NMDR online browsing, data upload and analysis tools

Overview

- **Metabolomics workbench**
- **Data Repository**
  - **Browse/Search Studies**
  - **Analyze Studies**
  - **Upload/Manage Studies**
- **Databases**
- **Protocols**
- **Standards**

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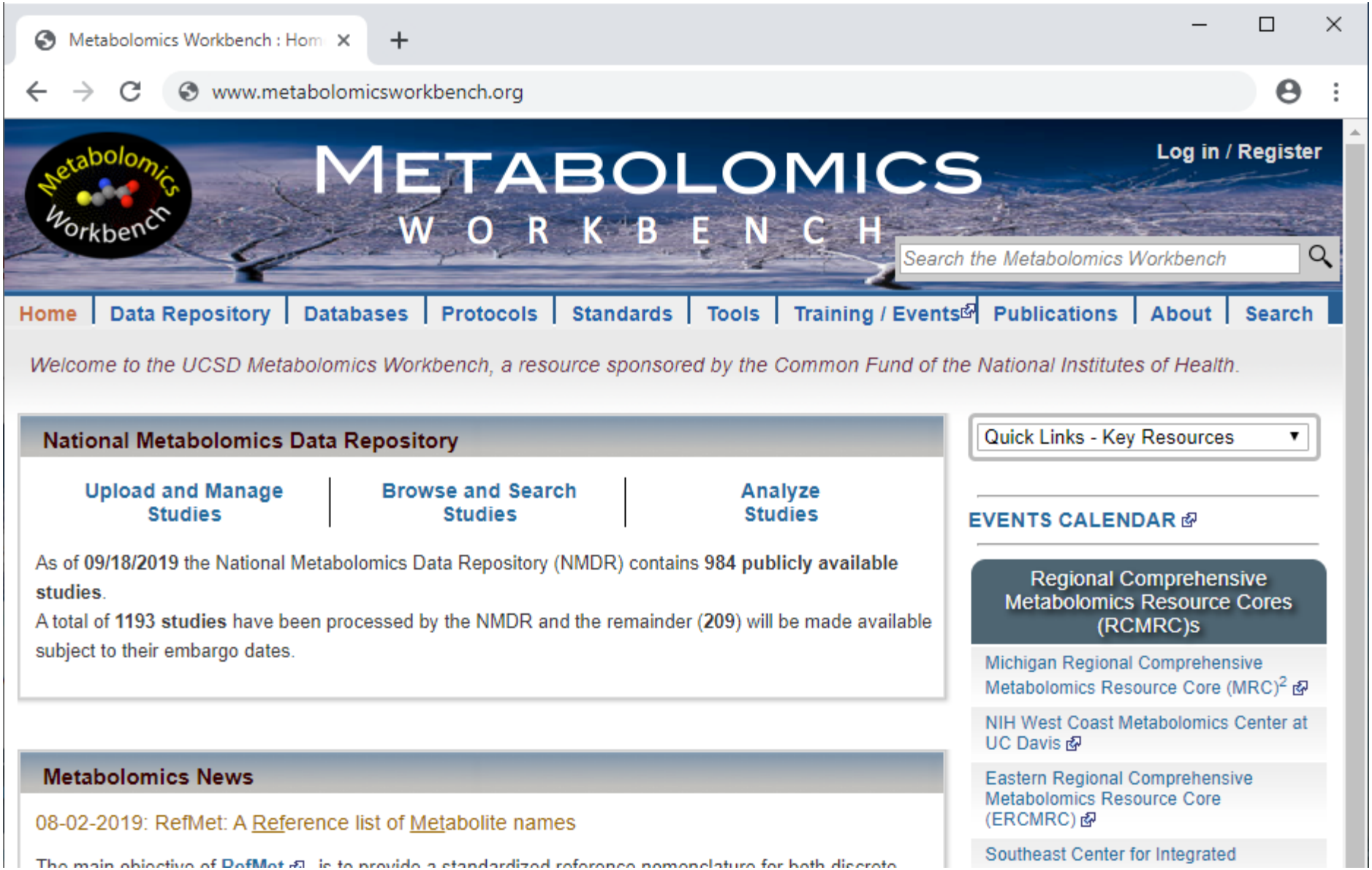
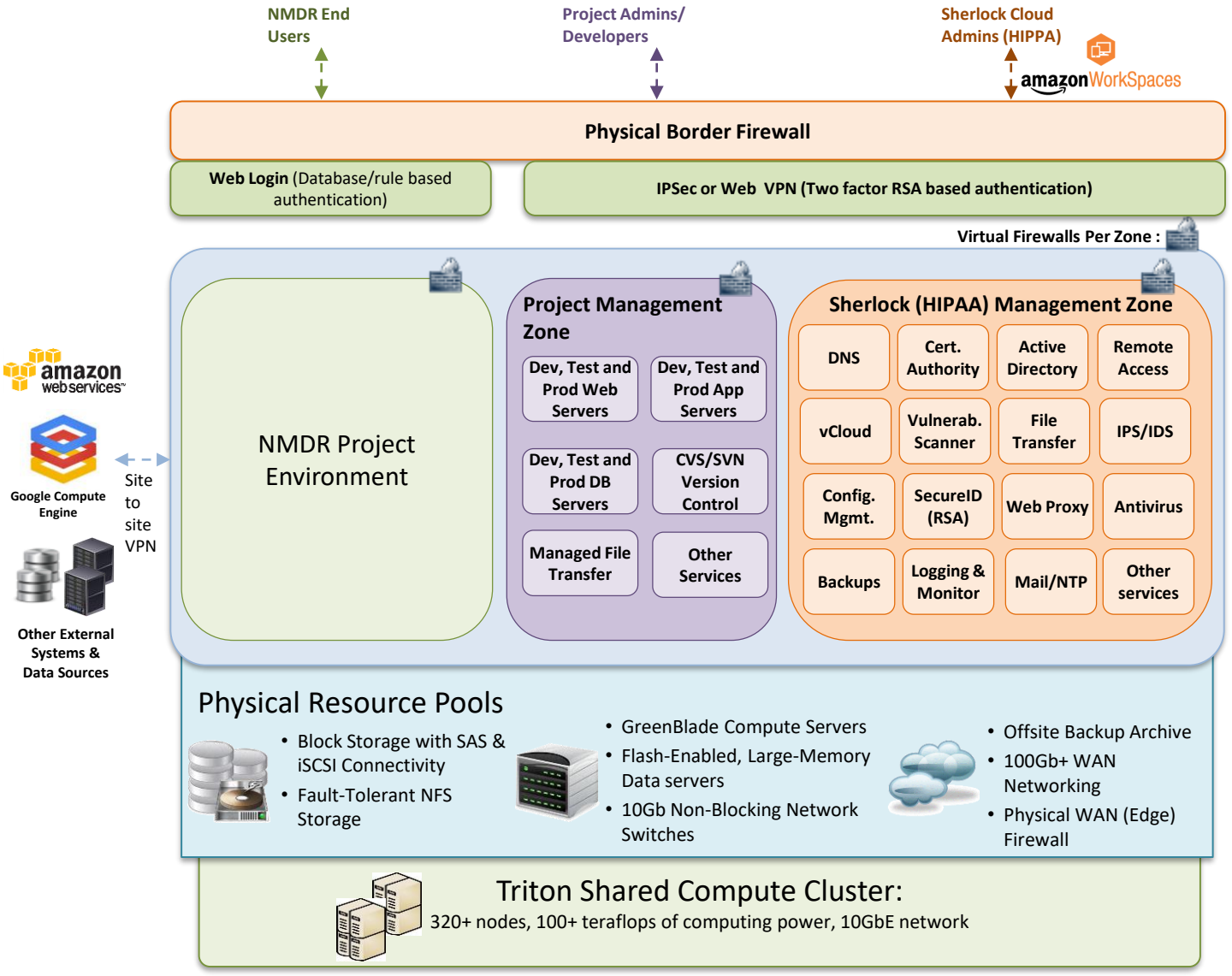
Metabolomics Workbench Home



Metabolomics vCloud infrastructure



Overview

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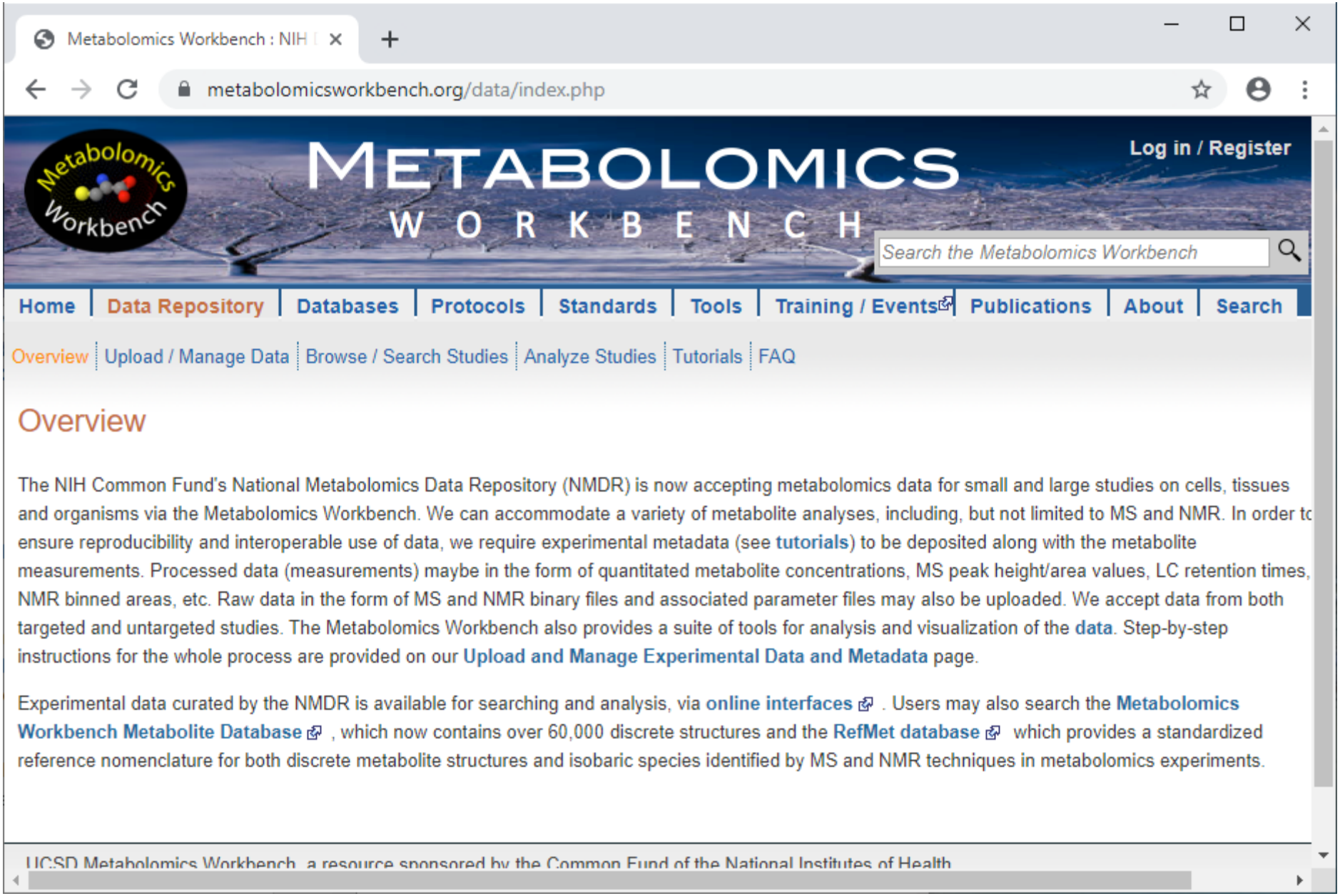
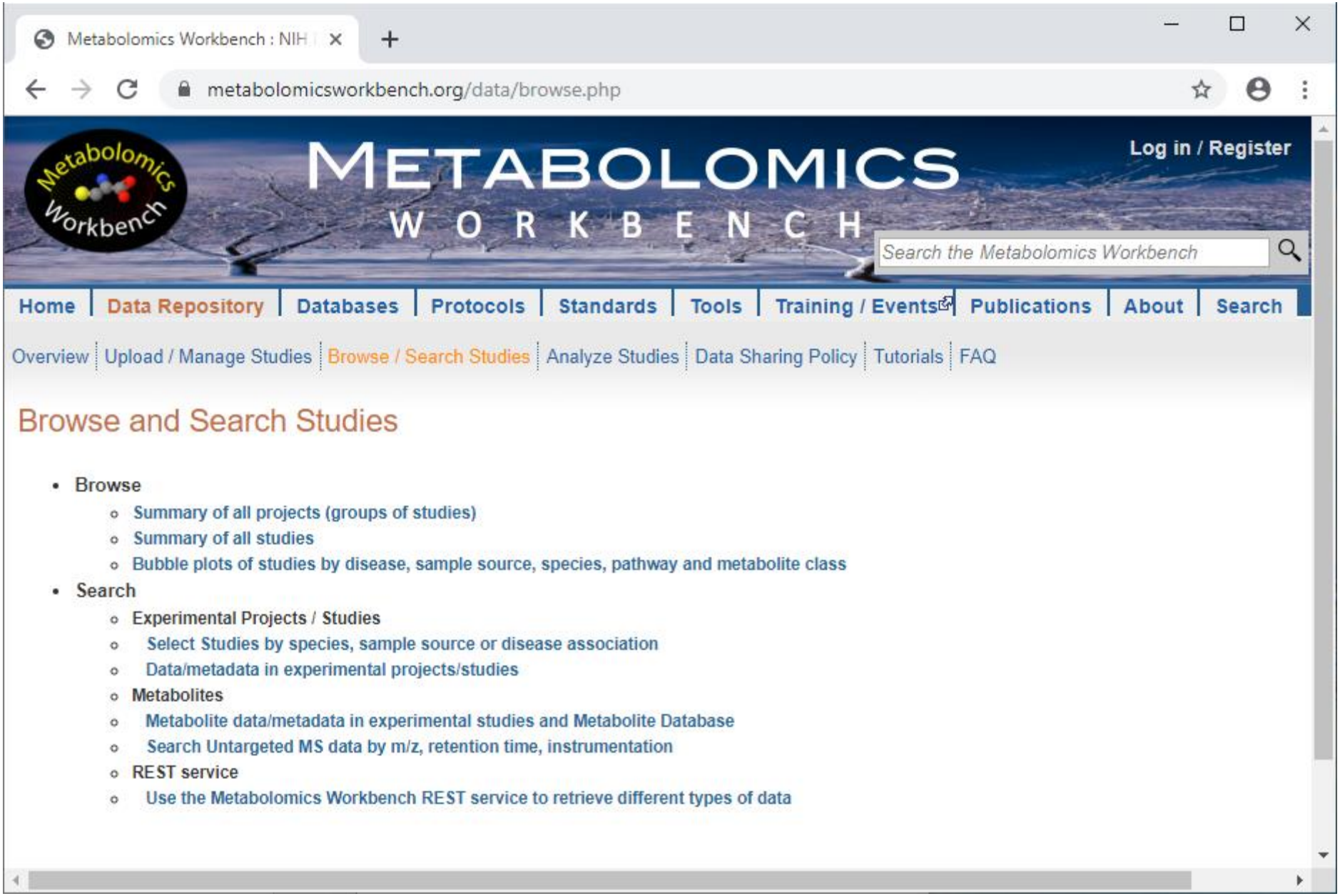
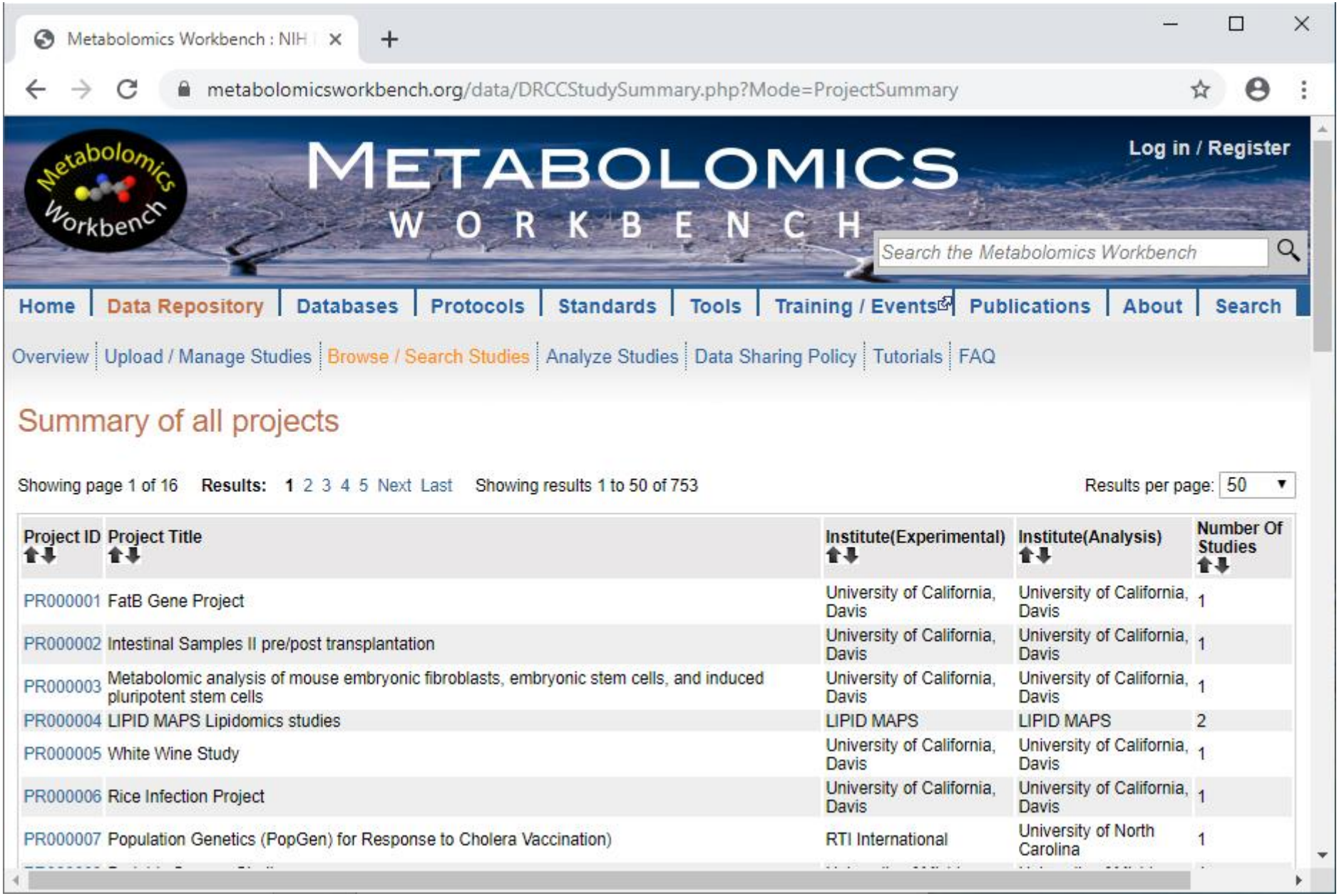
Data Repository



Browse/Search Studies

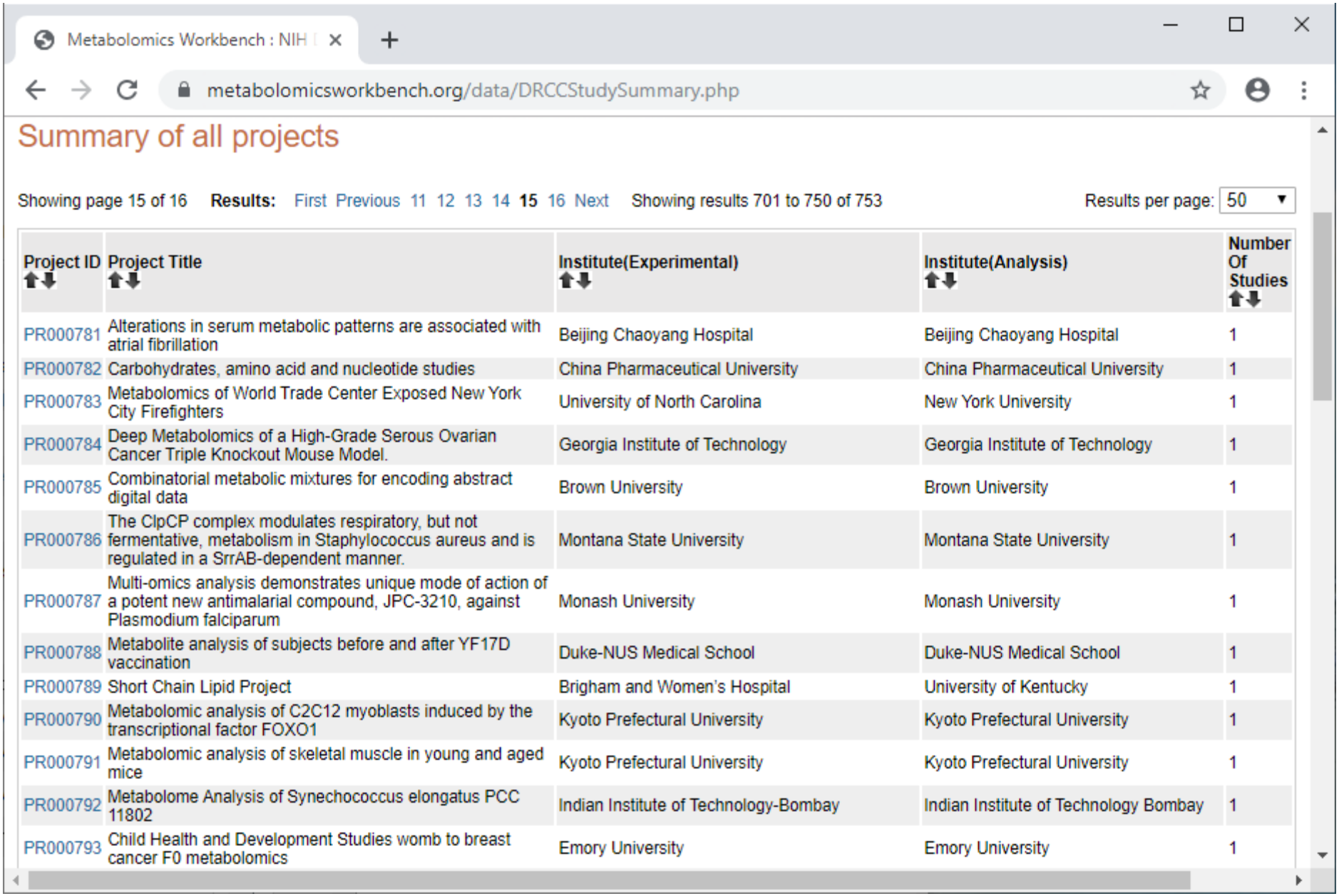


Data summary by projects



Project ID	Project Title	Institute(Experimental)	Institute(Analysis)	Number Of Studies
PR000001	FatB Gene Project	University of California, Davis	University of California, Davis	1
PR000002	Intestinal Samples II pre/post transplantation	University of California, Davis	University of California, Davis	1
PR000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	University of California, Davis	University of California, Davis	1
PR000004	LIPID MAPS Lipidomics studies	LIPID MAPS	LIPID MAPS	2
PR000005	White Wine Study	University of California, Davis	University of California, Davis	1
PR000006	Rice Infection Project	University of California, Davis	University of California, Davis	1
PR000007	Population Genetics (PopGen) for Response to Cholera Vaccination)	RTI International	University of North Carolina	1

Data summary by projects

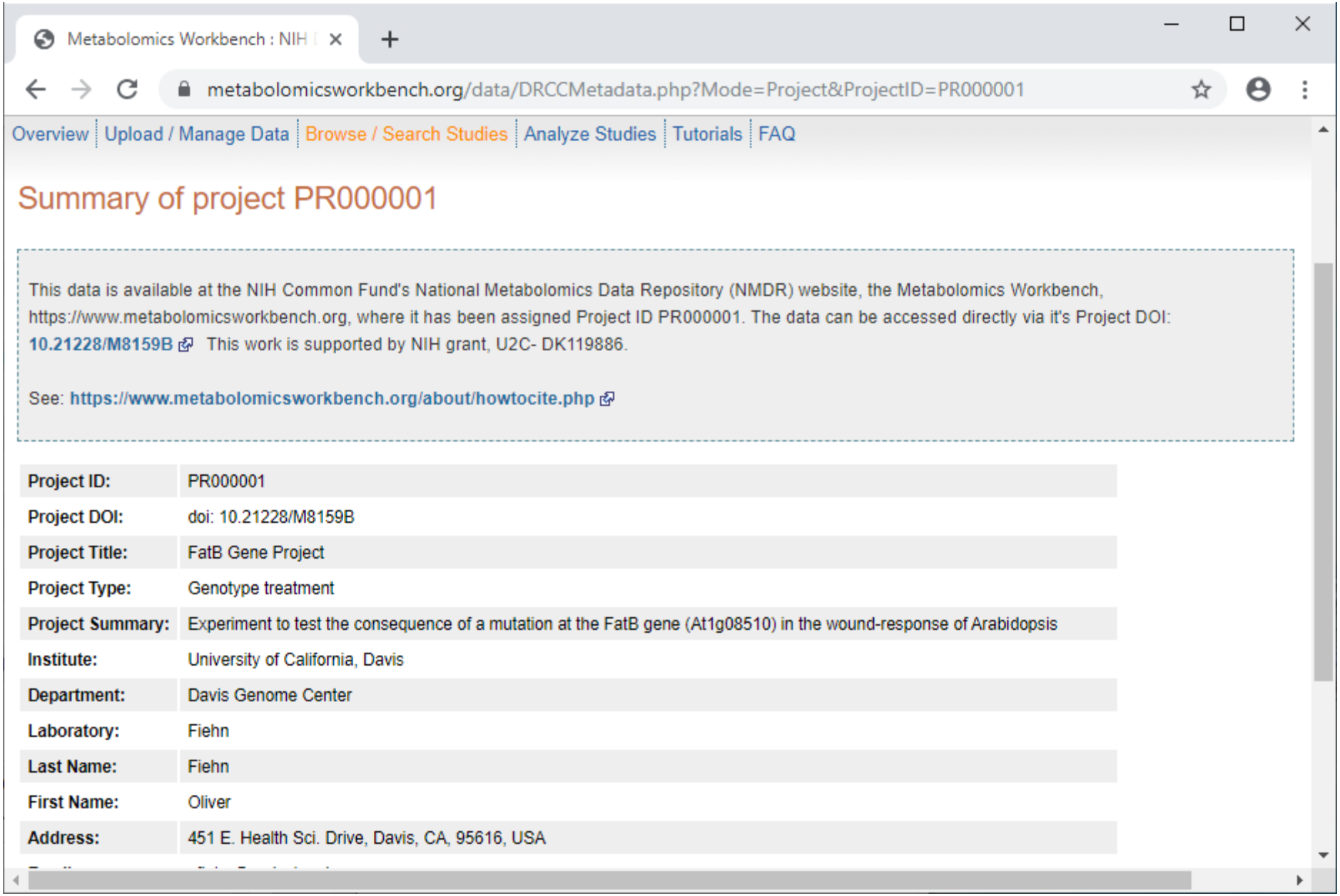


Summary of all projects

Showing page 15 of 16 **Results:** First Previous 11 12 13 14 **15** 16 Next Showing results 701 to 750 of 753 Results per page: 50

Project ID	Project Title	Institute(Experimental)	Institute(Analysis)	Number Of Studies
PR000781	Alterations in serum metabolic patterns are associated with atrial fibrillation	Beijing Chaoyang Hospital	Beijing Chaoyang Hospital	1
PR000782	Carbohydrates, amino acid and nucleotide studies	China Pharmaceutical University	China Pharmaceutical University	1
PR000783	Metabolomics of World Trade Center Exposed New York City Firefighters	University of North Carolina	New York University	1
PR000784	Deep Metabolomics of a High-Grade Serous Ovarian Cancer Triple Knockout Mouse Model.	Georgia Institute of Technology	Georgia Institute of Technology	1
PR000785	Combinatorial metabolic mixtures for encoding abstract digital data	Brown University	Brown University	1
PR000786	The ClpCP complex modulates respiratory, but not fermentative, metabolism in Staphylococcus aureus and is regulated in a SrrAB-dependent manner.	Montana State University	Montana State University	1
PR000787	Multi-omics analysis demonstrates unique mode of action of a potent new antimalarial compound, JPC-3210, against Plasmodium falciparum	Monash University	Monash University	1
PR000788	Metabolite analysis of subjects before and after YF17D vaccination	Duke-NUS Medical School	Duke-NUS Medical School	1
PR000789	Short Chain Lipid Project	Brigham and Women's Hospital	University of Kentucky	1
PR000790	Metabolomic analysis of C2C12 myoblasts induced by the transcriptional factor FOXO1	Kyoto Prefectural University	Kyoto Prefectural University	1
PR000791	Metabolomic analysis of skeletal muscle in young and aged mice	Kyoto Prefectural University	Kyoto Prefectural University	1
PR000792	Metabolome Analysis of Synechococcus elongatus PCC 11802	Indian Institute of Technology-Bombay	Indian Institute of Technology Bombay	1
PR000793	Child Health and Development Studies womb to breast cancer F0 metabolomics	Emory University	Emory University	1

Project details



Project details with multiple studies

Summary of project PR000830

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 PR000830. The data can be accessed directly via it's Project DOI: 10.21228/M8D68Q This work is supported by NIH grant, U2C- DK119886.

