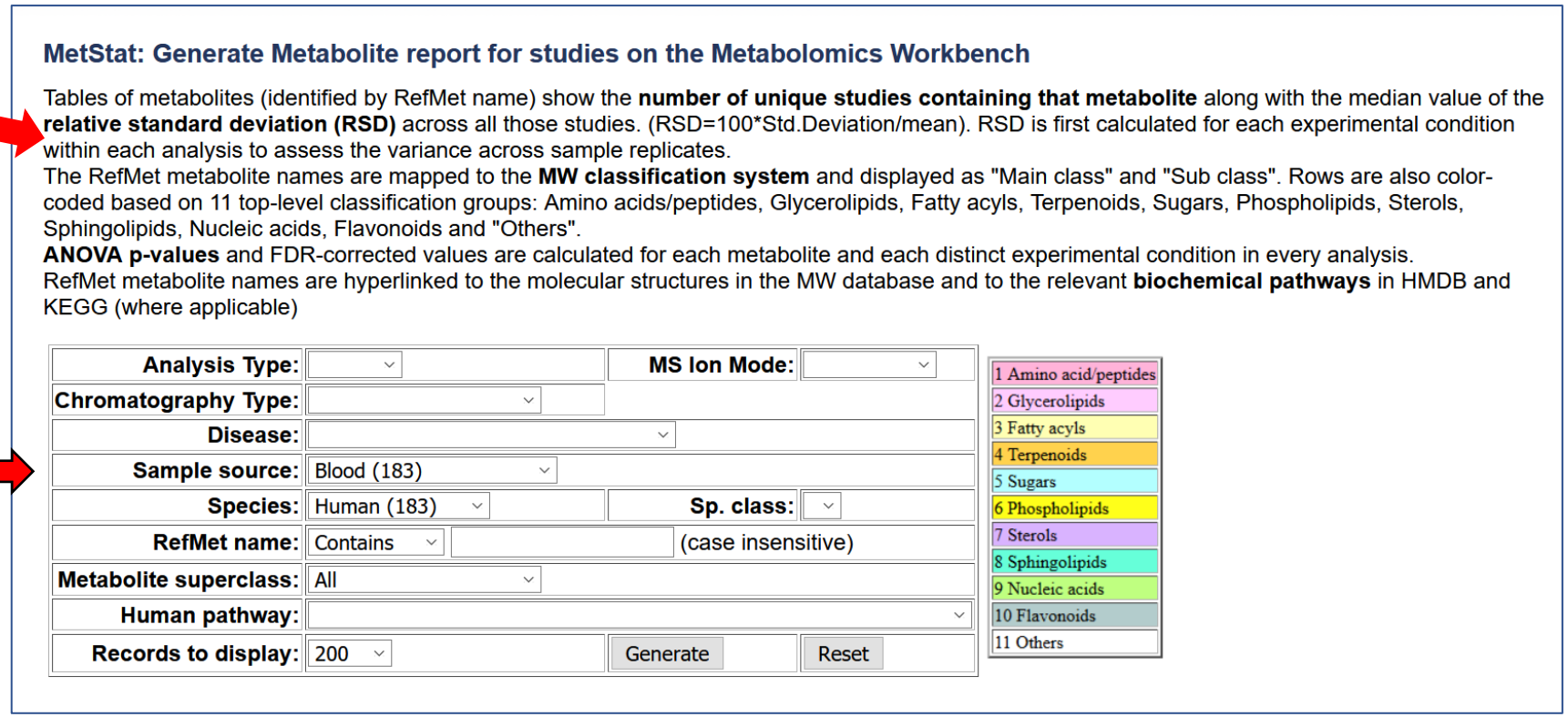


List of Studies



MetStat query buider: Select criteria, e.g. species, sample source, analysis type, ion mode, disease association, metabolite class.





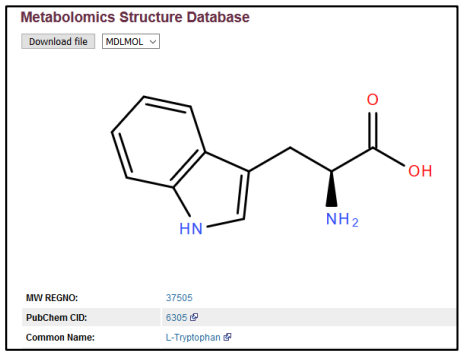
In this example, all human studies with blood* as the sample source are selected

*** "Blood" may refer to whole blood, serum or plasma-see individual study metadata for details**

MetStat summary table of human metabolites detected in blood

Sorted by number of studies in which that metabolite is reported

Structure (MW db)



MetStat: Search parameters: Source:Blood Species:Human | Most significant ANOVA measurements

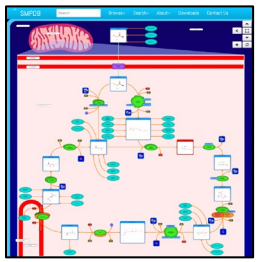
Refmet Name [Pathways]	Studies [Data Details]	RSD	Main Class	Sub Class
Proline [P]	111 [Data]	32.29	Amino acids and peptides	Amino acids
Tryptophan [P]	110 [Data]	22.04	Amino acids and peptides	Amino acids
Phenylalanine [P]	110 [Data]	21.72	Amino acids and peptides	Amino acids
Tyrosine [P]	108 [Data]	25.31	Amino acids and peptides	Amino acids
Valine [P]	108 [Data]	24.01	Amino acids and peptides	Amino acids
Glutamine [P]	105 [Data]	25.71	Amino acids and peptides	Amino acids
Histidine [P]	105 [Data]	25.80	Amino acids and peptides	Amino acids
Methionine [P]	105 [Data]	26.67	Amino acids and peptides	Amino acids
Lysine [P]	105 [Data]	26.12	Amino acids and peptides	Amino acids
Glutamic acid [P]	101 [Data]	43.28	Amino acids and peptides	Amino acids
Ornithine [P]	101 [Data]	34.02	Amino acids and peptides	Amino acids
Serine [P]	99 [Data]	26.11	Amino acids and peptides	Amino acids
Isoleucine [P]	99 [Data]	28.60	Amino acids and peptides	Amino acids
Leucine [P]	98 [Data]	27.90	Amino acids and peptides	Amino acids
Creatinine [P]	95 [Data]	29.39	Azolines	Imidazolines
Stearic acid [P]	94 [Data]	30.47	Fatty acids	Saturated FA
Alanine [P]	93 [Data]	26.38	Amino acids and peptides	Amino acids
Uric acid [P]	92 [Data]	25.65	Purines	Xanthines
Linoleic acid [P]	91 [Data]	50.53	Fatty acids	Unsaturated FA
Asparagine [P]	89 [Data]	25.38	Amino acids and peptides	Amino acids
Threonine [P]	88 [Data]	27.93	Amino acids and peptides	Amino acids
Palmitic acid [P]	88 [Data]	33.31	Fatty acids	Saturated FA
Oleic acid [P]	88 [Data]	49.22	Fatty acids	Unsaturated FA
Aspartic acid [P]	87 [Data]	39.78	Amino acids and peptides	Amino acids
Taurine [P]	84 [Data]	39.66	Sulfonic acids	Sulfonic acids
Arachidonic acid [P]	84 [Data]	42.06	Fatty acids	Unsaturated FA
Citrulline [P]	83 [Data]	29.88	Amino acids and peptides	Amino acids
Lactic acid [P]	82 [Data]	37.17	Short-chain acids	Short-chain acids
Citric acid [P]	82 [Data]	30.27	TCA acids	TCA acids
Palmitoleic acid [P]	82 [Data]	63.72	Fatty acids	Unsaturated FA
Myristic acid [P]	81 [Data]	42.07	Fatty acids	Saturated FA
Glycine [P]	81 [Data]	30.30	Amino acids and peptides	Amino acids
Arginine [P]	81 [Data]	26.07	Amino acids and peptides	Amino acids
Malic acid [P]	80 [Data]	35.52	TCA acids	TCA acids
Hypoxanthine [P]	80 [Data]	55.48	Purines	Hypoxanthines
Succinic acid [P]	80 [Data]	33.90	TCA acids	TCA acids
Cholesterol [P]	79 [Data]	24.16	Sterols	Cholesterols
Pyroglutamic acid [P]	78 [Data]	31.77	Pyrroline carboxylic acids	Pyrroline carboxylic acids
Kynurenine [P]	75 [Data]	30.52	Butyrophenones	Butyrophenones
LPC 16:0 [P]	74 [Data]	35.90	Glycerophosphocholines	LPC
Carnitine [P]	73 [Data]	23.34	Carnitines	Carnitines

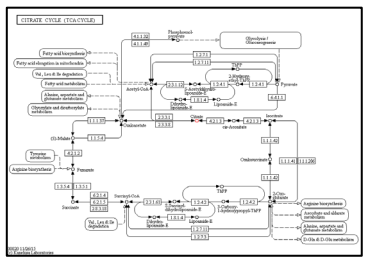
List of Studies

List of Studies

Study_id	Study_title
ST000009	Mixed meal tolerance
ST000010	Lung Cancer Cells 4
ST000011	African Metabolomics
ST000016	NPM-ALK metabolic regulation
ST000017	Rat HCR/LCR Stamina Study
ST000040	Heatshock response of C. elegans using IROA (I)
ST000041	High PUFA diet in humans
ST000042	BALF Control vs ALI by RPLC-MS
ST000043	MDA-MB-231 cells and p38 gamma knockdown

[P]:Human Pathways (SMP/KEGG)





Relative standard deviation (RSD) =100*Standard deviation/mean
The RSD is calculated separately for each experimental condition within each study.
It is a measure of the variance across sample replicates

MetStat “data” link displays a histogram of RSD data across all studies containing Valine

Additional data on ANOVA statistics in each study and RSD/replicate information

MetStat: Search parameters: Source:Blood Species:Human | Most significant ANOVA measurements

Refmet Name [Pathways]	Studies [Data Details]	RSD	Main Class	Sub Class
Proline [P]	111 [Data]	32.29	Amino acids and peptides	Amino acids
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Cholesterol [P]	79 [Data]	24.16	Sterols	Cholesterols
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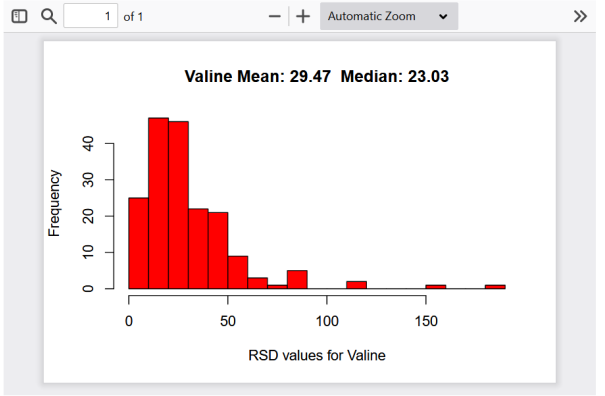
LPC 16:0 [P]	74 [Data]	35.90	Glycerophosphocholines	LPC
Carnitine [P]	73 [Data]	23.34	Carnitines	Carnitines

Histogram of RSD values for Valine(Name:Valine Source:Blood Species:Human)



Valine(Name:Valine Source:Blood Species:Human)
ANOVA results for this metabolite where p-value <=0.05

Name	Study_id	Analysis_id	ANOVA p-Value	FDR	Experimental Conditions (factors)
Valine	ST000589	AN000904	3.769E-270	5.905E-269	Plasma Volume Extracted;0 uL;100 uL;150 uL;200 uL;25 uL;300 ...
valine	ST001386	AN002314	1.642E-122	1.689E-121	cc;1;2;3;4;5;6
valine	ST000385	AN000620	3.140E-38	2.170E-37	Organ;Plasma;Serum;Serum or Plasma
Valine	ST000586	AN000901	2.250E-28	9.080E-28	Plasma Volume;0 uL;150 uL;700 uL
valine	ST001815	AN002944	1.722E-22	4.147E-22	Timepoint;-;3
valine	ST001842	AN002985	1.051E-23	8.249E-22	Organ;plasma;liver
VALINE (M+H)+	ST000842	AN001357	2.120E-21	7.450E-21	Sample type;Muscles;Plasma;Pooled sample
L-valine	ST000608	AN000931	7.270E-19	1.420E-18	Sample_Type;blotter;serum
Valine	ST000051	AN000087	2.540E-15	1.840E-14	As Exposure;high;low;Pooled-High;Pooled-Low;Pooled-Total
Valine 1 - CPMG-1	ST000892	AN001454	2.960E-15	2.360E-14	Sample type;Extracted plasma;Intact plasma
Valine 2 - CPMG-1	ST000892	AN001454	3.000E-15	2.360E-14	Sample type;Extracted plasma;Intact plasma
Valine 2 - CPMG-2	ST000892	AN001454	2.580E-15	2.360E-14	Sample type;Extracted plasma;Intact plasma
Valine 1 - PROJECT-1	ST000892	AN001454	5.080E-15	3.000E-14	Sample type;Extracted plasma;Intact plasma
Valine 2 - PROJECT-1	ST000892	AN001454	6.830E-15	3.230E-14	Sample type;Extracted plasma;Intact plasma
Valine 1 - CPMG-3	ST000892	AN001454	8.000E-15	3.360E-14	Sample type;Extracted plasma;Intact plasma
Valine 2 - CPMG-3	ST000892	AN001454	8.050E-15	3.360E-14	Sample type;Extracted plasma;Intact plasma
L-valine 1	ST000865	AN001390	1.080E-13	2.020E-13	Patient group;CIRR;HCC;Pool CIRR;Pool HCC;POSSIBLE CASE;-

Valine(Name:Valine Source:Blood Species:Human)
List of studies, analyses, submitted metabolite names, experimental conditions and RSD values

Replicate numbers reflect the number of replicates for each experimental condition where the measured value was not null

Name	Study_id	Analysis_id	Factors	Range(RSD)	Replicates
Valine	ST000046	AN000079	Cognitive Status:AD	23.56	30
Valine	ST000046	AN000079	Cognitive Status:CN	17.51	30
Valine	ST000046	AN000079	Cognitive Status:MCI	20.69	30
Valine	ST000051	AN000087	As Exposure:high	19.32	25
Valine	ST000051	AN000087	As Exposure:low	18.43	25
valine	ST000062	AN000100	Source:Group 1 - Score 0	19.37	48
valine	ST000062	AN000100	Source:Group 2 - Score 50	18.63	49
Val_Valine	ST000091	AN000145	Treatment:Control	16.59	9
Val_Valine	ST000091	AN000145	Treatment:Insulin Deprived	22.96	8
Val_Valine	ST000091	AN000145	Treatment:Insulin Treatment	20.16	9

List of human studies on blood that report Proline

List of Studies (Metabolite:Proline Source:Blood Species:Human)

Study_id	Analysis_id	Study_title	Source	Species	Disease	Institute	Units(range)
ST001037	AN001698	High Resolution GC-MS and FID Metabolomics of Human Serum	Blood	Human		Wake Forest Baptist Medical Center	Abundance
ST000450	AN000705	Metabolic features of chronic fatigue syndrome	Blood	Human	Chronic fatigue syndrome	University of California, San Diego	Area under curve
ST000617	AN000947	Validation of the application of targeted metabolomic appraoch in the diagnosis of CFS	Blood	Human	Chronic fatigue syndrome	University of California, San Diego	Area under curve
ST000041	AN000062	High PUFA diet in humans	Blood	Human		University of Michigan	Counts
ST000041	AN000063	High PUFA diet in humans	Blood	Human		University of Michigan	Counts
ST000105	AN000173	SCOR Metabolomics	Blood	Human		University of Chicago	Counts
ST000105	AN000174	SCOR Metabolomics	Blood	Human		University of Chicago	Counts
ST000106	AN000175	IWMS Study 1:Weight comparison of obese and lean patients	Blood	Human	Obesity	University of Michigan	Counts
ST000106	AN000176	IWMS Study 1:Weight comparison of obese and lean patients	Blood	Human	Obesity	University of Michigan	Counts
ST000368	AN000602	Investigation of metabolomic blood biomarkers for detection of adenocarcinoma lung cancer	Blood	Human	Cancer	University of California, Davis	Counts

...

ST001515	AN002511	A Metabolomic Signature of Glucagon Action in Healthy Individuals with Overweight/Obesity Humans	Blood	Human	Obesity	Translational Research Institute-AdventHealth Orlando	scaled units
ST000091	AN000145	Quantitative Metabolomics by 1H-NMR and LC-MS/MS Confirms Altered Metabolic Pathways in Diabetes	Blood	Human	Diabetes	Mayo Clinic	uM
ST000137	AN000219	Metabolomics in sarcoidosis	Blood	Human	Sarcoidosis	Wayne State University	uM
ST000168	AN000262	Effect of Insulin Sensitizer Therapy on Amino Acids and Their Metabolites	Blood	Human	Diabetes	Mayo Clinic	uM
ST000435	AN000685	Quantitative measurements of amino acids in T1D poor control, good control, and controls.	Blood	Human	Diabetes	Mayo Clinic	uM
ST000483	AN000749	Amino Acid Quantifcation of obese patients on a 16 week caloric restriction from Plasma	Blood	Human	Obesity	Mayo Clinic	uM
ST000491	AN000757	Sleep apnea and cardiovascular samples amino acid metabolites	Blood	Human	Sleep apnea	Mayo Clinic	uM
ST000524	AN000802	Effects of Curcumin Supplementation on the Amino Acid Concentration of Older Adults: Relation to Vascular Function	Blood	Human	Heart disease	Mayo Clinic	uM
ST000605	AN000926	Whole blood reveals more metabolic detail of the human metabolome than serum as measured by 1H-NMR spectroscopy: Implications for sepsis metabolomics	Blood	Human		University of Michigan	uM
ST000641	AN000973	Targeted Amino Acids in American Indian Adolescents (part II)	Blood	Human	Diabetes	Mayo Clinic	uM
ST000783	AN001239	Absolute Quantification of 180 metabolites in serum from african american and european american in prostate cancer and case control samples	Blood	Human	Cancer	Baylor College of Medicine	uM
ST000785	AN001244	Pharmacometabolomics of L-Carnitine Treatment Response Phenotypes in Patients with Septic Shock	Blood	Human	Sepsis	University of Michigan	uM
ST000825	AN001311	CHEAR Christiani Biocrates	Blood	Human		RTI International	uM
ST000826	AN001414	CHEAR Christiani NMR	Blood	Human		RTI International	uM
ST000876	AN001413	Human serum for a patient with neuropathy being treated with L-serine.	Blood	Human	Neuropathy	University of Helsinki	uM
ST000944	AN001549	Amino Acids, Acylcarnitine, & Insulin for P20 Participants	Blood	Human		University of Michigan	uM
ST000995	AN001624	Amino Acid Concentrations of Primary Sclerosing Cholangitis (part I)	Blood	Human		Mayo Clinic	uM
ST001012	AN001654	Amino Acid Concentrations in Serum for Muscle Wasting in Cancer Cachexia (part-VII)	Blood	Human	Cachexia	Mayo Clinic	uM
ST001097	AN001785	Metabolomics of Metabolic Risk in Patients Taking Atypical Antipsychotics	Blood	Human	Schizophrenia	University of Michigan	uM
ST001176	AN001952	Metabolite changes in human plasma before and after YF17D vaccination in symptomatic and asymptomatic subjects	Blood	Human	Yellow fever	Duke-NUS Medical School	uM
ST001295	AN002156	Estimating Platelet Mitochondrial Function in Patients with Sepsis - WB NMRs (part-II)	Blood	Human	Sepsis	University of Michigan, University of Mississippi, University of Minnesota	uM
ST001319	AN002195	Pre-treatment L-Carnitine Pharmacometabolomics in Sepsis (CaPS) Patients	Blood	Human	Sepsis	University of Michigan	uM
ST001354	AN002253	48 hours post-treatment L-Carnitine Pharmacometabolomics in Sepsis (CaPS) Patients	Blood	Human	Sepsis	University of Michigan	uM
ST001521	AN002533	Plasma metabolites of known identity profiled using hybrid nontargeted methods (part-III)	Blood	Human		Broad Institute of MIT and Harvard	unitless peak areas

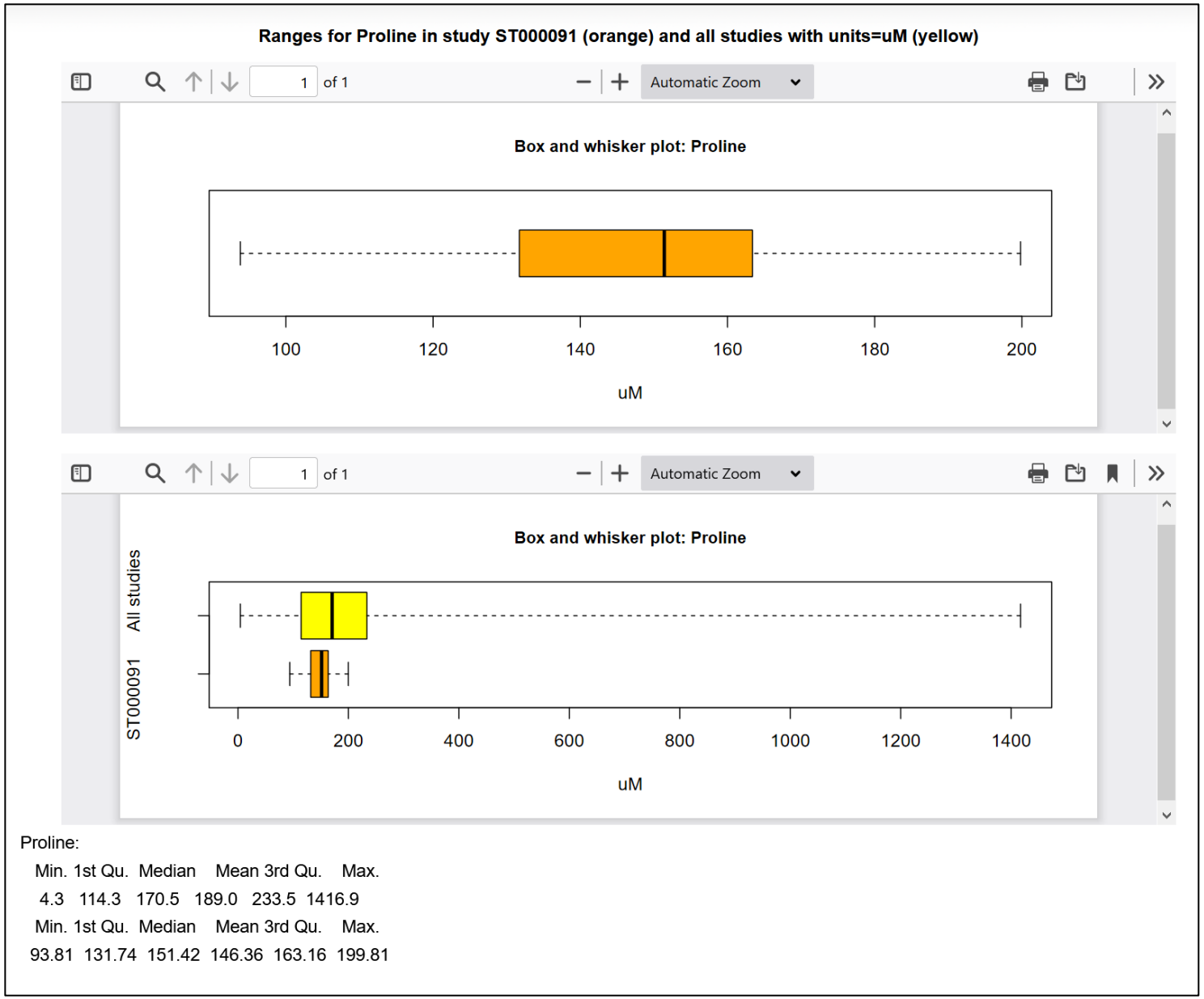
Click on a study link in the “Units(range) column

Focus on the targeted assays that report quantitative results (untargeted assays that report peak intensity, area, etc. are no good)

Boxplot for Proline in human blood

Study ST000091

Comparison with all studies (yellow) that report proline in human blood.
Notice the outlier(s) since many different studies are involved. However, the median is not significantly affected.

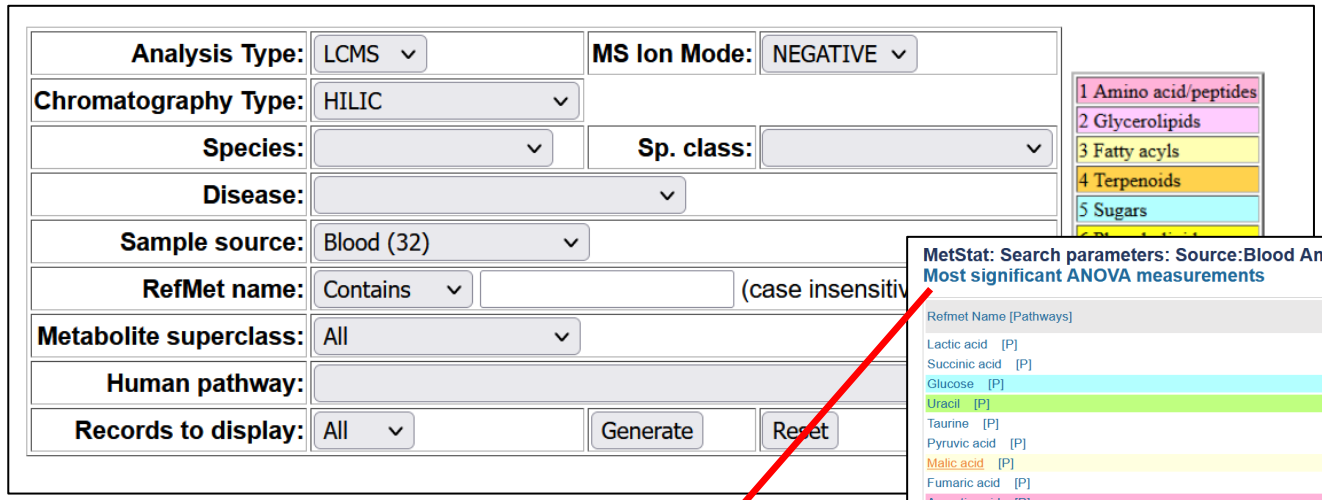


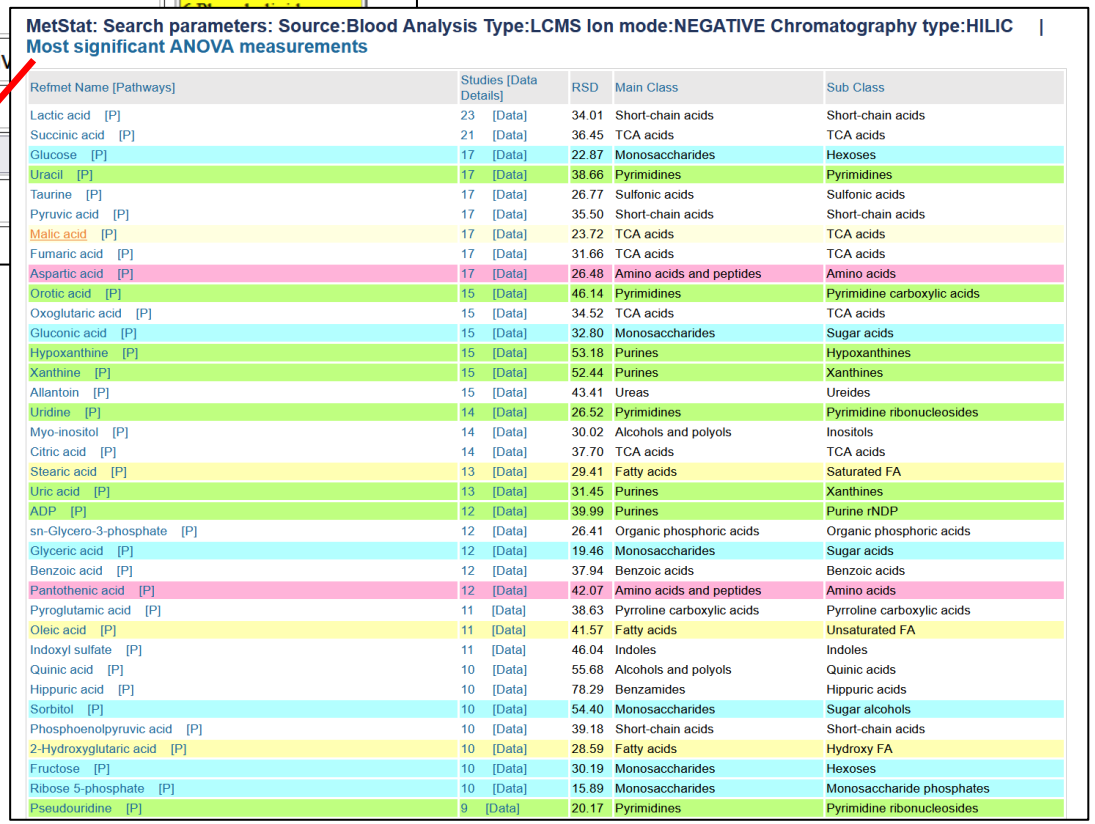
Proline:

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
4.3	114.3	170.5	189.0	233.5	1416.9

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
93.81	131.74	151.42	146.36	163.16	199.81

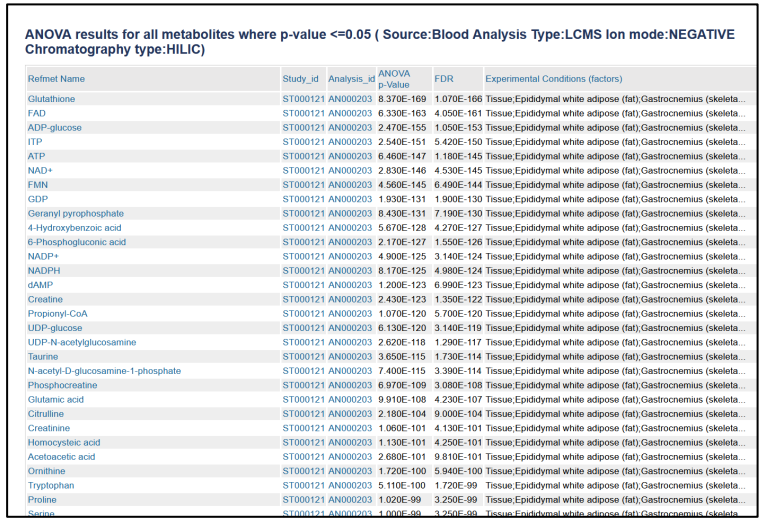
MetStat query buider: Select criteria, e.g. species, sample source, analysis type, ion mode, disease association, metabolite class.





MetStat: Search parameters: Source:Blood Analysis Type:LCMS Ion mode:NEGATIVE Chromatography type:HILIC |
Most significant ANOVA measurements

Refmet Name [Pathways]	Studies [Data Details]	RSD	Main Class	Sub Class
Lactic acid [P]	23 [Data]	34.01	Short-chain acids	Short-chain acids
Succinic acid [P]	21 [Data]	36.45	TCA acids	TCA acids
Glucose [P]	17 [Data]	22.87	Monosaccharides	Hexoses
Uracil [P]	17 [Data]	38.66	Pyrimidines	Pyrimidines
Taurine [P]	17 [Data]	26.77	Sulfonic acids	Sulfonic acids
Pyruvic acid [P]	17 [Data]	35.50	Short-chain acids	Short-chain acids
Malic acid [P]	17 [Data]	23.72	TCA acids	TCA acids
Fumaric acid [P]	17 [Data]	31.66	TCA acids	TCA acids
Aspartic acid [P]	17 [Data]	26.48	Amino acids and peptides	Amino acids
Orotic acid [P]	15 [Data]	46.14	Pyrimidines	Pyrimidine carboxylic acids
Oxoglutaric acid [P]	15 [Data]	34.52	TCA acids	TCA acids
Gluconic acid [P]	15 [Data]	32.80	Monosaccharides	Sugar acids
Hypoxanthine [P]	15 [Data]	53.18	Purines	Hypoxanthines
Xanthine [P]	15 [Data]	52.44	Purines	Xanthines
Allantoin [P]	15 [Data]	43.41	Ureas	Ureides
Uridine [P]	14 [Data]	26.52	Pyrimidines	Pyrimidine ribonucleosides
Myo-inositol [P]	14 [Data]	30.02	Alcohols and polyols	Inositols
Citric acid [P]	14 [Data]	37.70	TCA acids	TCA acids
Stearic acid [P]	13 [Data]	29.41	Fatty acids	Saturated FA
Uric acid [P]	13 [Data]	31.45	Purines	Xanthines
ADP [P]	12 [Data]	39.99	Purines	Purine rNDP
sn-Glycero-3-phosphate [P]	12 [Data]	26.41	Organic phosphoric acids	Organic phosphoric acids
Glyceric acid [P]	12 [Data]	19.46	Monosaccharides	Sugar acids
Benzoic acid [P]	12 [Data]	37.94	Benzoic acids	Benzoic acids
Pantothenic acid [P]	12 [Data]	42.07	Amino acids and peptides	Amino acids
Pyroglutamic acid [P]	11 [Data]	38.63	Pyrroline carboxylic acids	Pyrroline carboxylic acids
Oleic acid [P]	11 [Data]	41.57	Fatty acids	Unsaturated FA
Indoxyl sulfate [P]	11 [Data]	46.04	Indoles	Indoles
Quinic acid [P]	10 [Data]	55.68	Alcohols and polyols	Quinic acids
Hippuric acid [P]	10 [Data]	78.29	Benzamides	Hippuric acids
Sorbitol [P]	10 [Data]	54.40	Monosaccharides	Sugar alcohols
Phosphoenolpyruvic acid [P]	10 [Data]	39.18	Short-chain acids	Short-chain acids
2-Hydroxyglutaric acid [P]	10 [Data]	28.59	Fatty acids	Hydroxy FA
Fructose [P]	10 [Data]	30.19	Monosaccharides	Hexoses
Ribose 5-phosphate [P]	10 [Data]	15.89	Monosaccharides	Monosaccharide phosphates
Pseudouridine [P]	9 [Data]	20.17	Pyrimidines	Pyrimidine ribonucleosides

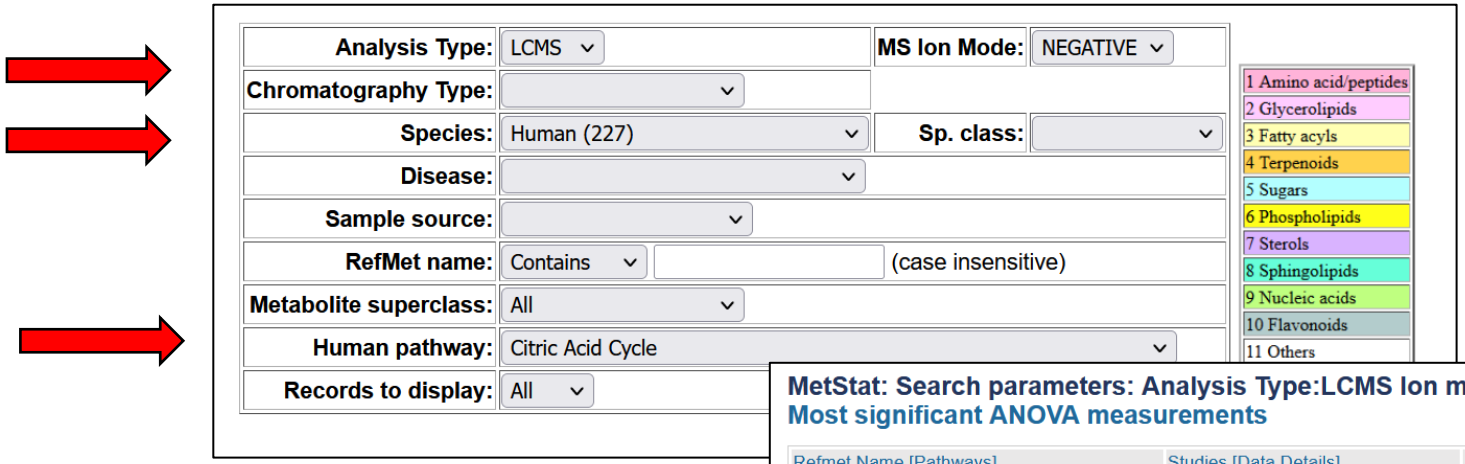


ANOVA results for all metabolites where p-value <=0.05 (Source:Blood Analysis Type:LCMS Ion mode:NEGATIVE Chromatography type:HILIC)

Refmet Name	Study_id	Analysis_id	ANOVA p-Value	FDR	Experimental Conditions (factors)
Glutathione	ST000121	AN000203	8.370E-169	1.070E-166	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
FAD	ST000121	AN000203	6.330E-163	4.050E-161	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
ADP-glucose	ST000121	AN000203	2.470E-155	1.050E-153	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
ITP	ST000121	AN000203	2.540E-151	5.420E-150	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
ATP	ST000121	AN000203	6.460E-147	1.180E-145	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
NAD+	ST000121	AN000203	2.830E-146	4.530E-145	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
FMN	ST000121	AN000203	4.560E-145	6.490E-144	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
GDP	ST000121	AN000203	1.930E-131	1.900E-130	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Geranyl pyrophosphate	ST000121	AN000203	8.430E-131	7.190E-130	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
4-Hydroxybenzoic acid	ST000121	AN000203	5.670E-128	4.270E-127	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
6-Phosphogluconic acid	ST000121	AN000203	2.170E-127	1.550E-126	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
NADP+	ST000121	AN000203	4.900E-125	3.140E-124	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
NADPH	ST000121	AN000203	8.170E-125	4.980E-124	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
dAMP	ST000121	AN000203	1.200E-123	6.990E-123	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Creatine	ST000121	AN000203	2.430E-123	1.350E-122	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Propionyl-CoA	ST000121	AN000203	1.070E-120	5.700E-120	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
UDP-glucose	ST000121	AN000203	6.130E-120	3.140E-119	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
UDP-N-acetylglucosamine	ST000121	AN000203	2.620E-118	1.290E-117	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Taurine	ST000121	AN000203	3.650E-115	1.730E-114	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
N-acetyl-D-glucosamine-1-phosphate	ST000121	AN000203	7.400E-115	3.390E-114	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Phosphocreatine	ST000121	AN000203	6.970E-109	3.080E-108	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Glutamic acid	ST000121	AN000203	9.910E-108	4.230E-107	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Citrulline	ST000121	AN000203	2.180E-104	9.000E-104	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Creatinine	ST000121	AN000203	1.060E-101	4.130E-101	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Homocysteic acid	ST000121	AN000203	1.130E-101	4.250E-101	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Acetoacetic acid	ST000121	AN000203	2.680E-101	9.810E-101	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Ornithine	ST000121	AN000203	1.720E-100	5.940E-100	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Tryptophan	ST000121	AN000203	5.110E-100	1.720E-99	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Proline	ST000121	AN000203	1.020E-99	3.250E-99	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...
Serine	ST000121	AN000203	1.000E-99	3.250E-99	Tissue;Epididymal white adipose (fat);Gastrocnemius (skeleta...

In this example, all studies with blood as the sample source using LCMS and HILIC chromatography in negative ion mode are selected

MetStat query buider: Select criteria, e.g. species, sample source, analysis type, ion mode, disease association, metabolite class.



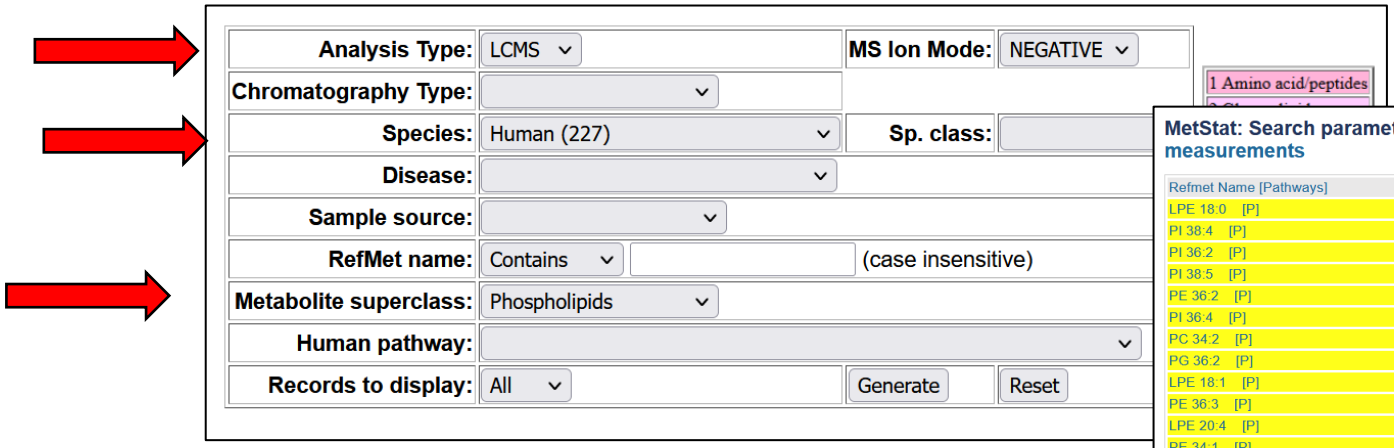
MetStat: Search parameters: Analysis Type:LCMS Ion mode:NEGATIVE Species:Human Pathway ID:SMP00057

Most significant ANOVA measurements

Refmet Name [Pathways]	Studies [Data Details]	RSD	Main Class	Sub Class
Malic acid [P]	107 [Data]	32.79	TCA acids	TCA acids
Citric acid [P]	84 [Data]	30.89	TCA acids	TCA acids
Succinic acid [P]	79 [Data]	32.84	TCA acids	TCA acids
ADP [P]	62 [Data]	35.86	Purines	Purine rNDP
Fumaric acid [P]	61 [Data]	35.13	TCA acids	TCA acids
Pyruvic acid [P]	60 [Data]	37.81	Short-chain acids	Short-chain acids
Oxoglutaric acid [P]	60 [Data]	49.35	TCA acids	TCA acids
ATP [P]	52 [Data]	41.12	Purines	Purine rNTP
NAD+ [P]	40 [Data]	34.97	Nicotinamides	Nicotinamide dinucleotides
FAD [P]	35 [Data]	31.58	Flavins	Flavin nucleotides
NADH [P]	34 [Data]	36.65	Nicotinamides	Nicotinamide dinucleotides
cis-Aconitic acid [P]	30 [Data]	39.01	TCA acids	TCA acids
Oxaloacetic acid [P]	26 [Data]	25.02	TCA acids	TCA acids
GDP [P]	25 [Data]	40.99	Purines	Purine rNDP
Acetyl-CoA [P]	22 [Data]	37.03	Fatty esters	Acyl CoAs
GTP [P]	17 [Data]	29.44	Purines	Purine rNTP
Biotin [P]	11 [Data]	20.08	Heterocyclic compounds	Biotin
Coenzyme A [P]	5 [Data]	30.56	Purines	Coenzyme A
Lipoamide [P]	3 [Data]	69.53	Fatty amides	Primary amides
Thiamine diphosphate [P]	3 [Data]	80.85	Pyrimidines	Thiamine phosphates

In this example, human studies using LCMS in negative ion mode for Citric acid cycle metabolites are selected

MetStat query buider: Select criteria, e.g. species, sample source, analysis type, ion mode, disease association, metabolite class.



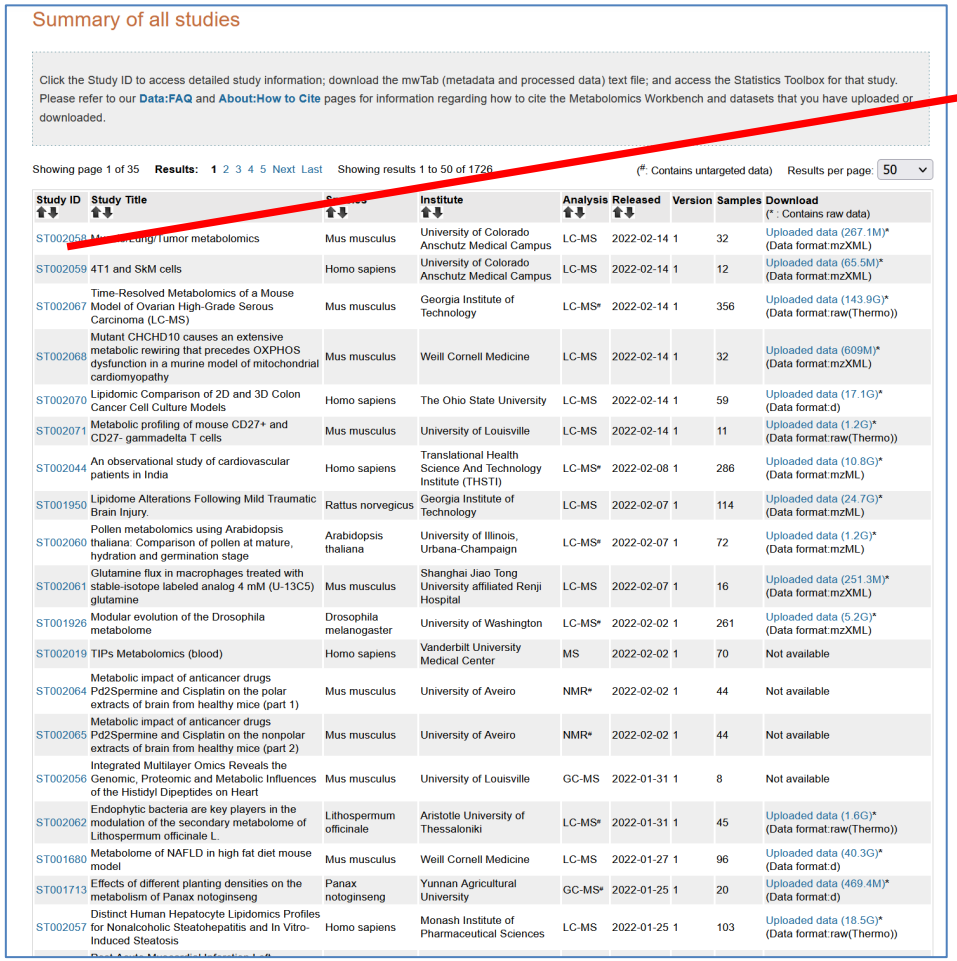
MetStat: Search parameters: Analysis Type:LCMS Ion mode:NEGATIVE Species:Human | Most significant ANOVA measurements

Refmet Name [Pathways]	Studies [Data Details]	RSD	Main Class	Sub Class
LPE 18:0 [P]	63 [Data]	40.01	Glycerophosphoethanolamines	LPE
PI 38:4 [P]	49 [Data]	34.81	Glycerophosphoinositols	PI
PI 36:2 [P]	48 [Data]	37.79	Glycerophosphoinositols	PI
PI 38:5 [P]	43 [Data]	36.94	Glycerophosphoinositols	PI
PE 36:2 [P]	42 [Data]	40.28	Glycerophosphoethanolamines	PE
PI 36:4 [P]	42 [Data]	36.92	Glycerophosphoinositols	PI
PC 34:2 [P]	40 [Data]	30.16	Glycerophosphocholines	PC
PG 36:2 [P]	40 [Data]	40.47	Glycerophosphoglycerols	PG
LPE 18:1 [P]	40 [Data]	48.15	Glycerophosphoethanolamines	LPE
PE 36:3 [P]	39 [Data]	46.77	Glycerophosphoethanolamines	PE
LPE 20:4 [P]	39 [Data]	40.00	Glycerophosphoethanolamines	LPE
PE 34:1 [P]	39 [Data]	42.35	Glycerophosphoethanolamines	PE
PI 38:3 [P]	38 [Data]	37.90	Glycerophosphoinositols	PI
PC 32:2 [P]	38 [Data]	35.95	Glycerophosphocholines	PC
LPE 16:0 [P]	38 [Data]	43.83	Glycerophosphoethanolamines	LPE
PI 34:2 [P]	38 [Data]	38.63	Glycerophosphoinositols	PI
PC 32:1 [P]	38 [Data]	38.07	Glycerophosphocholines	PC
PE 36:1 [P]	38 [Data]	39.51	Glycerophosphoethanolamines	PE
PC 36:3 [P]	37 [Data]	25.61	Glycerophosphocholines	PC
PC 32:0 [P]	37 [Data]	23.45	Glycerophosphocholines	PC
PE 38:4 [P]	37 [Data]	42.16	Glycerophosphoethanolamines	PE
PC 38:4 [P]	37 [Data]	31.52	Glycerophosphocholines	PC
PC 38:5 [P]	37 [Data]	27.02	Glycerophosphocholines	PC
PE 34:2 [P]	36 [Data]	45.35	Glycerophosphoethanolamines	PE
PC 36:1 [P]	36 [Data]	25.44	Glycerophosphocholines	PC
PC 36:2 [P]	36 [Data]	28.93	Glycerophosphocholines	PC
PE 38:6 [P]	36 [Data]	47.87	Glycerophosphoethanolamines	PE
PC 38:2 [P]	35 [Data]	25.95	Glycerophosphocholines	PC
PC 38:3 [P]	35 [Data]	31.71	Glycerophosphocholines	PC
PC 33:1 [P]	35 [Data]	31.10	Glycerophosphocholines	PC
LPE 18:2 [P]	35 [Data]	39.54	Glycerophosphoethanolamines	LPE
PC 34:3 [P]	35 [Data]	30.71	Glycerophosphocholines	PC
PI 40:5 [P]	35 [Data]	42.30	Glycerophosphoinositols	PI
PI 34:1 [P]	35 [Data]	40.51	Glycerophosphoinositols	PI
PI 36:1 [P]	35 [Data]	35.54	Glycerophosphoinositols	PI
LPE 22:6 [P]	34 [Data]	44.92	Glycerophosphoethanolamines	LPE
PC 40:6 [P]	34 [Data]	33.55	Glycerophosphocholines	PC
PC 34:1 [P]	34 [Data]	27.20	Glycerophosphocholines	PC
PC 40:5 [P]	34 [Data]	32.55	Glycerophosphocholines	PC
PC 36:4 [P]	34 [Data]	31.47	Glycerophosphocholines	PC
PS 38:4 [P]	34 [Data]	51.02	Glycerophosphoserines	PS
PE 32:1 [P]	34 [Data]	62.88	Glycerophosphoethanolamines	PE

In this example, human studies using LCMS in negative ion mode containing Phospholipids are selected

NMDR:Study-level analysis options

Study summary page



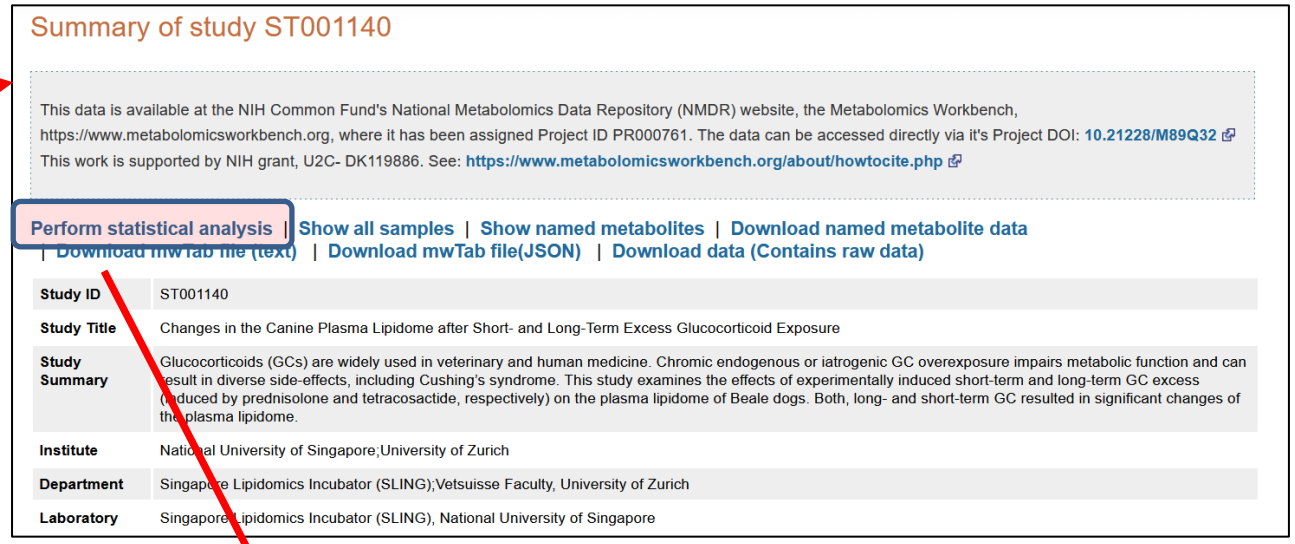
Summary of all studies

Click the Study ID to access detailed study information; download the mwTab (metadata and processed data) text file; and access the Statistics Toolbox for that study. Please refer to our **Data:FAQ** and **About:How to Cite** pages for information regarding how to cite the Metabolomics Workbench and datasets that you have uploaded or downloaded.