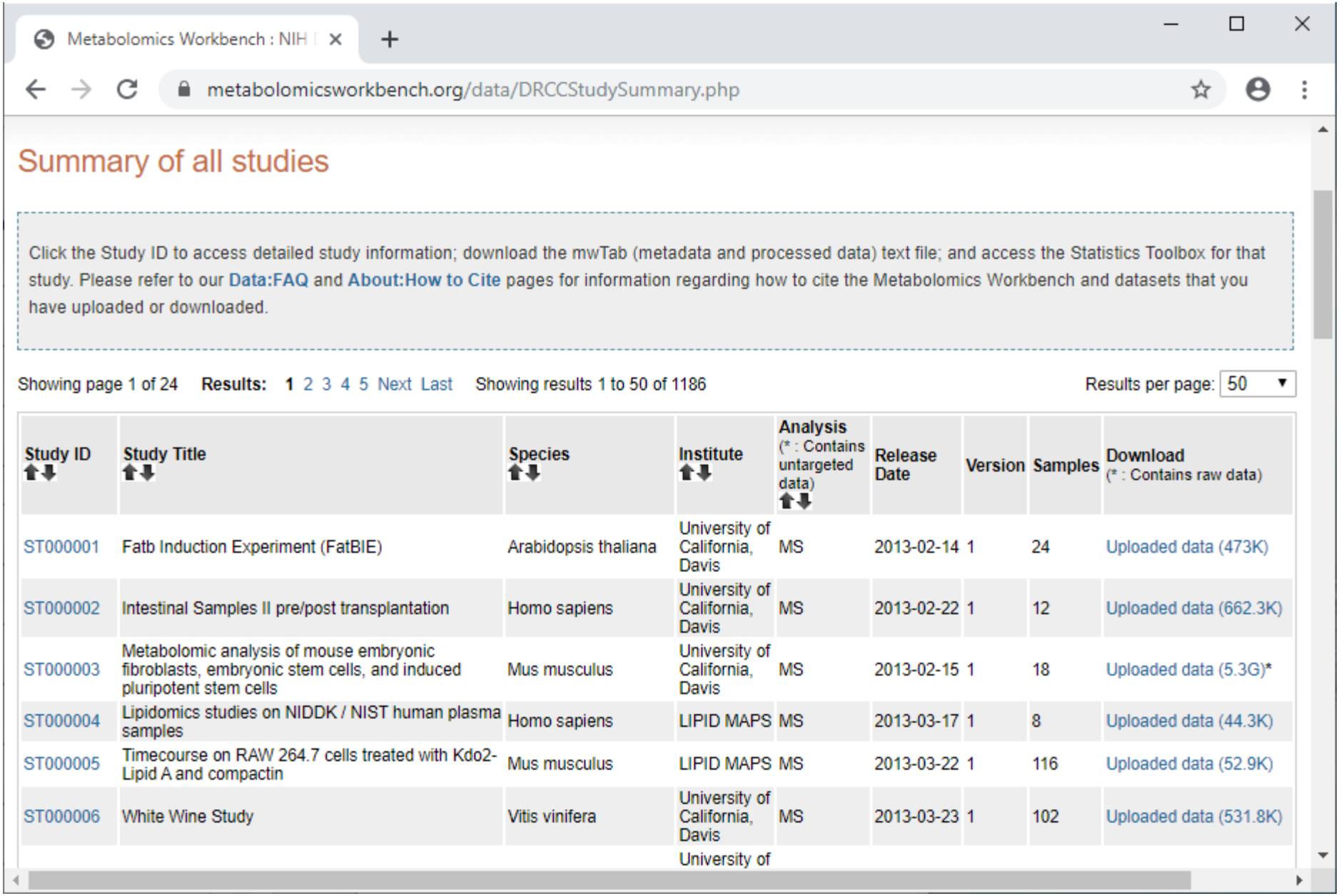
See: https://www.metabolomicsworkbench.org/about/howtocite.php

Project ID:	PR000830
Project DOI:	doi: 10.21228/M8D68Q
Project Title:	Trisomy 21 activates the kynurenine pathway via increased dosage of interferon receptors
Project Summary:	Trisomy 21 (T21) causes Down syndrome (DS), affecting immune and neurological function by unknown mechanisms. We report here a large metabolomics study of plasma and cerebrospinal fluid showing that people with DS produce elevated levels of kynurenine and quinolinic acid, two tryptophan catabolites with potent immunosuppressive and neurotoxic properties, respectively. We demonstrate that immune cells of people with DS overexpress IDO1, the rate-limiting enzyme in the kynurenine pathway (KP) and a known interferon (IFN)-stimulated gene. Furthermore, we show positive correlations among levels of IFN-inducible cytokines and KP dysregulation. Using metabolic tracing assays, we determine that IFN stimulation causes IDO1 overexpression and kynurenine overproduction in cells with T21, dependent on overexpression of IFN receptors encoded on chromosome 21. Finally, we show a mouse model of DS carrying triplication of the IFN receptors exhibits KP dysregulation. Altogether, these results reveal a mechanism by which T21 could drive

Summary of all studies in project PR000830

Study ID	Study Title	Species	Institute	Analysis (* : Contains Untargted data)	Release Date	Version	Samples	Download (* : Contains raw data)
ST001240	Global Metabolic Analysis Trisomy 21 - Cohort 2	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	388	Uploaded data (8.6G)*
ST001241	Global Metabolic Analysis Trisomy 21 - Cohort 3, Plasma	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	516	Uploaded data (6.5G)*
ST001242	Global Metabolic Analysis Trisomy 21 - Cohort 3, CSF	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	400	Uploaded data (5G)*
ST001243	Global Metabolic Analysis Trisomy 21 - Cohort 1	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	392	Uploaded data (7.8G)*

Data summary by studies



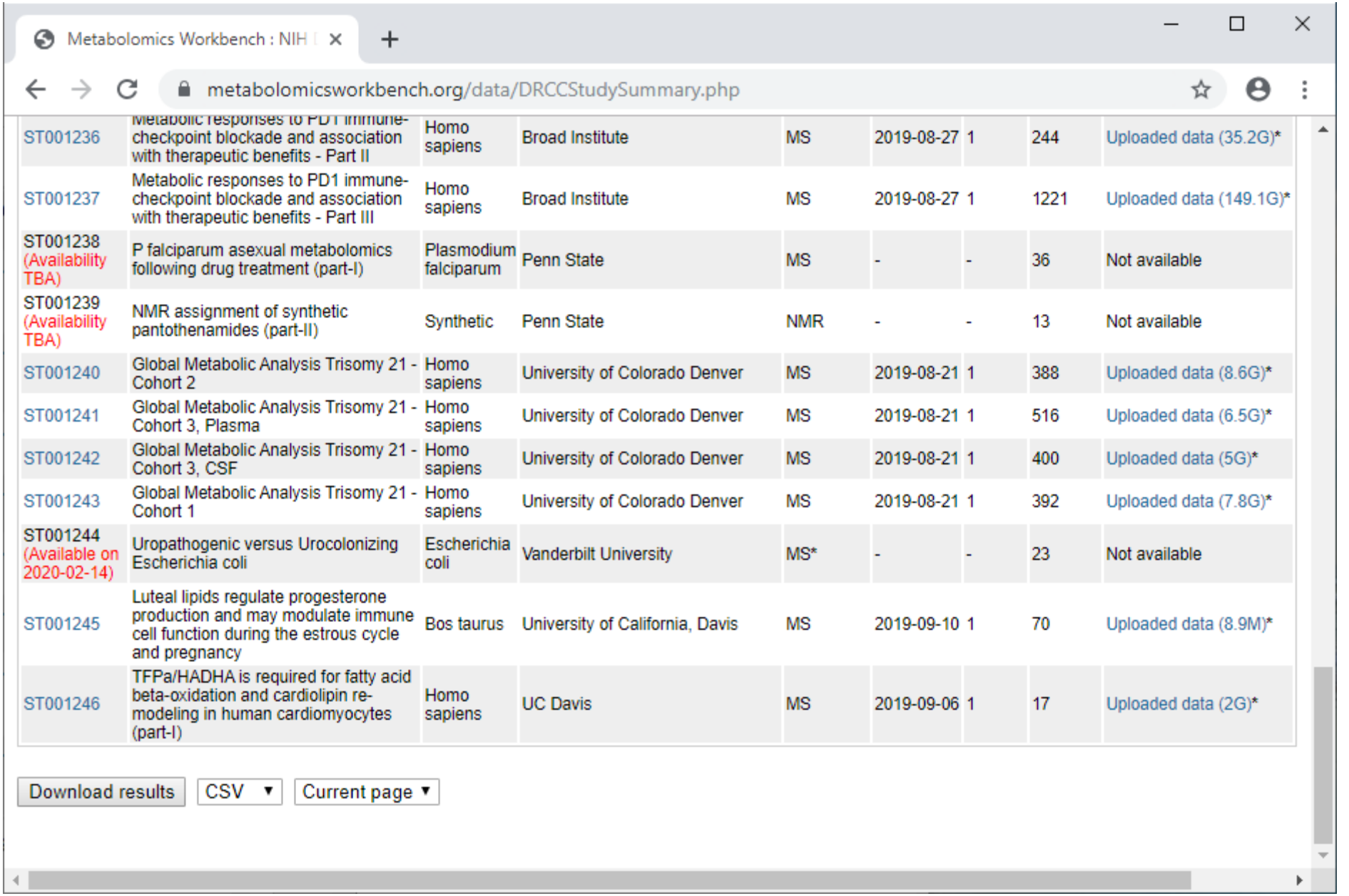
Summary of all studies

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 24 **Results:** **1** 2 3 4 5 Next Last Showing results 1 to 50 of 1186 Results per page: 50

Study ID	Study Title	Species	Institute	Analysis (* : Contains untargeted data)	Release Date	Version	Samples	Download (* : Contains raw data)
ST000001	Fatb Induction Experiment (FatBIE)	Arabidopsis thaliana	University of California, Davis	MS	2013-02-14	1	24	Uploaded data (473K)
ST000002	Intestinal Samples II pre/post transplantation	Homo sapiens	University of California, Davis	MS	2013-02-22	1	12	Uploaded data (662.3K)
ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	Mus musculus	University of California, Davis	MS	2013-02-15	1	18	Uploaded data (5.3G)*
ST000004	Lipidomics studies on NIDDK / NIST human plasma samples	Homo sapiens	LIPID MAPS	MS	2013-03-17	1	8	Uploaded data (44.3K)
ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Mus musculus	LIPID MAPS	MS	2013-03-22	1	116	Uploaded data (52.9K)
ST000006	White Wine Study	Vitis vinifera	University of California, Davis	MS	2013-03-23	1	102	Uploaded data (531.8K)
			University of					

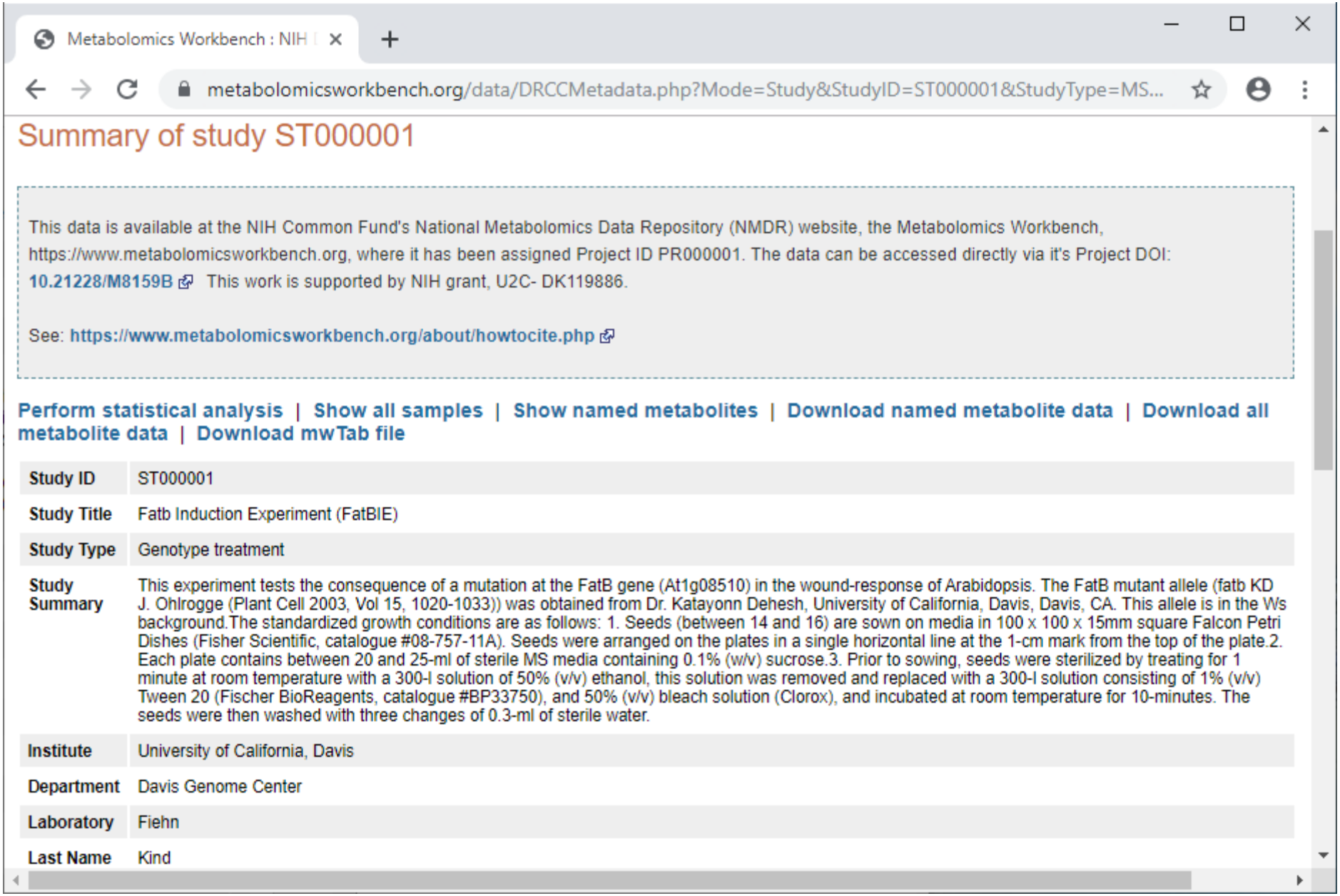
Data summary by studies



ST001236	Metabolic responses to PD1 immune-checkpoint blockade and association with therapeutic benefits - Part II	Homo sapiens	Broad Institute	MS	2019-08-27	1	244	Uploaded data (35.2G)*
ST001237	Metabolic responses to PD1 immune-checkpoint blockade and association with therapeutic benefits - Part III	Homo sapiens	Broad Institute	MS	2019-08-27	1	1221	Uploaded data (149.1G)*
ST001238 (Availability TBA)	P falciparum asexual metabolomics following drug treatment (part-I)	Plasmodium falciparum	Penn State	MS	-	-	36	Not available
ST001239 (Availability TBA)	NMR assignment of synthetic pantothenamides (part-II)	Synthetic	Penn State	NMR	-	-	13	Not available
ST001240	Global Metabolic Analysis Trisomy 21 - Cohort 2	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	388	Uploaded data (8.6G)*
ST001241	Global Metabolic Analysis Trisomy 21 - Cohort 3, Plasma	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	516	Uploaded data (6.5G)*
ST001242	Global Metabolic Analysis Trisomy 21 - Cohort 3, CSF	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	400	Uploaded data (5G)*
ST001243	Global Metabolic Analysis Trisomy 21 - Cohort 1	Homo sapiens	University of Colorado Denver	MS	2019-08-21	1	392	Uploaded data (7.8G)*
ST001244 (Available on 2020-02-14)	Uropathogenic versus Urocolonizing Escherichia coli	Escherichia coli	Vanderbilt University	MS*	-	-	23	Not available
ST001245	Luteal lipids regulate progesterone production and may modulate immune cell function during the estrous cycle and pregnancy	Bos taurus	University of California, Davis	MS	2019-09-10	1	70	Uploaded data (8.9M)*
ST001246	TFPa/HADHA is required for fatty acid beta-oxidation and cardiolipin re-modeling in human cardiomyocytes (part-I)	Homo sapiens	UC Davis	MS	2019-09-06	1	17	Uploaded data (2G)*

Download results | CSV | Current page

Study details



Summary of study ST000001

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 PR000001. The data can be accessed directly via it's Project DOI: 10.21228/M8159B 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 all metabolite data | Download mwTab file

Study ID	ST000001
Study Title	Fatb Induction Experiment (FatBIE)
Study Type	Genotype treatment
Study Summary	This experiment tests the consequence of a mutation at the FatB gene (At1g08510) in the wound-response of Arabidopsis. The FatB mutant allele (fatb KD J. Ohlrogge (Plant Cell 2003, Vol 15, 1020-1033)) was obtained from Dr. Katayonn Dehesh, University of California, Davis, Davis, CA. This allele is in the Ws background.The standardized growth conditions are as follows: 1. Seeds (between 14 and 16) are sown on media in 100 x 100 x 15mm square Falcon Petri Dishes (Fisher Scientific, catalogue #08-757-11A). Seeds were arranged on the plates in a single horizontal line at the 1-cm mark from the top of the plate.2. Each plate contains between 20 and 25-ml of sterile MS media containing 0.1% (w/v) sucrose.3. Prior to sowing, seeds were sterilized by treating for 1 minute at room temperature with a 300-l solution of 50% (v/v) ethanol, this solution was removed and replaced with a 300-l solution consisting of 1% (v/v) Tween 20 (Fischer BioReagents, catalogue #BP33750), and 50% (v/v) bleach solution (Clorox), and incubated at room temperature for 10-minutes. The seeds were then washed with three changes of 0.3-ml of sterile water.
Institute	University of California, Davis
Department	Davis Genome Center
Laboratory	Fiehn
Last Name	Kind

Study metadata details

Summary of study ST000001

Select appropriate tab below to view additional metadata details:

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

Project:

Project ID:	PR000001
Project DOI:	doi: 10.21228/M8159B
Project Title:	FatB Gene Project
Project Type:	Genotype treatment
Project Summary:	Experiment to test the consequence of a mutation at the FatB gene (At1g08510) in the wound-response of Arabidopsis
Institute:	University of California, Davis
Department:	Davis Genome Center
Laboratory:	Fiehn
Last Name:	Fiehn
First Name:	Oliver
Address:	451 E. Health Sci. Drive, Davis, CA, 95616, USA
Email:	ofiehn@ucdavis.edu
Publications:	Quality control for plant metabolomics: reporting MSI-compliant studies. DOI: 10.1111/j.1365-313X.2007.03387.x PubMed

Factors:

Study metadata details

Summary of study ST000001

Select appropriate tab below to view additional metadata details:

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

Factors:

Subject type: Plant; **Subject species:** *Arabidopsis thaliana* (Factor headings shown in green)

mb_sample_id	local_sample_id	Arabidopsis Genotype	Plant Wounding Treatment
SA000019	LabF_115904	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000020	LabF_115909	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000021	LabF_115914	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000022	LabF_115919	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000023	LabF_115924	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000024	LabF_115929	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000007	LabF_115842	fatb-ko KD; At1g08510	Wounded
SA000008	LabF_115847	fatb-ko KD; At1g08510	Wounded
SA000009	LabF_115852	fatb-ko KD; At1g08510	Wounded
SA000010	LabF_115857	fatb-ko KD; At1g08510	Wounded
SA000011	LabF_115862	fatb-ko KD; At1g08510	Wounded
SA000012	LabF_115867	fatb-ko KD; At1g08510	Wounded
SA000013	LabF_115873	Wassilewskija (Ws)	Control - Non-Wounded
SA000014	LabF_115878	Wassilewskija (Ws)	Control - Non-Wounded
SA000015	LabF_115883	Wassilewskija (Ws)	Control - Non-Wounded
SA000016	LabF_115888	Wassilewskija (Ws)	Control - Non-Wounded
SA000017	LabF_115893	Wassilewskija (Ws)	Control - Non-Wounded

Study metadata details

Summary of study ST000001

Select appropriate tab below to view additional metadata details:

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

Treatment:

Treatment ID:	TR000001
Treatment:	Abiotic
Treatment Route:	Wounded
Treatment Dose:	Ten punches
Treatment Doseduration:	3 min wounding period; 2 h response perioid before harvest
Plant Growth Support:	Fourteen to sixteen seeds were sown on 2025 ml of sterile Murashige and Skoog basal salt mixture (MS medium) containing 0.1% w/v sucrose and 1 liquid vitamin solution (Sigma, http://www.sigmaaldrich.com/) containing 15 g l)1 bacto agar (BD) in 100 100 15 mm square Falcon Petri dishes (Thermo Fisher Scientific; http:// www.thermofisher.com). Seeds were arranged on the plates in a single horizontal line 1 cm from the top of the plate. Prior to sowing, seeds were sterilized by treating for 1 min at room temperature with 300 ll of 50% v/v ethanol; this solution was then removed and replaced by 300 ll of a solution consisting of 1% v/v Tween-20 (Thermo Fisher Scientific) and 50% v/v bleach (Clorox; http://www.clorox. com), and incubated at room temperature for 10 min. The seeds were then washed with three changes of 0.3 ml of sterile water. After sowing the seeds, the plates were wrapped using micropore tape (3 M Health Care; http://www.3m.com), and then stored horizontally for 4 days at 4 C in the dark. On the 5th day, plates were moved to the growth room, and held in a vertical position in Plexiglass holders for 12 days.
Plant Growth Location:	Controlled-environment facility at Iowa State University, Nikolau laboratory.
Plant Plot Design:	Each genotype and replicate were grown on individual plates and placed randomly in the Plexiglass holders.
Plant Light Period:	24 h day at 82 micromol/m**2 s (light source Sylvania; http://www.sylvania.com), F34CW/SS/ECO/RP)
Plant Humidity:	Day 100%, night 100%
Plant Temp:	Day 24 C, night 24 C
Plant Watering	No further watering, plates remained closed

Study metadata details

Summary of study ST000001

Select appropriate tab below to view additional metadata details:

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

Collection:

Collection ID:	CO000001
Sample Type:	Plant
Volumeoramount Collected:	50 mg

Sample Preparation:

Sampleprep ID:	SP000001
Processing Storage Conditions:	Frozen tissues were kept in 2 ml round-bottomed Eppendorf tubes equipped with one 3 mm diameter steel ball, and homogenized using a Retsch (http://www.retch-us.com) ball mill for 30 sec at 25/sec
Extraction Method:	Ground tissue powder was kept in liquid nitrogen between homogenization and extraction. The extraction solvent was prepared by mixing isopropanol/ acetonitrile/water at the volume ratio 3:3:2 and degassing this mixture by directing a gentle stream of nitrogen through the solvent for 5 min. The solvent was cooled to)20 C prior to extraction. Randomly processing all samples of the study, 1 ml of cold solvent per 20 mg of ground tissue was added, vortexed for 10 sec, and shaken at 4 C for 5 min to extract metabolites and simultaneously precipitate proteins. After centrifugation at 12 800 g for 2 min, 90% of the supernatant was removed, taking are not to remove any residues from the pellet
Extract Concentration Dilution:	The supernatant was separated into two equal aliquots and concentrated to dryness in a Centrivap cold trap vacuum concentrator (http://www. labconco.com) at room temperature for 4 h
Extract Cleanup:	In order to fractionate complex lipids and waxes, the residue was re-suspended in 500 ll 50% aqueous acetonitrile and centrifuged at 12 800 g for 2 min. The supernatant was transferred to a 1.5 ml Eppendorf tube and concentrated to dryness in a vacuum concentrator
Extract Storage:	Dried extracts can be kept under nitrogen at -80 C for up to 4 weeks. In the study presented here, extracts were immediately derivatized for GCTOF mass spectrometry
Organ Specification:	Rosette leaf

Study metadata details

Summary of study ST000001

Select appropriate tab below to view additional metadata details:

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

Combined analysis:

Analysis ID	AN000001
Analysis type	MS
Chromatography type	GC
Chromatography system	Agilent 6890N
Column	
MS Type	EI
MS instrument type	GC-TOF
MS instrument name	Leco Pegasus III GC TOF
Ion Mode	POSITIVE

Chromatography:

Chromatography ID:	CH000001
Methods Filename:	nihms161442.pdf
Instrument Name:	Agilent 6890N
Chromatography Type:	GC

MS:

MS ID:	MS000001

Study samples data

Summary of study ST000001

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download all metabolite data | Download mwTab file

Samples for study ST000001

Species: *Arabidopsis thaliana* (Factor headings shown in green)

mb_sample_id	Subject name	Sample name	Arabidopsis Genotype	Plant Wounding Treatment
SA000019	-	LabF_115904	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000020	-	LabF_115909	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000021	-	LabF_115914	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000022	-	LabF_115919	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000023	-	LabF_115924	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000024	-	LabF_115929	fatb-ko KD; At1g08510	Control - Non-Wounded
SA000007	-	LabF_115842	fatb-ko KD; At1g08510	Wounded
SA000008	-	LabF_115847	fatb-ko KD; At1g08510	Wounded
SA000009	-	LabF_115852	fatb-ko KD; At1g08510	Wounded
SA000010	-	LabF_115857	fatb-ko KD; At1g08510	Wounded
SA000011	-	LabF_115862	fatb-ko KD; At1g08510	Wounded
SA000012	-	LabF_115867	fatb-ko KD; At1g08510	Wounded
SA000013	-	LabF_115873	Wassilewskija (Ws)	Control - Non-Wounded
SA000014	-	LabF_115878	Wassilewskija (Ws)	Control - Non-Wounded
SA000015	-	LabF_115883	Wassilewskija (Ws)	Control - Non-Wounded
SA000016	-	LabF_115888	Wassilewskija (Ws)	Control - Non-Wounded
SA000017	-	LabF_115893	Wassilewskija (Ws)	Control - Non-Wounded
SA000018	-	LabF_115898	Wassilewskija (Ws)	Control - Non-Wounded
SA000001	-	LabF_115811	Wassilewskija (Ws)	Wounded
SA000002	-	LabF_115816	Wassilewskija (Ws)	Wounded
SA000003	-	LabF_115821	Wassilewskija (Ws)	Wounded
SA000004	-	LabF_115826	Wassilewskija (Ws)	Wounded
SA000005	-	LabF_115831	Wassilewskija (Ws)	Wounded

Study sample details

MB Sample ID: SA000019

Select appropriate tab below to view additional metadata details:

All | Factors | Treatment | Collection | Sample Preparation | Chromatography | Analysis | MS

Factors:

Local Sample ID	MB Sample ID	Factor Level ID	Level Value	Factor Name
LabF_115904	SA000019	FL000004	Control - Non-Wounded	Plant Wounding Treatment
LabF_115904	SA000019	FL000004	fatb-ko KD; At1g08510	Arabidopsis Genotype

Download named metabolite data for a study

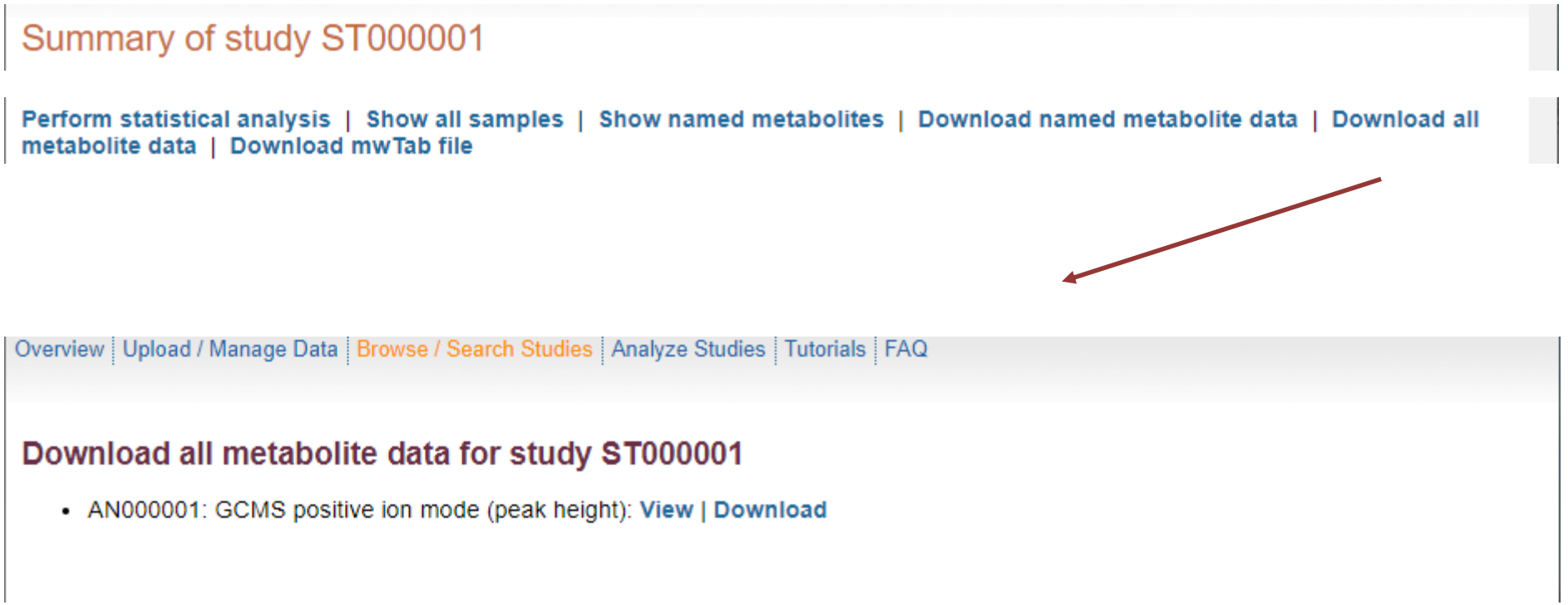
Summary of study ST000001

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download all metabolite data | Download mwTab file

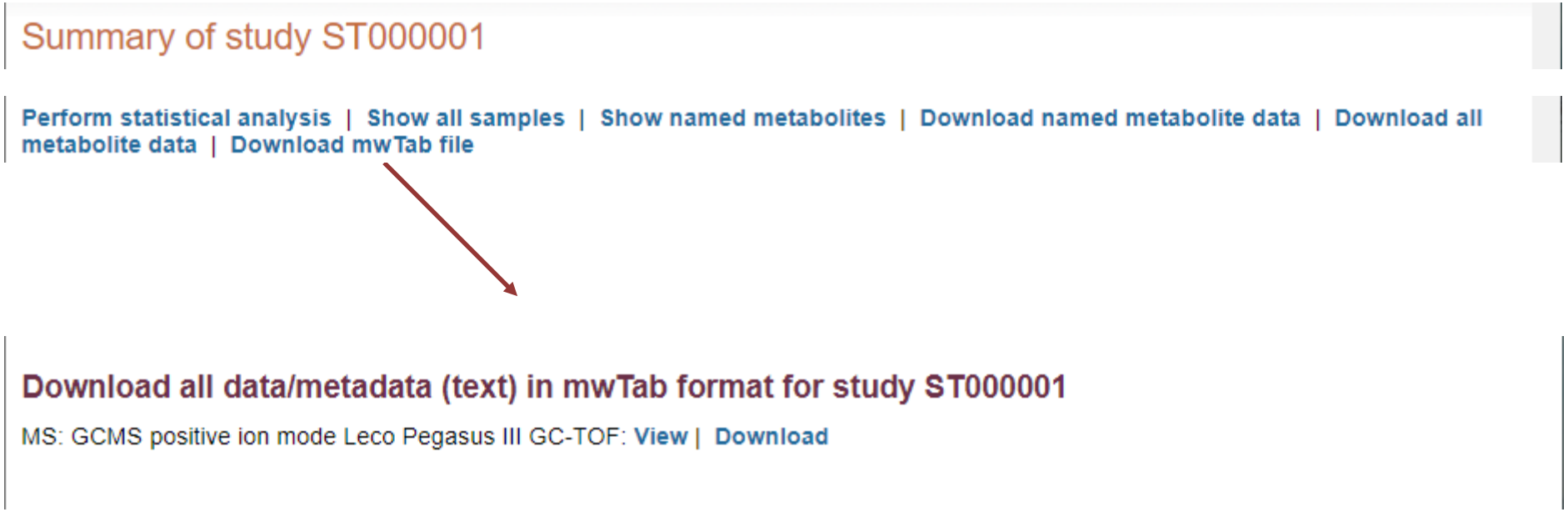
Download data matrix(Fatb Induction Experiment (FatBIE) GCMS positive ion mode)

Analysis	Samples	Factors	Units
GCMS positive ion mode	LabF_115904	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115909	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115914	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115919	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115924	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115929	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115842	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115847	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115852	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115857	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115862	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115867	Arabidopsis Genotype:fatb-ko KD; At1g08510 | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115873	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115878	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115883	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115888	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115893	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115898	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Control - Non-Wounded	peak height
GCMS positive ion mode	LabF_115811	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115816	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115821	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115826	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115831	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Wounded	peak height
GCMS positive ion mode	LabF_115836	Arabidopsis Genotype:Wassilewskija (Ws) | Plant Wounding Treatment:Wounded	peak height

Download all metabolite data for a study



Download mwTab data for a study



Named metabolites for a study of interest

Summary of study ST000001

Perform statistical analysis | Show all samples | Show named metabolites | Download named metabolite data | Download all metabolite data | Download mwTab file

Analysis: GCMS positive ion mode

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

Select	Metabolite Name	Refmet Name	WorkBench Metabolite_ID	PubChem Compound_ID	Kegg Id	Retention time/index	m/z ratio	Other Id	Other Id Type
☐	1,2,4-benzenetriol	1,2,4-benzenetriol	ME000097	10787	C02814	522741	239	205673	BinBase
☐	1-monostearin	MG(18:0/0:0/0:0)	ME000096	107036	D01947	959625	399	202835	BinBase
☐	2-hydroxyvaleric acid	DL-2-hydroxy valeric acid	ME000098	98009	-	310750	131	218773	BinBase
☐	3-phosphoglycerate	3-Phosphoglyceric acid	ME000095	724	C00597	611619	299	217821	BinBase
☐	5-hydroxynorvaline NIST	-	ME001834	95562	-	494838	142	200384	BinBase
☐	adenosine	Adenosine	ME000092	60961	C00212	917818	236	211944	BinBase
☐	adenosine-5-monophosphate	AMP	ME000091	6083	C00020	1040943	169	213958	BinBase
☐	adipic acid	Adipic acid	ME000090	196	C06104	475399	111	218815	BinBase
☐	agmatine	Agmatine	ME000089	199	C00179	587051	157	212007	BinBase
☐	alanine	Alanine	ME000088	5950	C00041	243537	116	199651	BinBase
☐	alpha ketoglutaric acid	Oxoglutaric acid	ME000087	51	C00026	507734	198	200425	BinBase
☐	arabinose	Arabinose	ME000086	7044039	C00216	546892	217	202065	BinBase
☐	arginine + ornithine	-	ME000085	6322	C00062	619420	142	199796	BinBase

Analyze metabolite of interest

tryptophan values for ST000014 (Units: peak height)

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

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

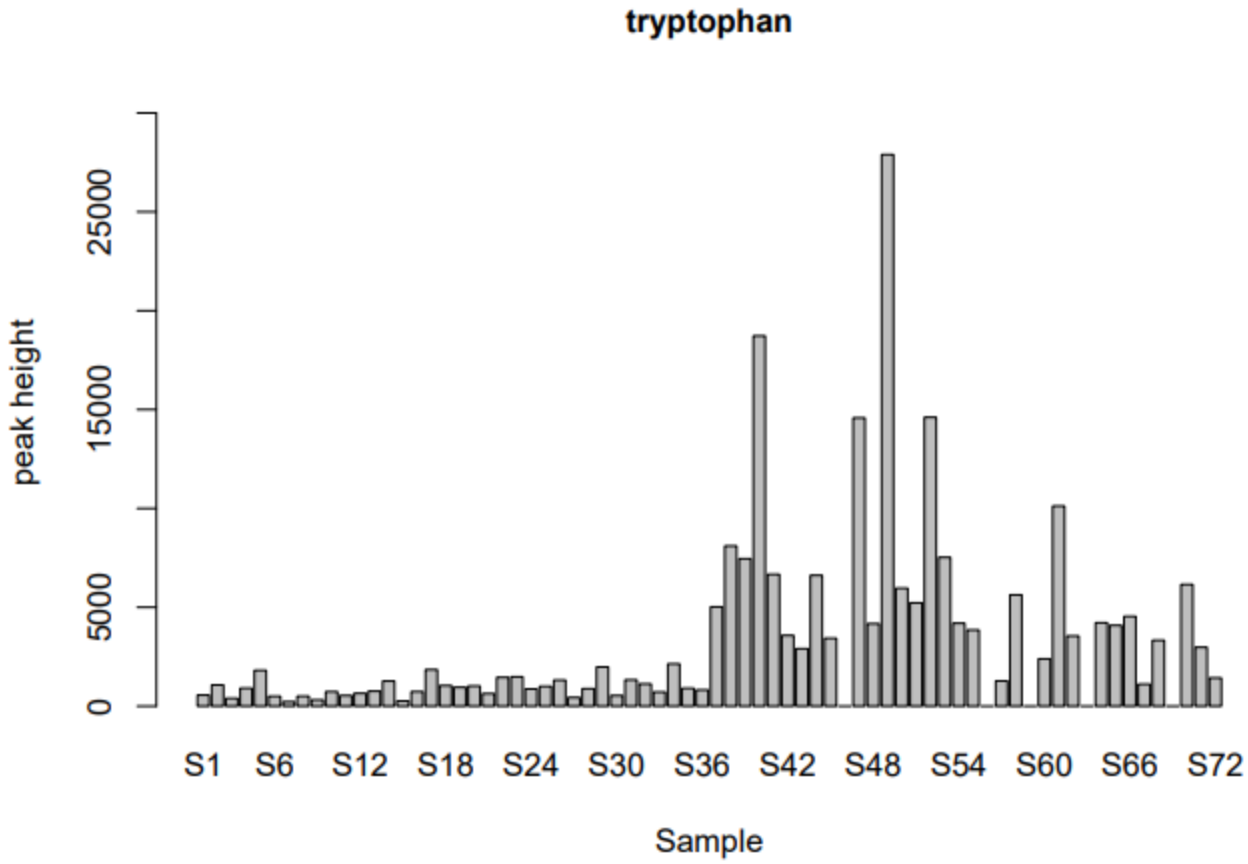
Sample	Tryptophan	Factors	Units
103879	558	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103884	1071	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103889	395	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103894	907	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103899	1810	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103904	497	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
104003	223	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104008	502	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104013	313	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104018	729	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104023	536	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104028	647	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104127	756	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height
104132	1268	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height
104137	262	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height
104142	732	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height
104147	1846	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height
104152	1038	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height
103941	952	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103946	1018	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103951	633	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103956	1454	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height

Analysis tools for a metabolite of interest

- **Bar graph of sample measurements for that metabolite**
- **Box-and-whisker plot of measurement ranges for the metabolite**
- **Bar graph of mean values for each factor level**
- **Tabular and graphical display by factor/factor level of interest**
- **Two-way ANOVA analysis of data for a metabolite**
- **T-test analysis of data for a metabolite**
- **Z-score analysis of data for a metabolite**

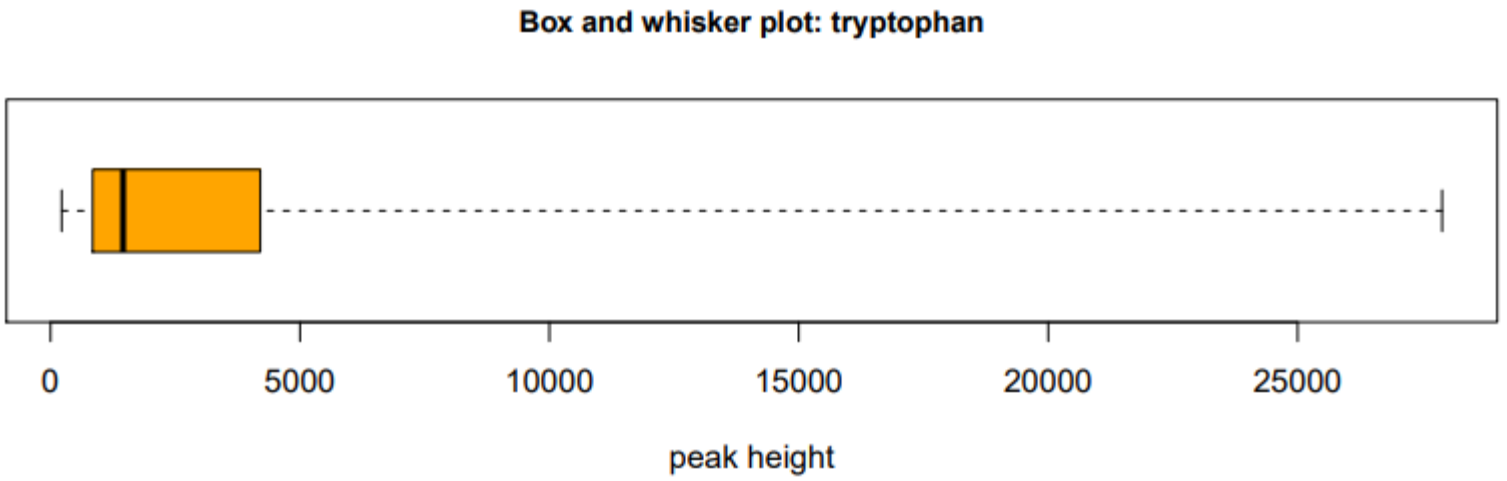
Analysis tools for a metabolite of interest

Bar graph of sample measurements for that metabolite



Analysis tools for a metabolite of interest

Box-and-whisker plot of measurement ranges for the metabolite

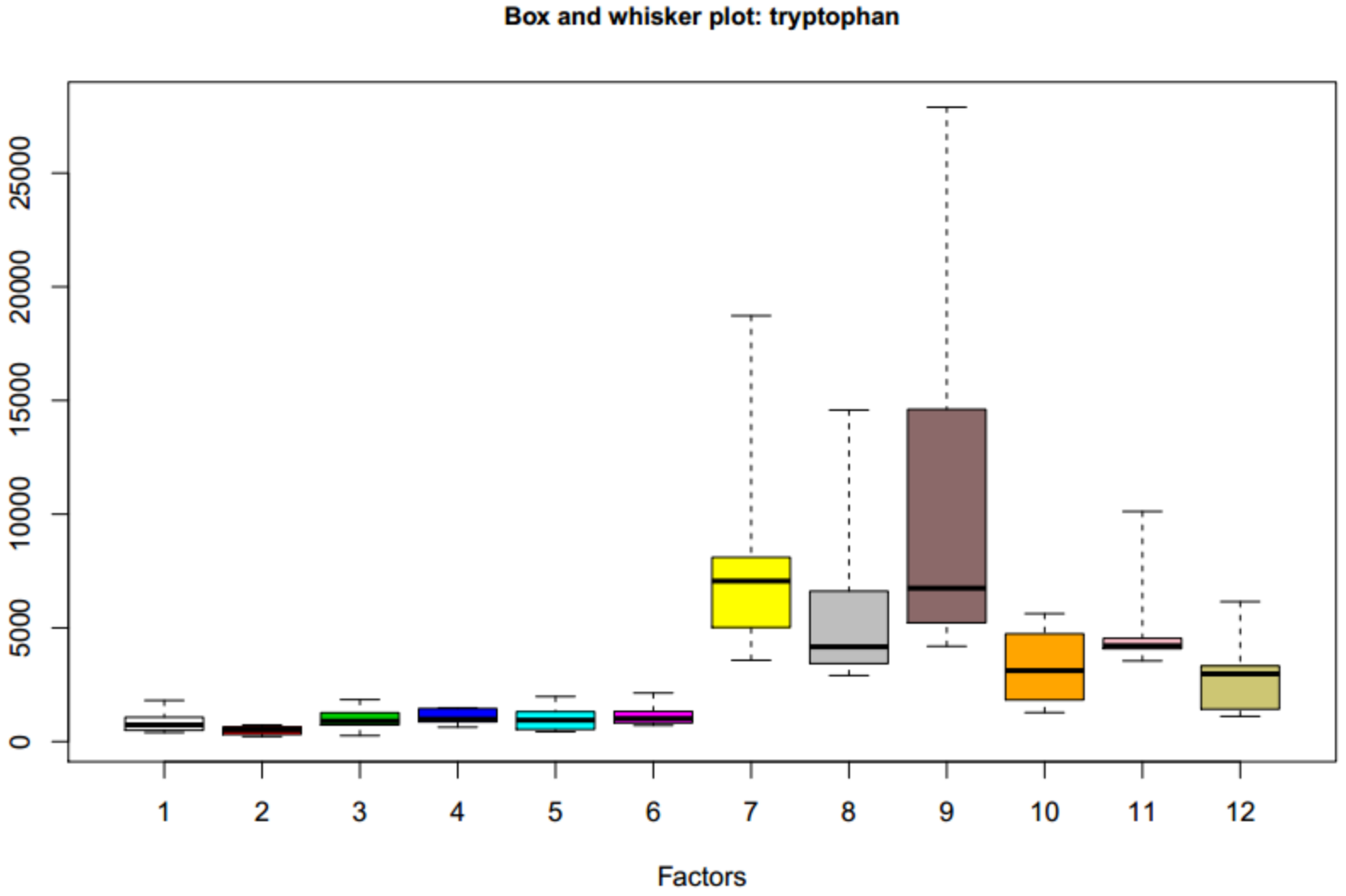


tryptophan:

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.	NA's
223	844	1454	3507	4204	27896	5

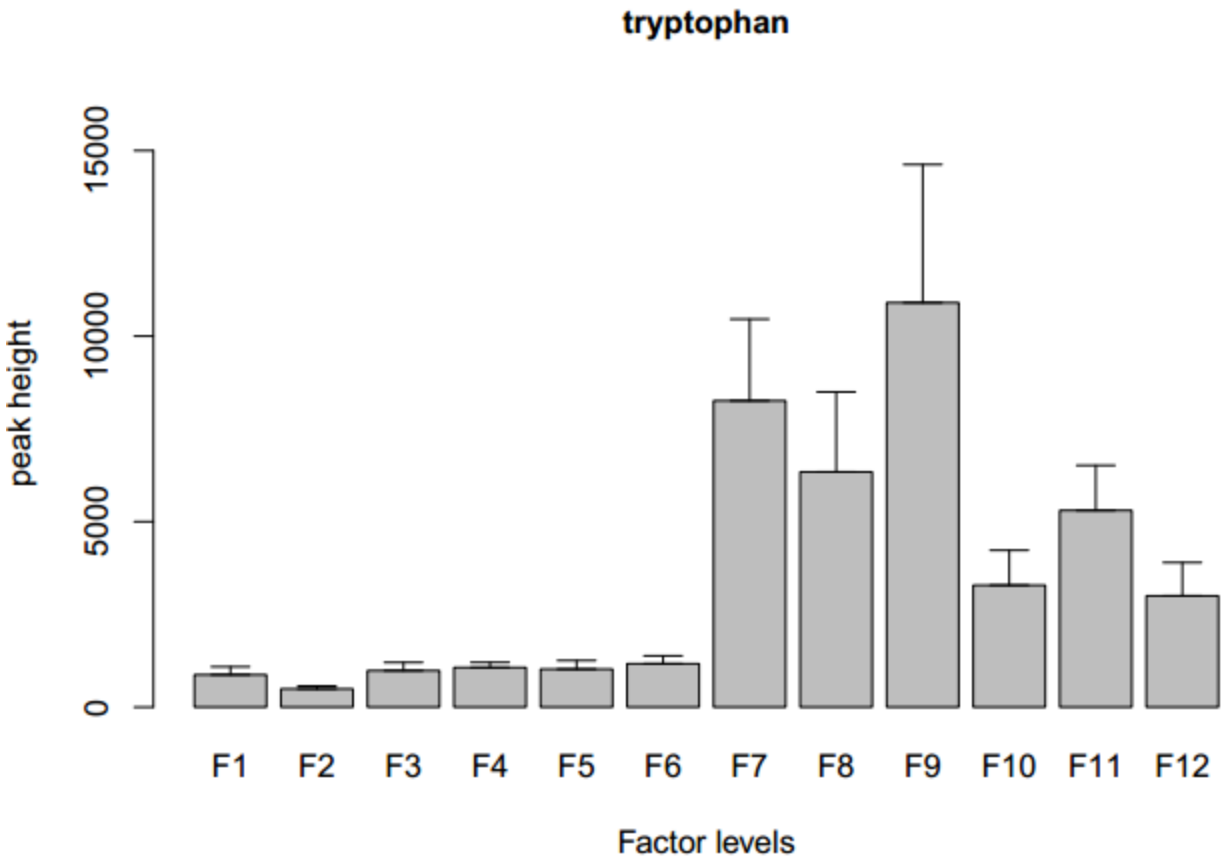
Analysis tools for a metabolite of interest

Box-and-whisker plot of measurement ranges for the metabolite



Analysis tools for a metabolite of interest

Bar graph of mean values for each factor level



Factor level F1:	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
Factor level F2:	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
Factor level F3:	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM

View metabolite data for a selected factor (from pulldown menu)

tryptophan values for ST000014 (Units: peak height)
Run ANOVA on this analyte | Run t-test on this analyte| Calculate z-scores for this analyte

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

Compartment
Minutes
Skeletal Muscle Treatment

Sample	Tryptophan	Factors	
103879	558	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak heigh
103884	1071	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak heigh

New menu appear for each additional factor (constrain these as needed)

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

Apply additional constraints Minutes: 20 Skeletal Muscle Treatment: palmitic acid 9.6 uM Show data table

Sample	Tryptophan	Factors	Units
103879	558	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak heigh

User-defined data subset

Study ST000014: tryptophan values for factor:Compartment
(Constraints: Minutes:20 Skeletal Muscle Treatment:palmitic acid 9.6 uM) (Units: peak height)

Bar graph of values (by sample)	Bar graph of values for Compartment
Bar graph (samples)	Display bar graph for Compartment

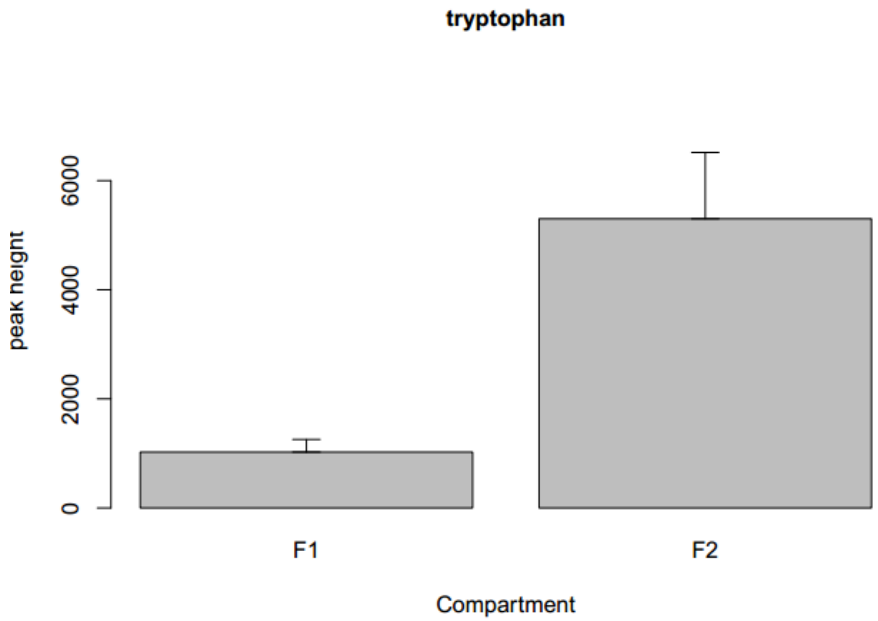
Sample	Tryptophan	Factor:Compartment
104065	999	cytosol
104070	1315	cytosol

Examine a specific factor for a metabolite of interest

Study ST000014: tryptophan values for factor:Compartment
(Constraints: Minutes:20 Skeletal Muscle Treatment:palmitic acid 9.6 uM) (Units: peak height)

Bar graph of values (by sample)	Bar graph of values for Compartment
Bar graph (samples)	Display bar graph for Compartment

Sample	Tryptophan	Factor:Compartment
104065	999	cytosol
104070	1315	cytosol



Analysis tools for a metabolite of interest

Two-way ANOVA analysis of data for a metabolite

ANOVA parameters for tryptophan in Study ST000014

This analysis uses the 'anova' function of the R statistics environment

Please specify the first order terms:

Compartment:	☑
Minutes:	☑
Skeletal_Muscle_Treatment:	☑

Please specify the second order terms:

	Compartment	Minutes	Skeletal_Muscle_Treatment
Compartment	-	☐	☐
Minutes	-	-	☐
Skeletal_Muscle_Treatment	-	-	-

Submit

ANOVA results for tryptophan in Study ST000014

ANALYTE	Compartment	Minutes	Skeletal_Muscle_Treatment
tryptophan	3.626E-6	1.127E-2	6.128E-1

(Green: p value<=0.05)

Analysis tools for a metabolite of interest

T-test analysis of data for a metabolite

T-test on tryptophan

Calculate all t-test p-values

Select	Factor
☐	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
☐	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
☐	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
☐	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
☐	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
☐	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
☐	Compartment:mito | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
☐	Compartment:mito | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
☐	Compartment:mito | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
☐	Compartment:mito | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
☐	Compartment:mito | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
☐	Compartment:mito | Minutes:20 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM

Calculate t-test p-value for 2 selected conditions Treat variances as equal: TRUE ▾

Perform t-test on pairs of factor levels or across all possible combinations

T-test on tryptophan (2-tailed test. Assumes equal variances)

Factors	f2	f3	f4	f5	f6	f7	f8	f9	f10	f11	f12
f1	1.27E-1	7.27E-1	4.62E-1	6.42E-1	3.50E-1	7.48E-3	2.11E-2	2.27E-2	1.59E-2	3.37E-3	3.29E-2
f2	-	6.23E-2	4.55E-3	5.44E-2	1.37E-2	5.47E-3	1.49E-2	1.89E-2	5.87E-3	1.79E-3	1.32E-2
f3	-	-	7.51E-1	9.01E-1	5.57E-1	8.15E-3	2.32E-2	2.39E-2	1.99E-2	3.95E-3	4.11E-2
f4	-	-	-	8.74E-1	6.96E-1	8.55E-3	2.44E-2	2.47E-2	1.98E-2	4.07E-3	4.38E-2
f5	-	-	-	-	6.53E-1	8.43E-3	2.41E-2	2.44E-2	2.21E-2	4.23E-3	4.52E-2
f6	-	-	-	-	-	9.39E-3	2.70E-2	2.60E-2	2.82E-2	5.05E-3	5.84E-2
f7	-	-	-	-	-	-	5.53E-1	5.54E-1	1.19E-1	2.97E-1	7.05E-2
f8	-	-	-	-	-	-	-	3.42E-1	2.75E-1	6.86E-1	1.90E-1
f9	-	-	-	-	-	-	-	-	1.45E-1	2.21E-1	9.22E-2
f10	-	-	-	-	-					2.50E-	8.33E-
f11	-	-	-	-	-						

f1	Compartment:cytosol | Minutes:0 | Ske
f2	Compartment:cytosol | Minutes:0 | Ske
f3	Compartment:cytosol | Minutes:0 | Ske

T-test 2-tailed with equal variances

Condition1:Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
Condition2:Compartment:mito | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM

p-value
7.48E-3

Green: p-value <= 0.05

Calculate z-scores for all samples for a metabolite of interest

Z-scores and measurements for tryptophan in Study ST000014 (Units: peak height)

Mean: 3507.090 Sample standard deviation: 4731.614

Sample	Value	z-score	Factors
103879	558	-0.623	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
103884	1071	-0.515	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
103889	395	-0.658	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
103894	907	-0.550	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
103899	1810	-0.359	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
103904	497	-0.636	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
104003	223	-0.694	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
104008	502	-0.635	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
104013	313	-0.675	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
104018	729	-0.587	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
104023	536	-0.628	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
104028	647	-0.604	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM
104127	756	-0.581	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
104132	1268	-0.473	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
104137	262	-0.686	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
104142	732	-0.586	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
104147	1846	-0.351	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
104152	1038	-0.522	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM
103941	952	-0.540	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM
103946	1018	-0.526	Compartment:cytosol | Minutes:20 | Skeletal Muscle Treatment:palmitic acid 2.4 uM

Analysis tools for 2 metabolites of interest

Note: Some different plotting/statistics items are displayed when 2 metabolites are selected (as opposed to a single metabolite)

- **Bar graph of sample ratios for the 2 metabolites**
- **Box-and-whisker plot of measurement ranges for the metabolites**
- **Bar graph of mean ratios for each factor level for the metabolites (A/B)**
- **Bar graph of mean inverse ratios for each factor level for the metabolites (B/A)**
- **Tabular and graphical display by factor/factor level of interest**

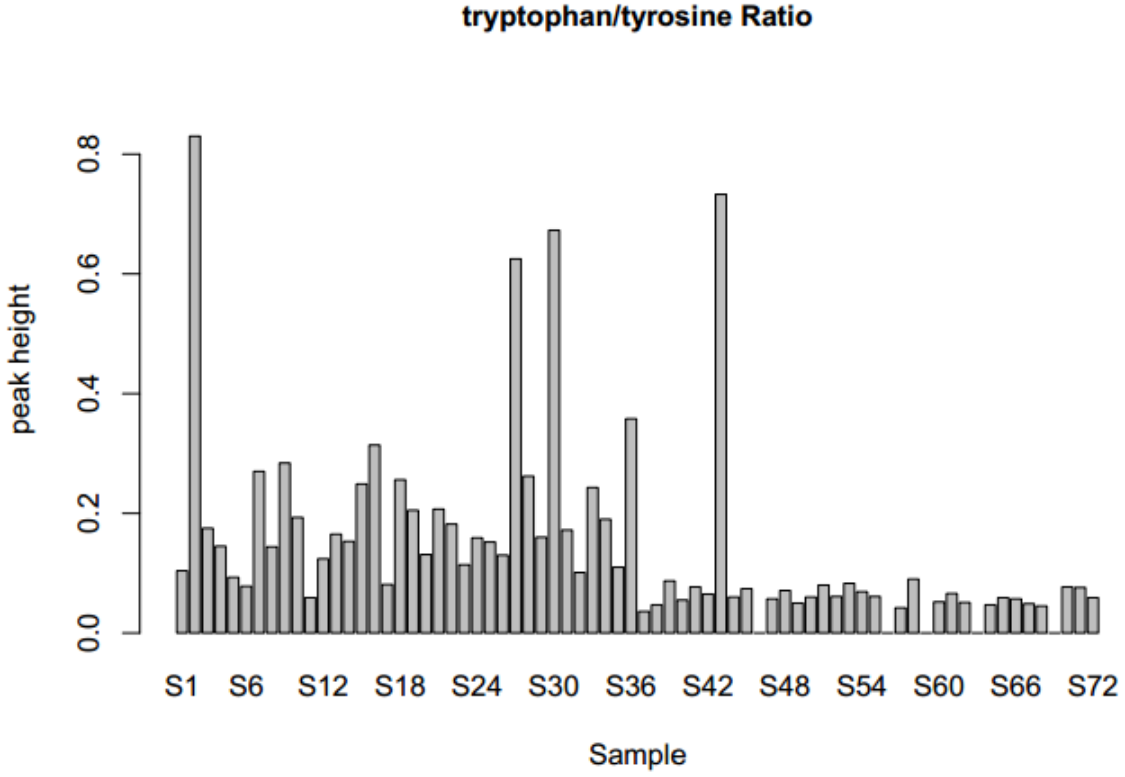
tryptophan/tyrosine Ratio values for ST000014 (Units: peak height)

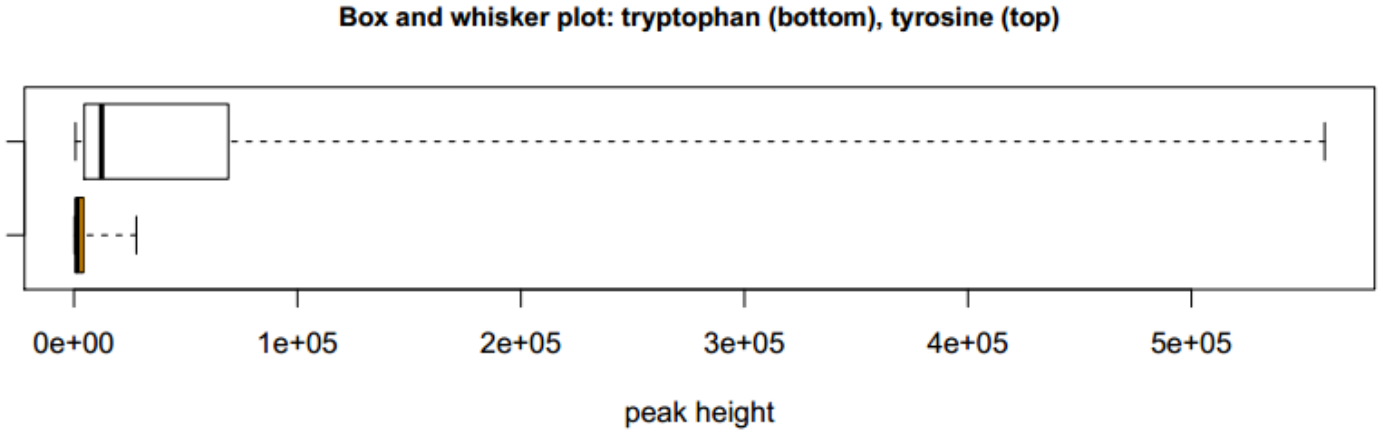
Calculate correlation coefficient for these 2 analytes

Bar graph by sample	Boxplot of 2 ranges	Bar graph of ratios for each factor level	Bar graph of inverse ratios for each factor level	View ratios for a selected factor
Bar graph (samples)	Box and whisker plot	Bar graph (factor level)	Bar graph (factor level) inverse	Factor:

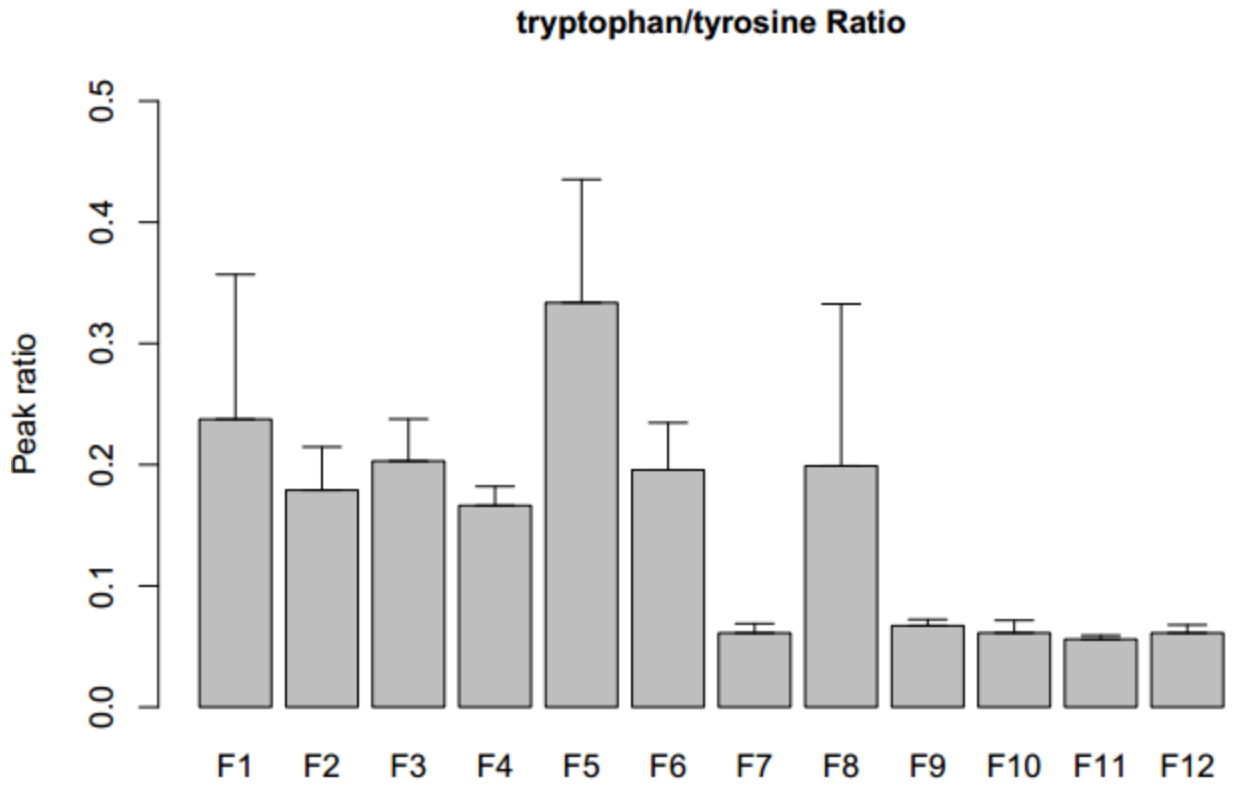
Sample	Tryptophan	Tyrosine	Tryptophan/tyrosine Ratio	Factors	Units
103879	558.0000	5351.0000	0.1043	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103884	1071.0000	1291.0000	0.8296	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103889	395.0000	2258.0000	0.1749	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103894	907.0000	6243.0000	0.1453	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103899	1810.0000	19460.0000	0.0930	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
103904	497.0000	6332.0000	0.0785	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 2.4 uM	peak height
104003	223.0000	826.0000	0.2700	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104008	502.0000	3476.0000	0.1444	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104013	313.0000	1104.0000	0.2835	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104018	729.0000	3772.0000	0.1933	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104023	536.0000	9033.0000	0.0593	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104028	647.0000	5238.0000	0.1235	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitic acid 9.6 uM	peak height
104127	756.0000	4592.0000	0.1646	Compartment:cytosol | Minutes:0 | Skeletal Muscle Treatment:palmitoyl carnitine 9.6 uM	peak height

Analysis tools for 2 metabolites of interest





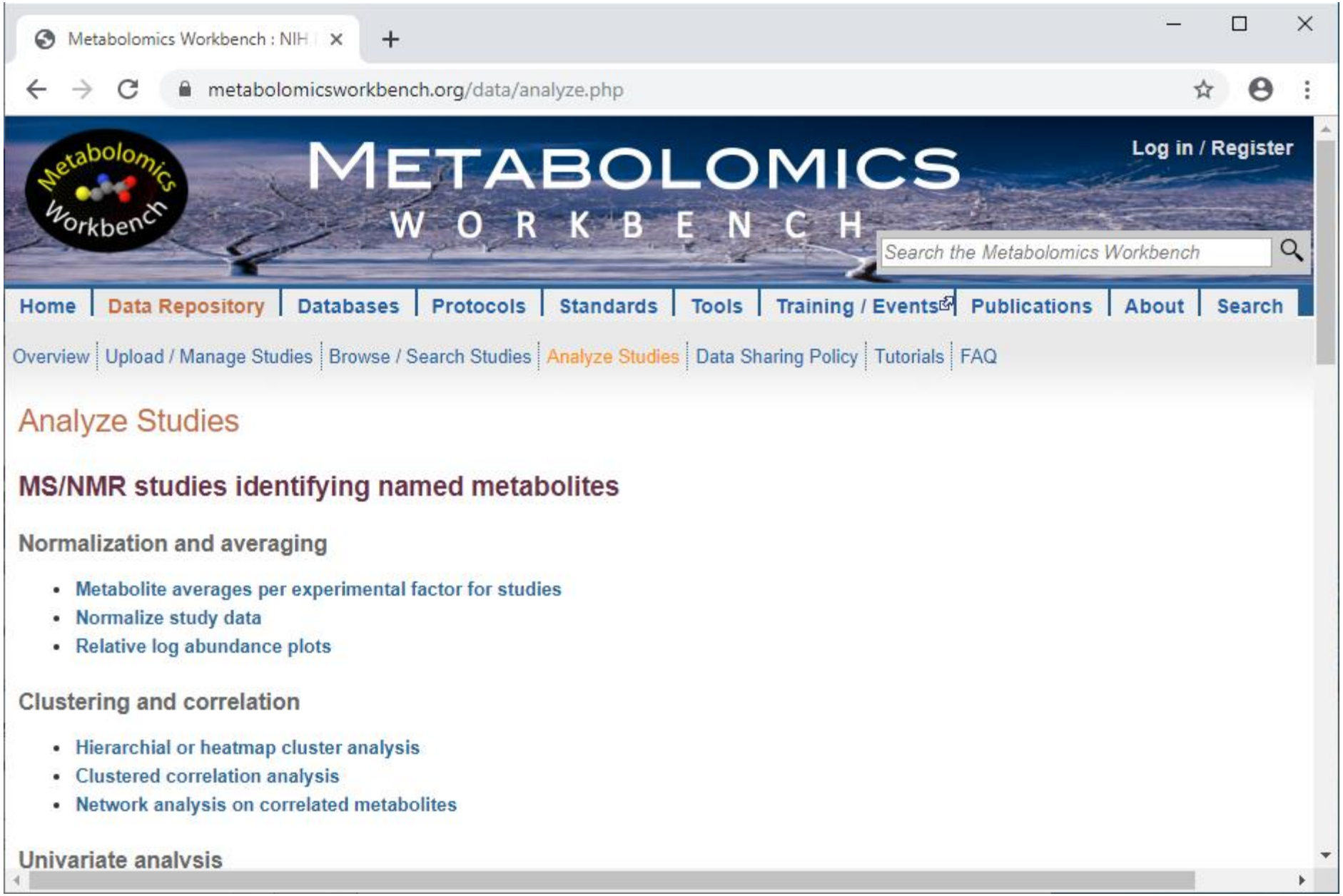
Analysis tools for 2 metabolites of interest