Showing page 1 of 35 **Results:** 1 2 3 4 5 Next Last Showing results 1 to 50 of 1726 (#: Contains untargeted data) Results per page: 50

Study ID	Study Title	Species	Institute	Analysis	Released	Version	Samples	Download (*: Contains raw data)
ST002058	M...eding/Tumor metabolomics	Mus musculus	University of Colorado Anschutz Medical Campus	LC-MS	2022-02-14	1	32	Uploaded data (267.1M)* (Data format:mzXML)
ST002059	4T1 and SkM cells	Homo sapiens	University of Colorado Anschutz Medical Campus	LC-MS	2022-02-14	1	12	Uploaded data (65.5M)* (Data format:mzXML)
ST002067	Time-Resolved Metabolomics of a Mouse Model of Ovarian High-Grade Serous Carcinoma (LC-MS)	Mus musculus	Georgia Institute of Technology	LC-MS*	2022-02-14	1	356	Uploaded data (143.9G)* (Data format:raw(Thermo))
ST002068	Mutant CHCHD10 causes an extensive metabolic rewiring that precedes OXPHOS dysfunction in a murine model of mitochondrial cardiomyopathy	Mus musculus	Weill Cornell Medicine	LC-MS	2022-02-14	1	32	Uploaded data (609M)* (Data format:mzXML)
ST002070	Lipidomic Comparison of 2D and 3D Colon Cancer Cell Culture Models	Homo sapiens	The Ohio State University	LC-MS	2022-02-14	1	59	Uploaded data (17.1G)* (Data format:d)
ST002071	Metabolic profiling of mouse CD27+ and CD27- gammadelta T cells	Mus musculus	University of Louisville	LC-MS	2022-02-14	1	11	Uploaded data (1.2G)* (Data format:raw(Thermo))
ST002044	An observational study of cardiovascular patients in India	Homo sapiens	Translational Health Science And Technology Institute (THSTI)	LC-MS*	2022-02-08	1	286	Uploaded data (10.8G)* (Data format:mzML)
ST001950	Lipidome Alterations Following Mild Traumatic Brain Injury.	Rattus norvegicus	Georgia Institute of Technology	LC-MS	2022-02-07	1	114	Uploaded data (24.7G)* (Data format:mzML)
ST002060	Pollen metabolomics using Arabidopsis thaliana: Comparison of pollen at mature, hydration and germination stage	Arabidopsis thaliana	University of Illinois, Urbana-Champaign	LC-MS*	2022-02-07	1	72	Uploaded data (1.2G)* (Data format:mzML)
ST002061	Glutamine flux in macrophages treated with stable-isotope labeled analog 4 mM (U-13C5) glutamine	Mus musculus	Shanghai Jiao Tong University affiliated Renji Hospital	LC-MS	2022-02-07	1	16	Uploaded data (251.3M)* (Data format:mzXML)
ST001926	Modular evolution of the Drosophila metabolome	Drosophila melanogaster	University of Washington	LC-MS*	2022-02-02	1	261	Uploaded data (5.2G)* (Data format:mzXML)
ST002019	TIPs Metabolomics (blood)	Homo sapiens	Vanderbilt University Medical Center	MS	2022-02-02	1	70	Not available
ST002064	Metabolic impact of anticancer drugs Pd2Spermine and Cisplatin on the polar extracts of brain from healthy mice (part 1)	Mus musculus	University of Aveiro	NMR*	2022-02-02	1	44	Not available
ST002065	Metabolic impact of anticancer drugs Pd2Spermine and Cisplatin on the nonpolar extracts of brain from healthy mice (part 2)	Mus musculus	University of Aveiro	NMR*	2022-02-02	1	44	Not available
ST002056	Integrated Multilayer Omics Reveals the Genomic, Proteomic and Metabolic Influences of the Histidyl Dipeptides on Heart	Mus musculus	University of Louisville	GC-MS	2022-01-31	1	8	Not available
ST002062	Endophytic bacteria are key players in the modulation of the secondary metabolome of Lithospermum officinale L.	Lithospermum officinale	Aristotle University of Thessaloniki	LC-MS*	2022-01-31	1	45	Uploaded data (1.6G)* (Data format:raw(Thermo))
ST001680	Metabolome of NAFLD in high fat diet mouse model	Mus musculus	Weill Cornell Medicine	LC-MS	2022-01-27	1	96	Uploaded data (40.3G)* (Data format:d)
ST001713	Effects of different planting densities on the metabolism of Panax notoginseng	Panax notoginseng	Yunnan Agricultural University	GC-MS*	2022-01-25	1	20	Uploaded data (469.4M)* (Data format:d)
ST002057	Distinct Human Hepatocyte Lipidomics Profiles for Nonalcoholic Steatohepatitis and In Vitro-Induced Steatosis	Homo sapiens	Monash Institute of Pharmaceutical Sciences	LC-MS	2022-01-25	1	103	Uploaded data (18.5G)* (Data format:raw(Thermo))

Study detail page



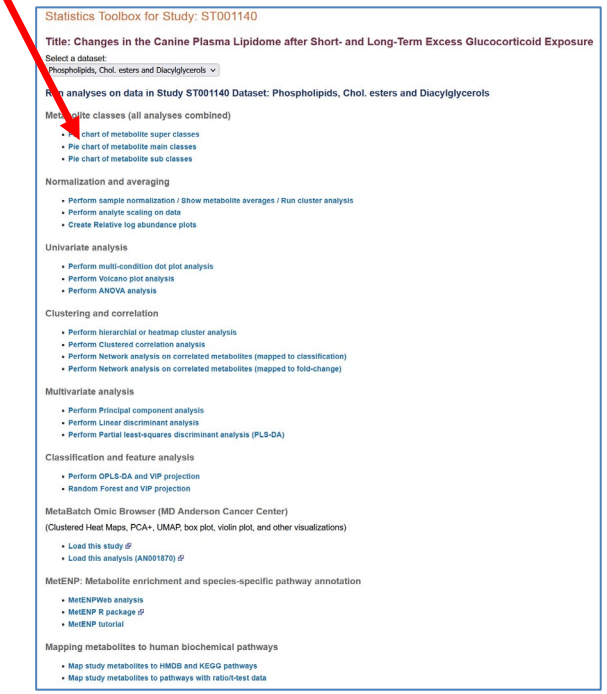
Summary of study ST001140

This data is available at the NIH Common Fund's National Metabolomics Data Repository (NMDR) website, the Metabolomics Workbench, https://www.metabolomicsworkbench.org, where it has been assigned Project ID PR000761. The data can be accessed directly via it's Project DOI: 10.21228/M89Q32
This work is supported by NIH grant, U2C- DK119886. See: https://www.metabolomicsworkbench.org/about/howtocite.php

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download mwTab file (text) | Download mwTab file(JSON) | Download data (Contains raw data)

Study ID	ST001140
Study Title	Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure
Study Summary	Glucocorticoids (GCs) are widely used in veterinary and human medicine. Chromic endogenous or iatrogenic GC overexposure impairs metabolic function and can result in diverse side-effects, including Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess (induced by prednisolone and tetracosactide, respectively) on the plasma lipidome of Beale dogs. Both, long- and short-term GC resulted in significant changes of the plasma lipidome.
Institute	National University of Singapore;University of Zurich
Department	Singapore Lipidomics Incubator (SLING);Vetsuisse Faculty, University of Zurich
Laboratory	Singapore Lipidomics Incubator (SLING), National University of Singapore

Study statistics page



Statistics Toolbox for Study: ST001140

Title: Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure

Select a dataset: Phospholipids, Chol. esters and Diacylglycerols

Run analyses on data in Study ST001140 Dataset: Phospholipids, Chol. esters and Diacylglycerols

Metabolite classes (all analyses combined)
- Pie chart of metabolite super classes
- Pie chart of metabolite main classes
- Pie chart of metabolite sub classes

Normalization and averaging
- Perform sample normalization / Show metabolite averages / Run cluster analysis
- Perform analyte scaling on data
- Create Relative log abundance plots

Univariate analysis
- Perform multi-condition dot plot analysis
- Perform Volcano plot analysis
- Perform ANOVA analysis

Clustering and correlation
- Perform hierarchial or heatmap cluster analysis
- Perform Clustered correlation analysis
- Perform Network analysis on correlated metabolites (mapped to classification)
- Perform Network analysis on correlated metabolites (mapped to fold-change)

Multivariate analysis
- Perform Principal component analysis
- Perform Linear discriminant analysis
- Perform Partial least-squares discriminant analysis (PLS-DA)

Classification and feature analysis
- Perform OPLS-DA and VIP projection
- Random Forest and VIP projection

MetaBatch Omic Browser (MD Anderson Cancer Center)
(Clustered Heat Maps, PCA+, UMAP, box plot, violin plot, and other visualizations)
- Load this study
- Load this analysis (AN001870)

MetENP: Metabolite enrichment and species-specific pathway annotation
- MetENPWeb analysis
- MetENP R package
- MetENP tutorial

Mapping metabolites to human biochemical pathways
- Map study metabolites to HMDB and KEGG pathways
- Map study metabolites to pathways with ratio/t-test data

Analysis tools applied to the data for the selected NMDR study
A study may have more than one analysis (dataset)

Metabolite classification
Pie chart of metabolite super classes
Pie chart of metabolite main classes
Pie chart of metabolite sub classes

Normalization and averaging
Show Metabolite averages per experimental factor
Perform normalization on data
Create Relative log abundance plots

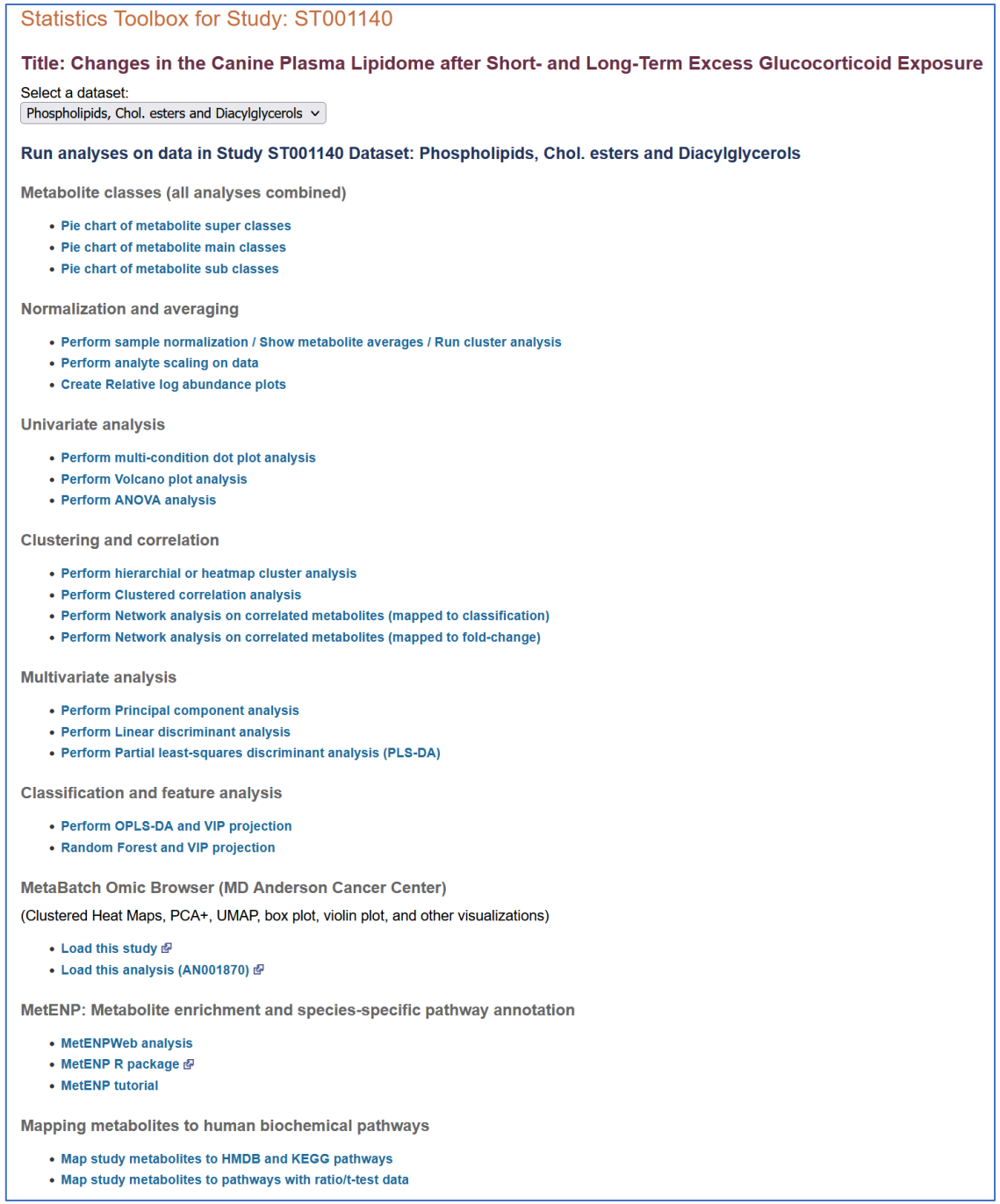
Univariate analysis
Perform multi-condition dot plot analysis
Perform Volcano plot analysis
Perform ANOVA analysis and class enrichment analysis
MetENP analysis

Clustering and correlation
Perform hierarchical or heatmap cluster analysis
Perform Clustered correlation analysis
Perform Network analysis on correlated metabolites (mapped to classification)
Perform Network analysis on correlated metabolites (mapped to fold-change)

Multivariate analysis
Perform Principal component analysis
Perform Linear discriminant analysis
Perform Partial least-squares discriminant analysis (PLS-DA)

Classification and feature analysis
Perform OPLS-DA and VIP projection
Random Forest and VIP projection

Mapping metabolites to human biochemical pathways
Map study metabolites to HMDB and KEGG pathways
Map study metabolites to pathways with ratio/t-test data



Study-specific analysis toolbox

Statistics Toolbox for Study: ST001140

Title: Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure

Select a dataset:

Phospholipids, Chol. esters and Diacylglycerols

Run analyses on data in Study ST001140 Dataset: Phospholipids, Chol. esters and Diacylglycerols

Metabolite classes (all analyses combined)

- Pie chart of metabolite super classes
- Pie chart of metabolite main classes
- Pie chart of metabolite sub classes

Normalization and averaging

- Perform sample normalization / Show metabolite averages / Run cluster analysis
- Perform analyte scaling on data
- Create Relative log abundance plots

Univariate analysis

- Perform multi-condition dot plot analysis
- Perform Volcano plot analysis
- Perform ANOVA analysis

Clustering and correlation

- Perform hierarchial or heatmap cluster analysis
- Perform Clustered correlation analysis
- Perform Network analysis on correlated metabolites (mapped to classification)
- Perform Network analysis on correlated metabolites (mapped to fold-change)

Multivariate analysis

- Perform Principal component analysis
- Perform Linear discriminant analysis
- Perform Partial least-squares discriminant analysis (PLS-DA)

Classification and feature analysis

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

MetaBatch Omic Browser (MD Anderson Cancer Center)

(Clustered Heat Maps, PCA+, UMAP, box plot, violin plot, and other visualizations)

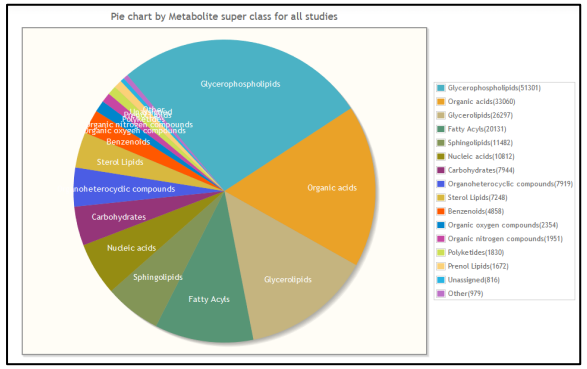
- Load this study
- Load this analysis (AN001870)

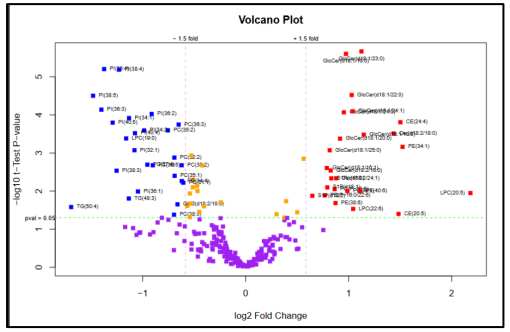
MetENP: Metabolite enrichment and species-specific pathway annotation

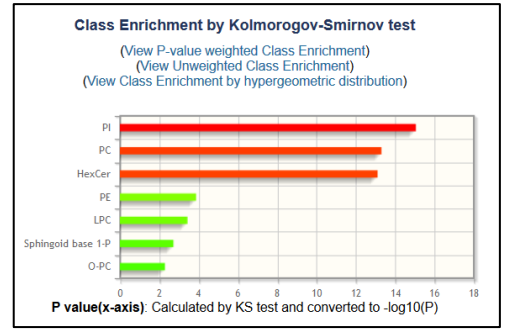
- MetENPWeb analysis
- MetENP R package
- MetENP tutorial

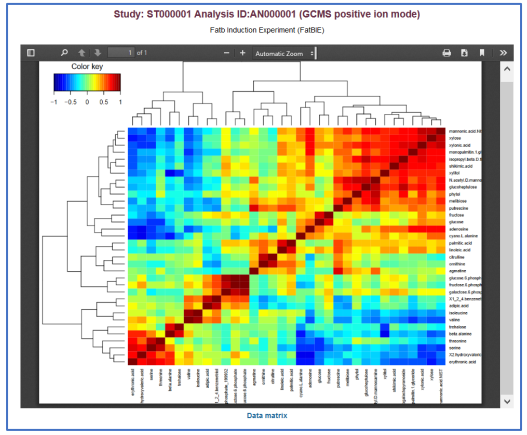
Mapping metabolites to human biochemical pathways

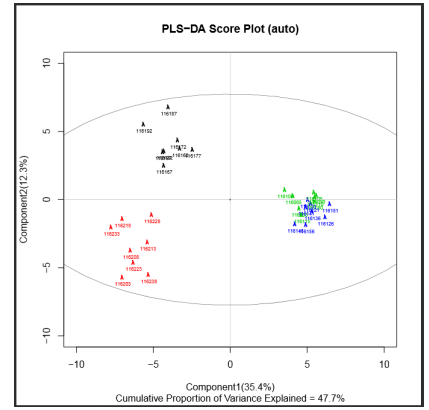
- Map study metabolites to HMDB and KEGG pathways
- Map study metabolites to pathways with ratio/t-test data





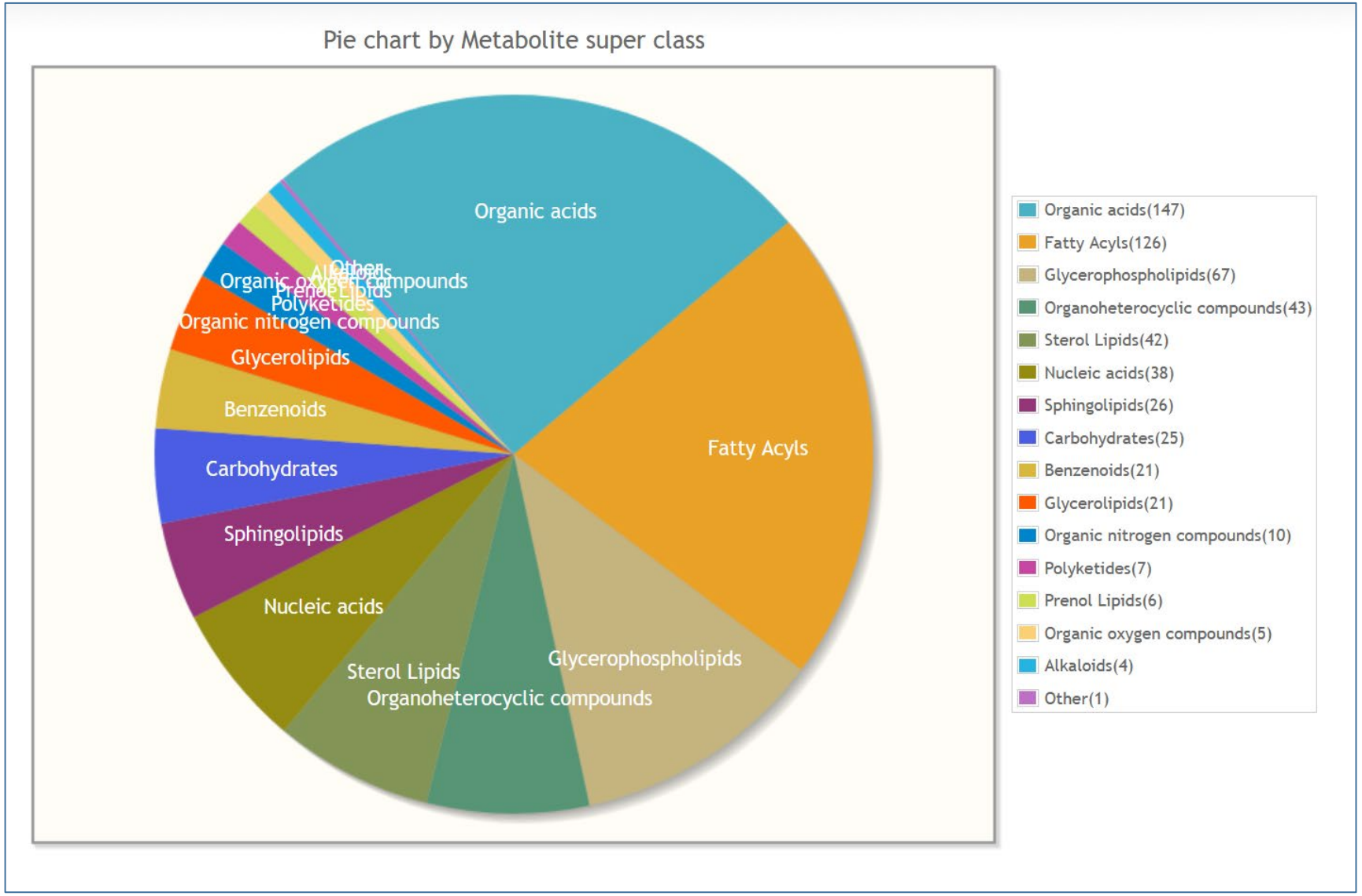




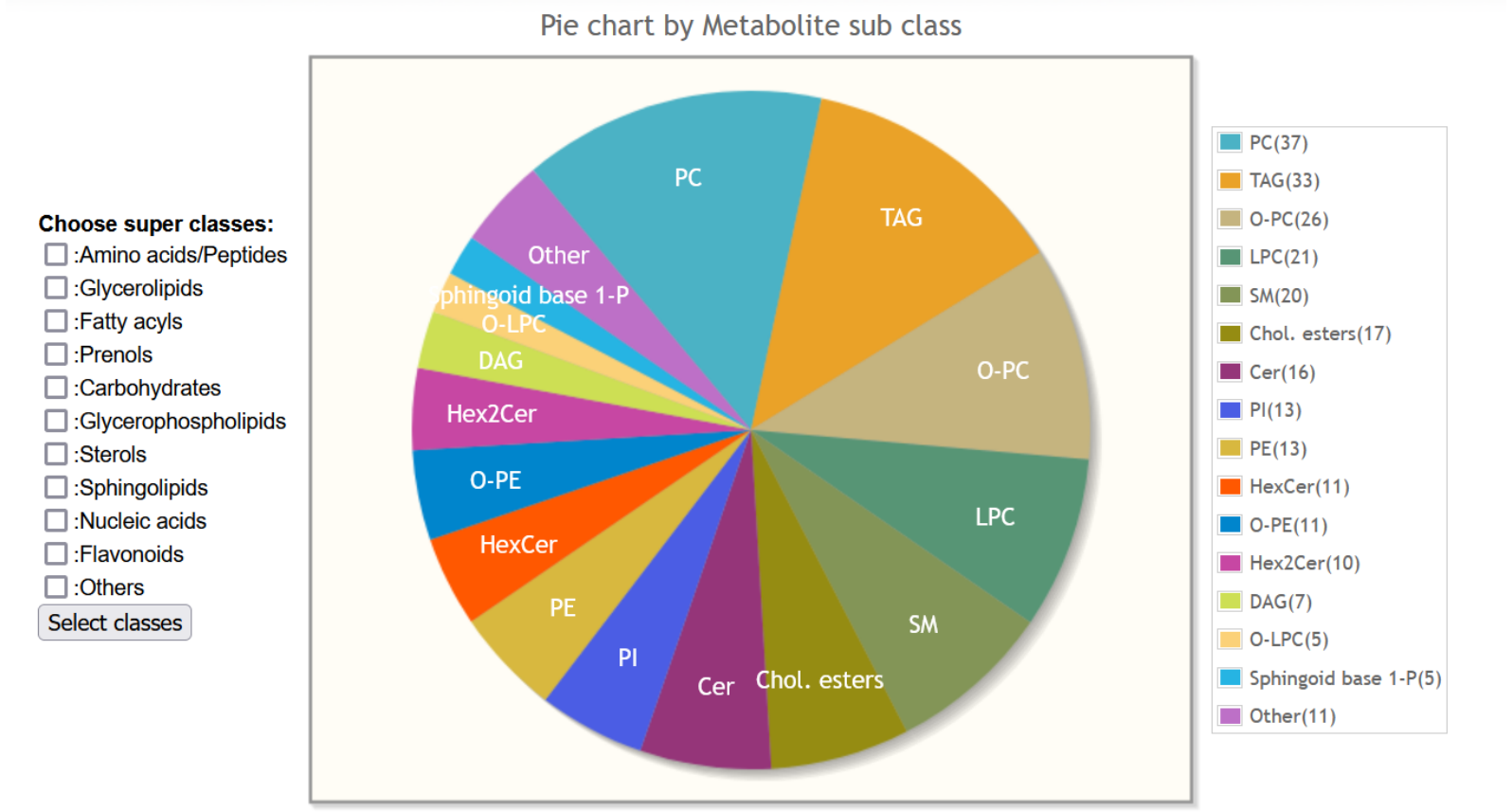


Pie-chart of metabolite super classes detected in a study

Metabolite names are mapped to RefMet which is linked to a chemical classification system

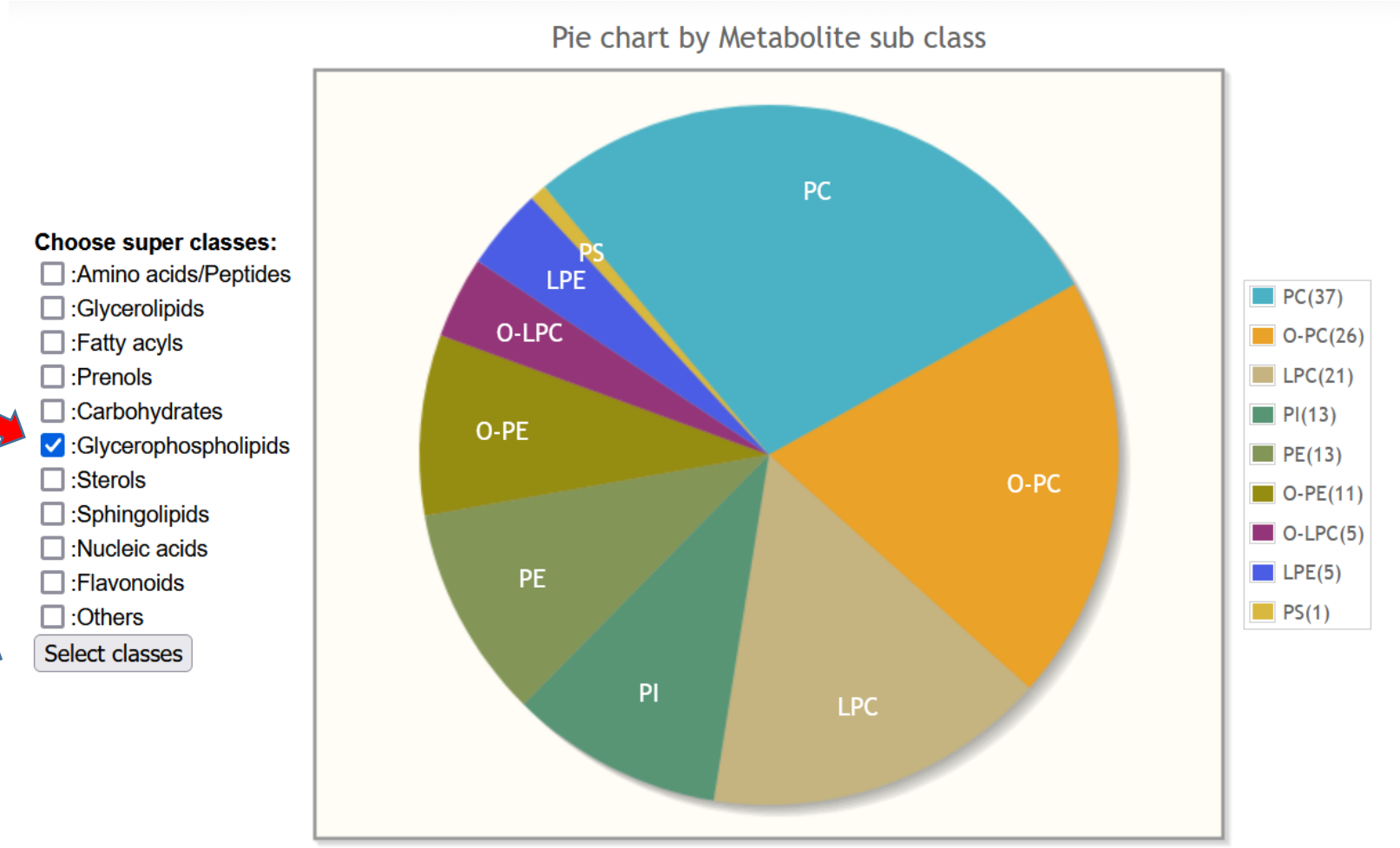


Pie-chart of metabolite sub classes detected in a study



Pie-chart of metabolite sub classes detected in a study

Restrict to a selected super class



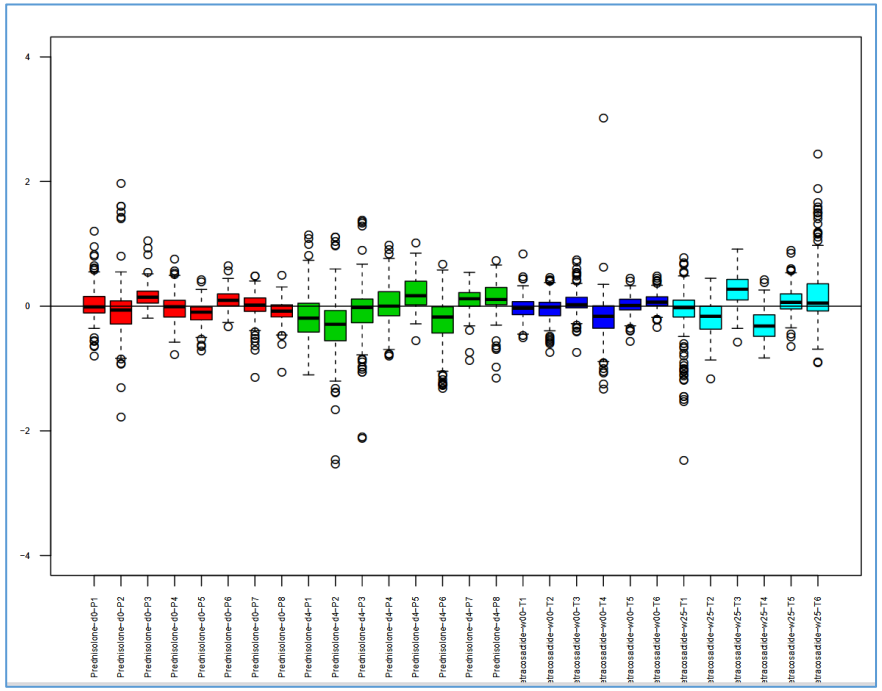
Normalization and averaging: Abundance plots

Normalization and averaging

- Perform sample normalization / Show metabolite averages / Run cluster analysis
- Perform analyte scaling on data
- Create Relative log abundance plots

Choose mode (within or across sample groups)

Map	Study ID	Mode	Study Title	MS Analysis Type
Run	ST001140	Within groups	Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure	Phospholipids, Chol. esters and Diacylglycerols
Run	ST001140	Within groups	Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure	Sphingolipids
Run	ST001140	Within groups	Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure	Triacylglycerols



Relative log Abundance plots

Volcano plot analysis tool

Most tools contain a form where the user selects appropriate experimental groups and analysis parameters prior to running the program

Univariate analysis

- Perform multi-condition dot plot analysis
- Perform Volcano plot analysis
- Perform ANOVA analysis

Volcano Plot analysis for Study ST001140

(Analysis All analyses used)

Select one or more experimental factors for Groups 1 and 2. The members of each group should be DIFFERENT.

Group1	Experimental factor	Group2
☑	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before (8)	☐
☐	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after (8)	☑
☐	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before (6)	☐
☐	TreatmentGroup:Tetracosactide | TreatmentDuration:25w | SamplingTimePoint:after (6)	☐

P-value cutoff: 0.05 **Fold-change cutoff:** 1.5 **Sample normalization:** None

Group by metabolite classification: Sub class **Use:** Submitted metabolite names

Maximum # of (most significant) metabolites per class to use in pvalue group calculation: All

Analysis: Phospholipids, Chol. esters and Diacylglycerols **Combine data for all analyses?:** ☑ Run Volcano Plot

In this case, samples before and after Prednisolone treatment are compared. This study contains 4 analyses (different metabolite classes) and all data will be combined. A p-value cutoff of 0.5 and fold-change cutoff of 1.5 are selected for the volcano plot analysis step. Metabolites will be classified by sub class (as opposed to main class). No sample normalization will be performed prior to analysis.

Analyses for this study:

Triacylglycerols
Sphingolipids
Phospholipids, Cholesterol esters and Diacylglycerols
Spingosine-1-phosphates

Volcano plot analysis results

Clickable icons

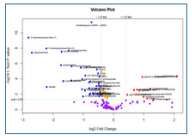
Columns are sortable

Table of results with log2 fold-change,t-test p-values and metabolite classification

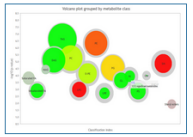
Default sort is by Main class/sub class

Click on “t-test P-value” heading to sort by that item

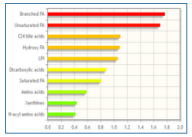
Experimental factors selected in each group			
Group1:	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	**Group2:**	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after



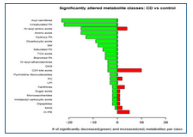
Volcano plot of all significant metabolites



Bubble plot of results grouped by metabolite class



Enrichment by metabolite class



Barplot of significant metabolites by metabolite class

List of significant metabolites (pvalue <=0.05 and fold-change >=1.5)

Metabolite	log2 Fold Change	t-Test P-value	FDR-adjusted P-value(BH)	Main class	Sub class
Cer(d18:2/24:1)	0.878	4.60e-3	3.08e-2	Ceramides	Cer
Cer(d18:2/18:0)	1.436	3.09e-4	4.22e-3	Ceramides	Cer
CE(20:5)	1.484	3.98e-2	1.50e-1	Sterol esters	Chol. esters
CE(24:4)	1.502	1.56e-4	3.03e-3	Sterol esters	Chol. esters
GlcCer(d18:1/16:1)	0.788	2.48e-3	1.91e-2	Glycosphingolipids	HexCer
GlcCer(d18:1/25:0)	0.816	8.50e-4	8.71e-3	Glycosphingolipids	HexCer
GlcCer(d18:2/16:0)	0.826	2.88e-3	2.11e-2	Glycosphingolipids	HexCer
GlcCer(d18:1/20:0)	0.916	4.21e-4	4.93e-3	Glycosphingolipids	HexCer
GlcCer(d18:1/24:0)	0.953	8.57e-5	2.33e-3	Glycosphingolipids	HexCer
GlcCer(d18:1/16:0)	0.974	2.51e-6	3.09e-4	Glycosphingolipids	HexCer
GlcCer(d18:1/22:0)	1.029	3.01e-5	1.29e-3	Glycosphingolipids	HexCer
GlcCer(d18:1/24:1)	1.040	8.03e-5	2.33e-3	Glycosphingolipids	HexCer
GlcCer(d18:1/23:0)	1.124	2.16e-6	3.09e-4	Glycosphingolipids	HexCer
GlcCer(d18:1/18:0)	1.147	3.31e-4	4.28e-3	Glycosphingolipids	HexCer
LPC(19:0)	-1.160	4.16e-4	4.93e-3	Glycerophosphocholines	LPC
LPC(22:6)	1.043	2.94e-2	1.16e-1	Glycerophosphocholines	LPC
LPC(20:5)	2.182	1.13e-2	5.65e-2	Glycerophosphocholines	LPC
PC(P-36:5)	0.864	8.89e-3	4.97e-2	Glycerophosphocholines	O-PC
PE(P-16:0/22:6)	0.768	1.30e-2	6.25e-2	Glycerophosphoethanolamines	O-PE
PC(37:4)	-0.954	2.02e-3	1.69e-2	Glycerophosphocholines	PC
PC(39:5)	-0.902	2.10e-3	1.69e-2	Glycerophosphocholines	PC
PC(35:2)	-0.755	2.54e-4	3.94e-3	Glycerophosphocholines	PC
PC(38:3)	-0.695	4.16e-2	1.53e-1	Glycerophosphocholines	PC
PC(32:2)	-0.692	1.32e-3	1.25e-2	Glycerophosphocholines	PC

Volcano plot analysis results (sorted by t-test p-value)

Metabolite sub classes (mean values)

Individual metabolites (sorted by p-value)

Table of results grouped by metabolite class (using most significant analytes per class)

Metabolite class	log2 Fold Change	-log10(P-value)	FDR-adjusted P-value(BH)	# of metabolites per class
LPC	-1.160	3.38	4.93e-3	-1(21)
PC	-0.719	2.65	3.22e-2	-10(37)
PI	-1.188	3.79	8.57e-3	-12(12)
TAG	-1.414	1.69	8.92e-2	-2(25)
Cer	1.157	2.92	1.75e-2	2(16)
Chol. esters	1.493	2.60	7.67e-2	2(17)
HexCer	0.961	3.90	6.47e-3	10(10)
LPC	1.613	1.74	8.65e-2	2(21)
O-PC	0.864	2.05	4.97e-2	1(26)
O-PE	0.768	1.89	6.25e-2	1(10)
PE	1.124	2.21	5.06e-2	4(12)
Sphingoid base 1-P	0.812	2.22	3.83e-2	2(5)

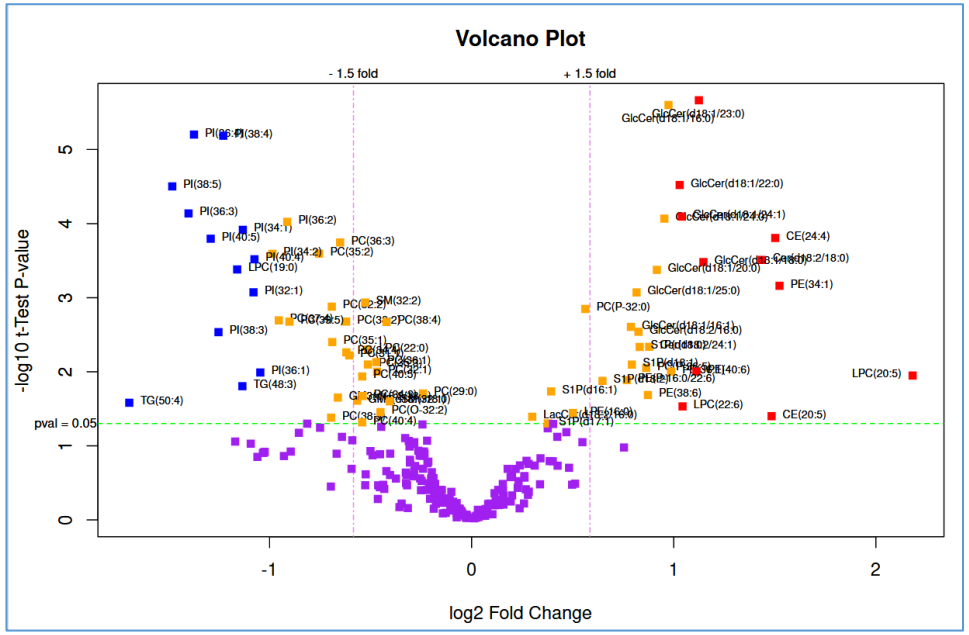
12 out of 12 PI's were significantly downregulated

4 out of 12 PE's were significantly upregulated

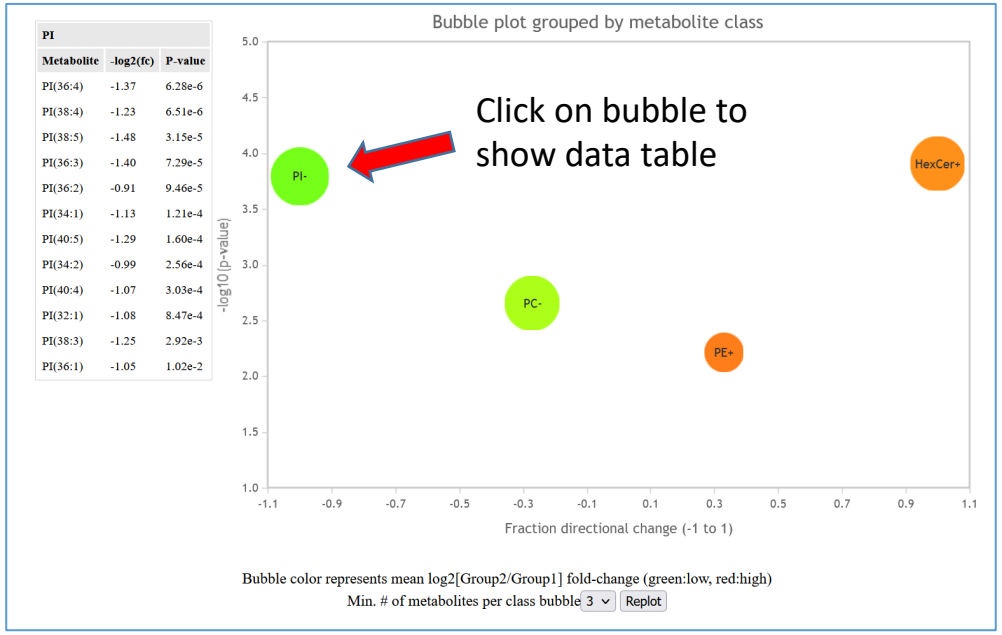
List of significant metabolites (pvalue <=0.05 and fold-change >=1.5)

Metabolite	log2 Fold Change	t-Test P-value	FDR-adjusted P-value(BH)	Main class	Sub class
GlcCer(d18:1/23:0)	1.124	2.16e-6	3.09e-4	Glycosphingolipids	HexCer
GlcCer(d18:1/16:0)	0.974	2.51e-6	3.09e-4	Glycosphingolipids	HexCer
PI(36:4)	-1.374	6.28e-6	4.01e-4	Glycerophosphoinositols	PI
PI(38:4)	-1.229	6.51e-6	4.01e-4	Glycerophosphoinositols	PI
GlcCer(d18:1/22:0)	1.029	3.01e-5	1.29e-3	Glycosphingolipids	HexCer
PI(38:5)	-1.481	3.15e-5	1.29e-3	Glycerophosphoinositols	PI
PI(36:3)	-1.401	7.29e-5	2.33e-3	Glycerophosphoinositols	PI
GlcCer(d18:1/24:1)	1.040	8.03e-5	2.33e-3	Glycosphingolipids	HexCer
GlcCer(d18:1/24:0)	0.953	8.57e-5	2.33e-3	Glycosphingolipids	HexCer
PI(36:2)	-0.912	9.46e-5	2.33e-3	Glycerophosphoinositols	PI
PI(34:1)	-1.132	1.21e-4	2.71e-3	Glycerophosphoinositols	PI
CE(24:4)	1.502	1.56e-4	3.03e-3	Sterol esters	Chol. esters
PI(40:5)	-1.291	1.60e-4	3.03e-3	Glycerophosphoinositols	PI
PC(36:3)	-0.651	1.80e-4	3.16e-3	Glycerophosphocholines	PC
PC(35:2)	-0.755	2.54e-4	3.94e-3	Glycerophosphocholines	PC
PI(34:2)	-0.986	2.56e-4	3.94e-3	Glycerophosphoinositols	PI
PI(40:4)	-1.075	3.03e-4	4.22e-3	Glycerophosphoinositols	PI
Cer(d18:2/18:0)	1.436	3.09e-4	4.22e-3	Ceramides	Cer
GlcCer(d18:1/18:0)	1.147	3.31e-4	4.28e-3	Glycosphingolipids	HexCer
LPC(19:0)	-1.160	4.16e-4	4.93e-3	Glycerophosphocholines	LPC
GlcCer(d18:1/20:0)	0.916	4.21e-4	4.93e-3	Glycosphingolipids	HexCer
PE(34:1)	1.523	6.91e-4	7.72e-3	Glycerophosphoethanolamines	PE
PI(32:1)	-1.079	8.47e-4	8.71e-3	Glycerophosphoinositols	PI
GlcCer(d18:1/25:0)	0.816	8.50e-4	8.71e-3	Glycosphingolipids	HexCer

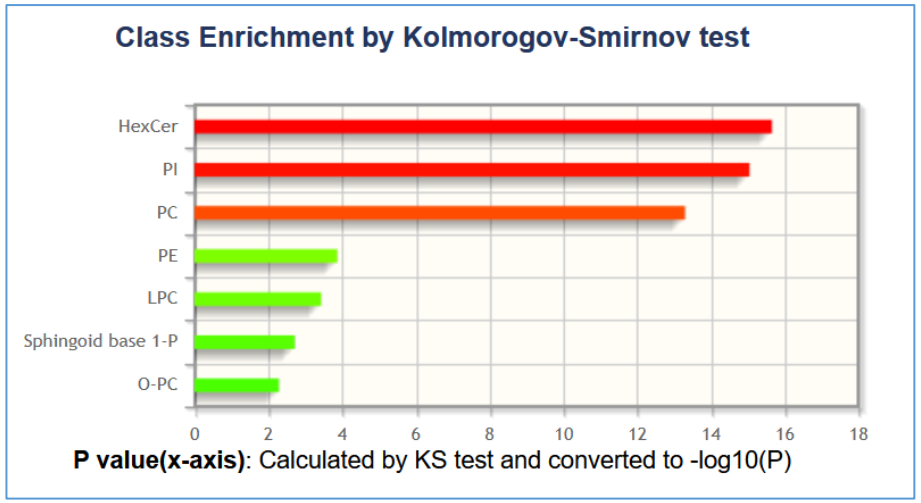
Volcano plot analysis results (click on icons)



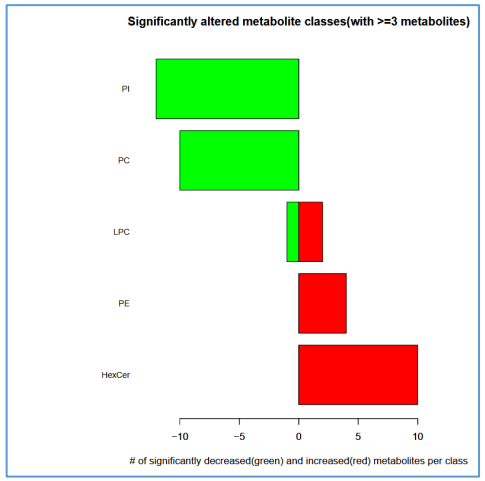
Volcano plot



Bubble plot of –log10 p-value vs fraction directional change



Class enrichment plot



Barplot of significantly altered metabolite classes

ANOVA analysis tool

Most tools contain a form where the user selects appropriate experimental groups and analysis parameters prior to running the program

Univariate analysis

- Perform multi-condition dot plot analysis
- Perform Volcano plot analysis
- Perform ANOVA analysis

ANOVA analysis for Study ST001140

ANOVA Setup	
Select Factor:	SamplingTimePoint
Analysis:	Phospholipids, Chol. esters and Diacylglycerols
P-value cutoff:	0.05
Group by metabolite classification:	Sub class
Maximum # of (most significant) metabolites per class to use in group calculation:	5

Run ANOVA

Choose experimental factor to analyze by ANOVA (in this case it is before and after drug treatment), analysis group, p-value cutoff and classification group.