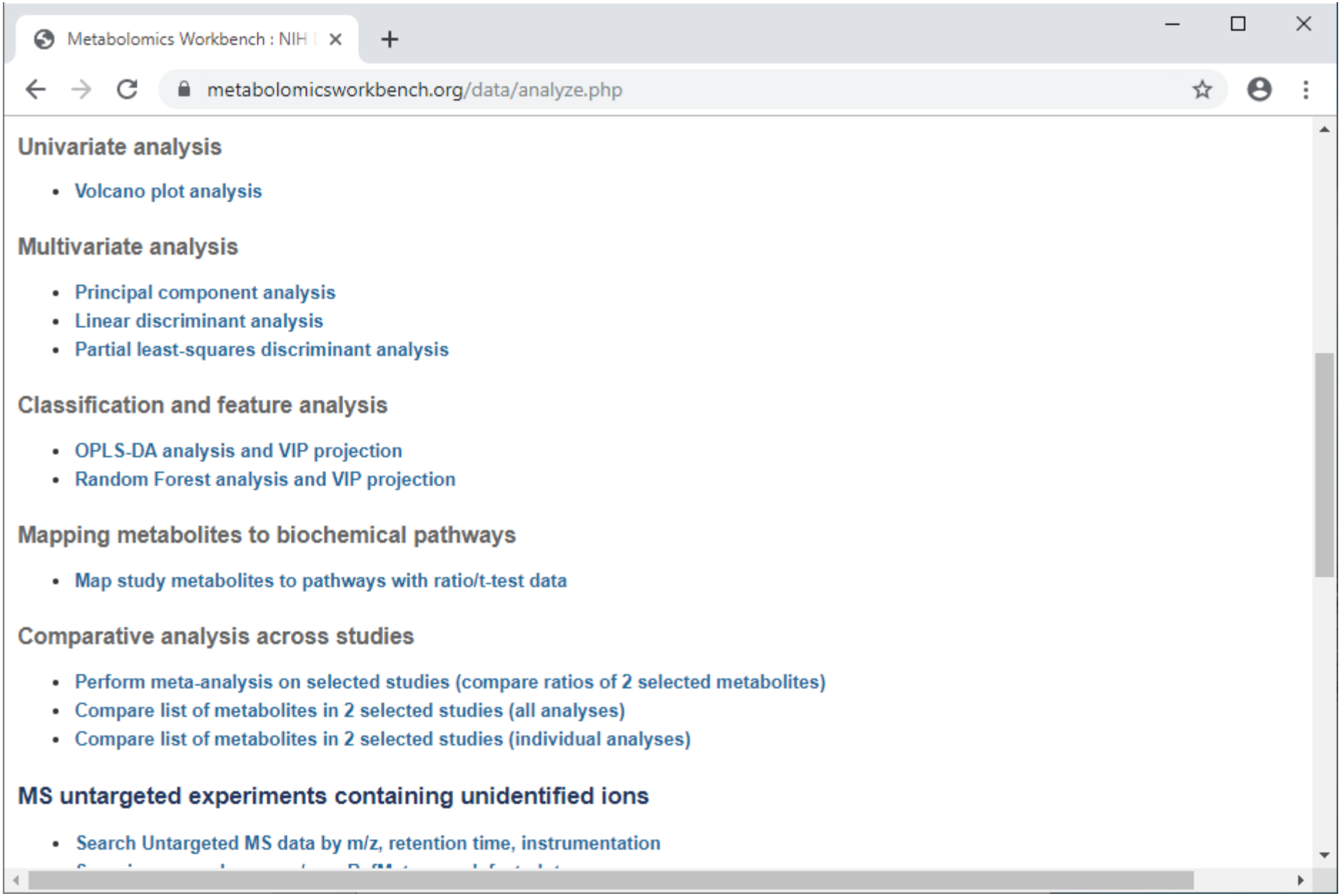
Overview

- Metabolomics workbench
- **Data Repository**
  - Browse/Search Studies
  - **Analyze Studies**
  - Upload/Manage Studies
- Databases
- Protocols
- Standards

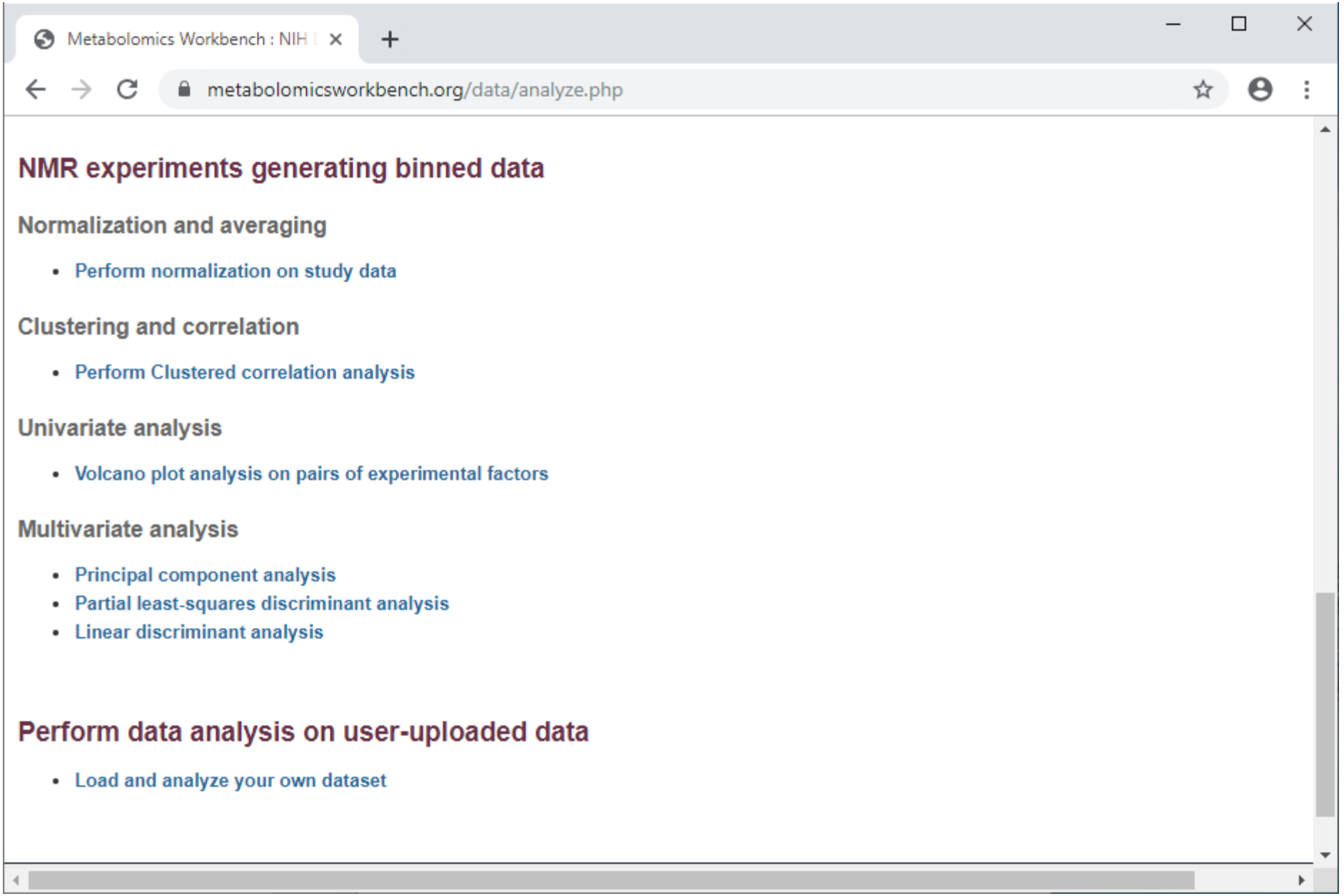
Tools for study-wide analysis



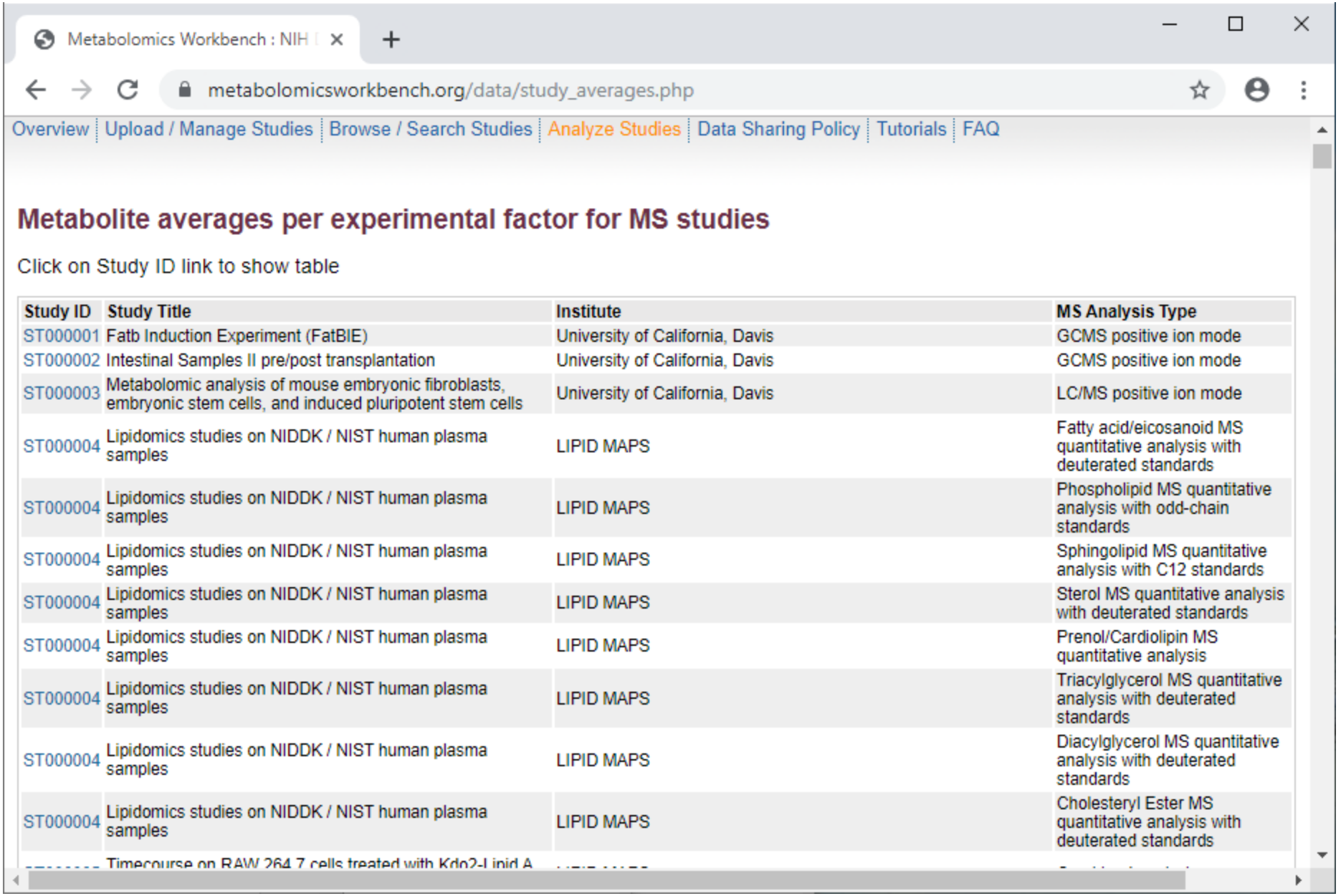
Tools for study-wide analysis



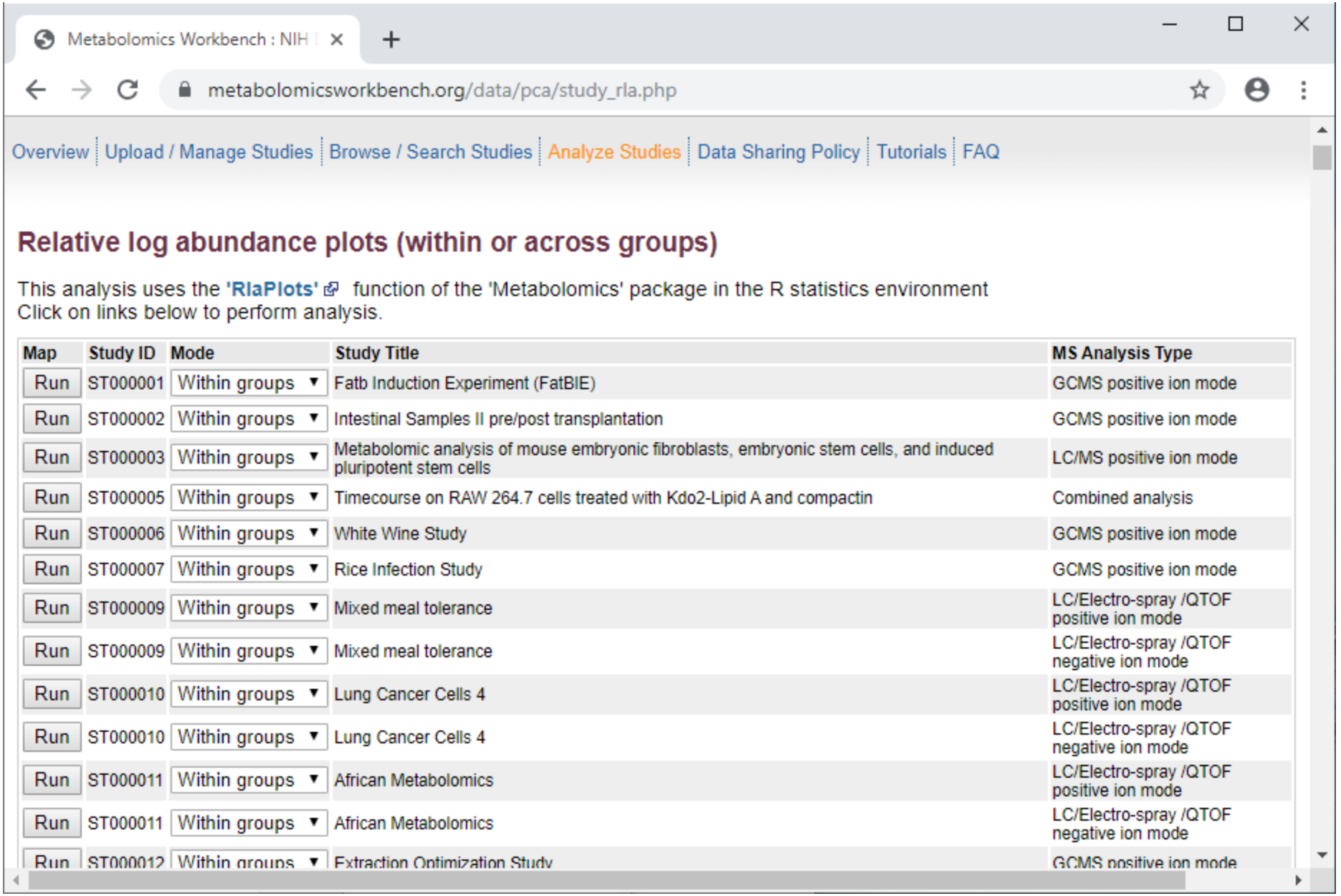
Tools for study-wide analysis



Tools for study-wide analysis

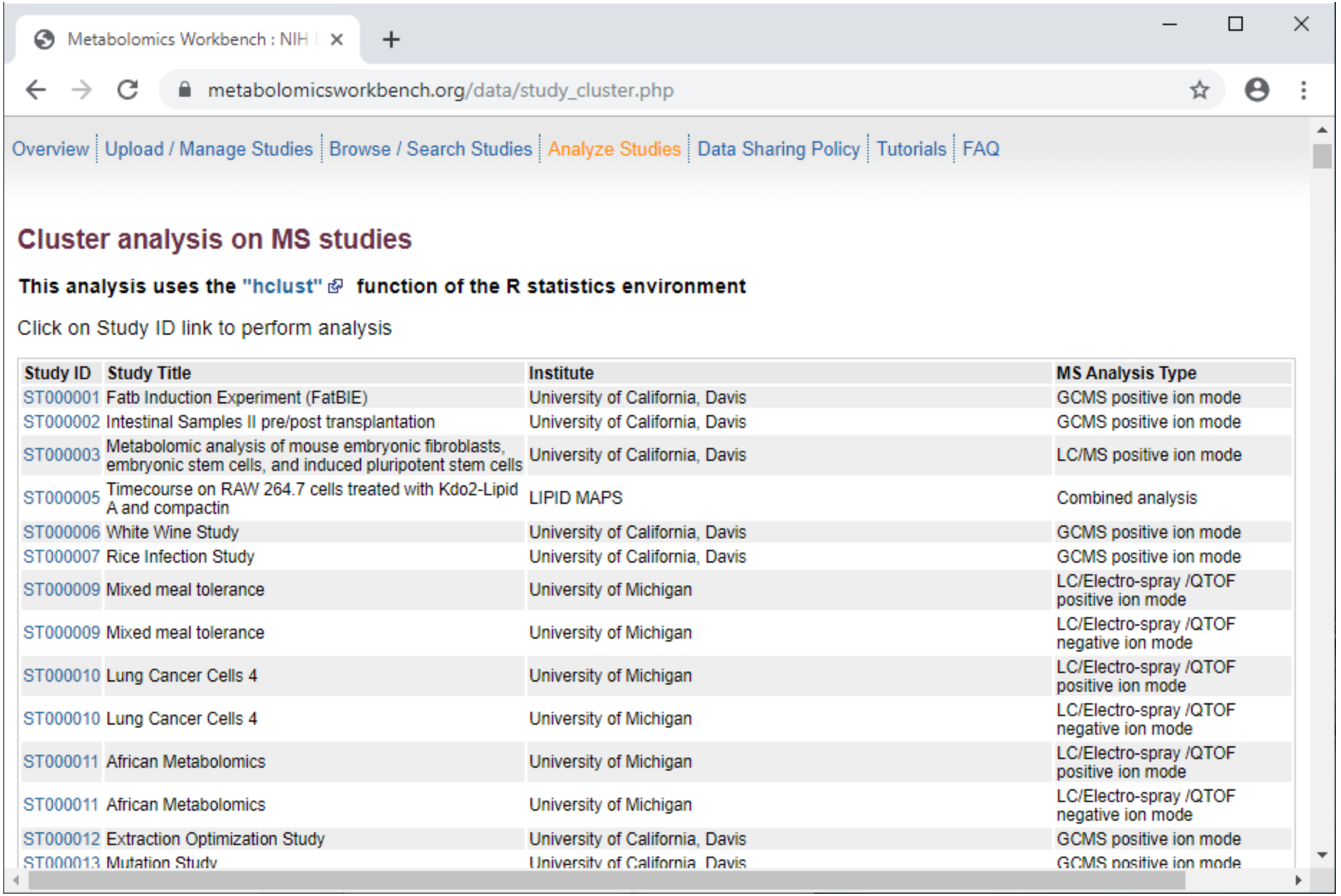


Tools for study-wide analysis



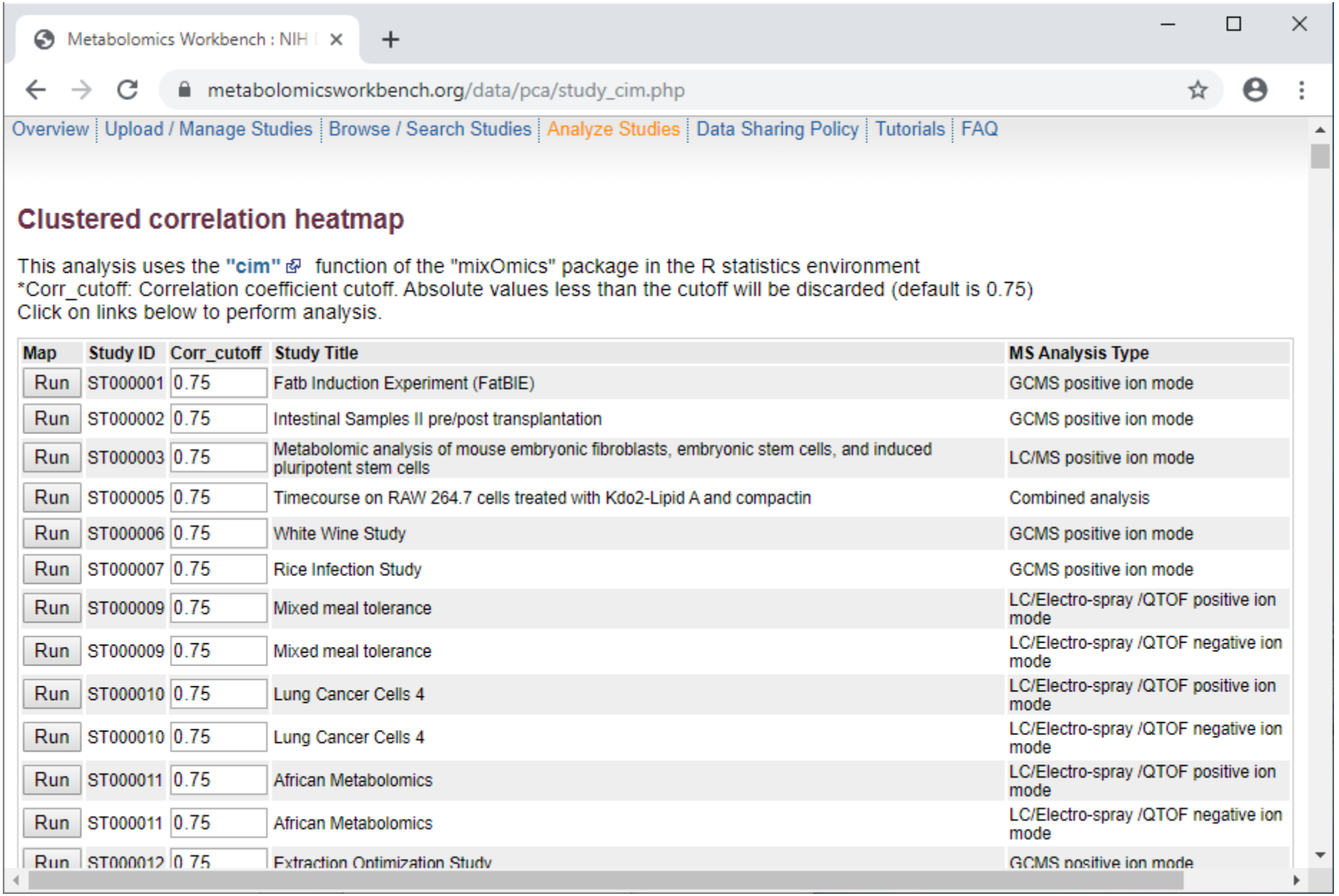
Map	Study ID	Mode	Study Title	MS Analysis Type
Run	ST000001	Within groups	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Within groups	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Within groups	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Within groups	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	Within groups	White Wine Study	GCMS positive ion mode
Run	ST000007	Within groups	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Within groups	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Within groups	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Within groups	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Within groups	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	Within groups	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	Within groups	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Within groups	Extraction Optimization Study	GCMS positive ion mode

Tools for study-wide analysis



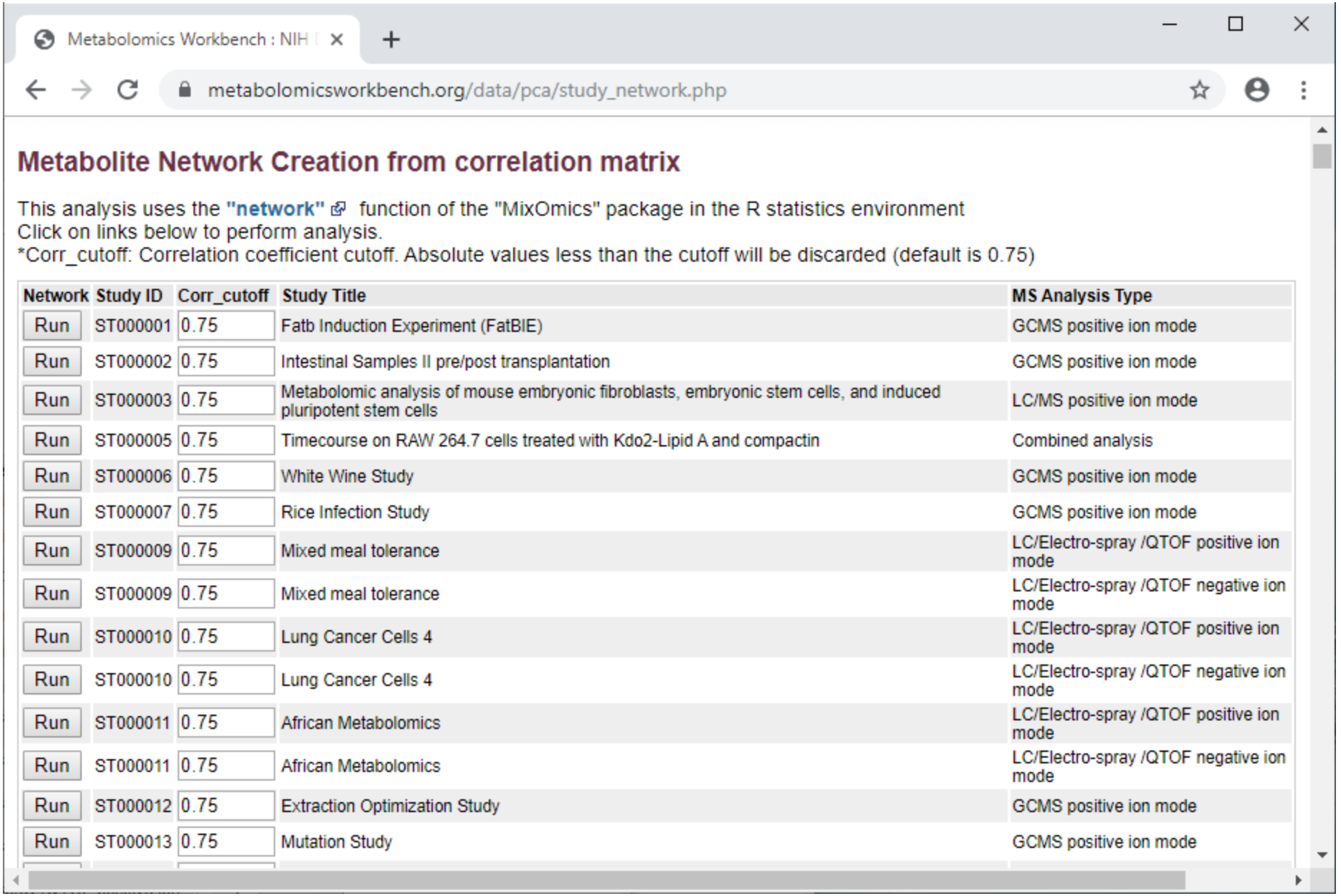
Study ID	Study Title	Institute	MS Analysis Type
ST000001	Fatb Induction Experiment (FatBIE)	University of California, Davis	GCMS positive ion mode
ST000002	Intestinal Samples II pre/post transplantation	University of California, Davis	GCMS positive ion mode
ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	University of California, Davis	LC/MS positive ion mode
ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	LIPID MAPS	Combined analysis
ST000006	White Wine Study	University of California, Davis	GCMS positive ion mode
ST000007	Rice Infection Study	University of California, Davis	GCMS positive ion mode
ST000009	Mixed meal tolerance	University of Michigan	LC/Electro-spray /QTOF positive ion mode
ST000009	Mixed meal tolerance	University of Michigan	LC/Electro-spray /QTOF negative ion mode
ST000010	Lung Cancer Cells 4	University of Michigan	LC/Electro-spray /QTOF positive ion mode
ST000010	Lung Cancer Cells 4	University of Michigan	LC/Electro-spray /QTOF negative ion mode
ST000011	African Metabolomics	University of Michigan	LC/Electro-spray /QTOF positive ion mode
ST000011	African Metabolomics	University of Michigan	LC/Electro-spray /QTOF negative ion mode
ST000012	Extraction Optimization Study	University of California, Davis	GCMS positive ion mode
ST000013	Mutation Study	University of California, Davis	GCMS positive ion mode

Tools for study-wide analysis



Map	Study ID	Corr_cutoff	Study Title	MS Analysis Type
Run	ST000001	0.75	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	0.75	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	0.75	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	0.75	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	0.75	White Wine Study	GCMS positive ion mode
Run	ST000007	0.75	Rice Infection Study	GCMS positive ion mode
Run	ST000009	0.75	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	0.75	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	0.75	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	0.75	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	0.75	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	0.75	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	0.75	Extraction Optimization Study	GCMS positive ion mode

Tools for study-wide analysis

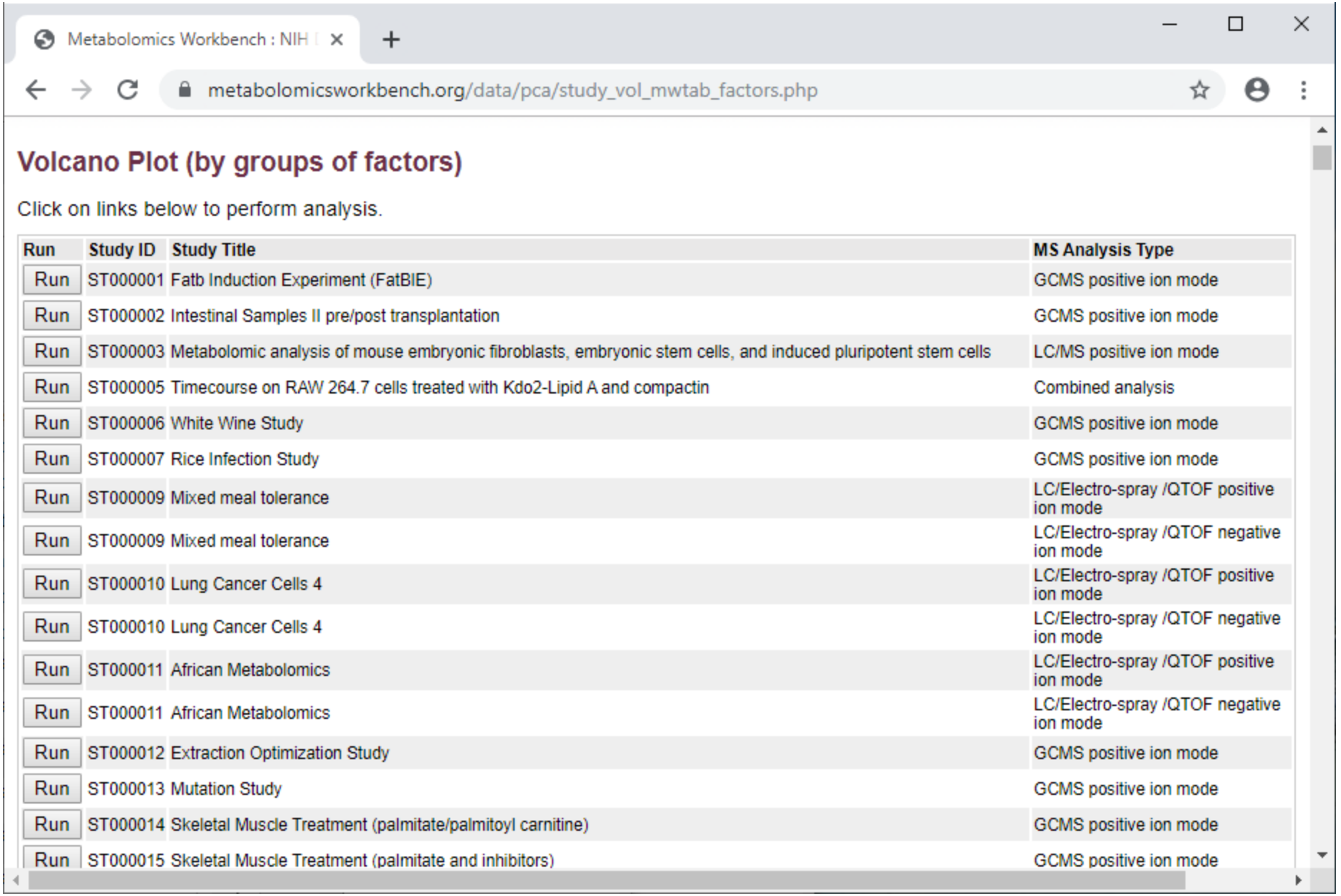


Metabolite Network Creation from correlation matrix

This analysis uses the "network" function of the "MixOmics" package in the R statistics environment
Click on links below to perform analysis.
*Corr_cutoff: Correlation coefficient cutoff. Absolute values less than the cutoff will be discarded (default is 0.75)