Analyses for this study:

Triacylglycerols
Sphingolipids
Phospholipids, Cholesterol esters and Diacylglycerols
Spingosine-1-phosphates

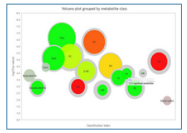
ANOVA analysis tool: Results

Most tools contain a form where the user selects appropriate experimental groups and analysis parameters prior to running the program

Metabolite sub classes (mean values)

Columns are sortable

Individual metabolites (sorted by p-value)



View Bubble plot of results grouped by metabolite classification

Table of results grouped by metabolite class (using 5 most significant analytes per class)

Metabolite class	F-value	-log10(P-value)	FDR-adjusted P-value(BH)	# of metabolites per class
PI	47.763	6.36	1.91e-4	11(13)
PC	38.360	5.56	1.26e-3	10(37)
O-PC	19.046	3.73	2.29e-3	19(26)
O-LPC	17.402	3.53	2.93e-3	1(5)
LPC	18.045	3.34	2.38e-2	10(21)
Chol. esters	19.437	2.92	3.18e-2	4(17)
O-PE	6.665	1.79	6.64e-2	3(11)
PE	6.261	1.72	6.68e-2	4(13)

(Analysis: AN001870)

Factor:SamplingTimePoint					
Metabolite	F value	P-value	FDR adjusted P-value	Main class	Sub class
PI(38:4)	78.118	2.597E-9	4.077E-7	Glycerophosphoinositols	PI
PC(37:4)	66.821	1.178E-8	6.267E-7	Glycerophosphocholines	PC
PI(38:5)	66.703	1.198E-8	6.267E-7	Glycerophosphoinositols	PI
PC(38:4)	44.981	4.079E-7	1.318E-5	Glycerophosphocholines	PC
PC(39:5)	44.828	4.197E-7	1.318E-5	Glycerophosphocholines	PC
PI(36:4)	42.527	6.506E-7	1.702E-5	Glycerophosphoinositols	PI
LPC(19:0)	41.711	7.627E-7	1.711E-5	Glycerophosphocholines	LPC
CE(24:4)	52.841	4.100E-6	8.047E-5	Sterol esters	Chol. esters
PI(40:5)	26.714	2.155E-5	3.759E-4	Glycerophosphoinositols	PI
PI(40:4)	24.754	3.587E-5	5.631E-4	Glycerophosphoinositols	PI
PC(O-32:2)	24.240	4.113E-5	5.668E-4	Glycerophosphocholines	O-PC
LPC(22:0)	24.047	4.332E-5	5.668E-4	Glycerophosphocholines	LPC
PC(40:4)	19.824	1.426E-4	1.723E-3	Glycerophosphocholines	PC
PC(P-34:2)	19.543	1.550E-4	1.739E-3	Glycerophosphocholines	O-PC
PC(P-34:1)	17.597	2.808E-4	2.929E-3	Glycerophosphocholines	O-PC
LPC(O-20:0)	17.402	2.985E-4	2.929E-3	Glycerophosphocholines	O-LPC
PC(O-34:3)	17.122	3.260E-4	3.011E-3	Glycerophosphocholines	O-PC
PC(P-36:2)	16.727	3.696E-4	3.224E-3	Glycerophosphocholines	O-PC
PC(O-34:1)	15.359	5.772E-4	4.549E-3	Glycerophosphocholines	O-PC
PC(40:5)	15.347	5.795E-4	4.549E-3	Glycerophosphocholines	PC
PC(P-34:3)	14.395	7.980E-4	5.966E-3	Glycerophosphocholines	O-PC

Bubble plot representation of significant ANOVA metabolite classes
Colored circles represent significant metabolites, gray circles represent all metabolites per class

Multi-condition dot-plot analysis

Useful for plotting time-course data or comparing multiple experimental conditions to controls

Univariate analysis

- Perform multi-condition dot plot analysis
- Perform Volcano plot analysis
- Perform ANOVA analysis

Example: Metabolite changes associated with methionine stress sensitivity of human breast cancer cells. Use 100uM Methionine group as control and compare 370uM Homocysteine groups at various timepoints.

Dot Plot analysis for Study ST000077

Select one or more experimental factors for control and test groups. The members of each group should be DIFFERENT.

Control(s)	Experimental factor	Test(s)
☑	Treatment:100uM Met | Timepoint:0 hours (4)	☐
☐	Treatment:370uM Hcy | Timepoint:2 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:4 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:8 hours (3)	☑
☐	Treatment:370uM Hcy | Timepoint:12 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:24 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:48 hours (4)	☑
☐	Treatment:quality check | Timepoint:quality check (3)	☐

x-axis labels: 2hr__4hr__8hr__12hr__24hr__48hr **Show a single class:**

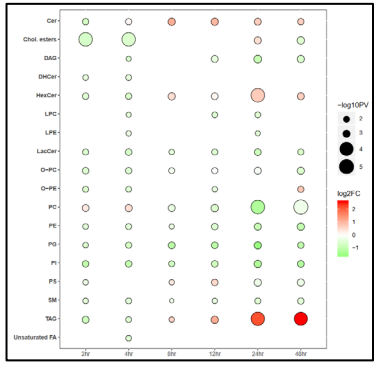
P-value cutoff: 0.05 **Fold-change cutoff:** 1.2 **Sample normalization:** Mean

Group by metabolite classification: Sub class **# of individual metabolites to display:** 30

Maximum # of (most significant) metabolites per class to use in group calculation: 5

Analysis: ESI/QTOF positive ion mode **Combine data for all analyses?:** ☑ Run Analysis

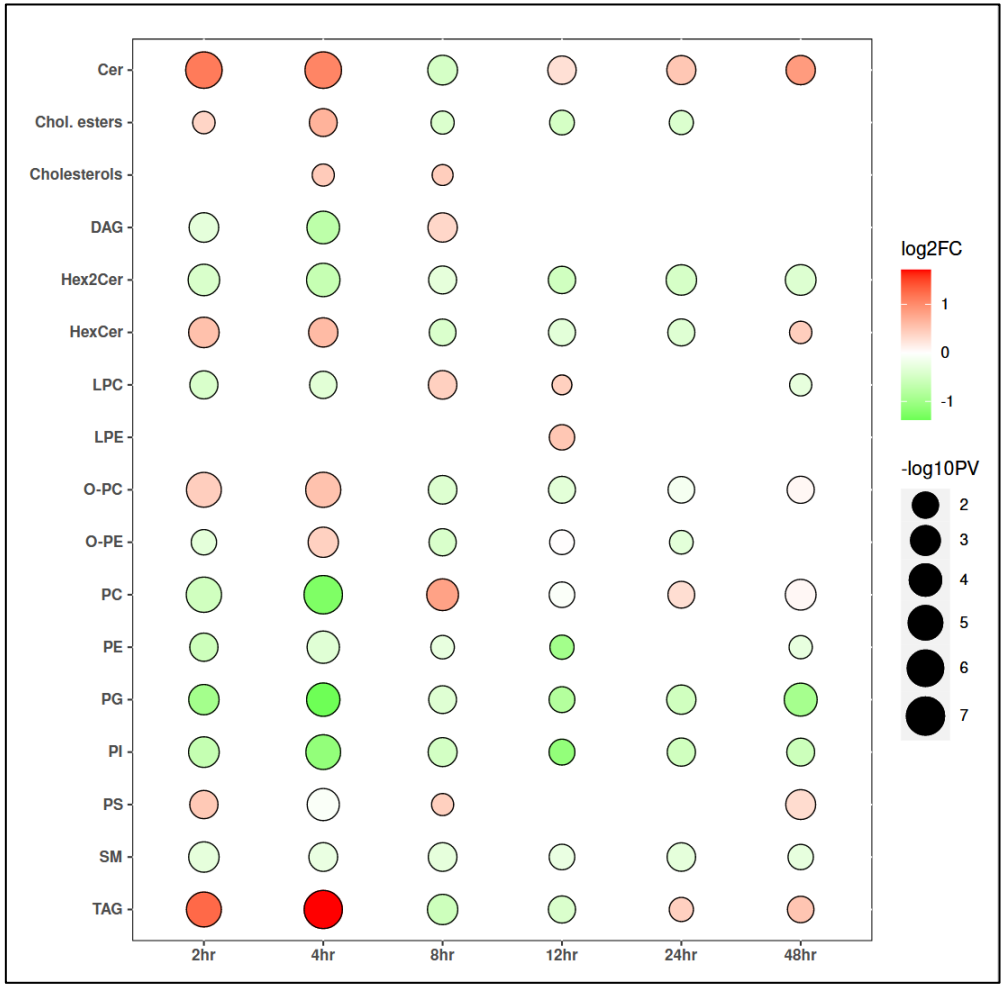
Query builder GUI



Plots

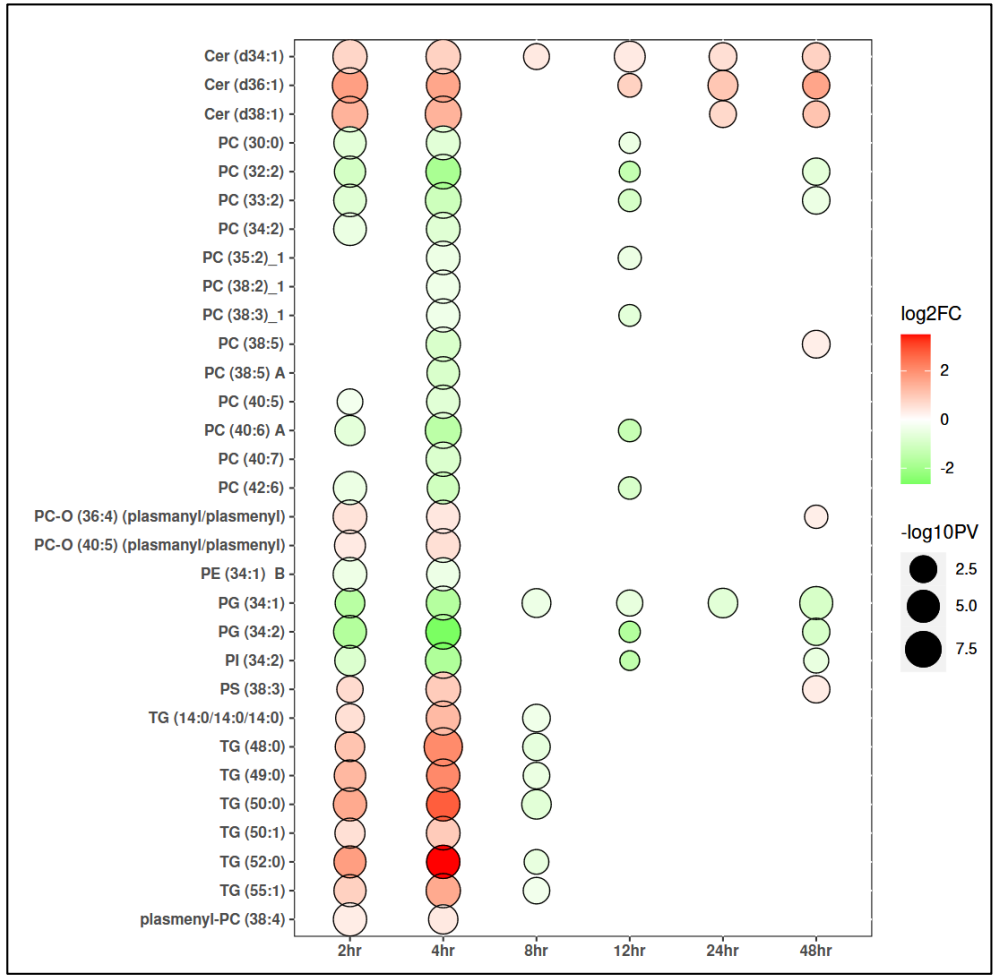
Multi-condition dot-plot analysis results

All groups are being compared to the control group (100uM Methionine treatment)



Increasing time ->

Metabolite class Plot



Increasing time ->

Individual metabolite Plot

Multi-condition dot-plot analysis

Useful for plotting time-course data or comparing multiple experimental conditions to controls

Dot Plot analysis for Study ST000077

Select one or more experimental factors for control and test groups. The members of each group should be DIFFERENT.

Control(s)	Experimental factor	Test(s)
☑	Treatment:100uM Met | Timepoint:0 hours (4)	☐
☐	Treatment:370uM Hcy | Timepoint:2 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:4 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:8 hours (3)	☑
☐	Treatment:370uM Hcy | Timepoint:12 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:24 hours (4)	☑
☐	Treatment:370uM Hcy | Timepoint:48 hours (4)	☑
☐	Treatment:quality check | Timepoint:quality check (3)	☐

x-axis labels ?: 2hr__4hr__8hr__12hr__24hr__48hr **Show a single class:** TAG

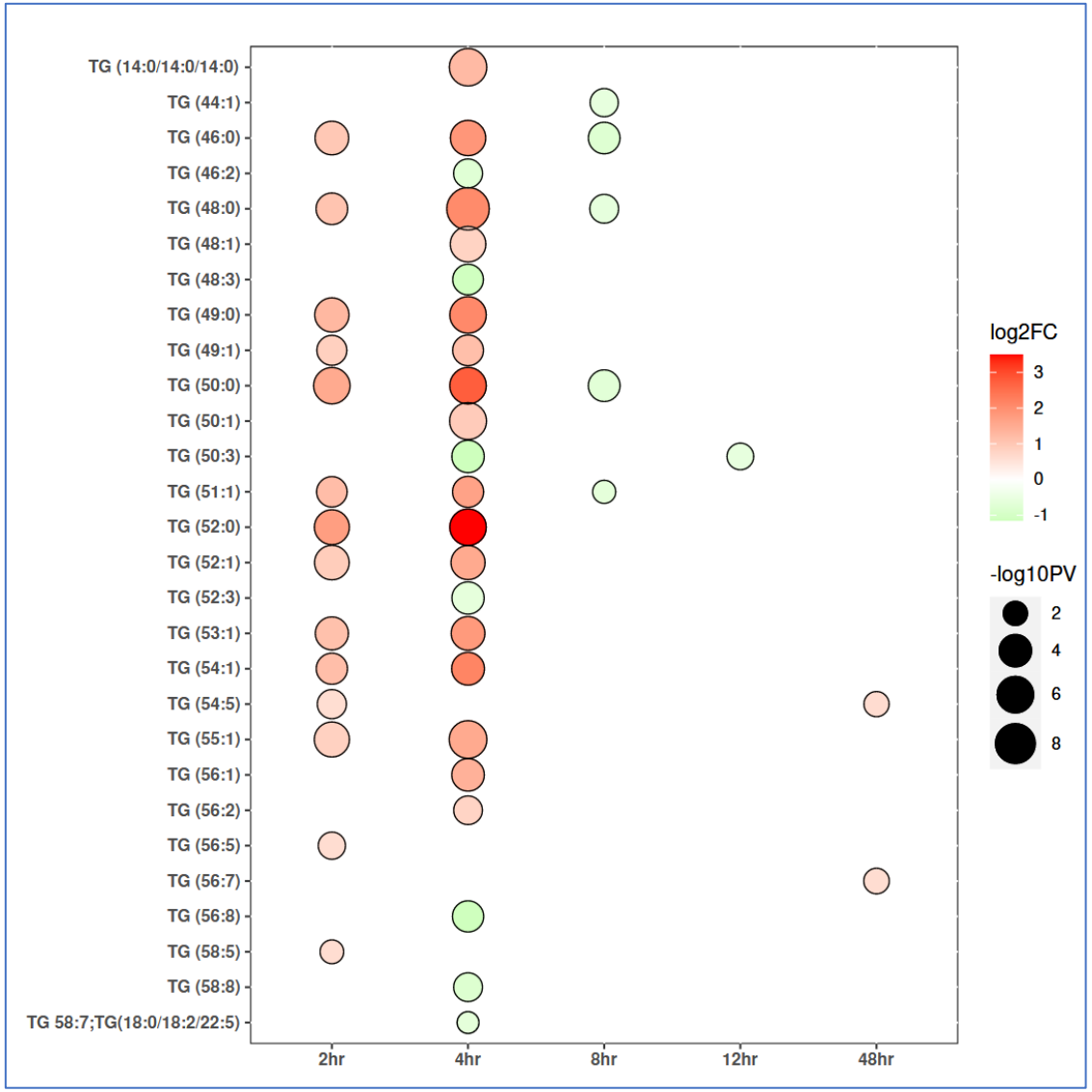
P-value cutoff: 0.05 **Fold-change cutoff:** 1.5 **Sample normalization:** None

Use: Submitted metabolite names **Maximum # of individual metabolites to display:** 30

Group by: Sub class **Maximum # of (most significant) metabolites per class to use in group calculation:** 5

Analysis: ESI/QTOF positive ion mode **Combine data for all analyses?:** ☑ Run Analysis

Restrict to a single class (triacylglycerols)



No significant changes compared to control in the TAG class were observed at the 24hr timepoint, so that column is absent in the plot.

Cluster analysis tools

Clustering and correlation

- Perform hierarchial or heatmap cluster analysis
- Perform Clustered correlation analysis
- Perform Network analysis on correlated metabolites (mapped to classification)
- Perform Network analysis on correlated metabolites (mapped to fold-change)

Data for (Study ST001140)

(Analysis AN001871)

Values for each metabolite have been scaled by dividing by the mean across all factors

Run Hierarchial cluster analysis on this study | Run Heatmap cluster analysis on this study

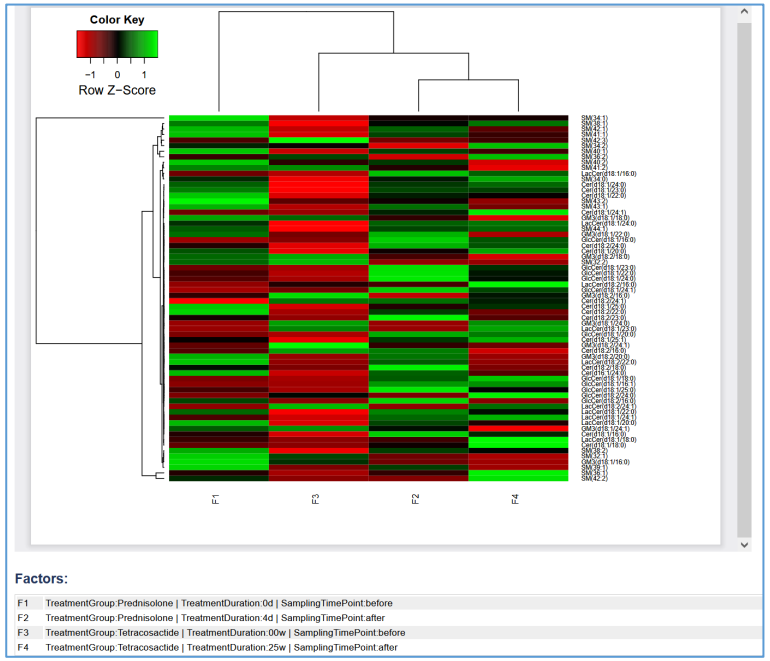
Metabolite	F1	F2	F3	F4
Cer(d16:1/24:0)	1.3232	1.1491	0.5756	0.7946
Cer(d18:1/16:0)	0.9360	1.2680	0.6926	1.0354
Cer(d18:1/18:0)	0.6867	0.9859	0.5171	1.9195
Cer(d18:1/20:0)	1.1739	0.9578	0.4702	2542
Cer(d18:1/22:0)	1.3841	1.0262	0.5037	0.949
Cer(d18:1/23:0)	1.1823	1.0882	0.5655	1.0739
Cer(d18:1/24:0)	1.1411	1.0774	0.5541	1.1545
Cer(d18:1/24:1)	0.8238	1.0613	0.7579	1.3952
Cer(d18:1/25:0)	1.3044	0.9207	0.6363	1.0637
Cer(d18:1/25:1)	0.9870	1.0916	0.5991	1.2960
Cer(d18:2/16:0)	0.9557	1.0655	1.0837	0.8881
Cer(d18:2/18:0)	0.5583	1.4417	NA	NA
Cer(d18:2/22:0)	1.3553	1.0771	0.6618	0.7618
Cer(d18:2/23:0)	0.9520	1.2847	0.8033	0.8811
Cer(d18:2/24:0)	0.9376	1.2327	0.6736	1.0994
Cer(d18:2/24:1)	0.6456	1.1770	1.1840	1.0526
GlcCer(d18:1/16:0)	0.7048	1.3701	0.7533	1.1468
GlcCer(d18:1/16:1)	0.7320	1.2868	0.6996	1.2754
GlcCer(d18:1/18:0)	0.6099	1.3018	0.4579	1.6599
GlcCer(d18:1/20:0)	0.7235	1.3584	0.6325	1.2584
GlcCer(d18:1/22:0)	0.7804	1.6101	0.4553	1.0241
GlcCer(d18:1/23:0)	0.7066	1.5278	0.5807	1.1067
GlcCer(d18:1/24:0)	0.7881	1.5167	0.5867	1.0069
GlcCer(d18:1/24:1)	0.6721	1.4048	0.7622	1.1354
GlcCer(d18:1/25:0)	0.8215	1.4817	0.6211	0.9747
GlcCer(d18:2/16:0)	0.7297	1.2703	NA	NA
GlcCer(d18:2/24:0)	NA	NA	0.5144	1.4856
GM3(d18:1/16:0)	1.1701	0.9053	1.0343	0.8651
GM3(d18:1/18:0)	1.3228	0.8800	1.1933	0.5362
GM3(d18:1/22:0)	1.1302	1.2234	0.8020	0.7264
GM3(d18:1/24:0)	NA	NA	1.0209	0.9791

Clustering data with hclust algorithm for (Study ST001140)

(Analysis AN001871)

Metabolite	Structure	F1	F2	F3	F4
GlcCer(d18:2/24:0)	ME272158	NA	NA	0.51	1.49
LacCer(d18:2/24:1)	ME272168	NA	NA	1.13	0.87
GM3(d18:1/24:0)	ME272142	NA	NA	1.02	0.98
LacCer(d18:1/23:0)	ME272163	NA	NA	0.94	1.06
GM3(d18:2/20:0)	ME272146	1.10	0.90	NA	NA
LacCer(d18:2/22:0)	ME272167	1.19	0.81	NA	NA
Cer(d18:2/18:0)	ME272134	0.56	1.44	NA	NA
GlcCer(d18:2/16:0)	ME272157	0.73	1.27	NA	NA
GM3(d18:1/18:0)	ME272140	1.32	0.88	1.19	0.54
GM3(d18:2/18:0)	ME272145	1.29	0.80	1.48	0.39
Cer(d18:2/24:1)	ME272138	0.65	1.18	1.18	1.05
GM3(d18:2/24:1)	ME272147	0.82	0.93	1.55	0.79
GM3(d18:2/16:0)	ME272144	0.95	0.75	1.34	1.05
SM(42:3)	ME272185	0.92	0.87	1.35	0.94
LacCer(d18:2/16:0)	ME272166	0.73	0.89	0.97	1.54
Cer(d18:1/24:1)	ME272130	0.82	1.06	0.76	1.40
SM(36:1)	ME272174	0.95	0.91	0.66	1.53
Cer(d18:1/18:0)	ME272125	0.69	0.99	0.52	1.92
GlcCer(d18:1/18:0)	ME272150	0.61	1.30	0.46	1.66
GlcCer(d18:1/16:0)	ME272148	0.70	1.37	0.75	1.15
GlcCer(d18:1/24:1)	ME272155	0.67	1.40	0.76	1.14
GlcCer(d18:1/16:1)	ME272149	0.73	1.29	0.70	1.28
GlcCer(d18:1/20:0)	ME272151	0.72	1.36	0.63	1.26
GlcCer(d18:1/22:0)	ME272152	0.78	1.61	0.46	1.02
GlcCer(d18:1/23:0)	ME272153	0.71	1.53	0.58	1.11
GlcCer(d18:1/24:0)	ME272154	0.79	1.52	0.59	1.01
GlcCer(d18:1/25:0)	ME272156	0.82	1.48	0.62	0.97
SM(32:2)	ME272170	1.16	0.80	1.27	0.79
GM3(d18:1/16:0)	ME272139	1.17	0.91	1.03	0.87
SM(32:1)	ME272169	1.17	0.90	1.05	0.85
GM3(d18:1/24:1)	ME272143	1.09	1.01	1.15	0.72

Hierarchial Cluster analysis



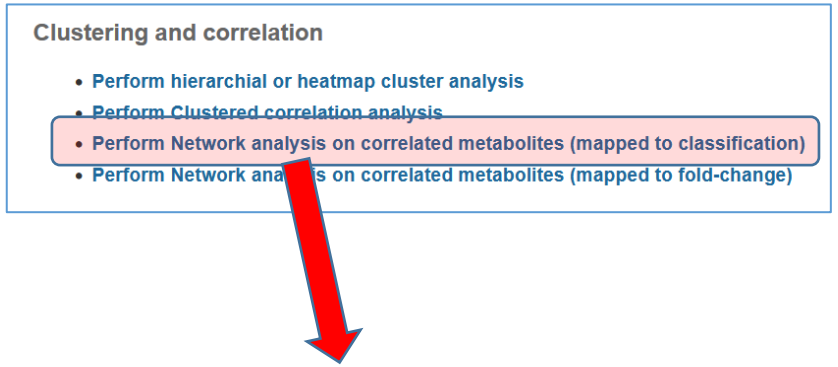
Factors:

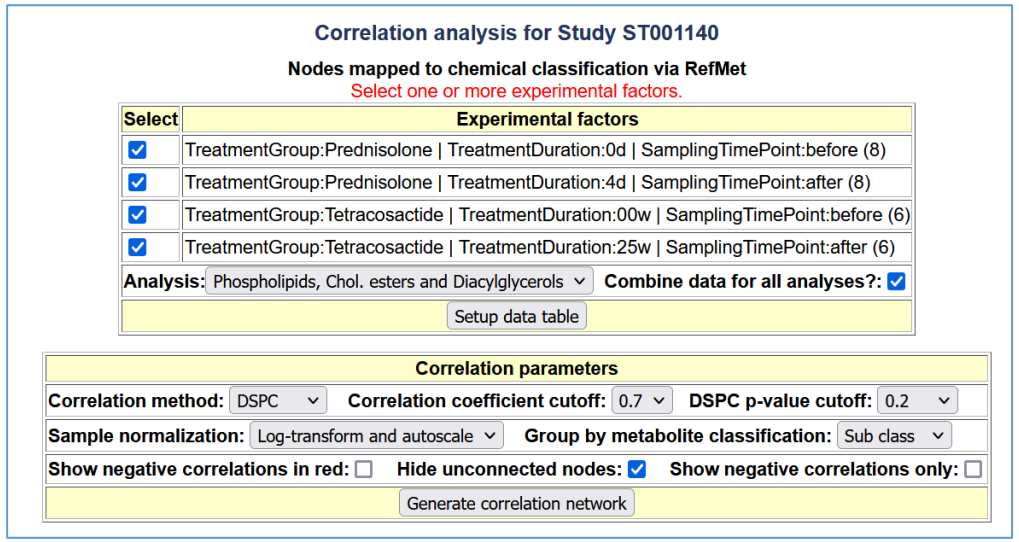
F1	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before
F2	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after
F3	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before
F4	TreatmentGroup:Tetracosactide | TreatmentDuration:25w | SamplingTimePoint:after

Heatmap Cluster analysis

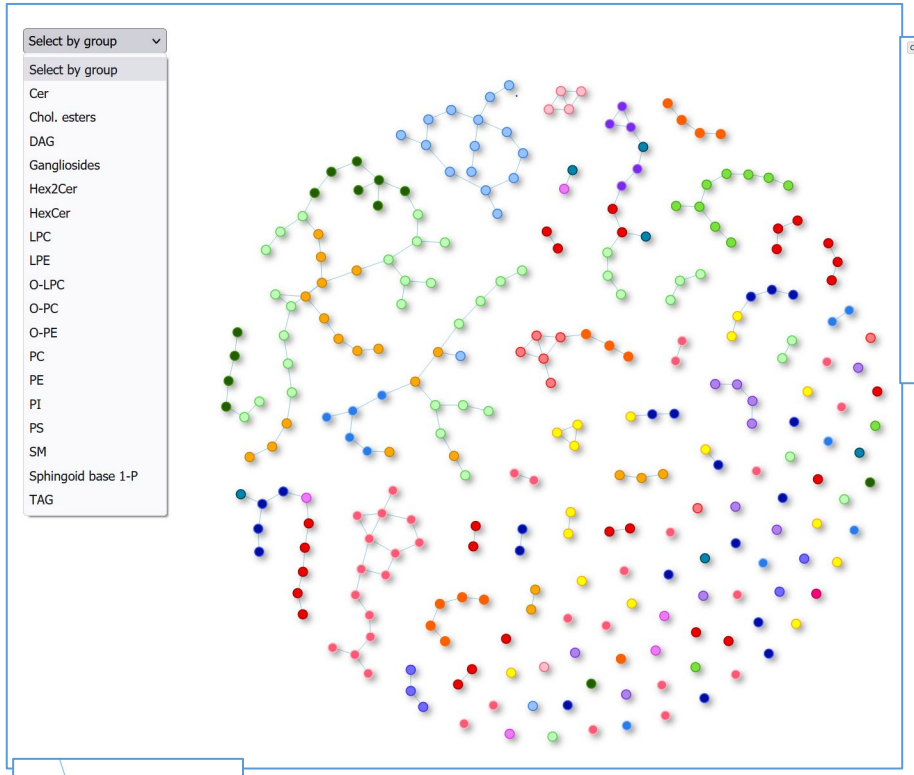
Network analysis tools (mapped to classification)

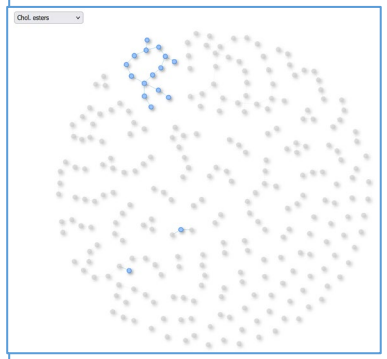
Pearson correlation or Debiased Sparse Partial Correlation (DSPC)



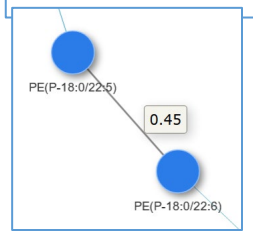


Select groups, correlation method, correlation value cutoff, DSPC p-value cutoff and sample normalization options

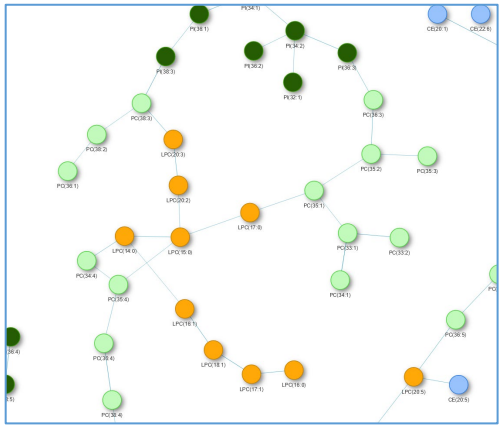


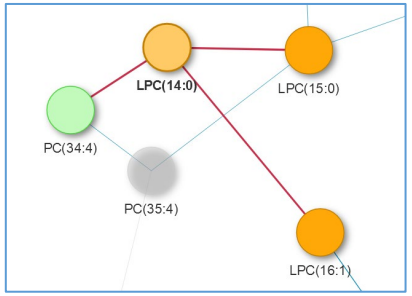


View a single metabolite class using group menu



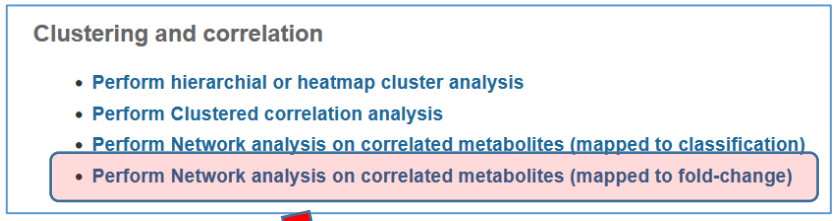
Hover over edge to display correlation coefficient

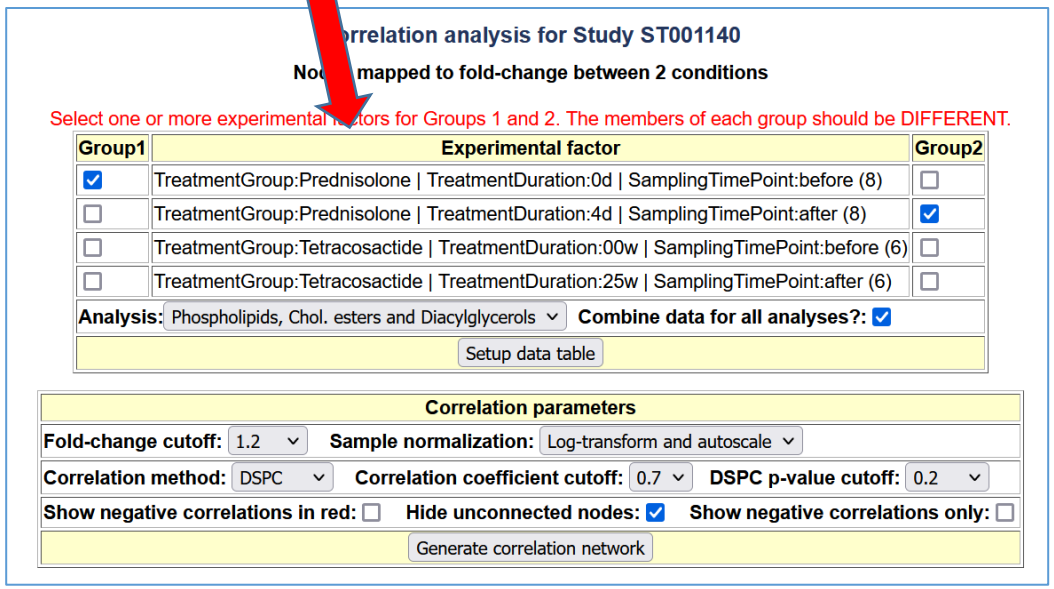




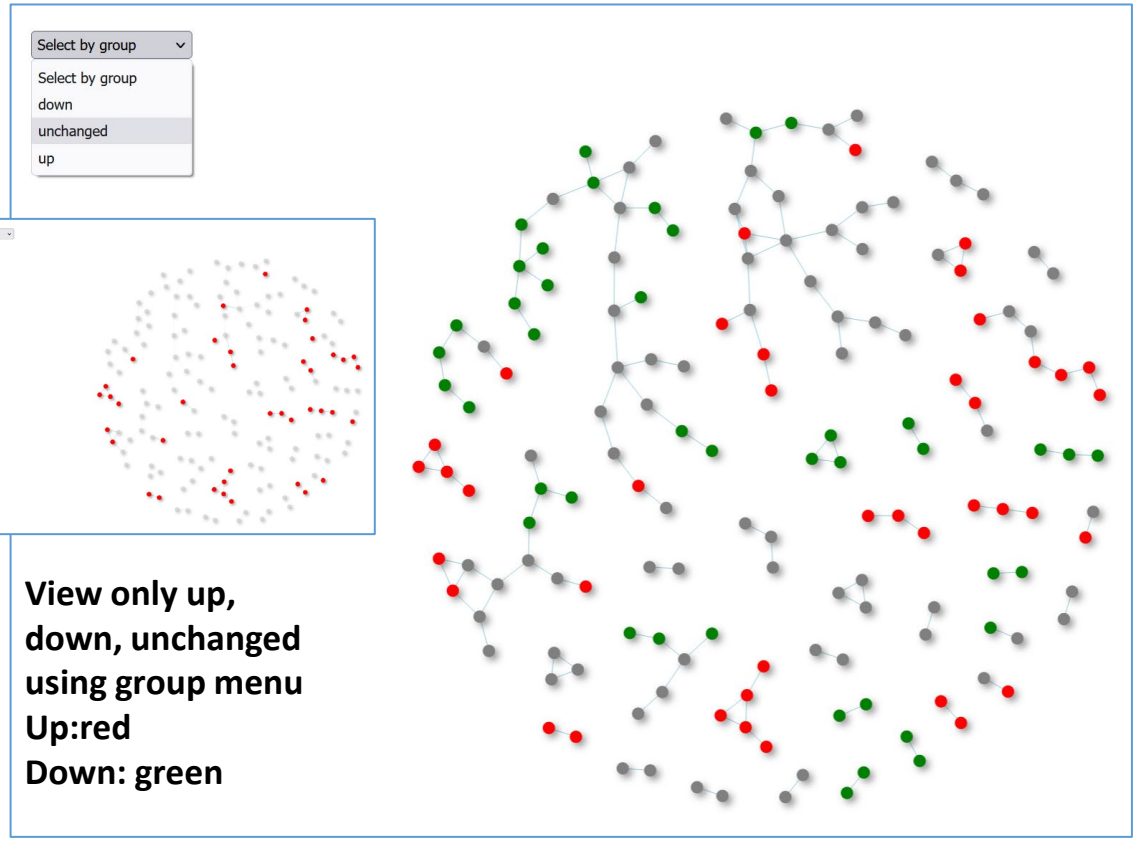
Zoom in to see metabolite labels

Network analysis tools (mapped to fold-change)

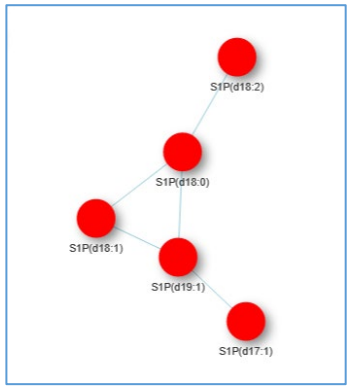




Select groups to compare by fold-change, correlation method, correlation value cutoff, DSPC p-value cutoff and sample normalization options



View only up, down, unchanged using group menu
Up:red
Down: green



Zoom in to see metabolite labels

Multivariate analysis tools (LDA example)

Multivariate analysis

- Perform Principal component analysis
- Perform Linear discriminant analysis
- Perform Partial least-squares discriminant analysis (PLS-DA)

Choose conditions to analyze

Alternatively, run LDA on all analysis groups in a study combined. This analysis is being run only one group (phospholipids/DAG/ CE)

LDA analysis for Study ST001140

(Analysis AN001870)

Select 3 or more experimental factors for PCA analysis.

Group	Experimental factor
☑	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before
☑	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after
☑	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before
☑	TreatmentGroup:Tetracosactide | TreatmentDuration:25w | SamplingTimePoint:after

Run LDA

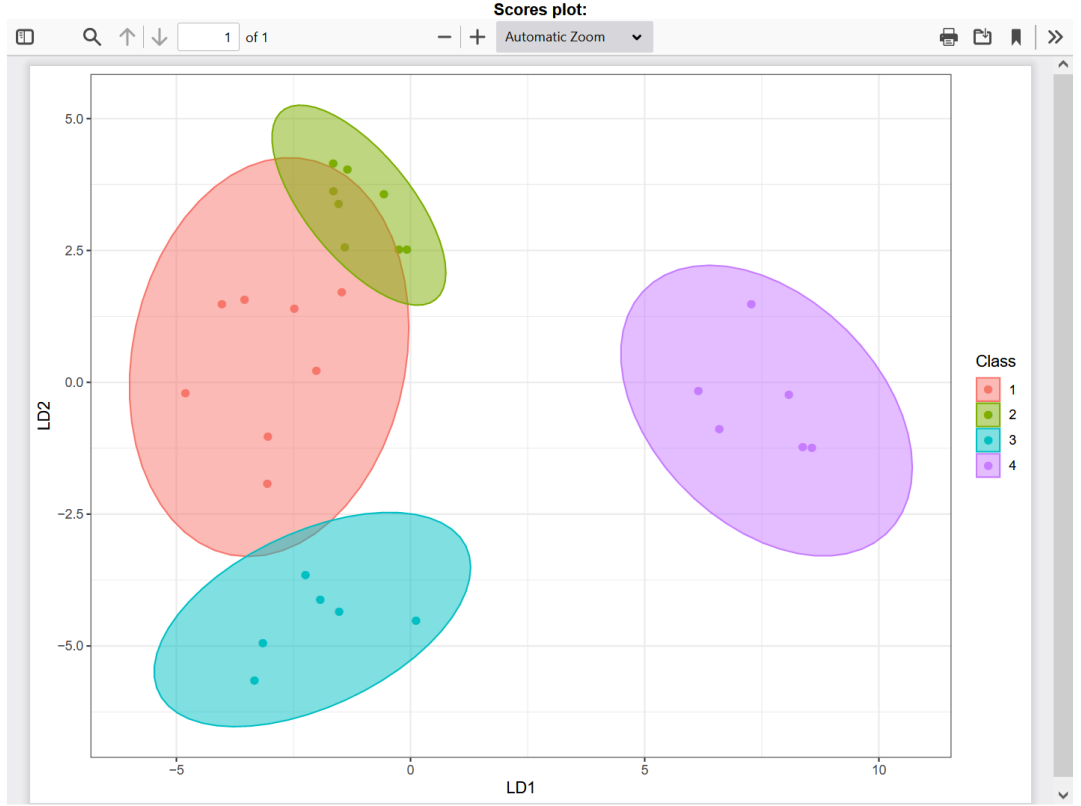
OR

Perform LDA on individual factors (all analyses in study)

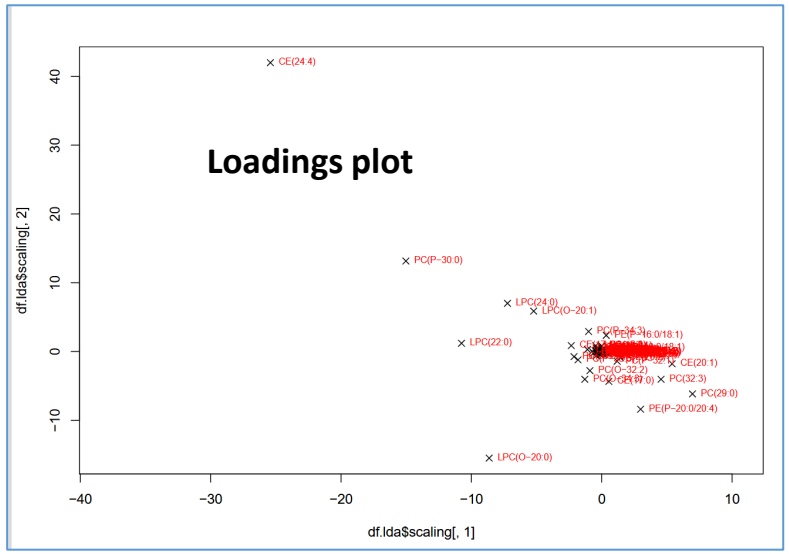
LDA analysis for (Study ST001140)

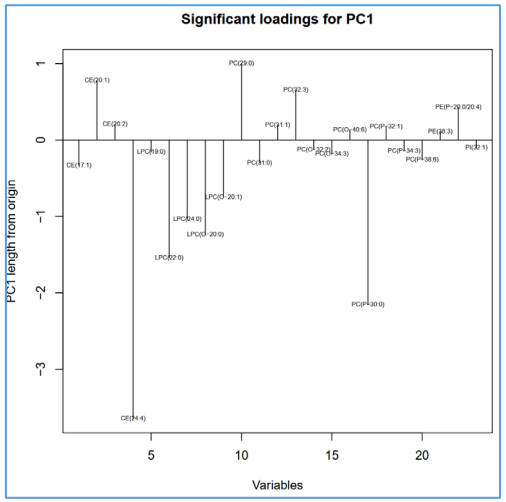
(Analysis AN001870)

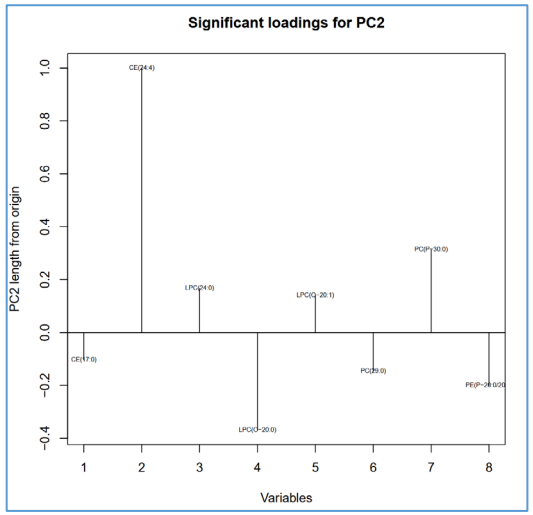
Scores plot:



Scores plot







Classification and feature analysis tools (OPLS-DA example)