Network	Study ID	Corr_cutoff	Study Title	MS Analysis Type
Run	ST000001	0.75	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	0.75	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	0.75	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	0.75	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	0.75	White Wine Study	GCMS positive ion mode
Run	ST000007	0.75	Rice Infection Study	GCMS positive ion mode
Run	ST000009	0.75	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	0.75	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	0.75	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	0.75	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	0.75	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	0.75	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	0.75	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	0.75	Mutation Study	GCMS positive ion mode

Tools for study-wide analysis

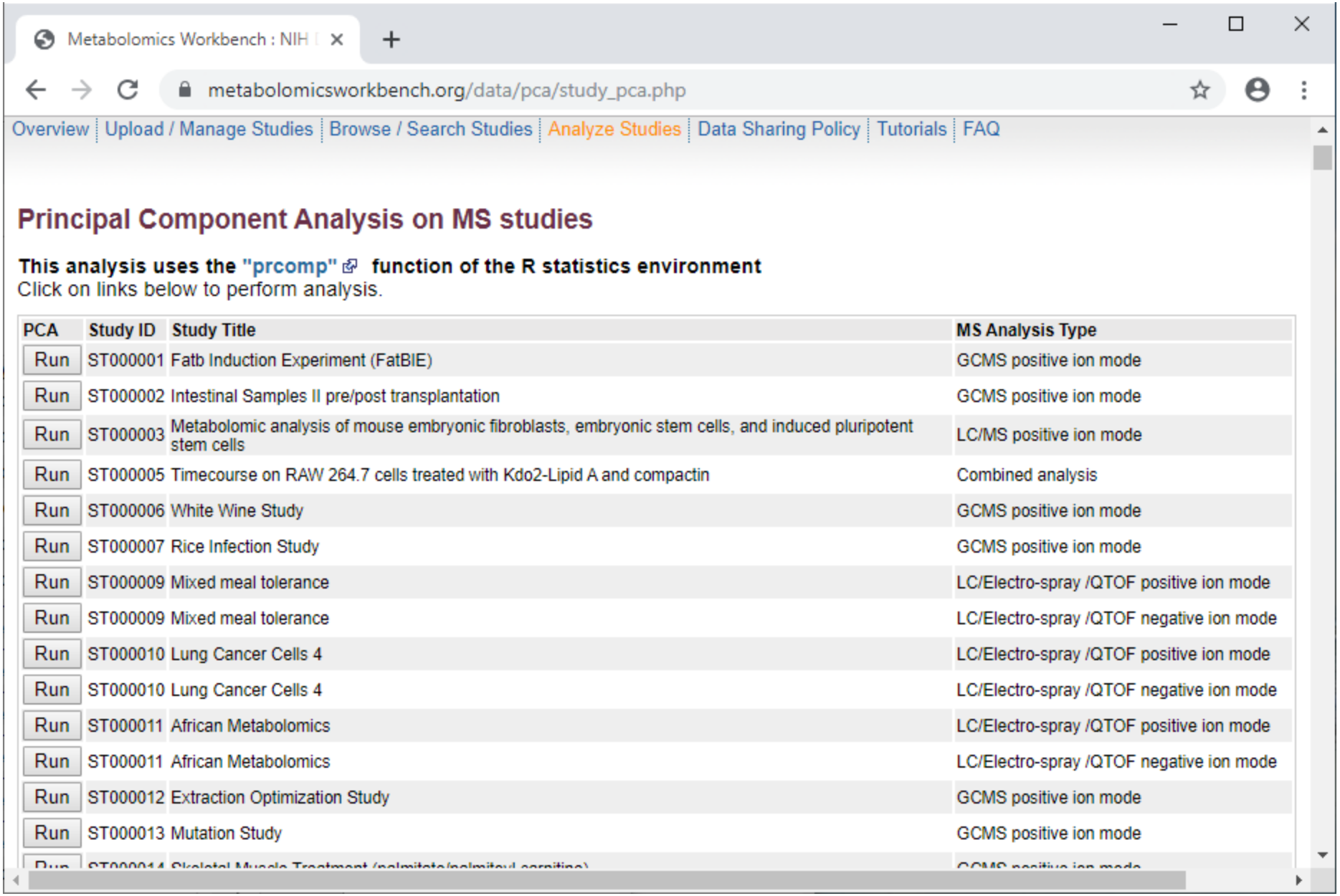


Volcano Plot (by groups of factors)

Click on links below to perform analysis.

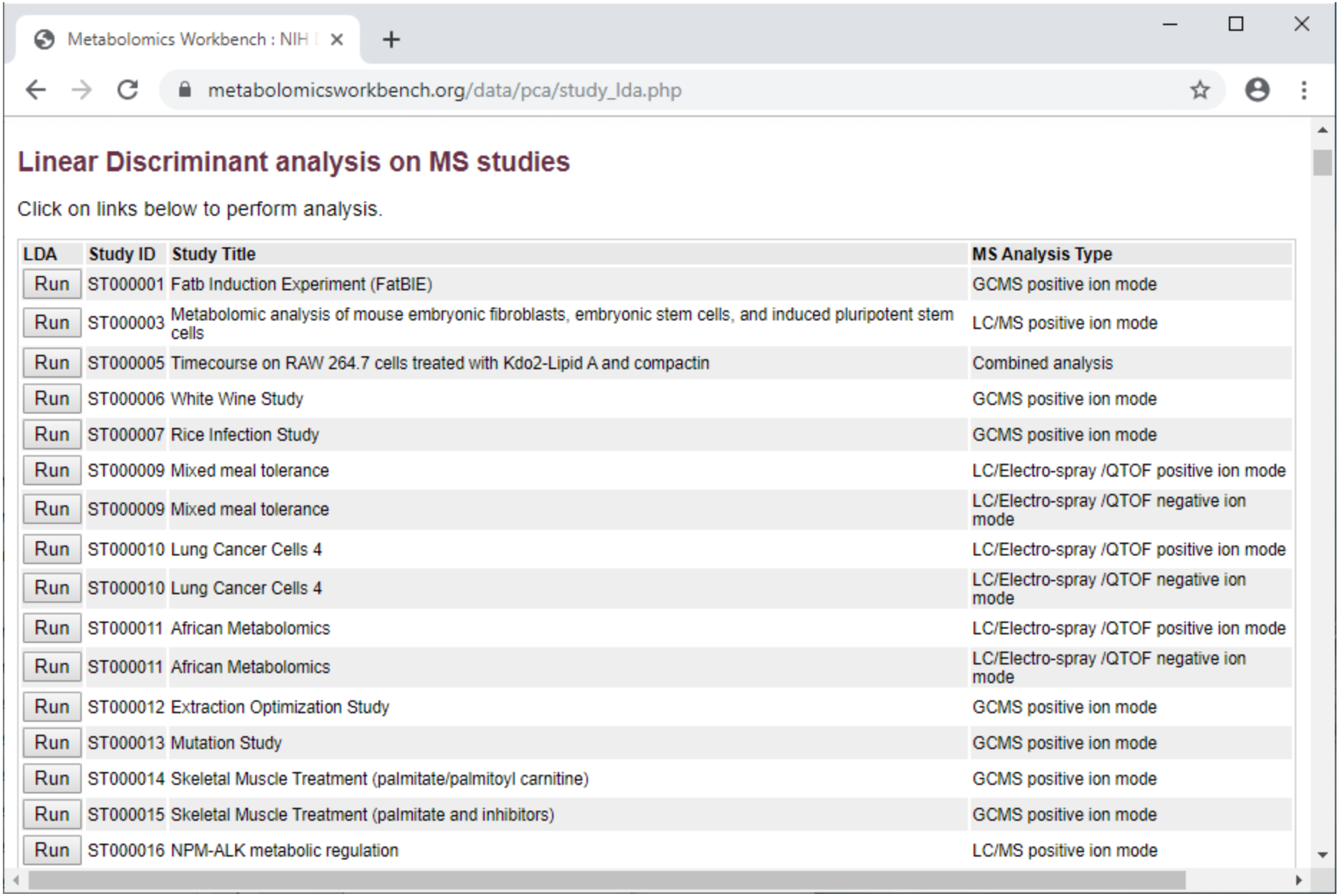
Run	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	White Wine Study	GCMS positive ion mode
Run	ST000007	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Mutation Study	GCMS positive ion mode
Run	ST000014	Skeletal Muscle Treatment (palmitate/palmitoyl carnitine)	GCMS positive ion mode
Run	ST000015	Skeletal Muscle Treatment (palmitate and inhibitors)	GCMS positive ion mode

Tools for study-wide analysis



PCA	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	White Wine Study	GCMS positive ion mode
Run	ST000007	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Mutation Study	GCMS positive ion mode

Tools for study-wide analysis

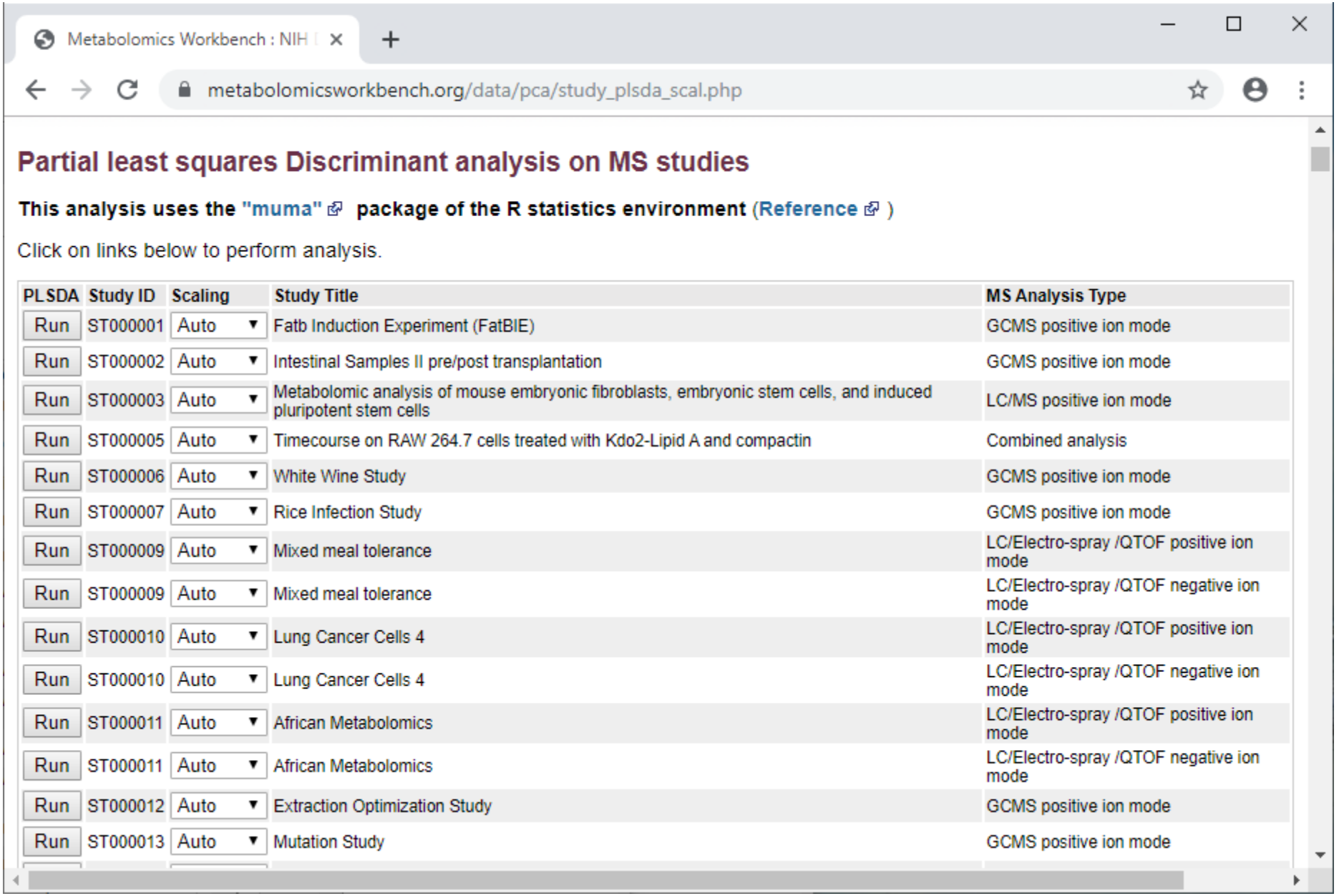


Linear Discriminant analysis on MS studies

Click on links below to perform analysis.

LDA	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	White Wine Study	GCMS positive ion mode
Run	ST000007	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Mutation Study	GCMS positive ion mode
Run	ST000014	Skeletal Muscle Treatment (palmitate/palmitoyl carnitine)	GCMS positive ion mode
Run	ST000015	Skeletal Muscle Treatment (palmitate and inhibitors)	GCMS positive ion mode
Run	ST000016	NPM-ALK metabolic regulation	LC/MS positive ion mode

Tools for study-wide analysis



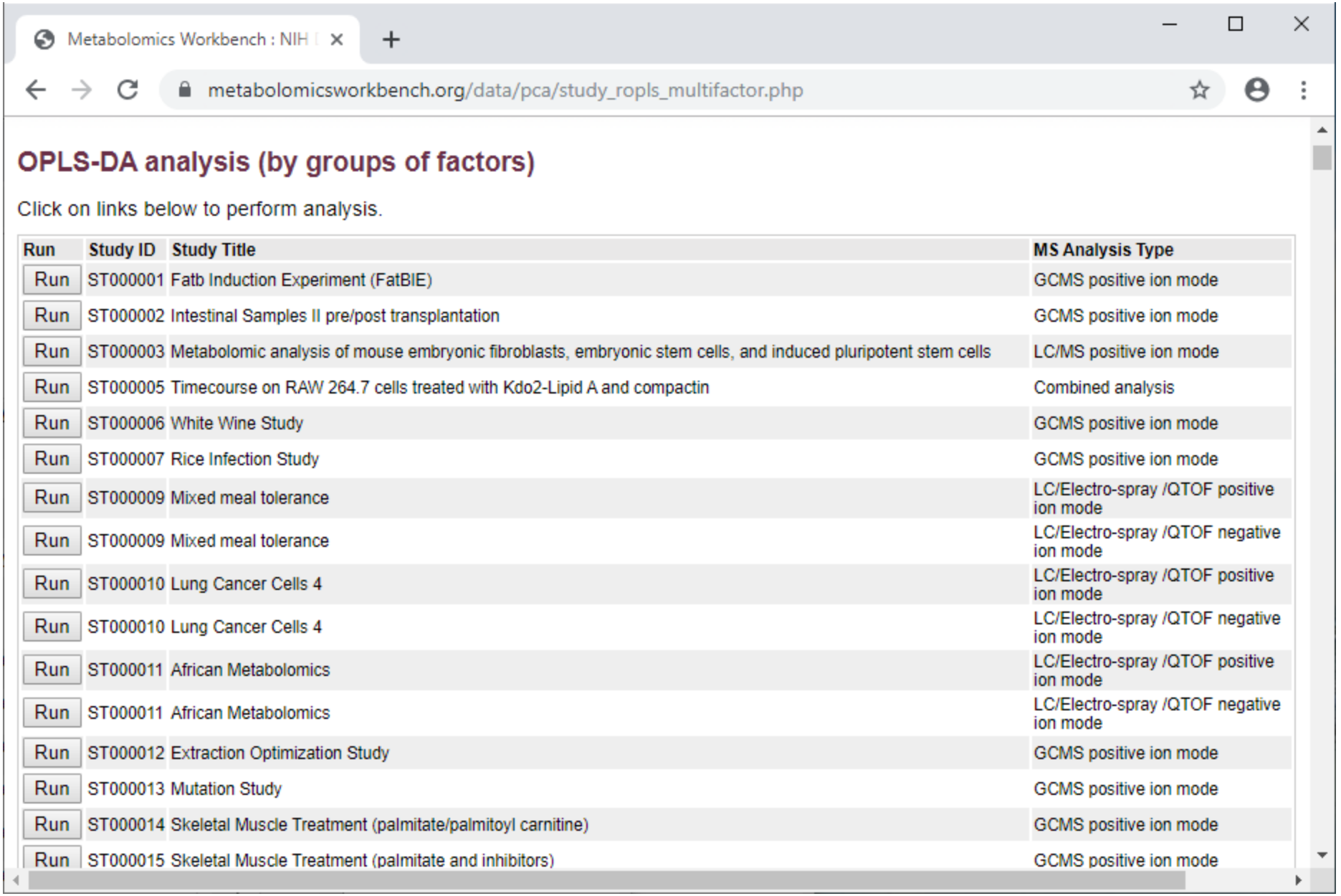
Partial least squares Discriminant analysis on MS studies

This analysis uses the "muma" package of the R statistics environment (Reference)

Click on links below to perform analysis.

PLSDA	Study ID	Scaling	Study Title	MS Analysis Type
Run	ST000001	Auto	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Auto	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Auto	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Auto	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	Auto	White Wine Study	GCMS positive ion mode
Run	ST000007	Auto	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Auto	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Auto	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Auto	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Auto	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	Auto	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	Auto	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Auto	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Auto	Mutation Study	GCMS positive ion mode

Tools for study-wide analysis

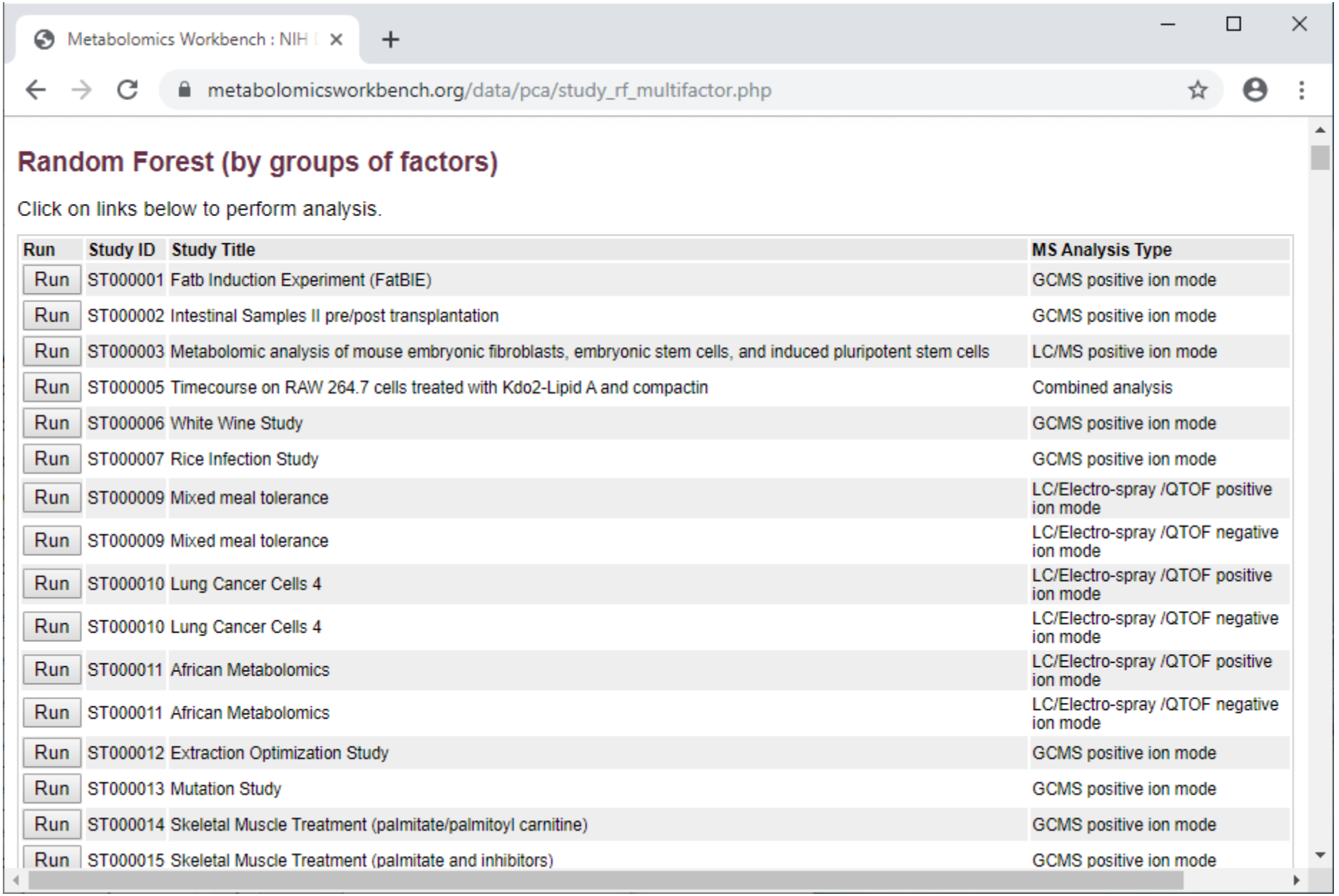


OPLS-DA analysis (by groups of factors)

Click on links below to perform analysis.

Run	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	White Wine Study	GCMS positive ion mode
Run	ST000007	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Mutation Study	GCMS positive ion mode
Run	ST000014	Skeletal Muscle Treatment (palmitate/palmitoyl carnitine)	GCMS positive ion mode
Run	ST000015	Skeletal Muscle Treatment (palmitate and inhibitors)	GCMS positive ion mode

Tools for study-wide analysis

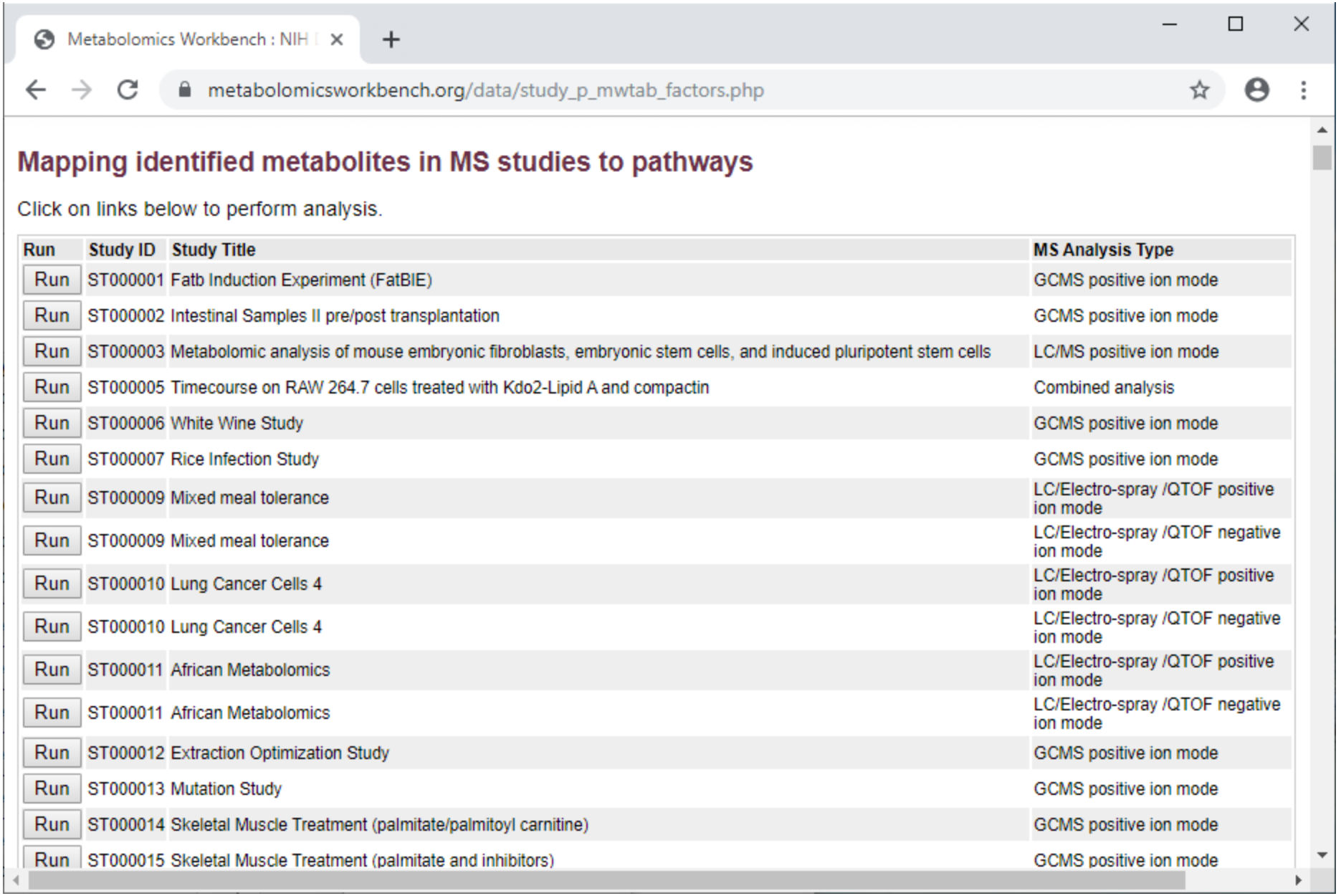


Random Forest (by groups of factors)

Click on links below to perform analysis.

Run	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	White Wine Study	GCMS positive ion mode
Run	ST000007	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Mutation Study	GCMS positive ion mode
Run	ST000014	Skeletal Muscle Treatment (palmitate/palmitoyl carnitine)	GCMS positive ion mode
Run	ST000015	Skeletal Muscle Treatment (palmitate and inhibitors)	GCMS positive ion mode

Tools for study-wide analysis

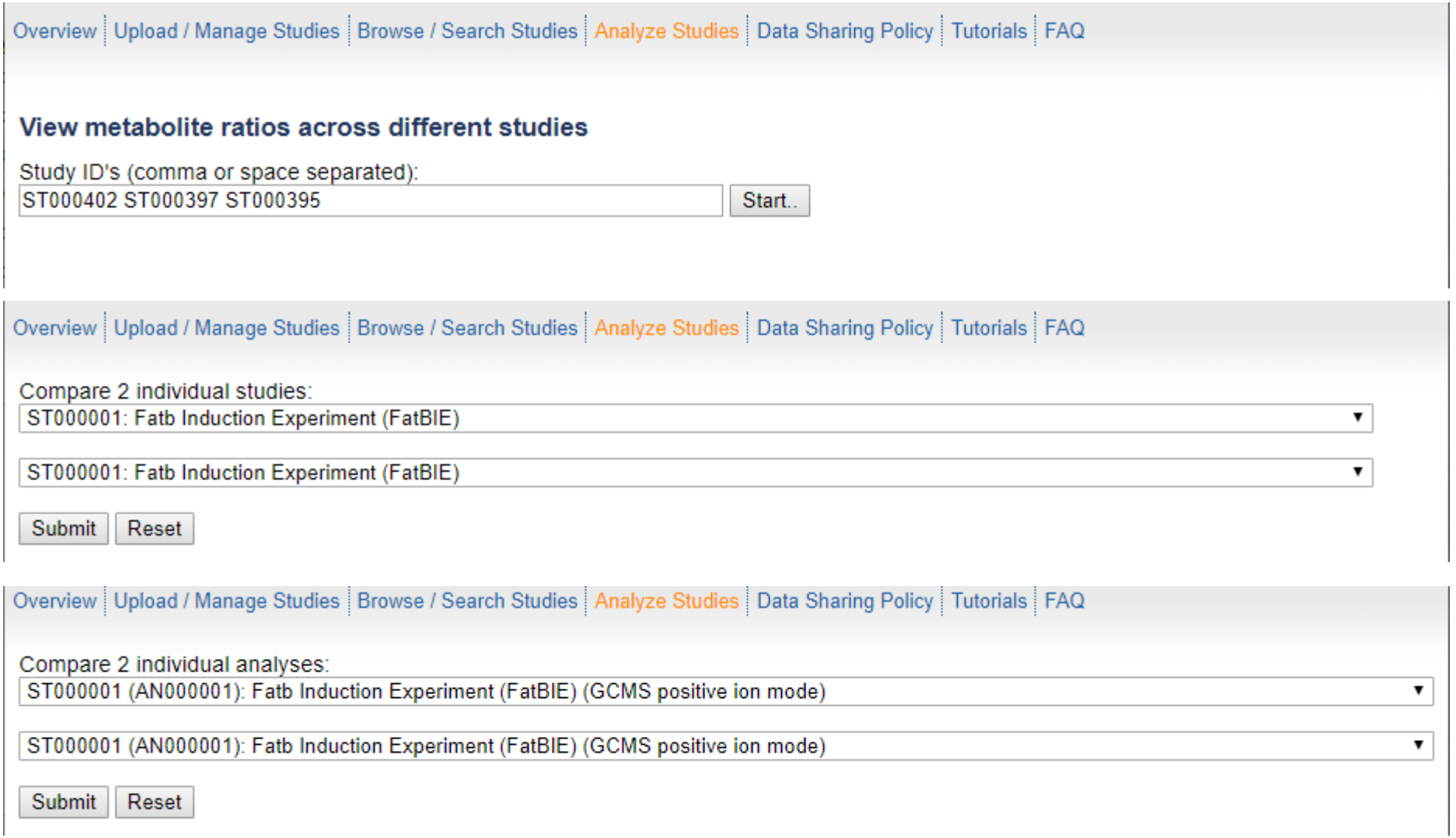


Mapping identified metabolites in MS studies to pathways

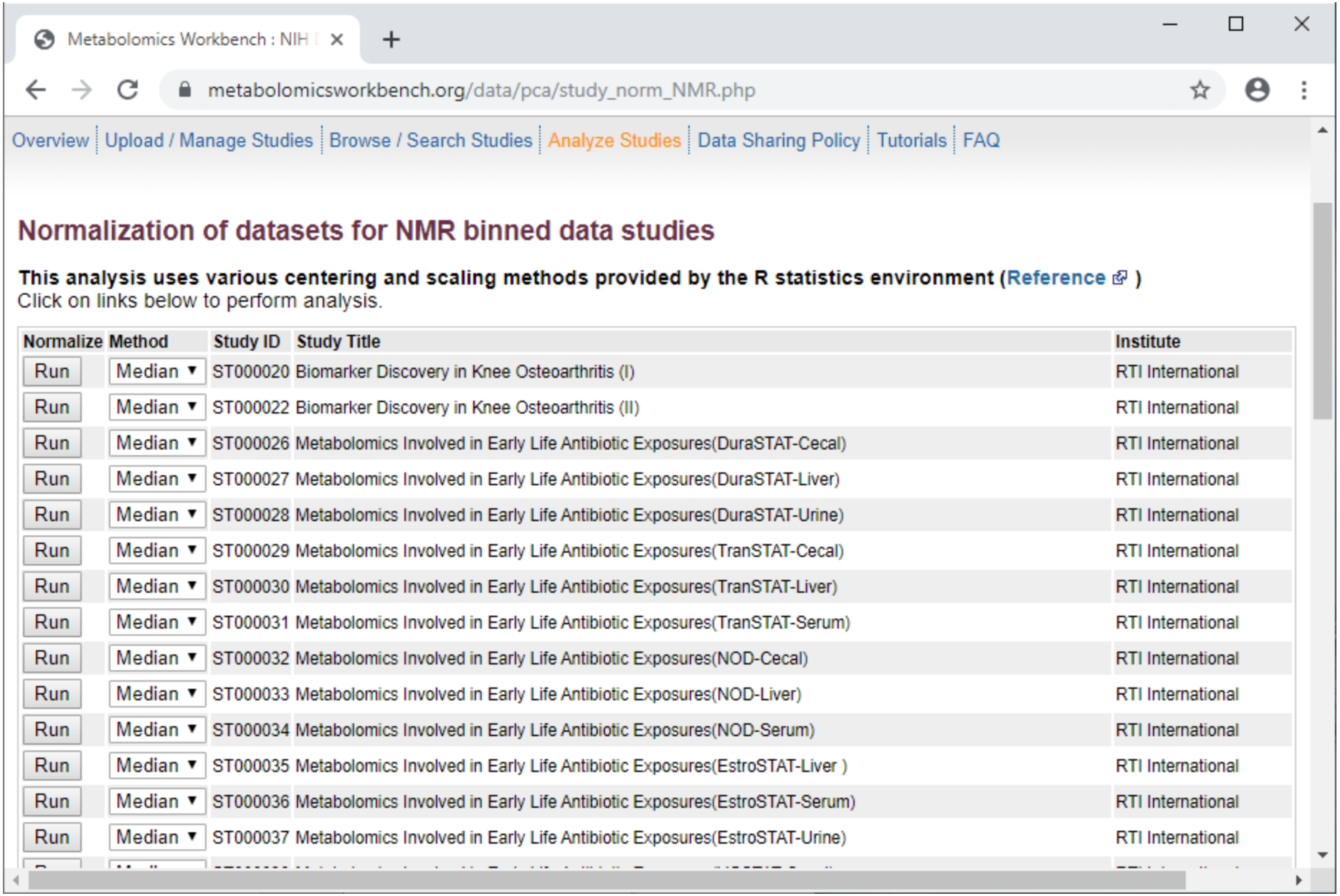
Click on links below to perform analysis.