Classification and feature analysis

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

Choose experimental conditions for the 2 groups being compared

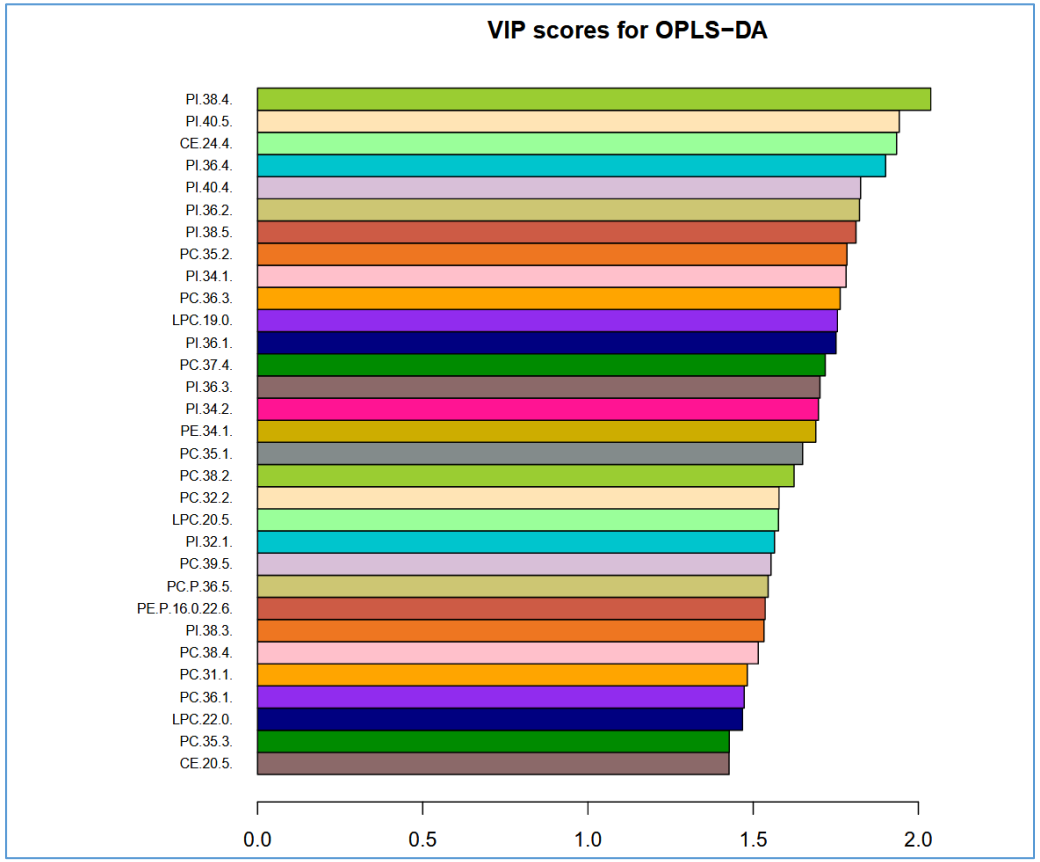
OPLS-DA analysis for Study ST001140

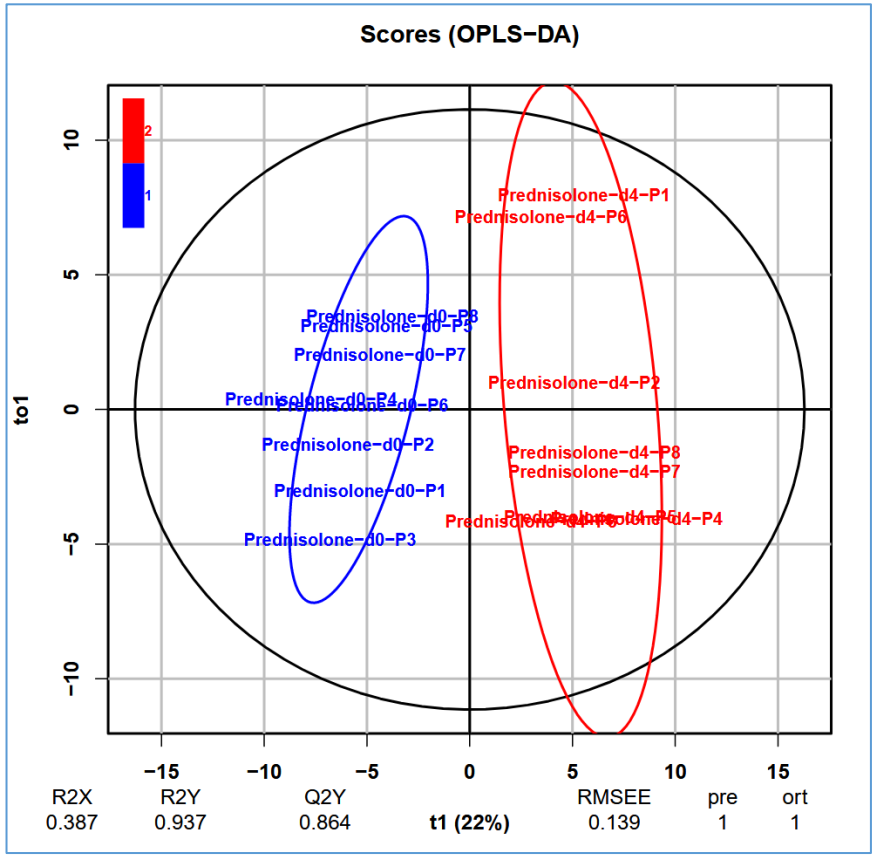
(Analysis AN001870)

Select one or more experimental factors for Groups 1 and 2. The members of each group should be DIFFERENT.

Group1	Experimental factor	Group2
☑	TreatmentGroup:Prednisolone | TreatmentDuration:0d | SamplingTimePoint:before	☐
☐	TreatmentGroup:Prednisolone | TreatmentDuration:4d | SamplingTimePoint:after	☑
☐	TreatmentGroup:Tetracosactide | TreatmentDuration:00w | SamplingTimePoint:before	☐
☐	TreatmentGroup:Tetracosactide | TreatmentDuration:25w | SamplingTimePoint:after	☐

Submit Query





Scores plot

Meta-analysis tools (across different studies)

Home | Data Repository | Databases | Protocols | Tools | Training / Events | About | Search

Overview | Upload / Manage Studies | Browse / Search Studies | Analyze Studies | Data Sharing Policy | Tutorials | FAQ

Analyze Studies

Analyze studies using **Jupyter Notebooks** or the following online tools.

MS/NMR studies identifying named metabolites

Select a study for analysis:

Select a study

Submit

Analysis tools may also be accessed from within each **study page** using the 'Perform statistical analysis' link

Comparative analysis across studies

- Perform meta-analysis on selected studies (compare ratios of 2 selected metabolites)
- Compare list of metabolites in 2 selected studies (all analyses)
- Compare list of metabolites in 2 selected studies (individual analyses)

View metabolite ratios across different studies

Study ID's (comma or space separated):

ST000402 ST000397 ST000395

Start..

Compare 2 individual studies:

ST000001: Fatb Induction Experiment (FatBIE)

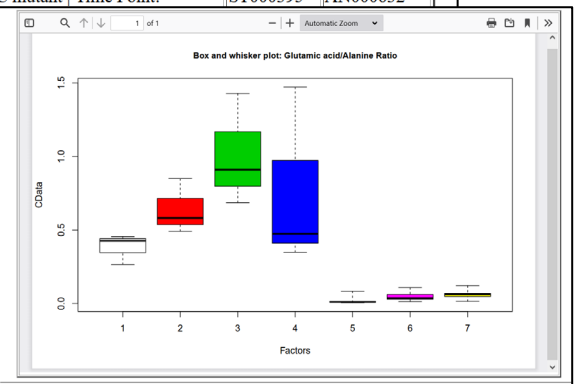
ST000002: Intestinal Samples II pre/post transplantation

Submit Reset

Alanine/Glutamic acid Ratio values (Units: AN000641)

Boxplot of ratio range	Boxplot of ratios for each factor level	Boxplot of inverse ratios for each factor level
Box and whisker plot	Boxplot by factor	Boxplot by factor (inverse)

Local Sample Id	Alanine	Glutamic Acid	Ratio	Factors	Study Id	Analysis Id
140619dlvsa01_1	24151	6385	3.782	Genotype:KaiC mutant | Time Point:-	ST000395	AN000632
140619dlvsa06_2	12244	5224	2.344	Genotype:Kai		
140619dlvsa07_2	13738	6254	2.197	Genotype:Kai		
140619dlvsa08_3	27389	23258	1.178	Genotype:Kai		
140619dlvsa09_2	21028	12228	1.720	Genotype:Kai		
140619dlvsa10_2	21827	10720	2.036	Genotype:Kai		
140619dlvsa03_1	11768	10707	1.099	Genotype:WT		
140619dlvsa05_1	10382	14825	0.700	Genotype:WT		
140619dlvsa11_1	8548	5864	1.458	Genotype:WT		
140619dlvsa02_1	17066	5947	2.870	Genotype:WT		
140619dlvsa04_1	10680	15722	0.679	Genotype:WT		
140619dlvsa12_2	11958	5660	2.113	Genotype:WT		
140421ajlsa01_1	36909	1576	23.419	Data:1		



Factor level F1: Genotype:KaiC mutant | Time Point:-
Factor level F2: Genotype:KaiC mutant | Time Point:4
Factor level F3: Genotype:WT | Time Point:-
Factor level F4: Genotype:WT | Time Point:4
Factor level F5: Data:1
Factor level F6: Glucose conc:0 g/L
Factor level F7: Glucose conc:10 g/L

Glutamic acid/Alanine Ratio

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
0.00500	0.01295	0.03970	0.09894	0.06530	1.47210

Metabolomics Tools:→Load and analyze your own dataset

Modular, portable suite of statistical tools for metabolomics analysis

- R statistics-based approach
  - **Normalization and scaling**
  - **Bar graphs and Boxplots**
  - **Univariate Analysis**
  - **Multivariate Analysis**
  - **Clustering and Correlation**
  - **Feature Analysis**
- Ability to select and combine groups of experimental conditions (factors)
- Applicable to targeted and untargeted datasets
- Workflow enables classification of metabolite names via RefMet
- Classified datasets are then amenable to class-specific and pathway-specific analysis

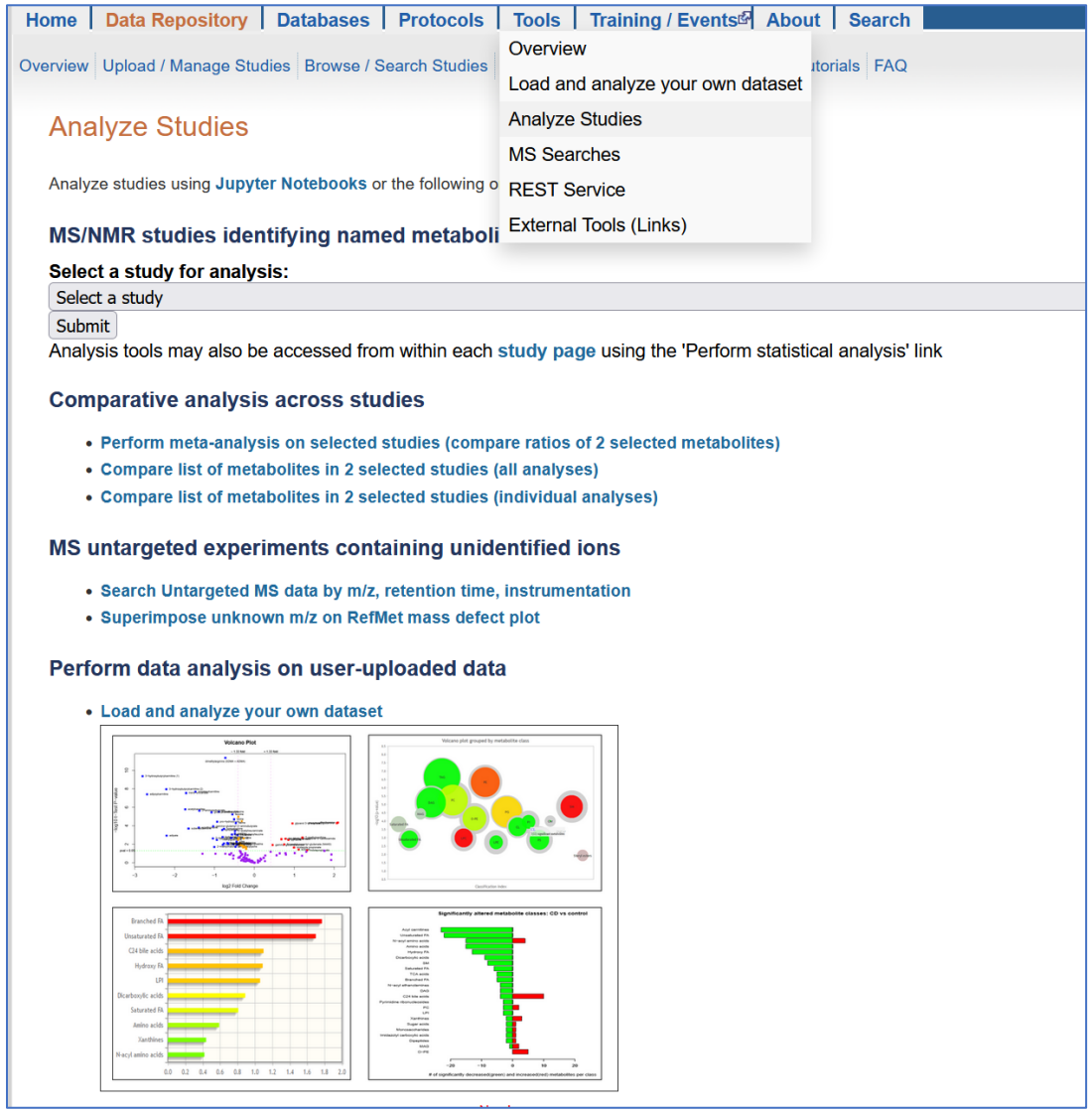
Metabolomics Tools:→Load and analyze your own dataset

https://www.metabolomicsworkbench.org/data/analyze.php

Samples	Group	CAR(16:0)		CAR(18:0)		CAR(18:1)		CAR(18:2)		CE(18:1)	
S001_2	Affected/Male	32592	7400	25164	16371	39797	461580	342255	241473	26379
S002_27	Affected/Male	37821	13552	40988	26845	51799	526923	409751	250720	41055
S007_51	Affected/Male	9201	6037	6219	10361	18848	461700	168391	125282	3802
S008_59	Affected/Male	132519	15845	245076	159627	24173	437630	326360	358552	21342
S009_39	Affected/Male	24407	9146	51668	32965	42774	337701	362332	204264	13970
S013_29	Affected/Male	30813	7299	35485	25603	58491	386359	385114	286028	30002
S014_22	Affected/Male	33082	8830	36894	21874	49050	542047	420069	256991	36641
S015_5	Affected/Male	29115	7472	38326	23507	35022	230142	298691	174860	9054
S016_31	Affected/Male	34081	7571	57646	48296	50157	498962	426752	266928	36812
S018_50	Affected/Male	58917	11048	101684	70157	45607	463558	429808	284710	18142
S021_21	Affected/Male	22655	6631	28896	22833	60510	567791	461084	409043	40955
S022_14	Affected/Male	23852	7132	33083	20959	56129	465535	475318	425279	17626
S023_41	Affected/Male	26156	6751	44201	26734	57518	482054	447923	338220	46731
S024_43	Affected/Male	24502	7108	36540	25172	37975	488013	379549	371133	21571
S025_33	Affected/Male	10231	5945	9475	14291	22012	391757	281674	189573	2667
S026_23	Affected/Male	31683	9410	39957	30026	40384	477841	385080	341657	19780
S027_18	Affected/Male	24153	5860	36417	28030	41637	476109	382987	348275	20344
S028_35	Affected/Male	32603	6541	64274	44075	62381	480321	527889	425970	32329
S029_34	Affected/Male	29696	7858	39767	36869	51518	483914	494792	379614	31195
S031_9	Affected/Male	30138	6312	26999	22104	40489	476062	401627	325777	30745
S032_64	Affected/Female	32551	9934	45279	30568	50255	329084	417248	412746	12094
S034_66	Affected/Female	40129	7901	54879	52292	51006	515113	355455	367787	28220
S037_46	Affected/Female	55349	7426	103693	35440	22463	173160	191218	172002	6157
S038_8	Affected/Female	16663	9111	9982	11166	49852	365320	332450	208024	3605
S040_26	Affected/Female	30737	11822	30133	19357	28450	464703	349594	352426	25960
S041_69	Affected/Female	20351	9616	33138	15191	60271	308696	365188	384615	18781
S042_61	Affected/Female	44531	10508	87680	70868	34093	507718	452632	536826	22587
S044_3	Affected/Female	26159	7195	34041	31696	33092	482180	363697	362897	29765
S045_58	Affected/Female	53023	9926	96073	71568	34687	403564	295048	467228	32331
S046_24	Affected/Female	21720	5712	23667	10882	41203	279409	267775	243040	17383
S047_16	Affected/Female	17094	5225	24567	17196	42917	349825	298969	278524	36062
S049_48	Affected/Female	55655	10899	63535	62495	42110	401089	387996	400073	17062
S051_44	Affected/Female	22293	5128	36012	26083	38486	475328	410951	371971	18243
S053_11	Affected/Female	12268	4303	24253	21592	52598	385859	259803	369865	16433
S057_1	Affected/Female	26327	7078	29278	21698	61240	504927	420130	390436	28532
S059_28	Affected/Female	3859	2676	1881	2439	31575	296196	186595	106324	2445

File format required:
Column 1: sample names
Column 2: group identifier (letters, numbers or text)
Columns 3 to n: Variables

This is an option to analyze your own dataset (as opposed to a submitted NMDR study)



Analysis tools available on user-uploaded data

(these are NOT submitted studies –a data table is uploaded via a form)

Normalization and scaling

- Sample normalization
- Analyte scaling
- Relative log abundance plot

Bargraphs and Boxplots

- Bargraph
- Bargraph ratio
- Boxplot

Univariate Analysis

- Volcano Plot
- ANOVA analysis
- Debiased sparse partial correlation analysis

Clustering and Correlation

- Hierarchical Cluster Analysis
- Pearson Correlation:
- Clustered correlation analysis

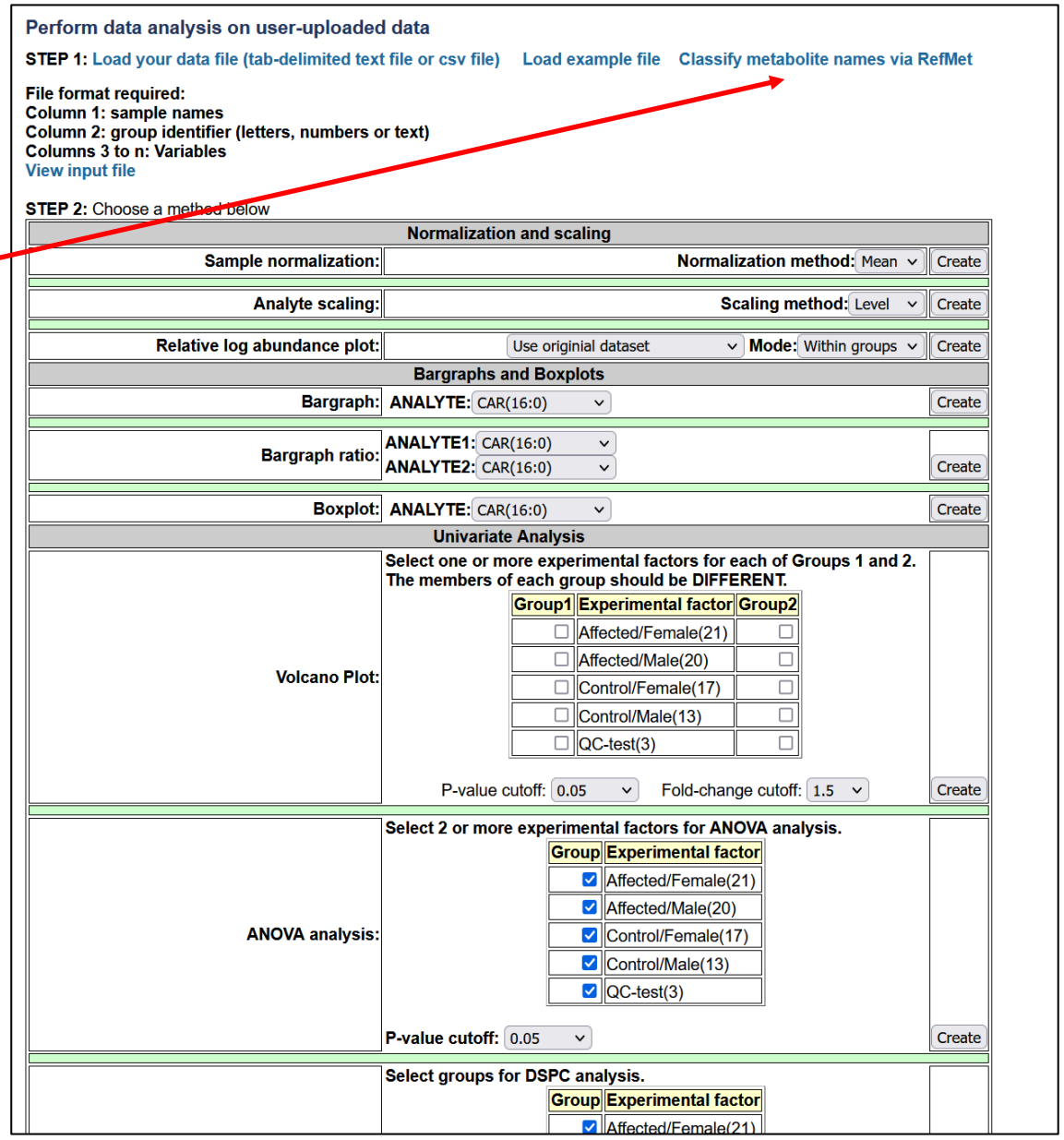
Multivariate Analysis

- Principal Component Analysis
- Linear Discriminant Analysis

Classification and Feature Analysis

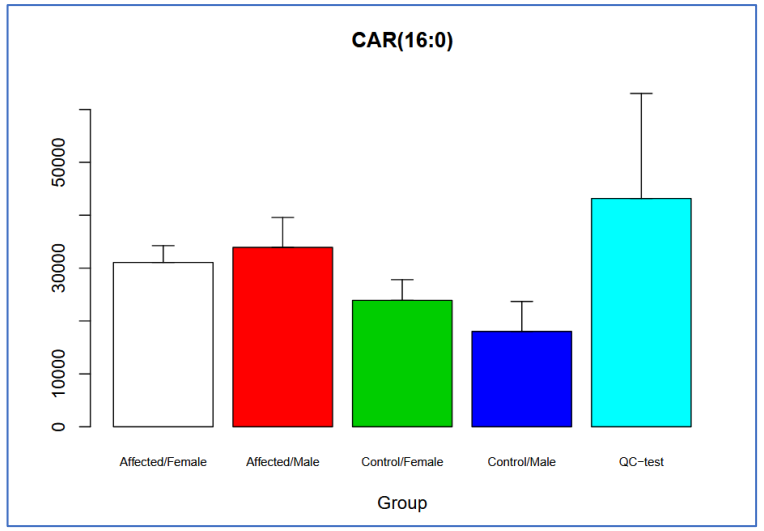
- OPLS-DA/VIP analysis
- Random Forest/VIP analysis

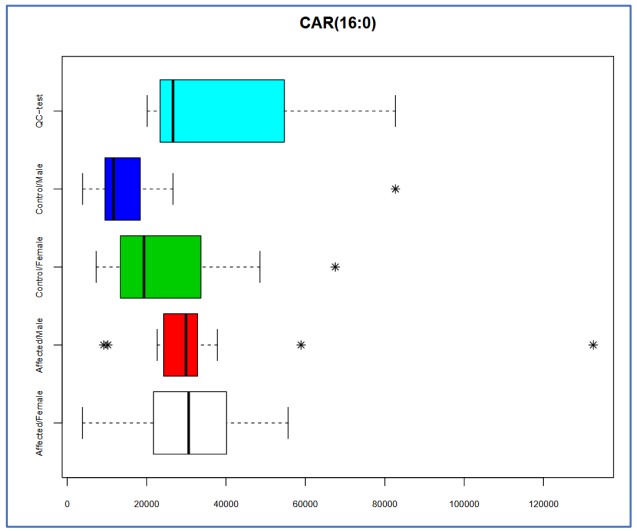
Mapping of input metabolite names to RefMet facilitates enables deployment of classification tools

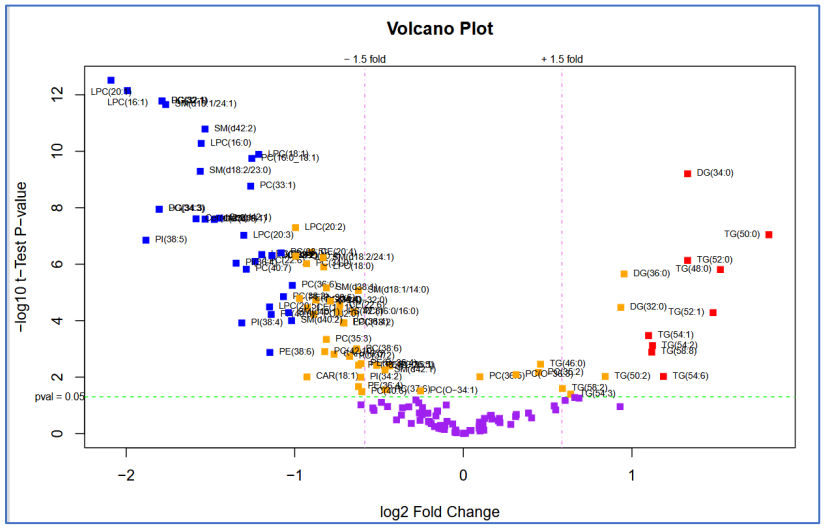


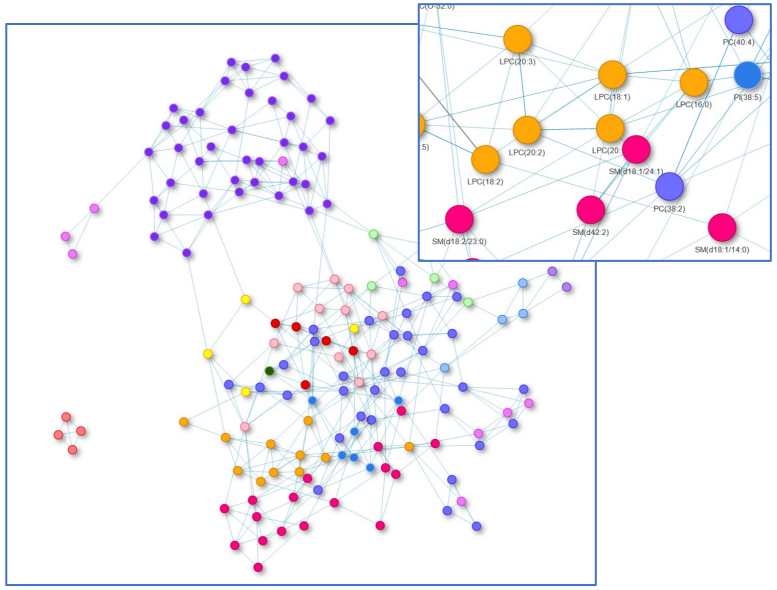
Metabolomics Tools:→Load and analyze your own dataset