Run	Study ID	Study Title	MS Analysis Type
Run	ST000001	Fatb Induction Experiment (FatBIE)	GCMS positive ion mode
Run	ST000002	Intestinal Samples II pre/post transplantation	GCMS positive ion mode
Run	ST000003	Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	LC/MS positive ion mode
Run	ST000005	Timecourse on RAW 264.7 cells treated with Kdo2-Lipid A and compactin	Combined analysis
Run	ST000006	White Wine Study	GCMS positive ion mode
Run	ST000007	Rice Infection Study	GCMS positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF positive ion mode
Run	ST000009	Mixed meal tolerance	LC/Electro-spray /QTOF negative ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF positive ion mode
Run	ST000010	Lung Cancer Cells 4	LC/Electro-spray /QTOF negative ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF positive ion mode
Run	ST000011	African Metabolomics	LC/Electro-spray /QTOF negative ion mode
Run	ST000012	Extraction Optimization Study	GCMS positive ion mode
Run	ST000013	Mutation Study	GCMS positive ion mode
Run	ST000014	Skeletal Muscle Treatment (palmitate/palmitoyl carnitine)	GCMS positive ion mode
Run	ST000015	Skeletal Muscle Treatment (palmitate and inhibitors)	GCMS positive ion mode

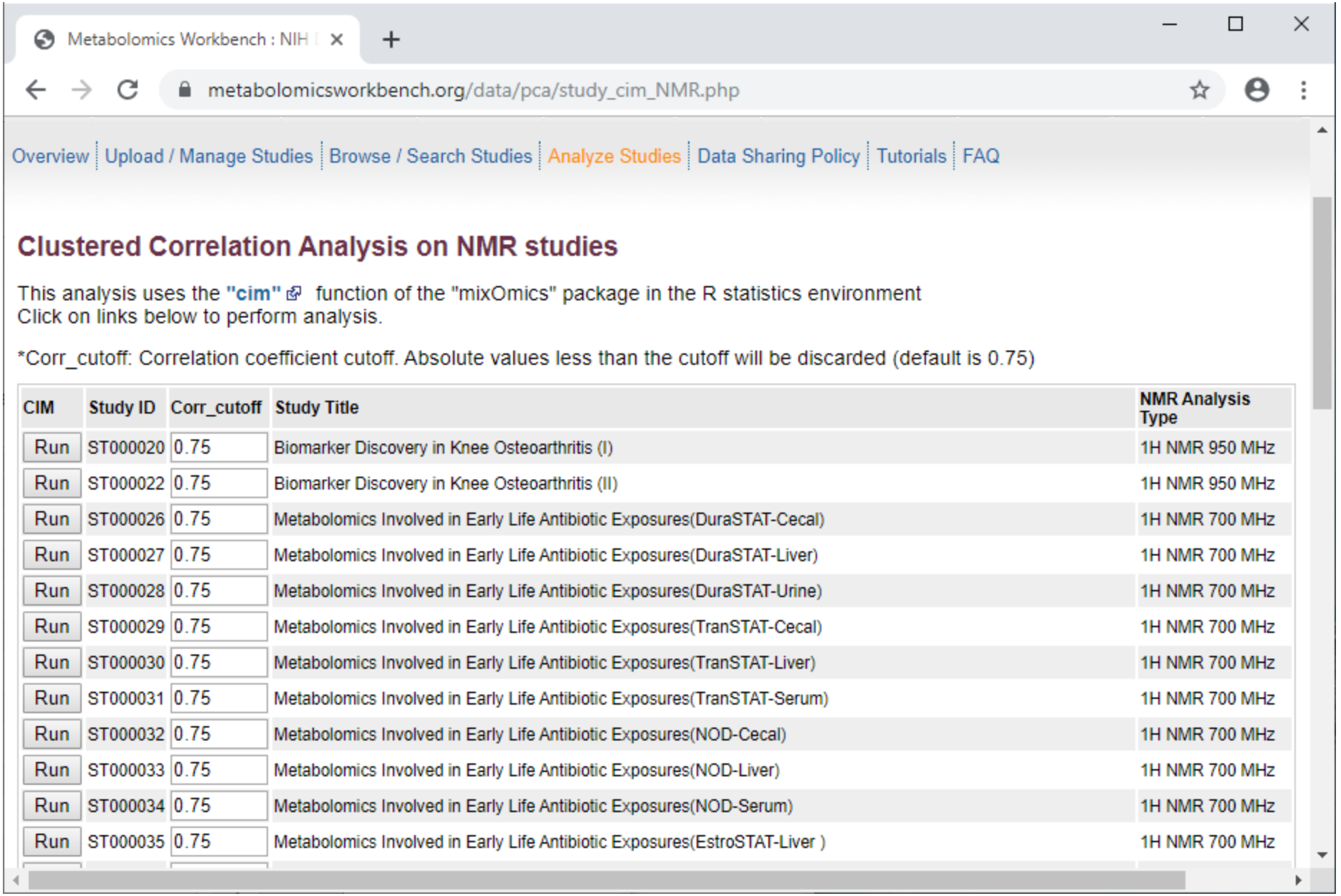
Tools for comparative analysis across studies



Tools for study-wide analysis

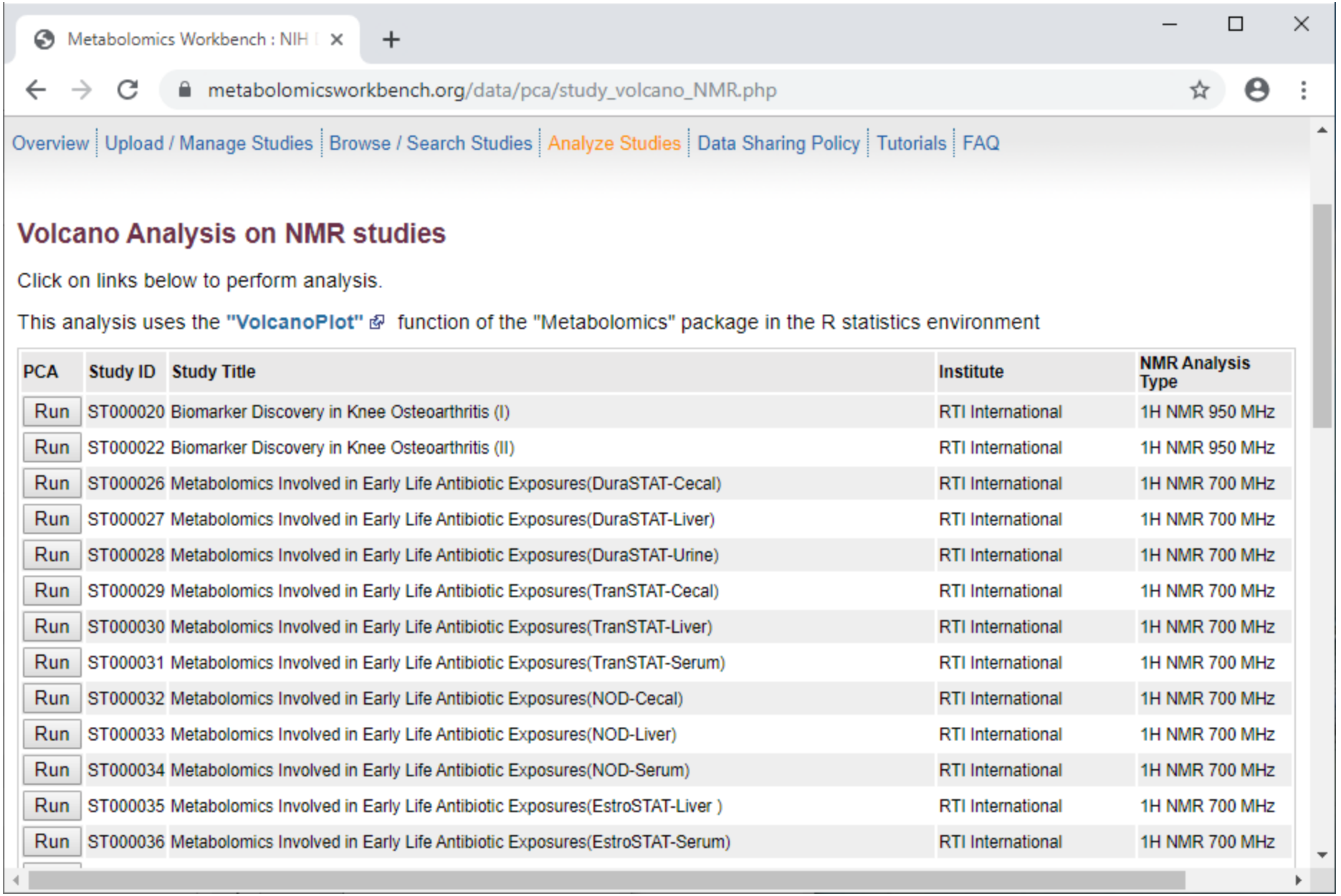


Tools for study-wide analysis



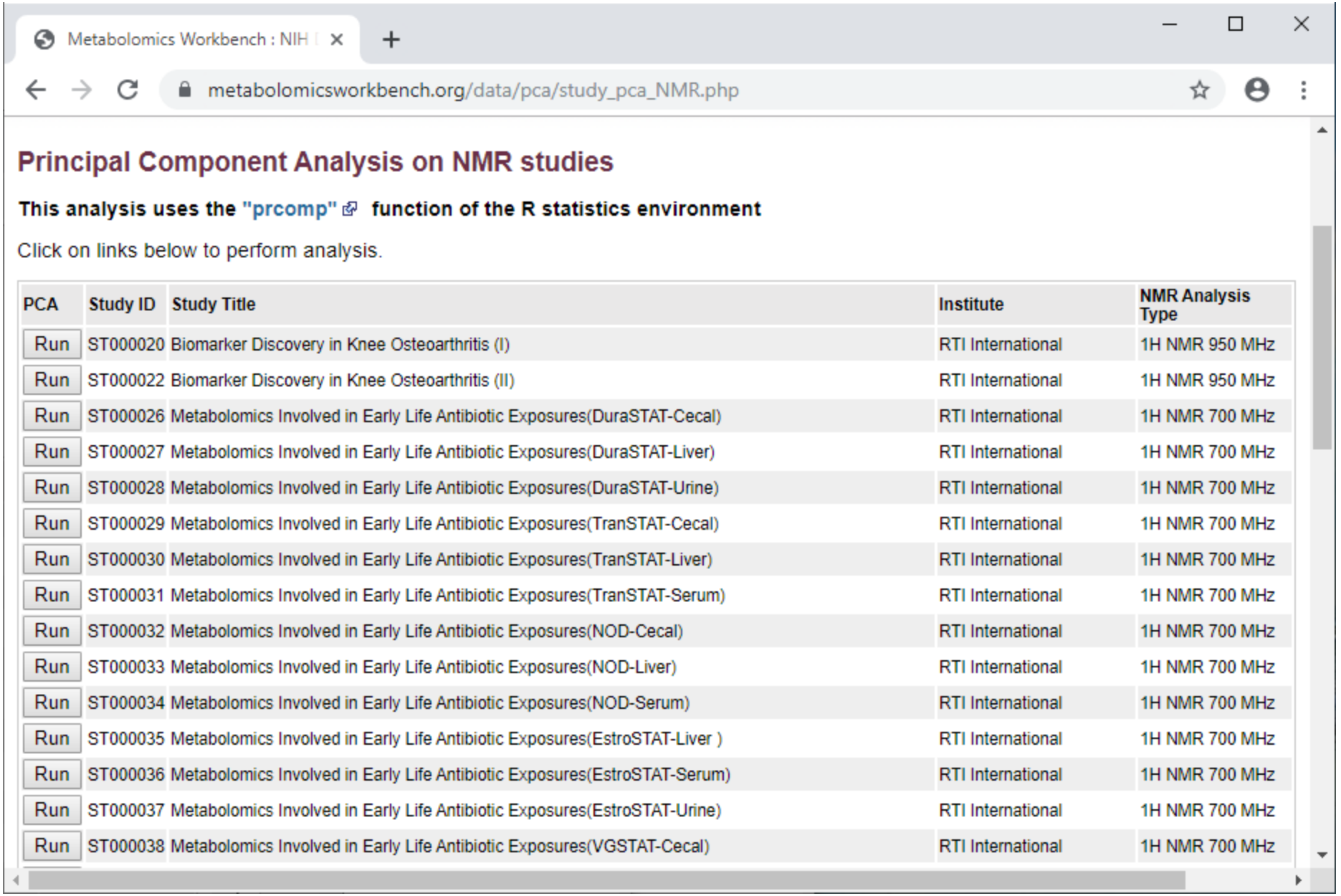
CIM	Study ID	Corr_cutoff	Study Title	NMR Analysis Type
Run	ST000020	0.75	Biomarker Discovery in Knee Osteoarthritis (I)	1H NMR 950 MHz
Run	ST000022	0.75	Biomarker Discovery in Knee Osteoarthritis (II)	1H NMR 950 MHz
Run	ST000026	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Cecal)	1H NMR 700 MHz
Run	ST000027	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Liver)	1H NMR 700 MHz
Run	ST000028	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Urine)	1H NMR 700 MHz
Run	ST000029	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Cecal)	1H NMR 700 MHz
Run	ST000030	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Liver)	1H NMR 700 MHz
Run	ST000031	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Serum)	1H NMR 700 MHz
Run	ST000032	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Cecal)	1H NMR 700 MHz
Run	ST000033	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Liver)	1H NMR 700 MHz
Run	ST000034	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Serum)	1H NMR 700 MHz
Run	ST000035	0.75	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Liver)	1H NMR 700 MHz

Tools for study-wide analysis



PCA	Study ID	Study Title	Institute	NMR Analysis Type
Run	ST000020	Biomarker Discovery in Knee Osteoarthritis (I)	RTI International	1H NMR 950 MHz
Run	ST000022	Biomarker Discovery in Knee Osteoarthritis (II)	RTI International	1H NMR 950 MHz
Run	ST000026	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000027	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000028	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Urine)	RTI International	1H NMR 700 MHz
Run	ST000029	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000030	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000031	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000032	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000033	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Liver)	RTI International	1H NMR 700 MHz
Run	ST000034	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Serum)	RTI International	1H NMR 700 MHz
Run	ST000035	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000036	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Serum)	RTI International	1H NMR 700 MHz

Tools for study-wide analysis



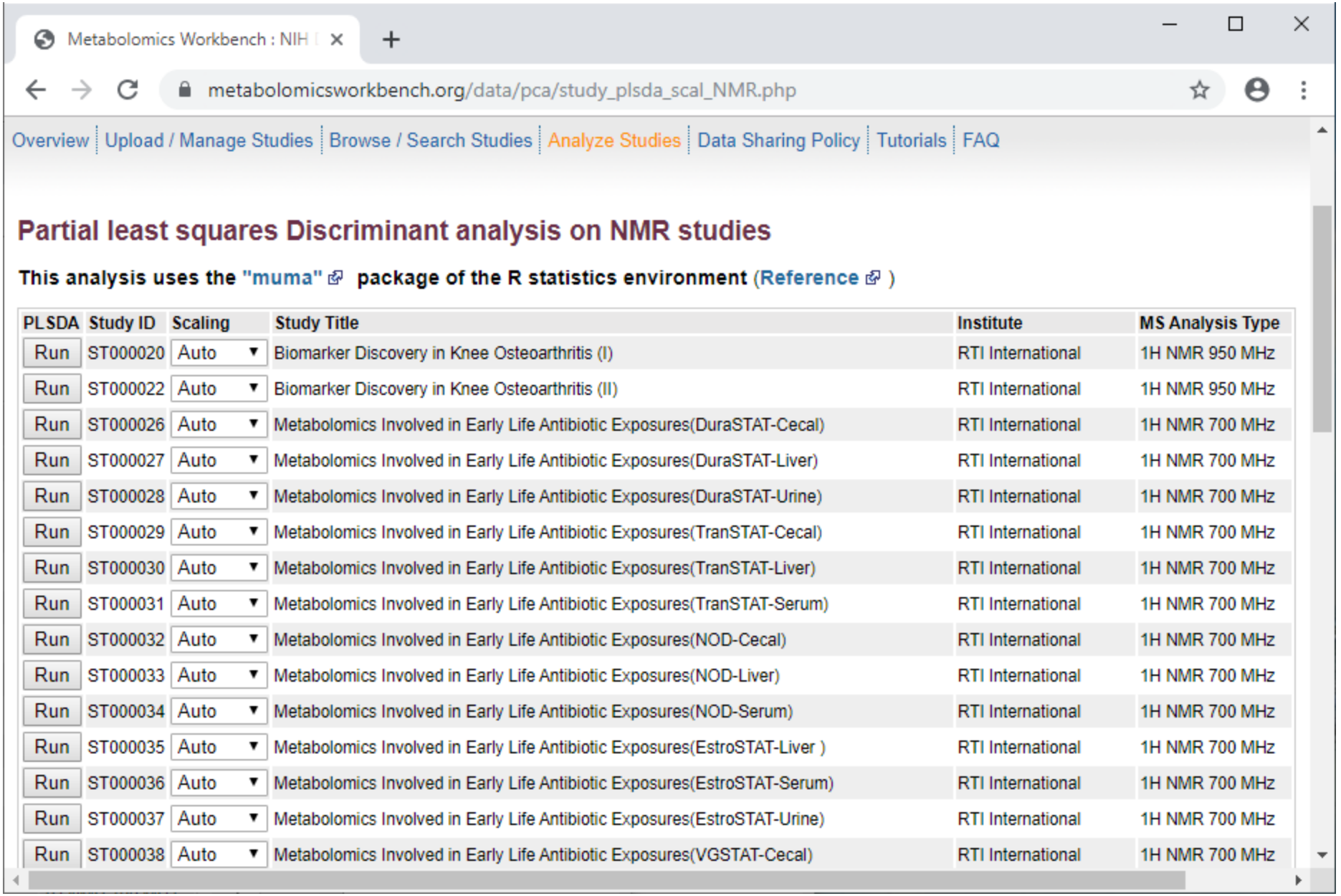
Principal Component Analysis on NMR studies

This analysis uses the "prcomp" function of the R statistics environment

Click on links below to perform analysis.

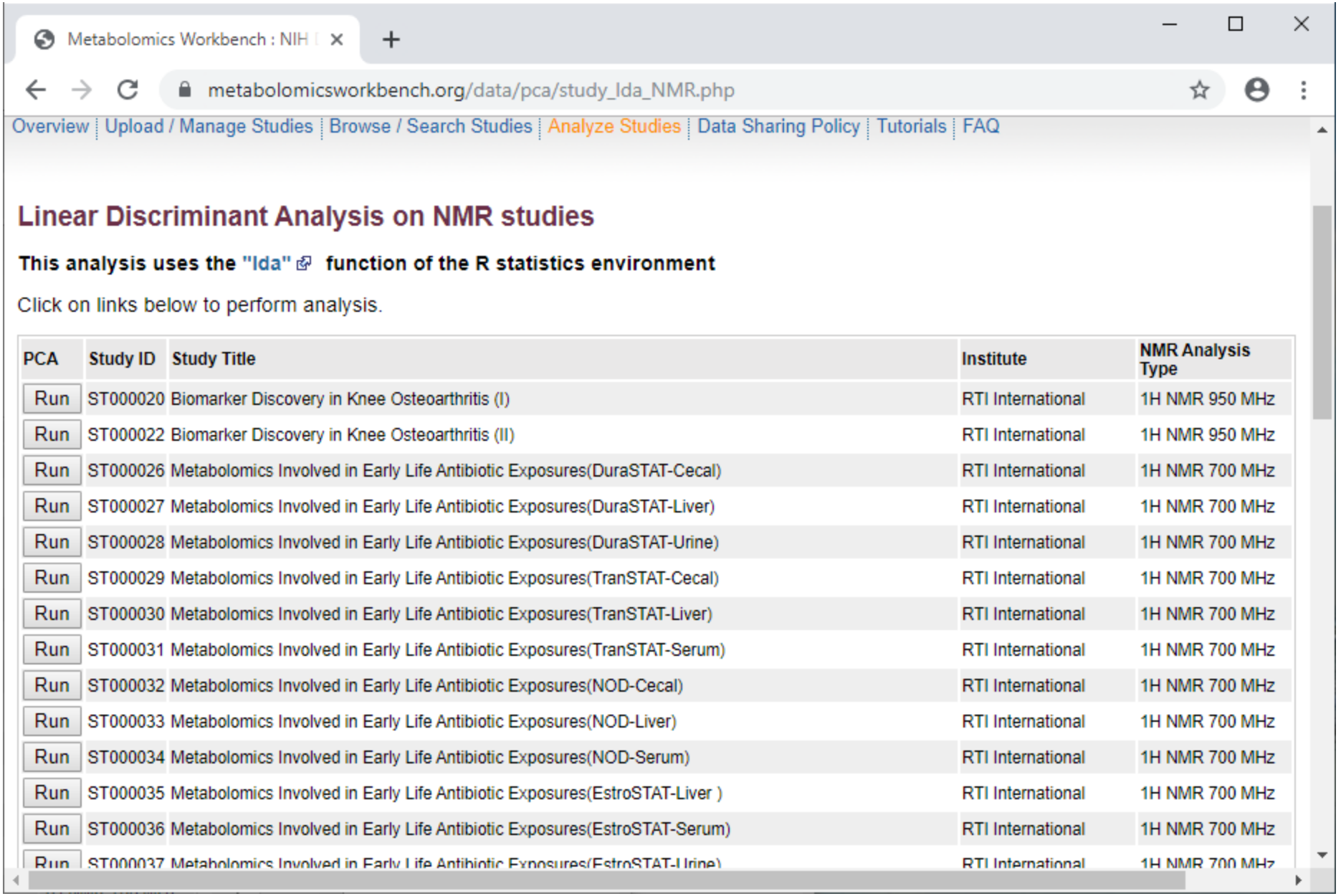
PCA	Study ID	Study Title	Institute	NMR Analysis Type
Run	ST000020	Biomarker Discovery in Knee Osteoarthritis (I)	RTI International	1H NMR 950 MHz
Run	ST000022	Biomarker Discovery in Knee Osteoarthritis (II)	RTI International	1H NMR 950 MHz
Run	ST000026	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000027	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000028	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Urine)	RTI International	1H NMR 700 MHz
Run	ST000029	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000030	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000031	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000032	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000033	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Liver)	RTI International	1H NMR 700 MHz
Run	ST000034	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Serum)	RTI International	1H NMR 700 MHz
Run	ST000035	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000036	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000037	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Urine)	RTI International	1H NMR 700 MHz
Run	ST000038	Metabolomics Involved in Early Life Antibiotic Exposures(VGSTAT-Cecal)	RTI International	1H NMR 700 MHz

Tools for study-wide analysis



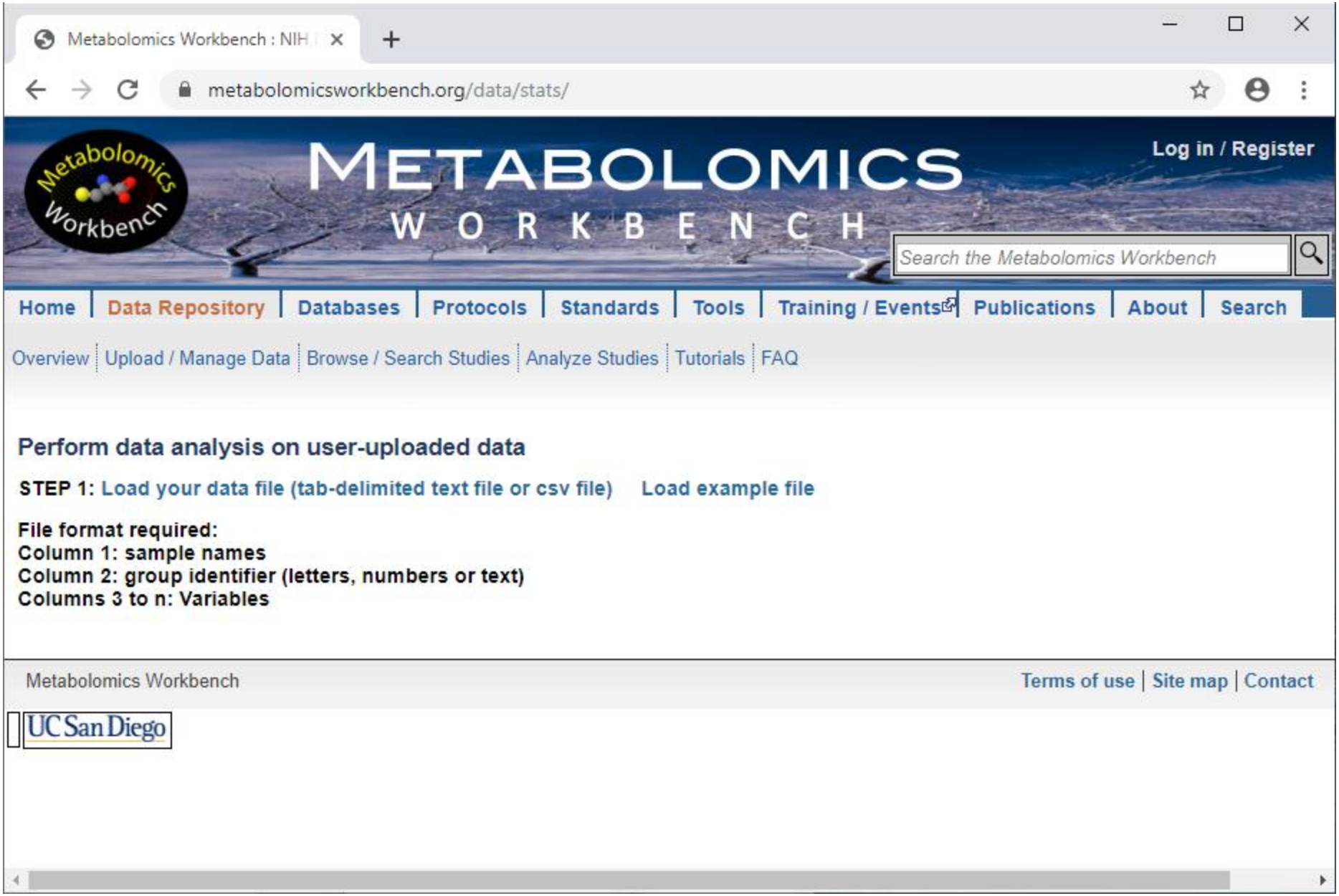
PLSDA	Study ID	Scaling	Study Title	Institute	MS Analysis Type
Run	ST000020	Auto	Biomarker Discovery in Knee Osteoarthritis (I)	RTI International	1H NMR 950 MHz
Run	ST000022	Auto	Biomarker Discovery in Knee Osteoarthritis (II)	RTI International	1H NMR 950 MHz
Run	ST000026	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000027	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000028	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Urine)	RTI International	1H NMR 700 MHz
Run	ST000029	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000030	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000031	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000032	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000033	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Liver)	RTI International	1H NMR 700 MHz
Run	ST000034	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Serum)	RTI International	1H NMR 700 MHz
Run	ST000035	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000036	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000037	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Urine)	RTI International	1H NMR 700 MHz
Run	ST000038	Auto	Metabolomics Involved in Early Life Antibiotic Exposures(VGSTAT-Cecal)	RTI International	1H NMR 700 MHz

Tools for study-wide analysis



PCA	Study ID	Study Title	Institute	NMR Analysis Type
Run	ST000020	Biomarker Discovery in Knee Osteoarthritis (I)	RTI International	1H NMR 950 MHz
Run	ST000022	Biomarker Discovery in Knee Osteoarthritis (II)	RTI International	1H NMR 950 MHz
Run	ST000026	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000027	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000028	Metabolomics Involved in Early Life Antibiotic Exposures(DuraSTAT-Urine)	RTI International	1H NMR 700 MHz
Run	ST000029	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000030	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000031	Metabolomics Involved in Early Life Antibiotic Exposures(TranSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000032	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Cecal)	RTI International	1H NMR 700 MHz
Run	ST000033	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Liver)	RTI International	1H NMR 700 MHz
Run	ST000034	Metabolomics Involved in Early Life Antibiotic Exposures(NOD-Serum)	RTI International	1H NMR 700 MHz
Run	ST000035	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Liver)	RTI International	1H NMR 700 MHz
Run	ST000036	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Serum)	RTI International	1H NMR 700 MHz
Run	ST000037	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Urine)	RTI International	1H NMR 700 MHz

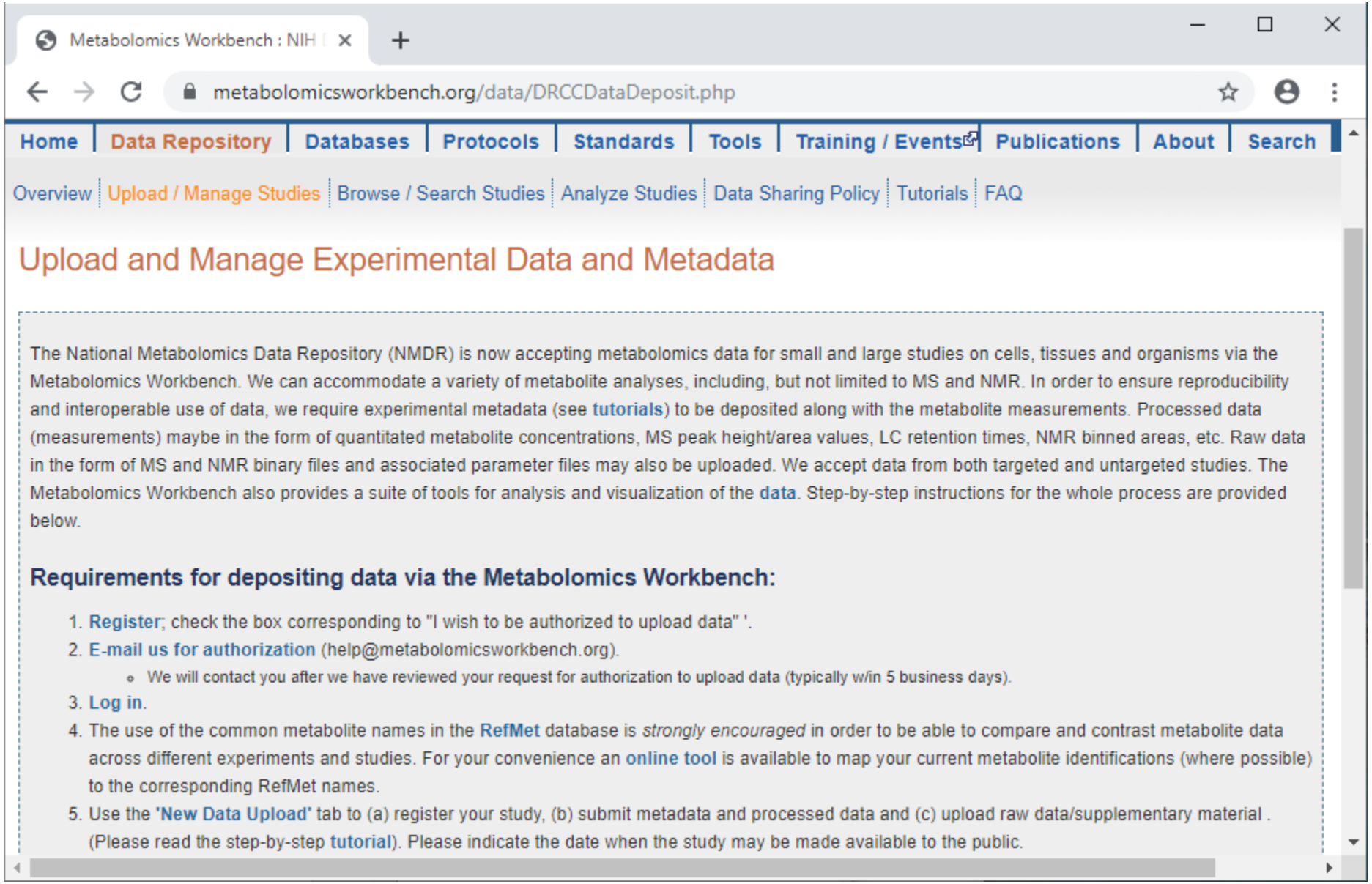
Tools for analysis of uploaded data



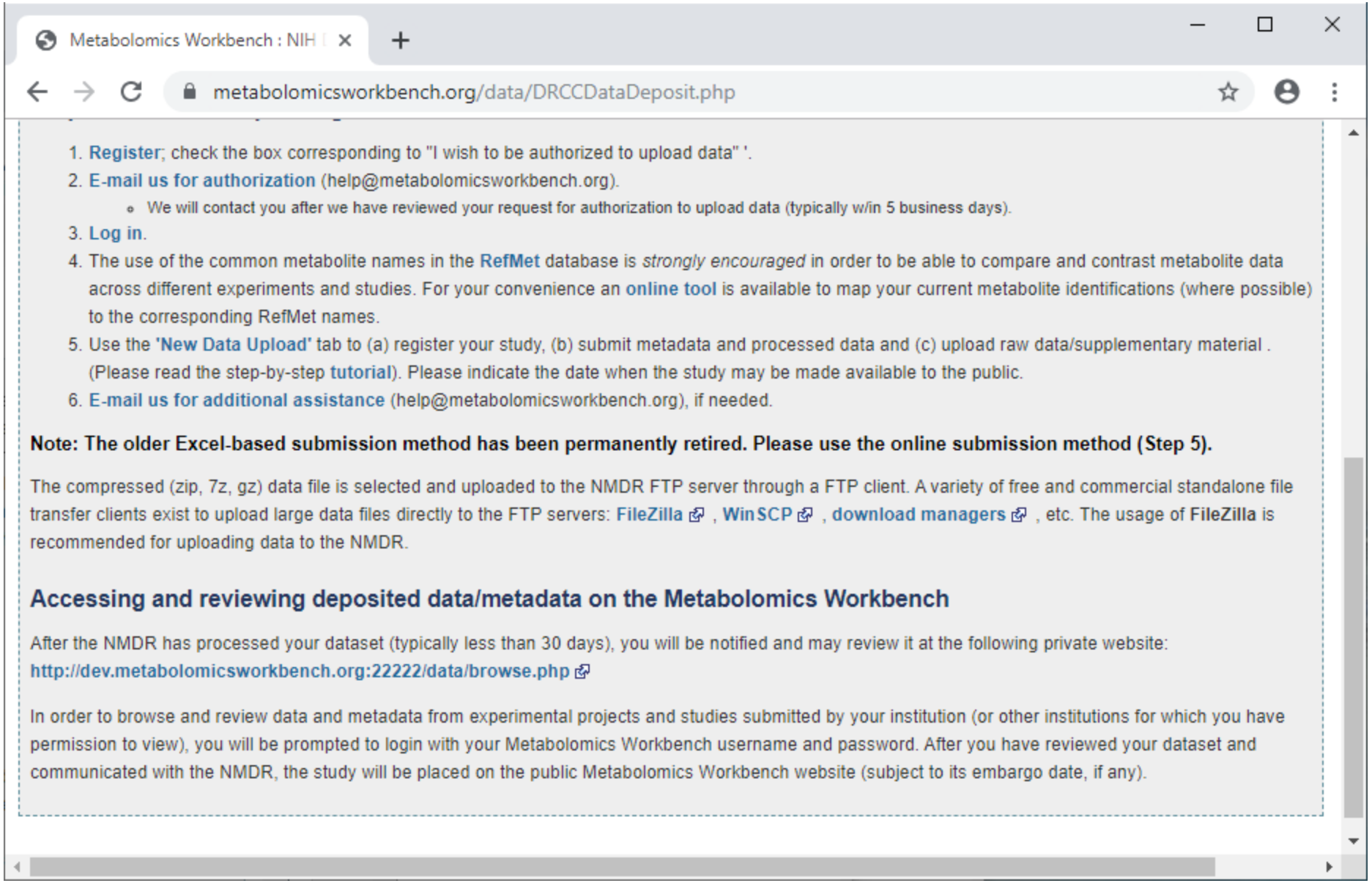
Overview

- Metabolomics workbench
- **Data Repository**
  - Browse/Search Studies
  - Analyze Studies
  - **Upload/Manage Studies**
- Databases
- Protocols
- Standards

Upload and manage data



Upload and manage data



1. Register; check the box corresponding to "I wish to be authorized to upload data" '.
2. E-mail us for authorization (help@metabolomicsworkbench.org).
    - We will contact you after we have reviewed your request for authorization to upload data (typically w/in 5 business days).
3. Log in.
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 read the step-by-step tutorial). 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.

Note: The older Excel-based submission method has been permanently retired. Please use the online submission method (Step 5).

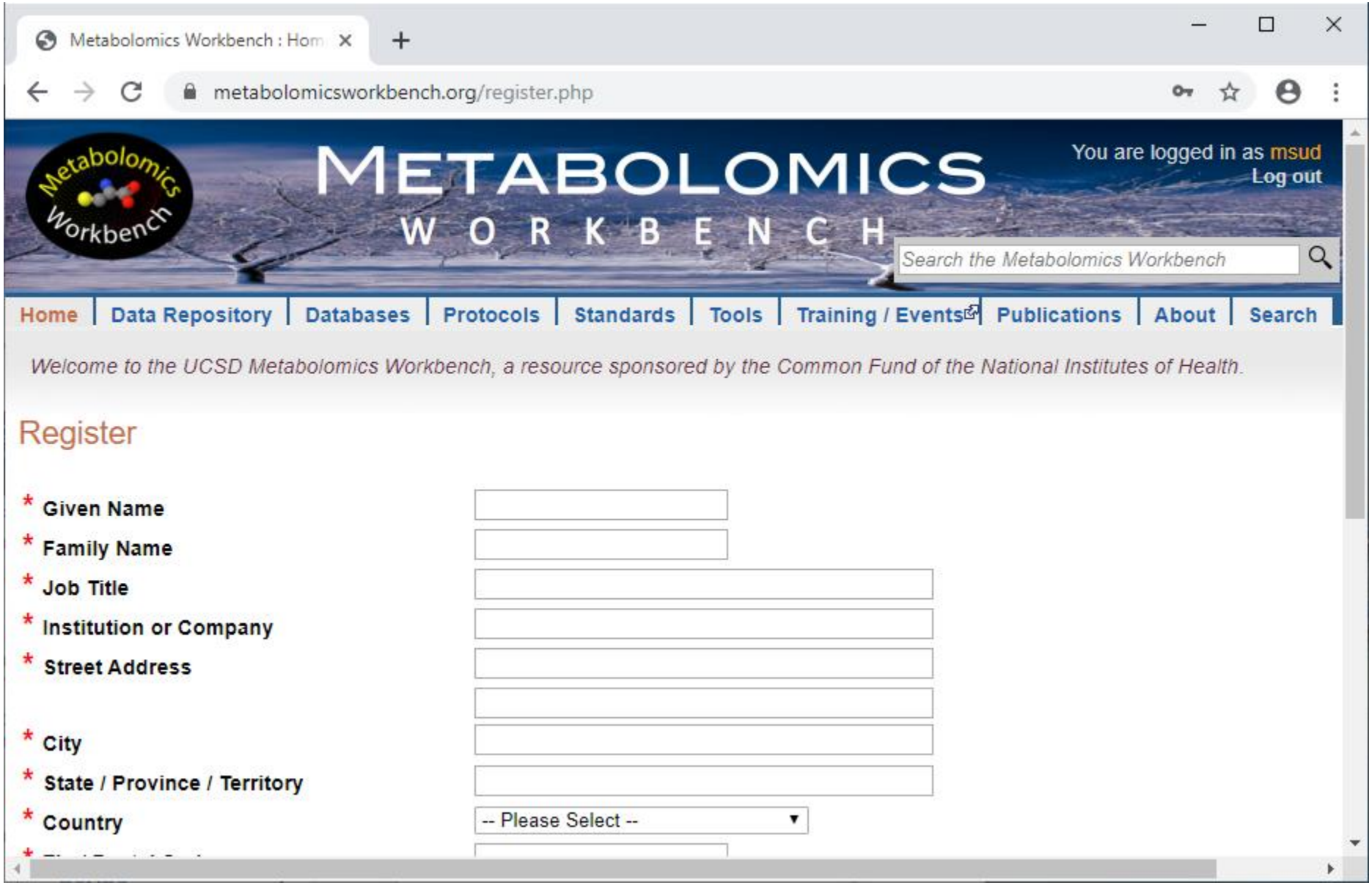
The compressed (zip, 7z, gz) data file is selected and uploaded to the NMDR FTP server through a FTP client. A variety of free and commercial standalone file transfer clients exist to upload large data files directly to the FTP servers: FileZilla , WinSCP , download managers , etc. The usage of **FileZilla** is recommended for uploading data to the NMDR.

Accessing and reviewing deposited data/metadata on the Metabolomics Workbench

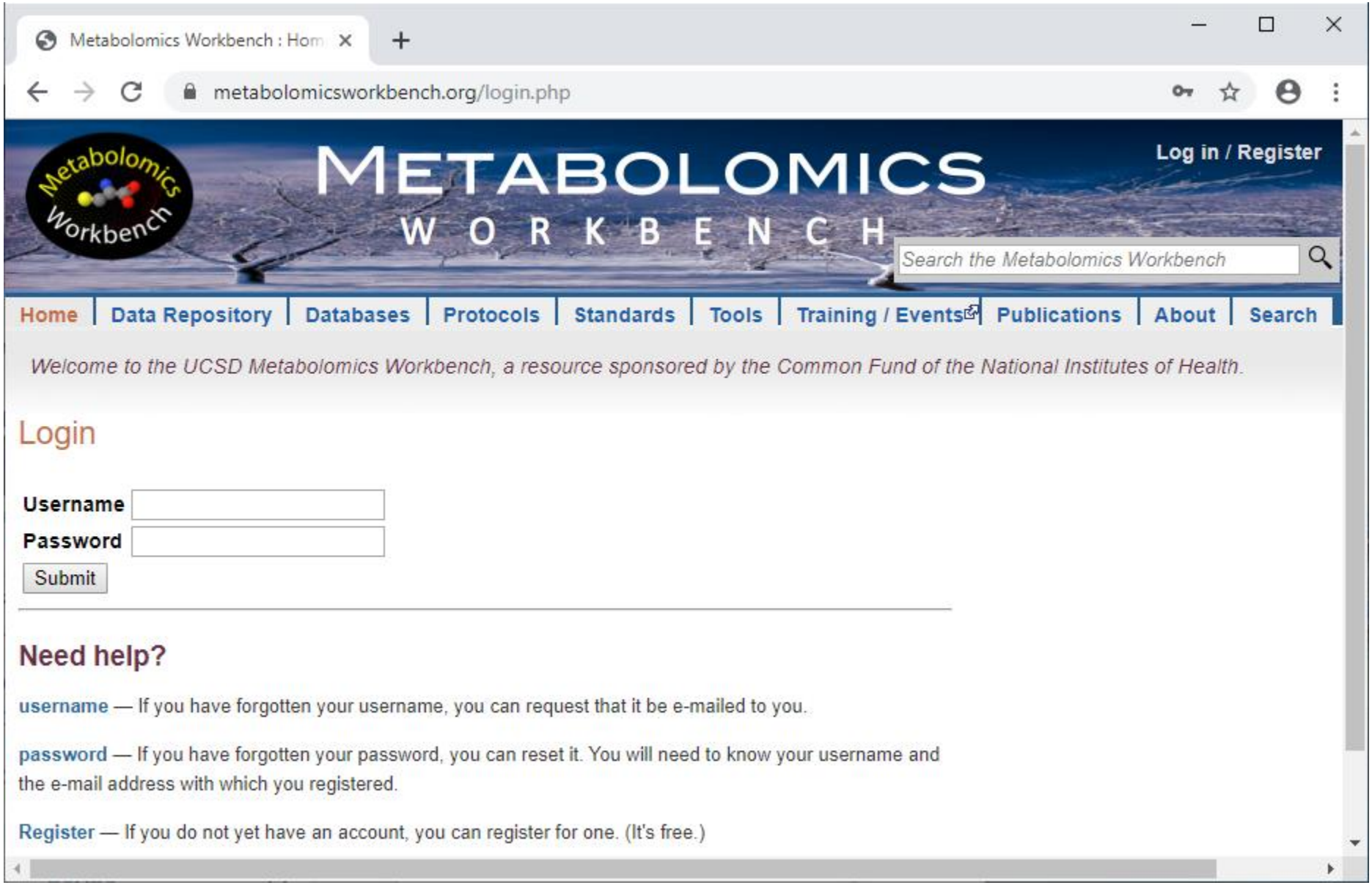
After the NMDR has processed your dataset (typically less than 30 days), you will be notified and may review it at the following private website: http://dev.metabolomicsworkbench.org:22222/data/browse.php

In order to browse and review data and metadata from experimental projects and studies submitted by your institution (or other institutions for which you have permission to view), you will be prompted to login with your Metabolomics Workbench username and password. After you have reviewed your dataset and communicated with the NMDR, the study will be placed on the public Metabolomics Workbench website (subject to its embargo date, if any).

Register to upload data (First time user)



Login to upload data



Upload and manage data (After login)

Upload and Manage Experimental Data and Metadata

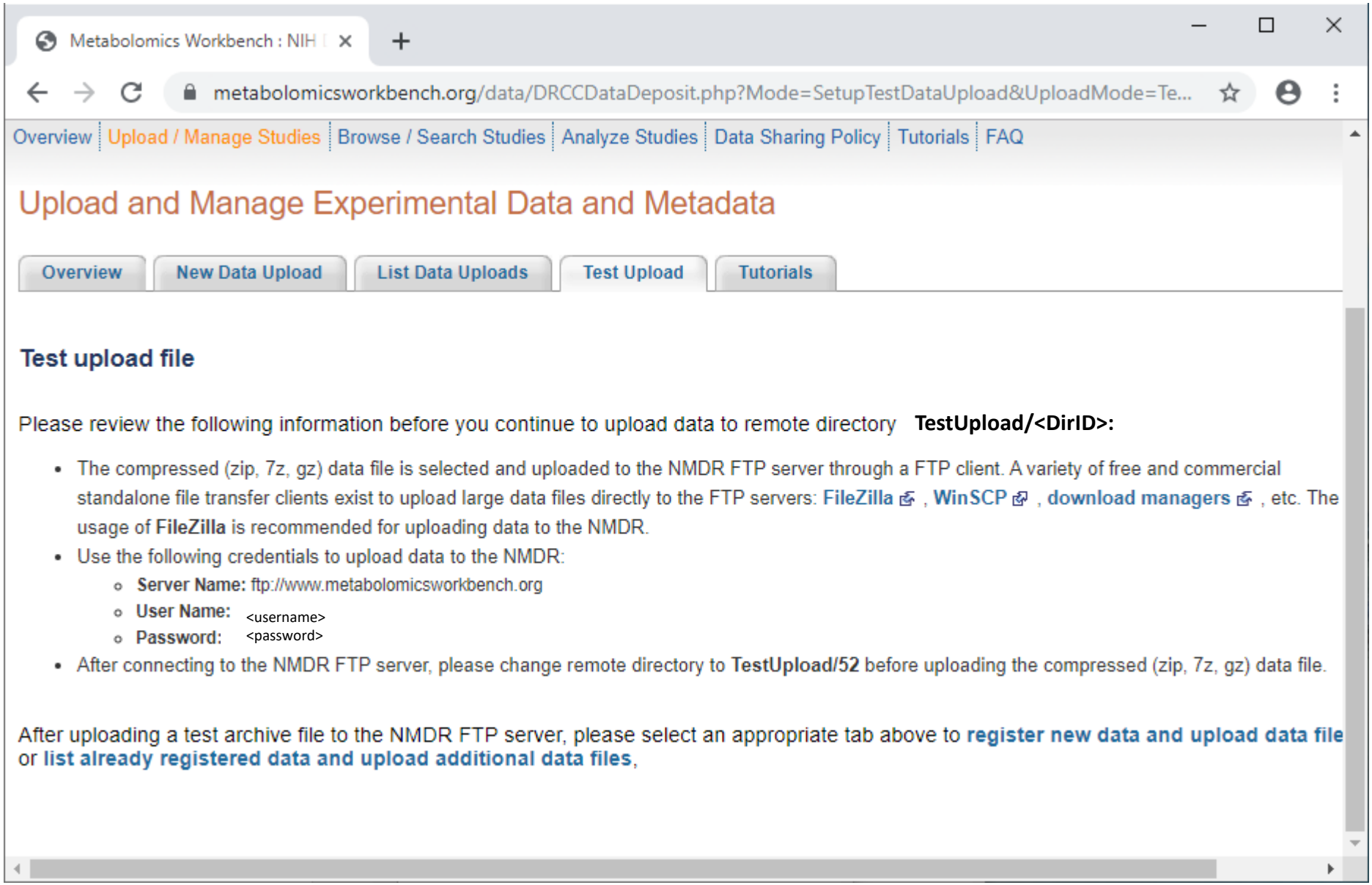
Overview | New Data Upload | List Data Uploads | Test Upload | Tutorials

The National Metabolomics Data Repository (NMDR) is now accepting metabolomics data for small and large studies on cells, tissues and organisms via the Metabolomics Workbench. We can accommodate a variety of metabolite analyses, including, but not limited to MS and NMR. In order to ensure reproducibility and interoperable use of data, we require experimental metadata (see **tutorials**) to be deposited along with the metabolite measurements. Processed data (measurements) maybe in the form of quantitated metabolite concentrations, MS peak height/area values, LC retention times, NMR binned areas, etc. Raw data in the form of MS and NMR binary files and associated parameter files may also be uploaded. We accept data from both targeted and untargeted studies. The Metabolomics Workbench also provides a suite of tools for analysis and visualization of the **data**. Step-by-step instructions for the whole process are provided below.

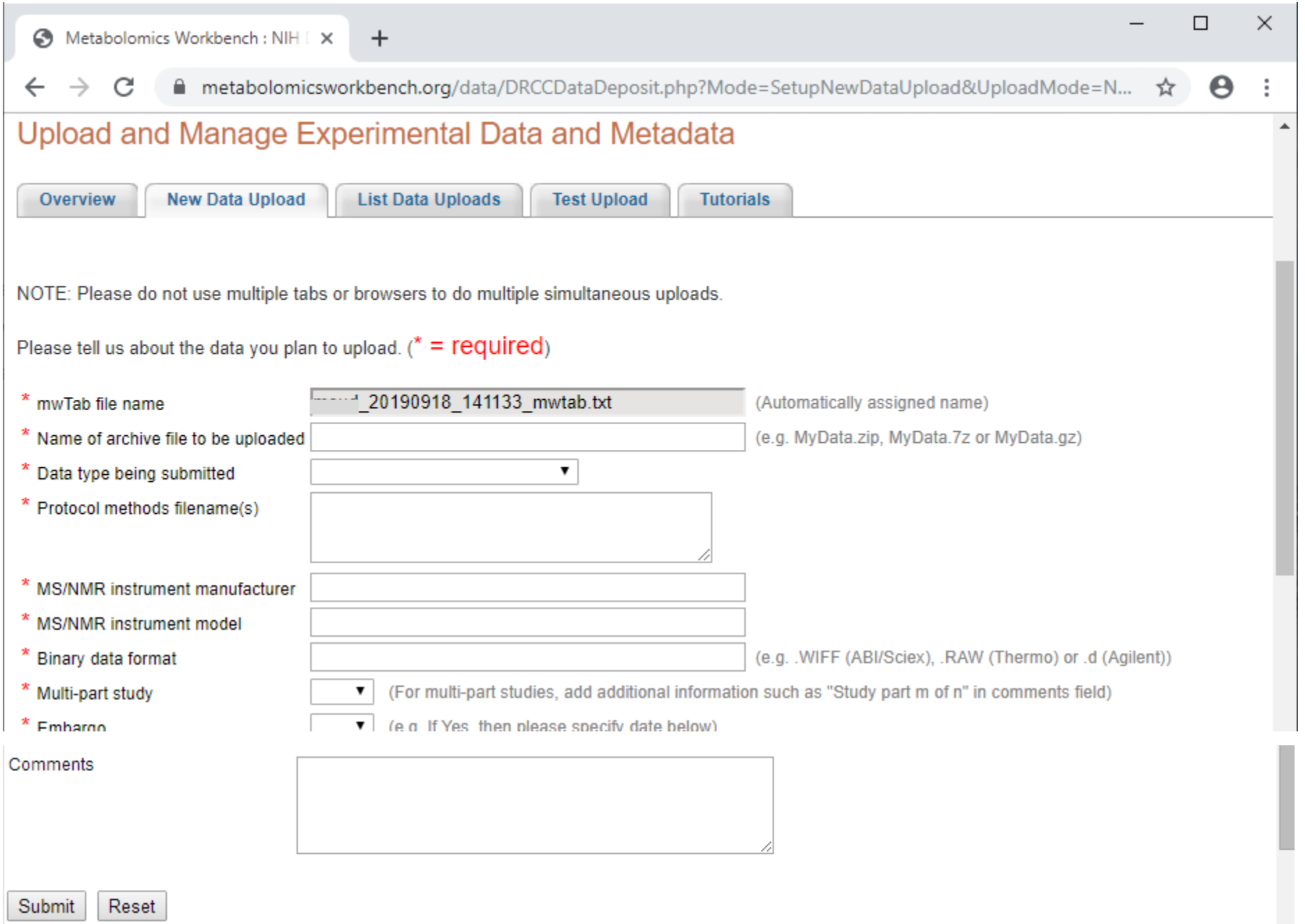
Requirements for depositing data via the Metabolomics Workbench:

1. **Register**; check the box corresponding to "I wish to be authorized to upload data" '.
2. **E-mail us for authorization** (help@metabolomicsworkbench.org).
    - We will contact you after we have reviewed your request for authorization to upload data (typically w/in 5 business days).
3. **Log in**.
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 read the step-by-step **tutorial**). 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.

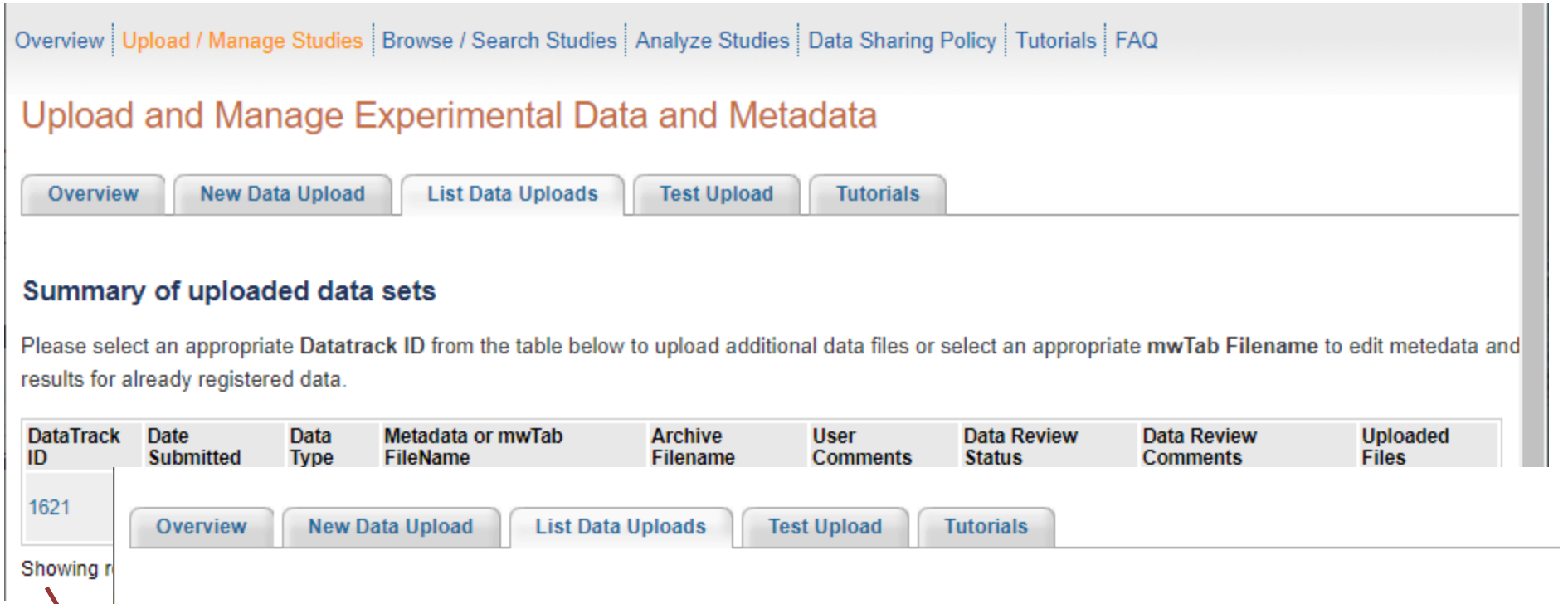
Test upload data (Recommended for first time users)



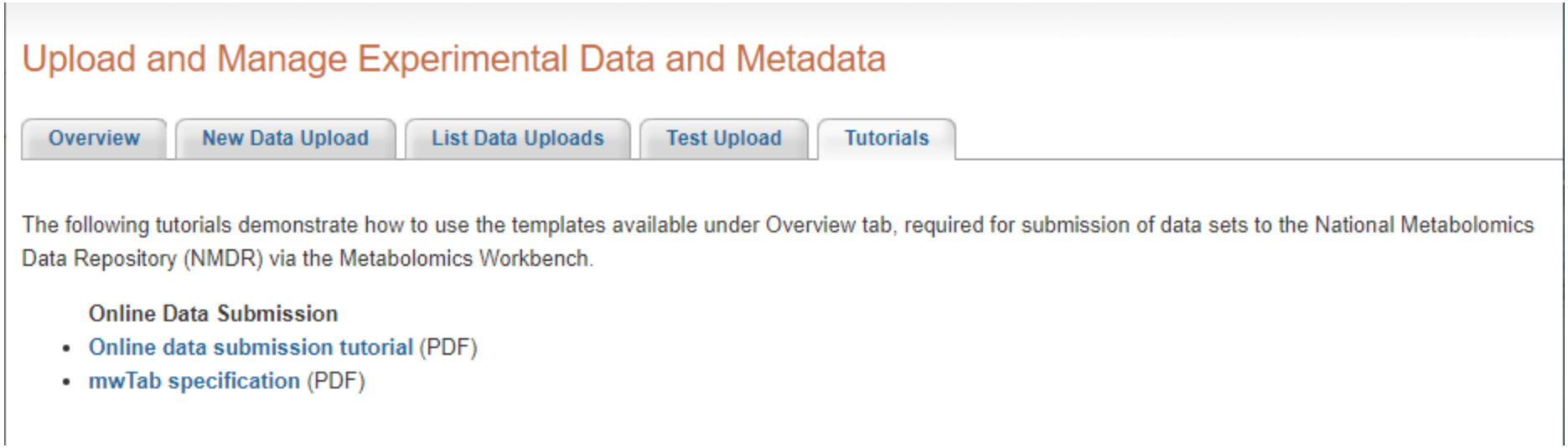
New data upload: Register data



Uploading additional data files for already registered data



Data upload tutorials



Overview

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- Protocols
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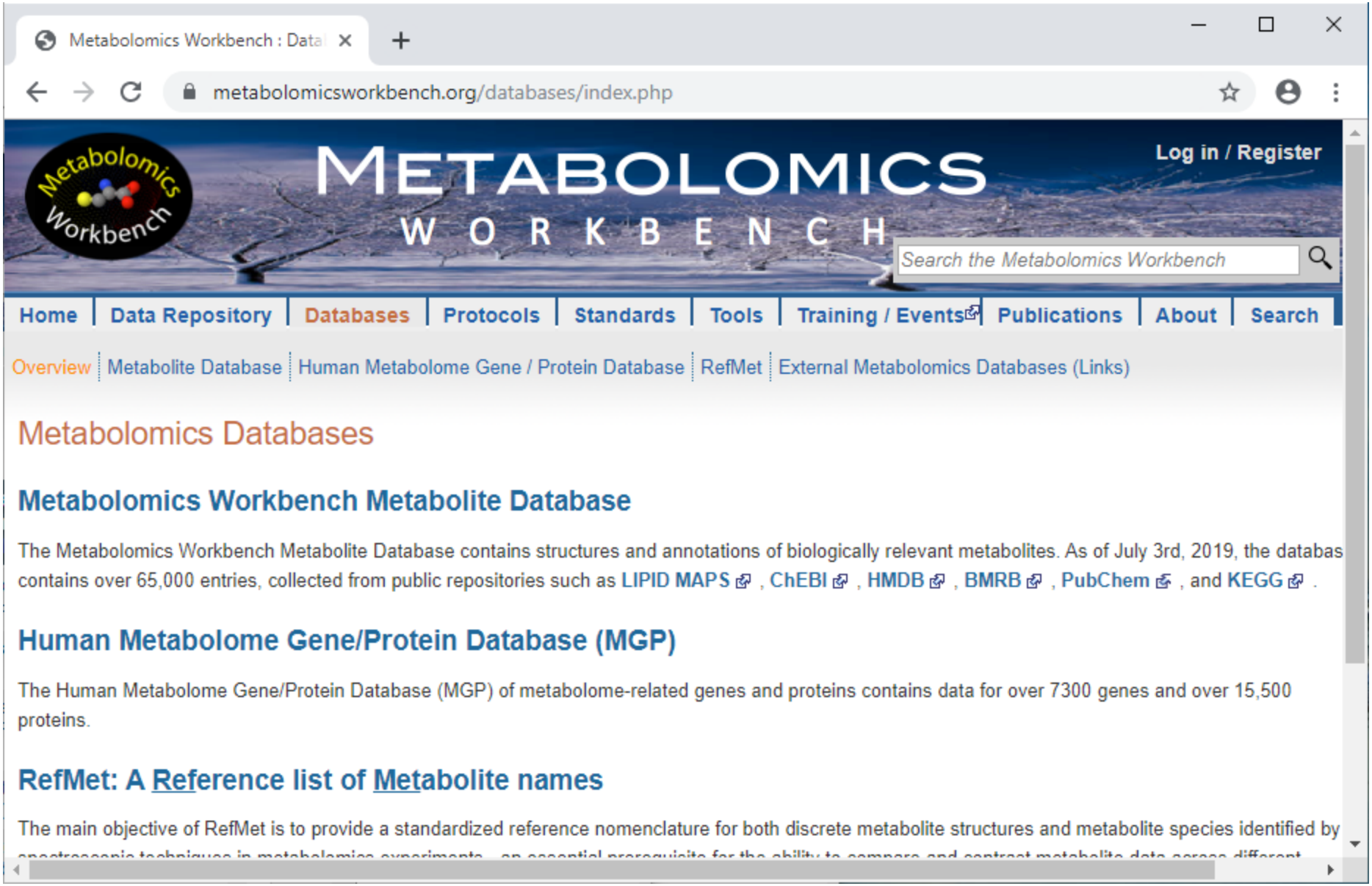
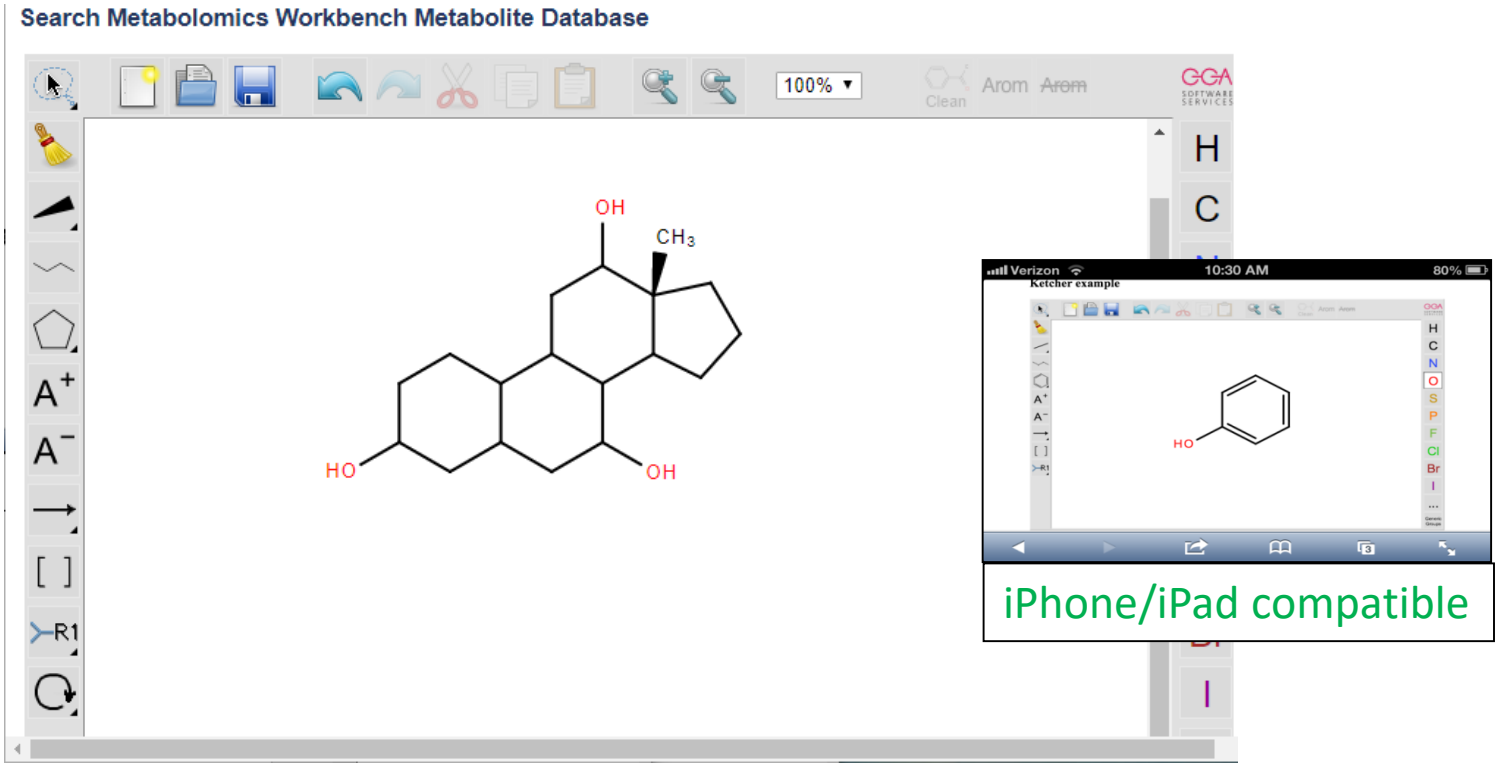
Databases