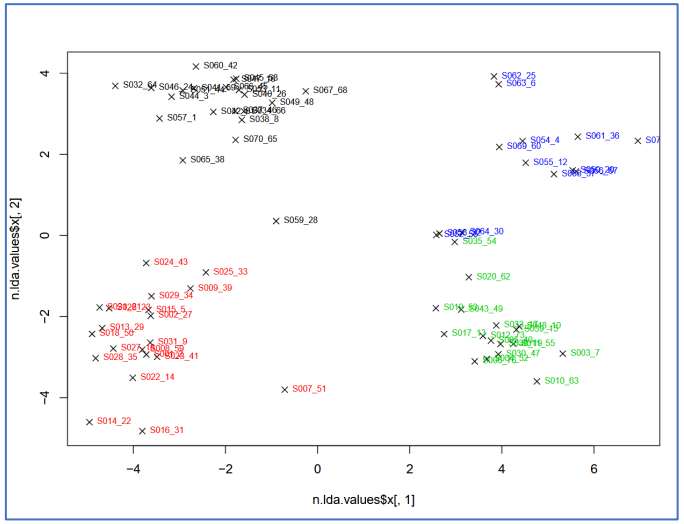
Examples of output from online tools

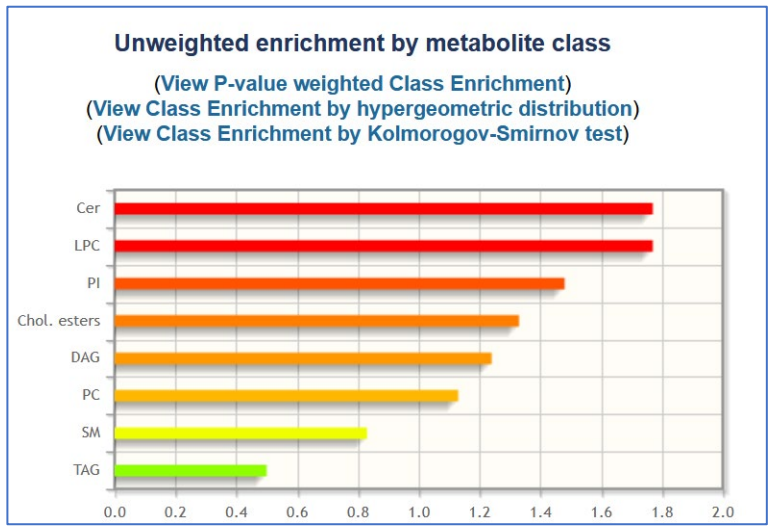












NMDR Tutorials

Tutorials and Documentation

NMDR Study Submission

- NMDR study submission tutorial (PDF)

NMDR Data Browsing/Searching/Analysis

- Metabolomics Workbench overview and infrastructure (PDF)
- NMDR browsing and searching tutorial (PDF)
- RefMet standardized nomenclature/Metabolite structure database tutorial (PDF)
- Metabolomics Workbench REST service tutorial (PDF)
- MetStat summary tool tutorial (PDF)
- NMDR analysis tools tutorial (PDF)

mwTab File Usage

- mwTab file specification (PDF)

REST service API

- REST service API (PDF)

Metabolomics Workbench collaborations with DTC's

Web tools

- **MetaBatch Omic Browser:** A web application developed at MD Anderson Cancer Center (John Weinstein group) for analysis and visualization of batch effects in NMDR datasets. Included are dynamically interactive Next-Generation Clustered Heat Maps, PCA+, UMAP, box plot, violin plot, and other visualizations for essentially all NMDR datasets.
- **Next-Generation Clustered Heat Map (NGCHM) Viewer:** A dynamically interactive web environment, developed at MD Anderson Cancer Center (John Weinstein group), for exploration of omic datasets with extreme zooming, panning, searches, covariate bars, dozens of link-outs, high-resolution graphics, and other features. Included is coordination with UMAP, t-SNE, PCA+, pathway, and other visualizations, with quantitative analyses. Updates are done periodically as additional datasets are added to NMDR. **https://www.biorxiv.org/content/10.1101/2020.10.31.363580v1.full.pdf** .
- **SIMPEL: (Stable Isotope assisted Metabolomics for Pathway ELucidation)** An R package for targeted extraction and analysis of isotopologue data developed by Jamey Young (Vanderbilt), Doug Allen (Danforth Center) and colleagues. The software works with any time-course labeling data and has been incorporated into a web application here. The R package may also be downloaded via **Github** . Please see the **tutorial** for details.

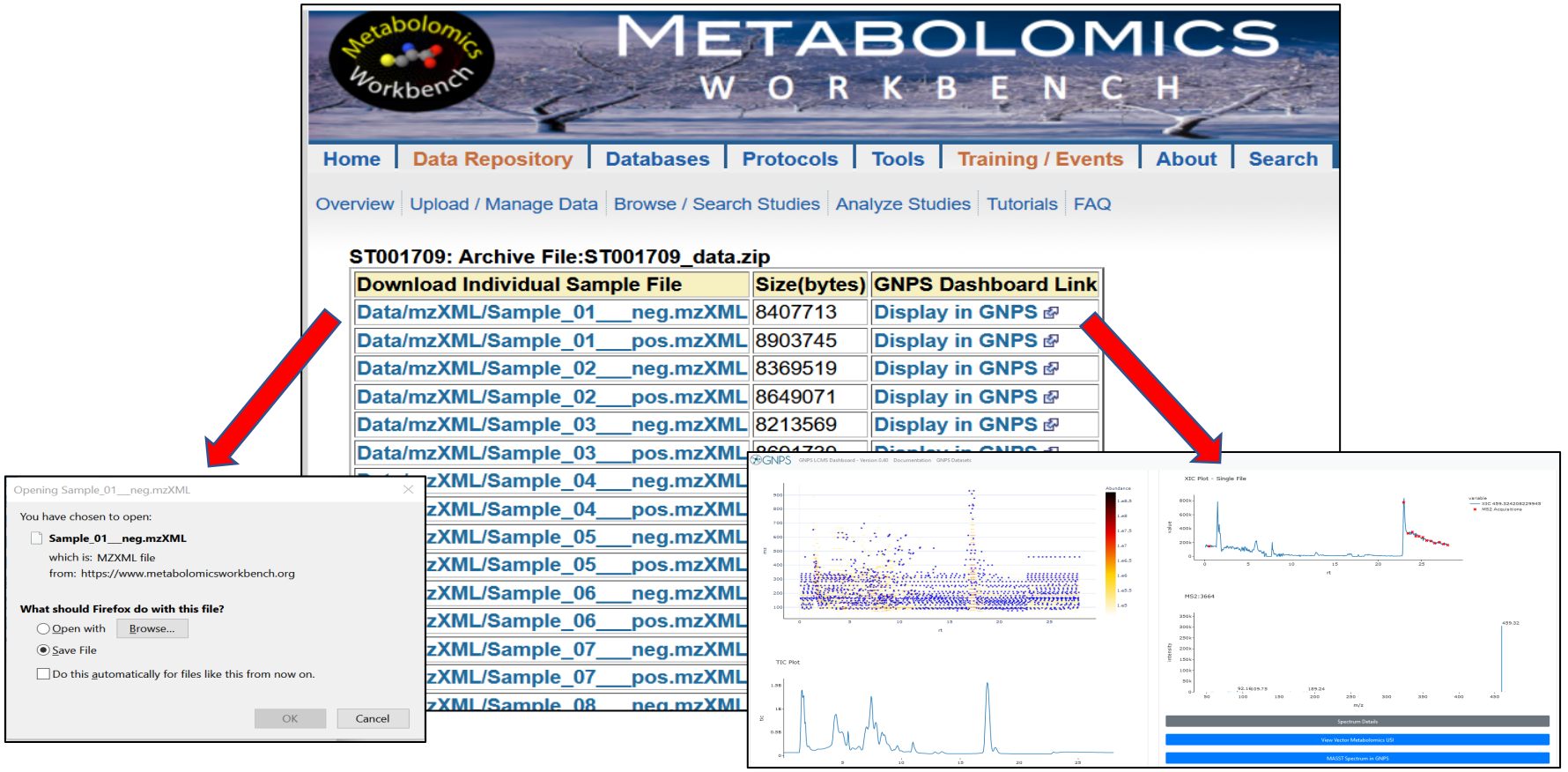
Docker tools

- **MSCAT:** A dockerized application developed by the group led by Katerina Kechris and Debashis Ghosh at the University of Colorado Anschutz Medical Campus in conjunction with the Metabolomics Workbench. The application provides a database of metabolomics software tools and allows one to generate potential software workflows using an online interface.

Shiny apps

- **RefMet name search:** A Shiny app developed by the Metabolomics Workbench to search the RefMet standardized metabolite nomenclature database by metabolite name.
- **RefMet MS search:** A Shiny app developed by the Metabolomics Workbench to search the RefMet standardized metabolite nomenclature database with a list of m/z values (Input is a text file with a single column of m/z values).
- **MetStat search:** A Shiny app developed by the Metabolomics Workbench to display summary information in NMDR based on analysis method, species, sample source and disease association.
- **PaIRKAT:** A Shiny app developed by the group led by Katerina Kechris and Debashis Ghosh at the University of Colorado Anschutz Medical Campus. PaIRKAT is a pathway integrated tool for improving testing power on high dimensional data by including graph topography in the kernel machine regression setting.
- **Marr:** A Shiny app developed by the group led by Katerina Kechris and Debashis Ghosh at the University of Colorado Anschutz Medical Campus which implements the method Maximum Rank Reproducibility (MaRR), a nonparametric approach that detects reproducible signals using a maximal rank statistic for high-dimensional biological data. An R package version is also available for download from **Github** .

Collaboration with Global Natural Product Social Molecular Networking (GNPS)



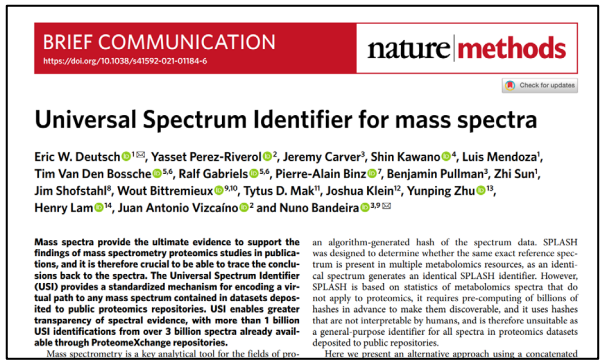
View spectral details of MS raw data files deposited in NMDR via the GNPS dashboard

GNPS Dashboard: Collaborative Analysis of Mass Spectrometry Data in the Web Browser

D. Petras et al, Nature Methods (2021) https://doi.org/10.1038/s41592-021-01339-5

Collaboration with Global Natural Product Social Molecular Networking (GNPS)

Universal spectrum Identifier for mass spectra



BRIEF COMMUNICATION
https://doi.org/10.1038/s41592-021-01184-6
nature methods

Universal Spectrum Identifier for mass spectra

Eric W. Deutsch, Yasset Perez-Riverol, Jeremy Carver, Shin Kawano, Luis Mendoza, Tim Van Den Bossche, Ralf Gabriels, Pierre-Alain Binz, Benjamin Pullman, Zhi Sun, Jim Shofstahl, Wout Bittremieux, Tytus D. Mak, Joshua Klein, Yunping Zhu, Henry Lam, Juan Antonio Vizcaíno and Nuno Bandeira

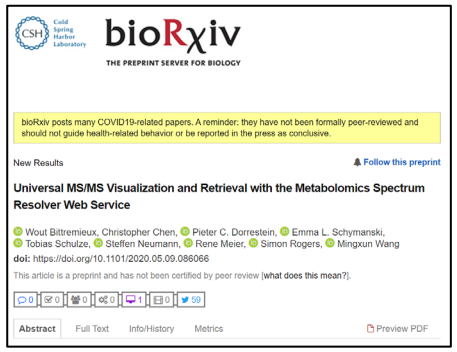
Mass spectra provide the ultimate evidence to support the findings of mass spectrometry proteomics studies in publications, and it is therefore crucial to be able to trace the conclusions back to the spectra. The Universal Spectrum Identifier (USI) provides a standardized mechanism for encoding a virtual path to any mass spectrum contained in datasets deposited to public proteomics repositories. USI enables greater transparency of spectral evidence, with more than 1 billion USI identifications from over 3 billion spectra already available through ProteomeXchange repositories.

Mass spectrometry is a key analytical tool for the fields of pro-

an algorithm-generated hash of the spectrum data. SPLASH was designed to determine whether the same exact reference spectrum is present in multiple metabolomics resources, as an identical spectrum generates an identical SPLASH identifier. However, SPLASH is based on statistics of metabolomics spectra that do not apply to proteomics, it requires pre-computing of billions of hashes in advance to make them discoverable, and it uses hashes that are not interpretable by humans, and is therefore unsuitable as a general-purpose identifier for all spectra in proteomics datasets deposited to public repositories.

Here we present an alternative approach using a concatenated

Proteomics data



bioRxiv
THE PREPRINT SERVER FOR BIOLOGY

bioRxiv posts many COVID19-related papers. A reminder: they have not been formally peer-reviewed and should not guide health-related behavior or be reported in the press as conclusive.

New Results — Follow this preprint

Universal MS/MS Visualization and Retrieval with the Metabolomics Spectrum Resolver Web Service

Wout Bittremieux, Christopher Chen, Pieter C. Dorrestein, Emma L. Schymanski, Tobias Schulze, Steffen Neumann, Rene Meier, Simon Rogers, Mingxun Wang

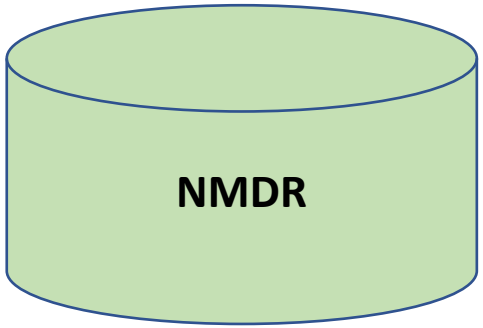
doi: https://doi.org/10.1101/2020.05.09.086066

This article is a preprint and has not been certified by peer review [what does this mean?].

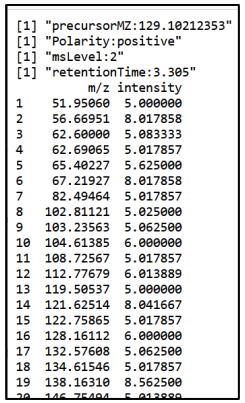
Abstract | Full Text | Info/History | Metrics | Preview PDF

Metabolomics data proposal

The Metabolomics Spectrum Resolver builds upon the USI standard developed by the HUPO.
USIs are formatted as follows:
mzspec:<collection>:<msRun>:<indexType>:<indexNumber>:<optional interpretation>
Example:mzspec:ST000003:iPSC-T1R1:scan:3

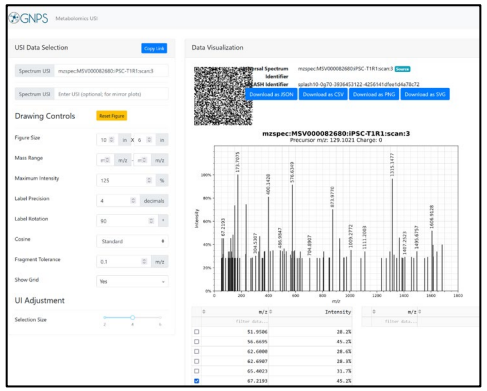


USI request from NMDR



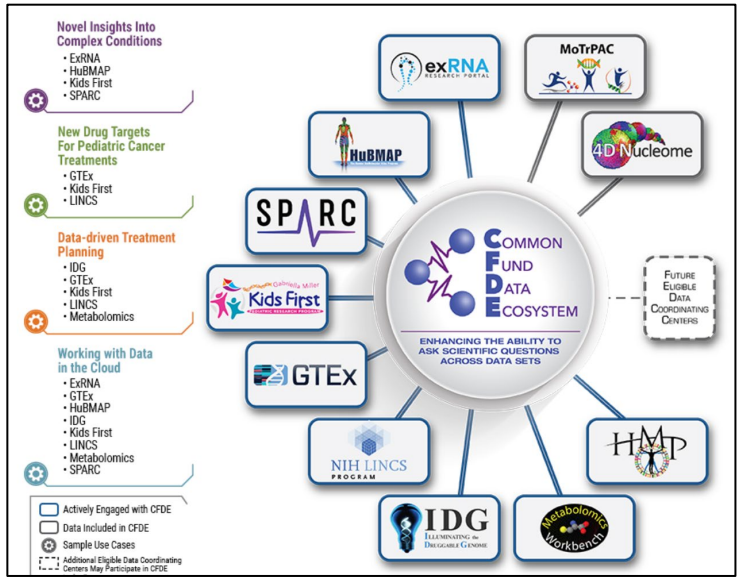
```
[1] "precursorMZ:129.10212353"
[1] "Polarity:positive"
[1] "msLevel:2"
[1] "retentionTime:3.305"
          m/z intensity
1    51.95060  5.000000
2    56.66951  8.017858
3    62.60000  5.083333
4    62.69065  5.017857
5    65.40227  5.625000
6    67.21927  8.017858
7    82.49464  5.017857
8   102.81121  5.025000
9   103.23563  5.062500
10  104.61385  6.000000
11  108.72567  5.017857
12  112.77679  6.013889
13  119.50537  5.000000
14  121.62514  8.041667
15  122.75865  5.017857
16  128.16112  6.000000
17  132.57608  5.062500
18  134.61546  5.017857
19  138.16310  8.562500
```

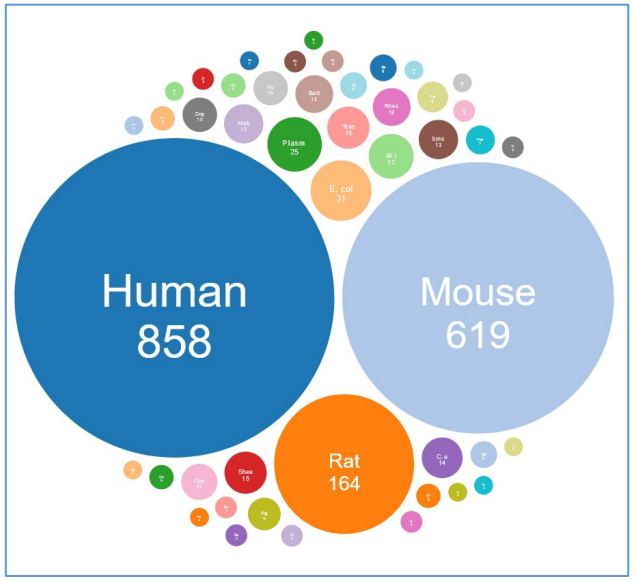
MS2 peaklist/metadata

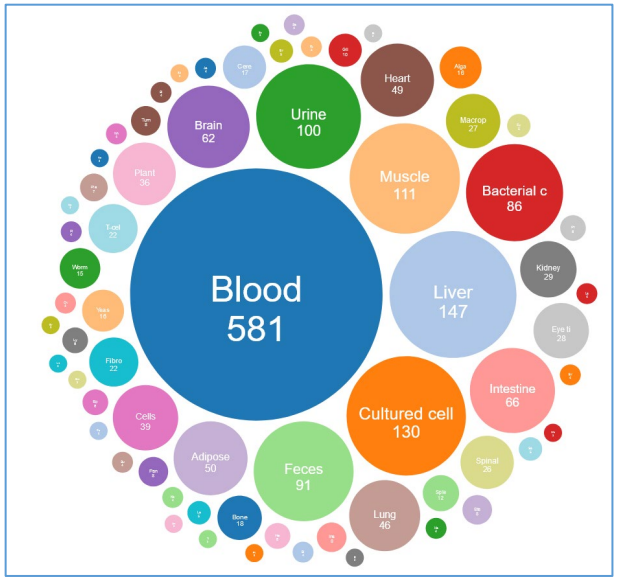


Metabolomics Spectrum Resolver Web Service

NIH's Common Fund Data Ecosystem







Ongoing efforts involve development of ontologies and parts lists of NMDR study data:
Specification of species designation and sample source at an **individual sample level** (>200,000 samples in NMDR)

REST service to retrieve sample data from NMDR

Sample context	
Fetch information for an individual sample in a study*New	https://www.metabolomicsworkbench.org/rest/sample/mb_sample_id/SA002633/all

Metabolomics Workbench/NMDR and FAIR principles

Findable:

DOIs are assigned to each submitted dataset/study.

schema.org formatted metadata is embedded in Metabolomicsworkbench.org which allows it to be found and indexed by search engines

MetabolomeXchange EBI: Omics Discovery Index

Accessible:

Metabolomics Workbench website: multiple browsing/download options

A REST API is provided for accessing data

Interoperable:

Using community standard **mwTAB** to describe data

mwTAB documented at fairsharing.org

Multiple positive outcomes via **RefMet** standardized nomenclature

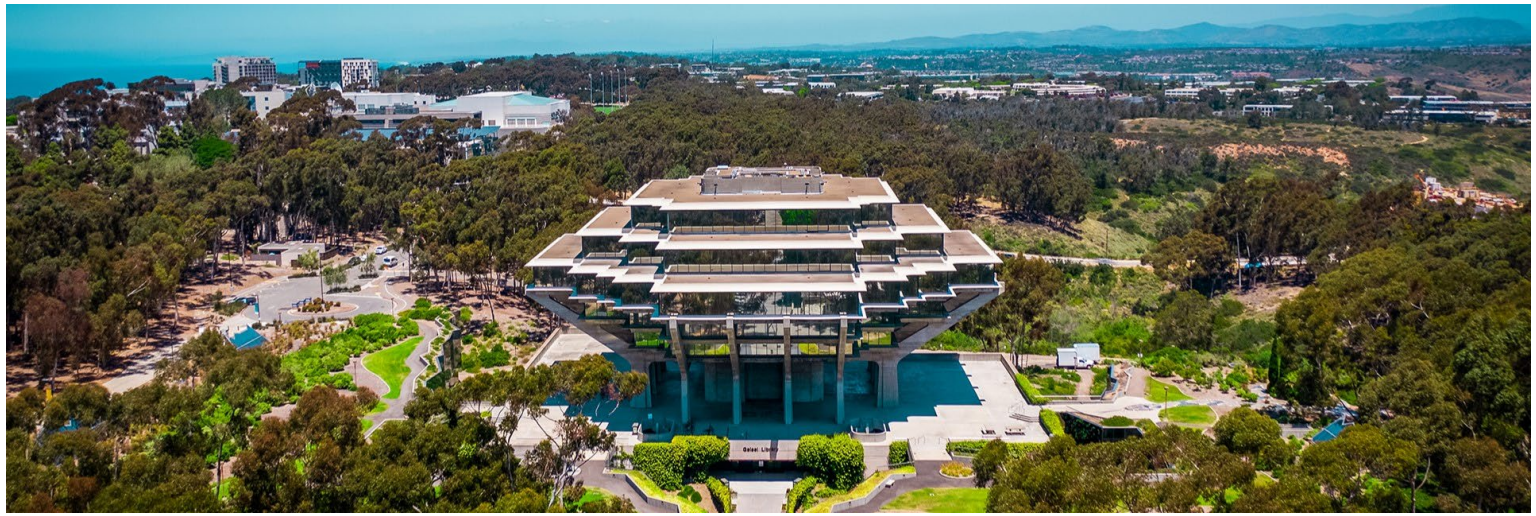
Reusable:

Download and re-process raw data from NMDR

Download and re-analyze processed data (multiple format options)

Jupyter notebooks illustrate how to (re)use the data

Thank you!



UCSD Main Library

UCSD Bioengineering

San Diego Supercomputer Center