Metabolomics Workbench : Data
metabolomicsworkbench.org/databases/index.php
METABOLOMICS
WORKBENCH
Log in / Register
Search the Metabolomics Workbench
Home
Data Repository
Databases
Protocols
Standards
Tools
Training / Events
Publications
About
Search
Overview
Metabolite Database
Human Metabolome Gene / Protein Database
RefMet
External Metabolomics Databases (Links)
Metabolomics Databases
Metabolomics Workbench Metabolite Database
The Metabolomics Workbench Metabolite Database contains structures and annotations of biologically relevant metabolites. As of July 3rd, 2019, the databas
contains over 65,000 entries, collected from public repositories such as LIPID MAPS , ChEBI , HMDB , BMRB , PubChem , and KEGG .
Human Metabolome Gene/Protein Database (MGP)
The Human Metabolome Gene/Protein Database (MGP) of metabolome-related genes and proteins contains data for over 7300 genes and over 15,500
proteins.
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

Search the metabolite database

Search the metabolite database of molecular structures



PUBCHEM_CID:

Name (Common, Systematic)

Sort by PUBCHEM_CID

Records per page: 20

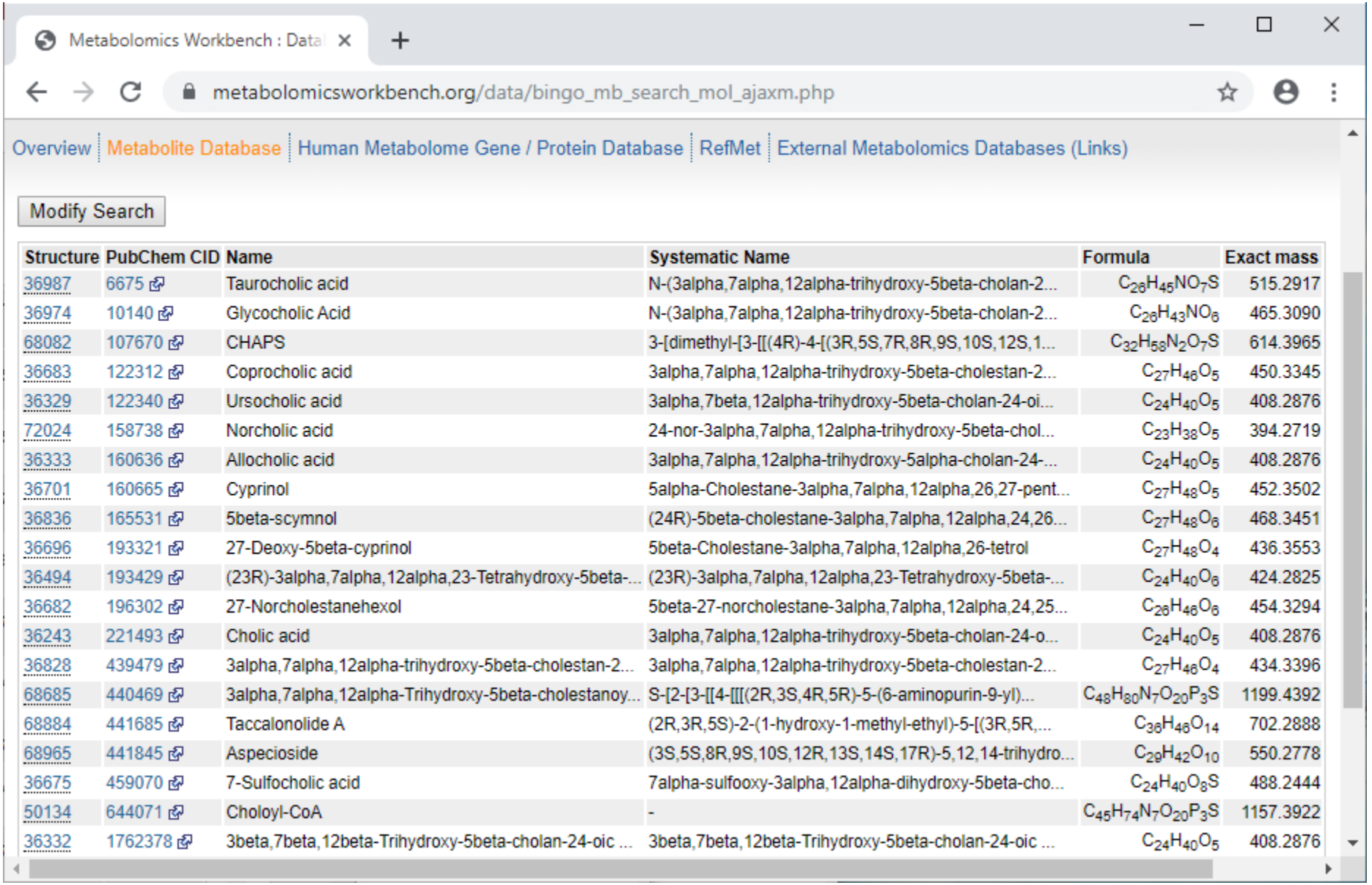
Submit

Search type: Substructure

Lower limit for Tanimoto: 0.95

Flags for Exact match: All(default)

Metabolite database: Substructure search results

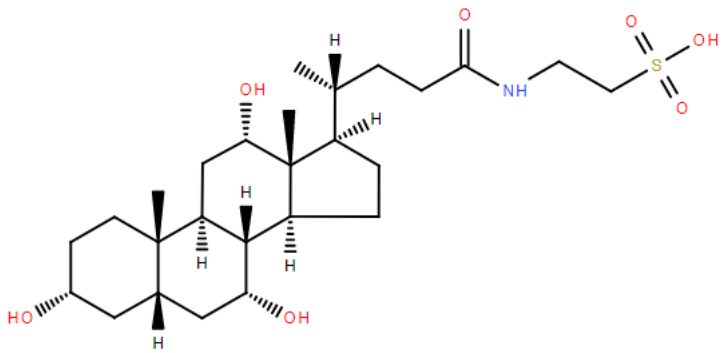


Structure	PubChem CID	Name	Systematic Name	Formula	Exact mass
36987	6675	Taurocholic acid	N-(3alpha,7alpha,12alpha-trihydroxy-5beta-cholan-2...	$C_{26}H_{45}NO_7S$	515.2917
36974	10140	Glycocholic Acid	N-(3alpha,7alpha,12alpha-trihydroxy-5beta-cholan-2...	$C_{26}H_{43}NO_6$	465.3090
68082	107670	CHAPS	3-[dimethyl-[3-[[(4R)-4-[(3R,5S,7R,8R,9S,10S,12S,1...	$C_{32}H_{58}N_2O_7S$	614.3965
36683	122312	Coprocholic acid	3alpha,7alpha,12alpha-trihydroxy-5beta-cholestan-2...	$C_{27}H_{46}O_5$	450.3345
36329	122340	Ursocholic acid	3alpha,7beta,12alpha-trihydroxy-5beta-cholan-24-oi...	$C_{24}H_{40}O_5$	408.2876
72024	158738	Norcholic acid	24-nor-3alpha,7alpha,12alpha-trihydroxy-5beta-chol...	$C_{23}H_{38}O_5$	394.2719
36333	160636	Allocholic acid	3alpha,7alpha,12alpha-trihydroxy-5alpha-cholan-24-...	$C_{24}H_{40}O_5$	408.2876
36701	160665	Cyprinol	5alpha-Cholestane-3alpha,7alpha,12alpha,26,27-pent...	$C_{27}H_{48}O_5$	452.3502
36836	165531	5beta-scymnol	(24R)-5beta-cholestane-3alpha,7alpha,12alpha,24,26...	$C_{27}H_{48}O_6$	468.3451
36696	193321	27-Deoxy-5beta-cyprinol	5beta-Cholestane-3alpha,7alpha,12alpha,26-tetrol	$C_{27}H_{48}O_4$	436.3553
36494	193429	(23R)-3alpha,7alpha,12alpha,23-Tetrahydroxy-5beta-...	(23R)-3alpha,7alpha,12alpha,23-Tetrahydroxy-5beta-...	$C_{24}H_{40}O_6$	424.2825
36682	196302	27-Norcholestanehexol	5beta-27-norcholestane-3alpha,7alpha,12alpha,24,25...	$C_{26}H_{46}O_6$	454.3294
36243	221493	Cholic acid	3alpha,7alpha,12alpha-trihydroxy-5beta-cholan-24-o...	$C_{24}H_{40}O_5$	408.2876
36828	439479	3alpha,7alpha,12alpha-trihydroxy-5beta-cholestan-2...	3alpha,7alpha,12alpha-trihydroxy-5beta-cholestan-2...	$C_{27}H_{46}O_4$	434.3396
68685	440469	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoy...	S-[2-[3-[[4-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)...	$C_{48}H_{80}N_7O_{20}P_3S$	1199.4392
68884	441685	Taccalonolide A	(2R,3R,5S)-2-(1-hydroxy-1-methyl-ethyl)-5-[(3R,5R,...	$C_{36}H_{46}O_{14}$	702.2888
68965	441845	Aspecioside	(3S,5S,8R,9S,10S,12R,13S,14S,17R)-5,12,14-trihydro...	$C_{29}H_{42}O_{10}$	550.2778
36675	459070	7-Sulfocholic acid	7alpha-sulfooxy-3alpha,12alpha-dihydroxy-5beta-cho...	$C_{24}H_{40}O_8S$	488.2444
50134	644071	Choloyl-CoA	-	$C_{45}H_{74}N_7O_{20}P_3S$	1157.3922
36332	1762378	3beta,7beta,12beta-Trihydroxy-5beta-cholan-24-oic ...	3beta,7beta,12beta-Trihydroxy-5beta-cholan-24-oic ...	$C_{24}H_{40}O_5$	408.2876

Metabolite database: Detail view

Metabolomics Structure Database

Download file | MDLMOL ▾



MW REGNO:	36987
PubChem CID:	6675
Common Name:	Taurocholic acid
Systematic Name:	N-(3alpha,7alpha,12alpha-trihydroxy-5beta-cholan-24-oyl)-taurine
Synonyms:	Taurocholic Acid [PubChem Synonyms]
Exact Mass:	515.2917 (neutral) Calculate m/z: (Select m/z) ▾
Formula:	$C_{26}H_{45}NO_7S$
InChIKey:	WBWWGRHZICKQGZ-HZAMXZRMSA-N
LIPID MAPS Category:	Sterol Lipids
LIPID MAPS mainclass:	Steroid conjugates
LIPID MAPS subclass:	Taurine conjugates
MoNA MS spectra:	View spectra
Studies:	Available studies

Select appropriate tab below to view additional details:

All | Database Links | Calculated Properties | Human Pathways

External database links:

LIPID MAPS ID:	LMST05040001
CHEBI ID:	28865
HMDB ID:	HMDB0000036
KEGG ID:	C05122
Chemspider ID:	-
METLIN ID:	-

Select appropriate tab below to view additional details:

All | Database Links | Calculated Properties | Human Pathways

Calculated physicochemical properties (?):

Heavy Atoms:	35
Rings:	4
Aromatic Rings:	0
Rotatable Bonds:	7
van der Waals Molecular volume:	497.32 $Å^3$ $molecule^{-1}$
Toplogical Polar Sufrace Area:	144.16 $Å^2$ $molecule^{-1}$
Hydrogen Bond Donors:	5
Hydrogen Bond Acceptors:	7
logP:	5.05
Molar Refractivity:	134.25
Fraction sp3 Carbons:	0.96
sp3 Carbons:	25

Select appropriate tab below to view additional details:

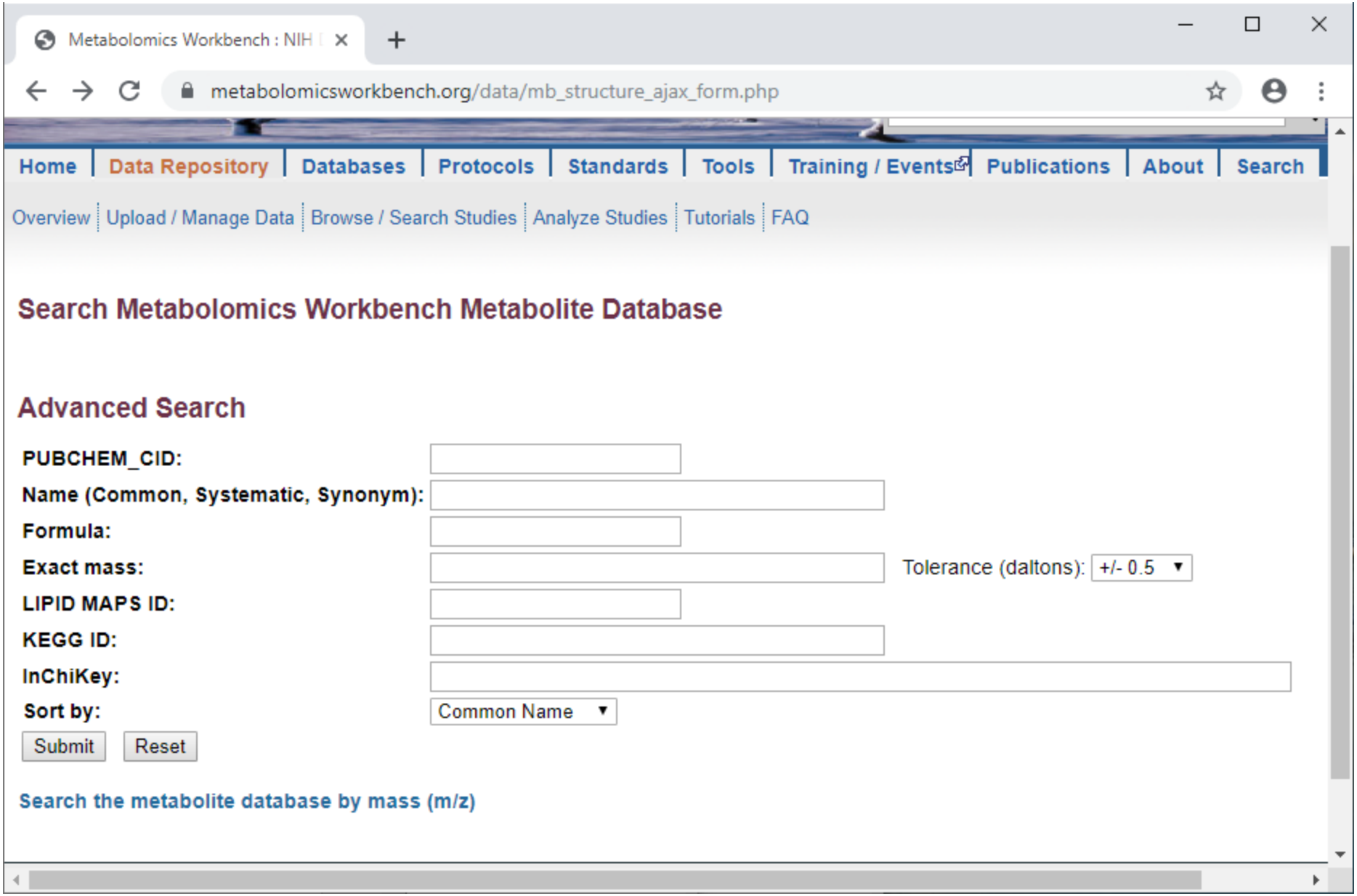
All | Database Links | Calculated Properties | Human Pathways

Human Pathway links:

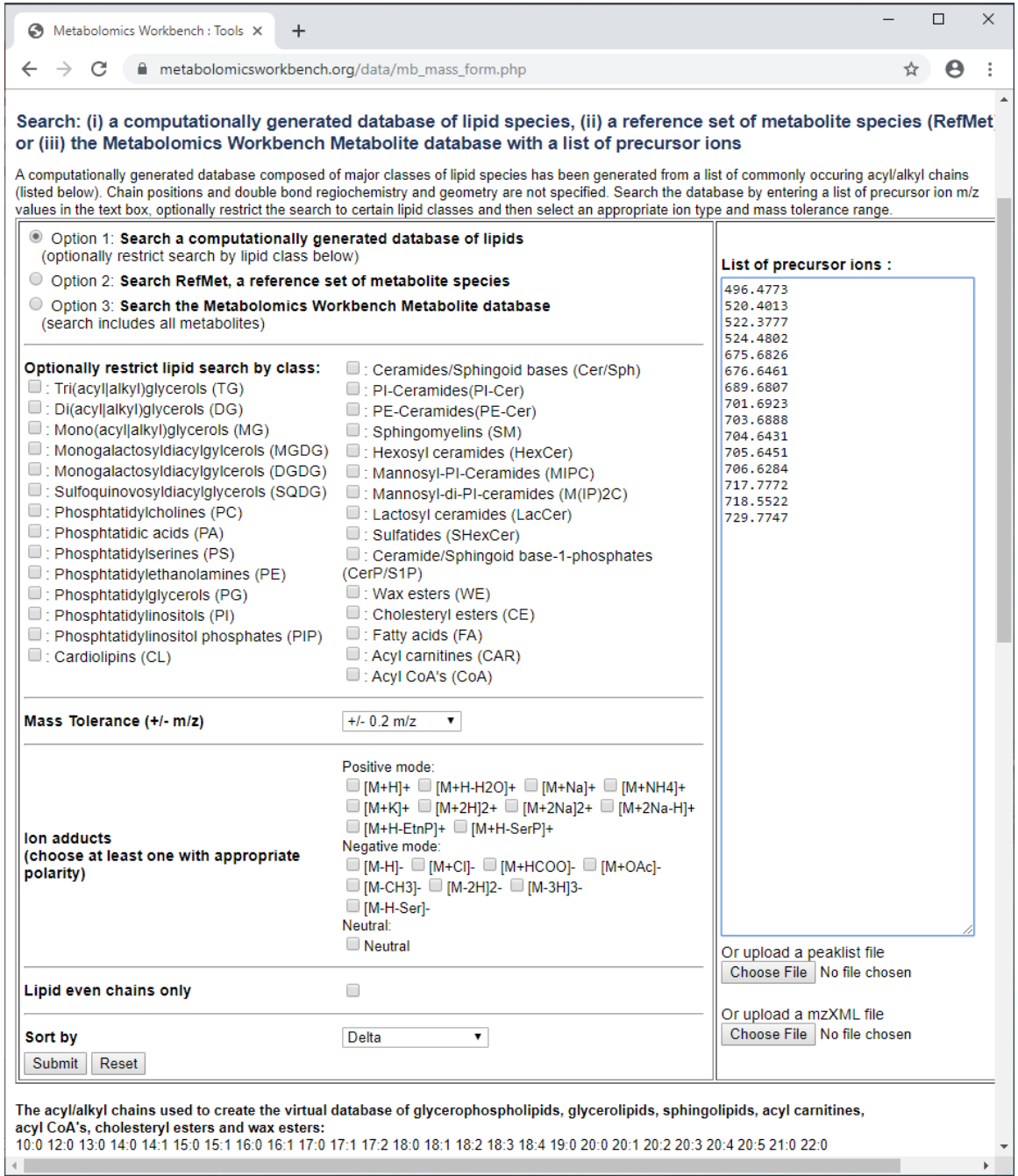
HMDB and KEGG pathways containing this metabolite

REACTOME pathways containing this metabolite

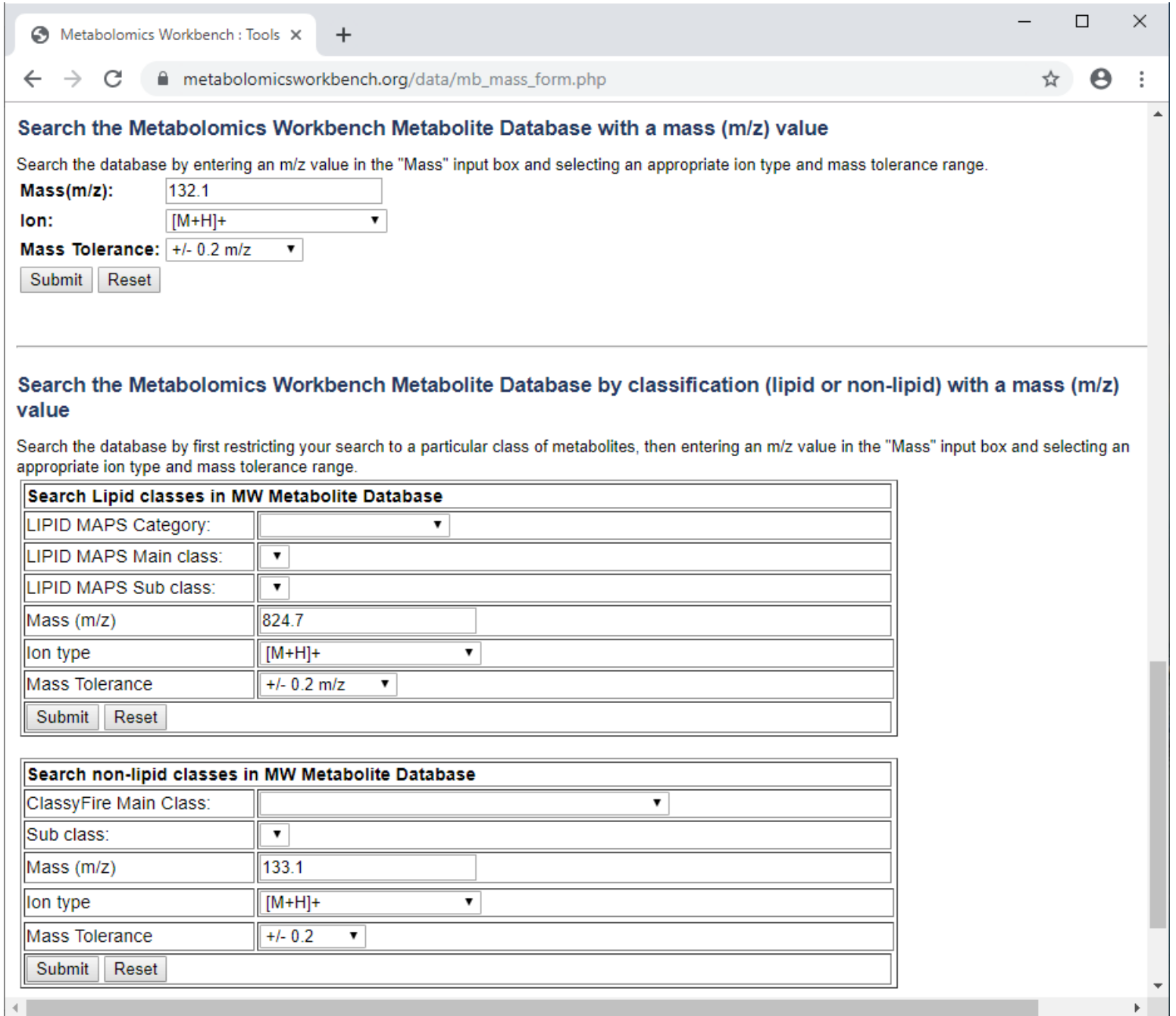
Search the metabolite database



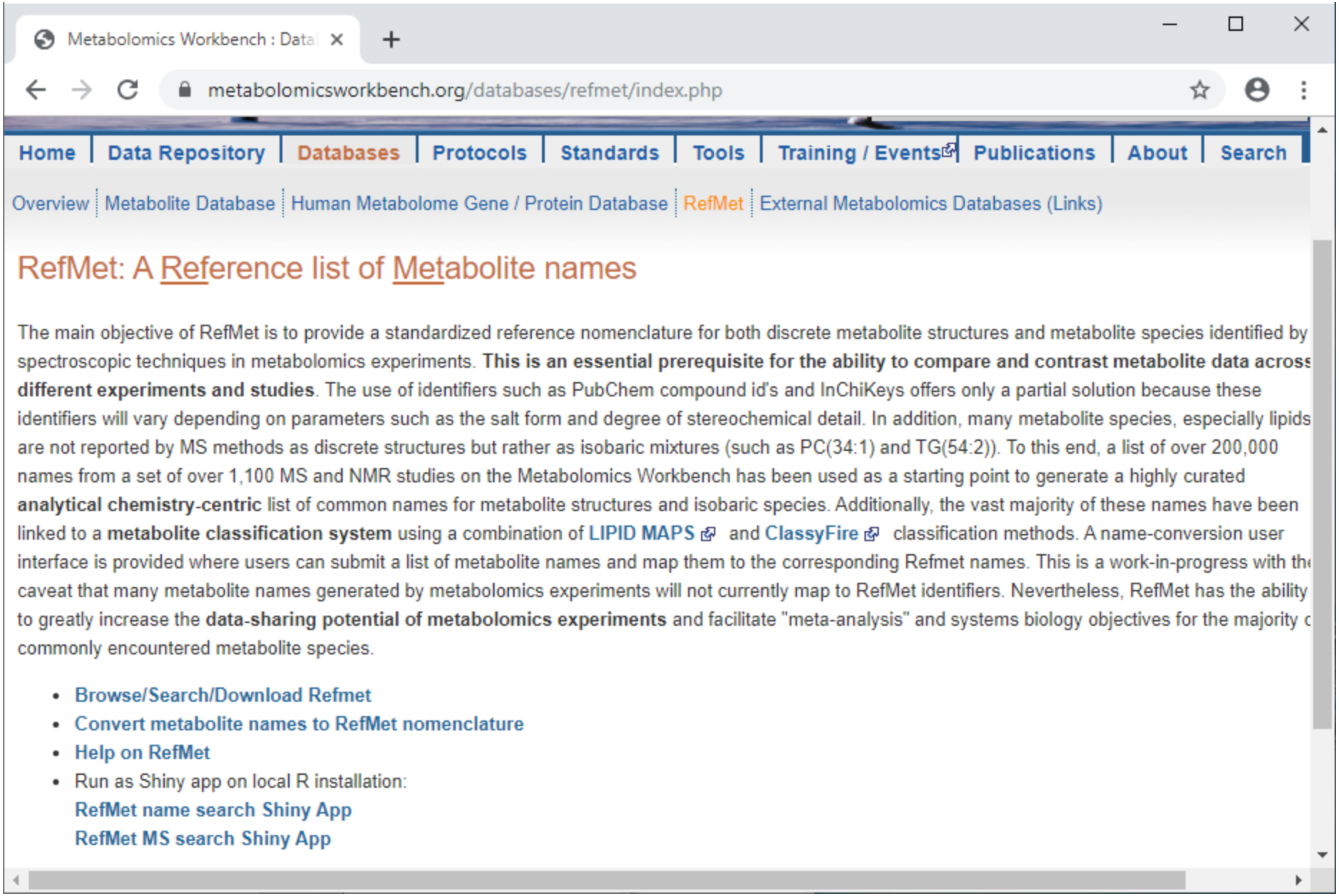
Search databases by mass



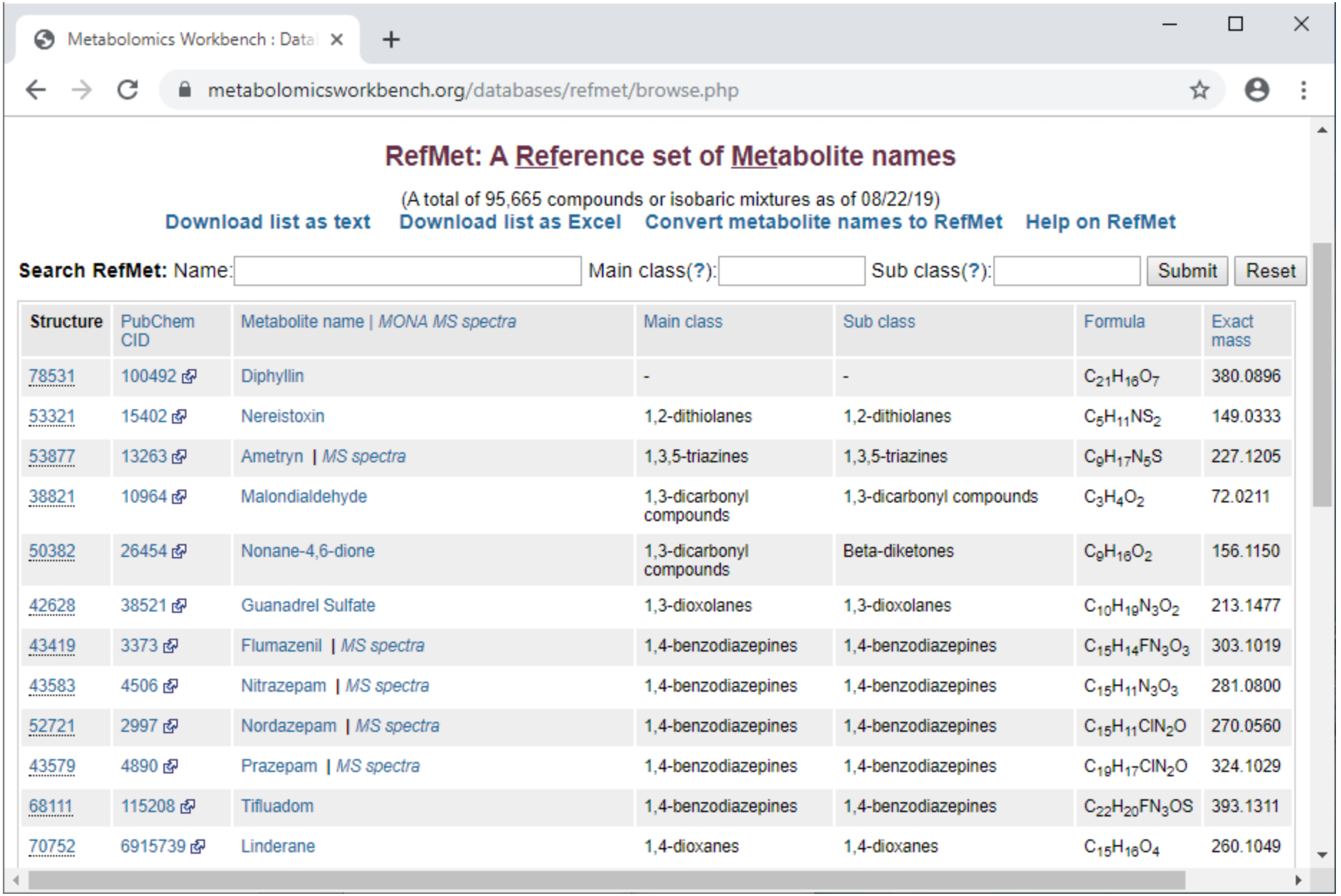
Search databases by mass



RefMet database



Search the RefMet database



RefMet: A Reference set of Metabolite names

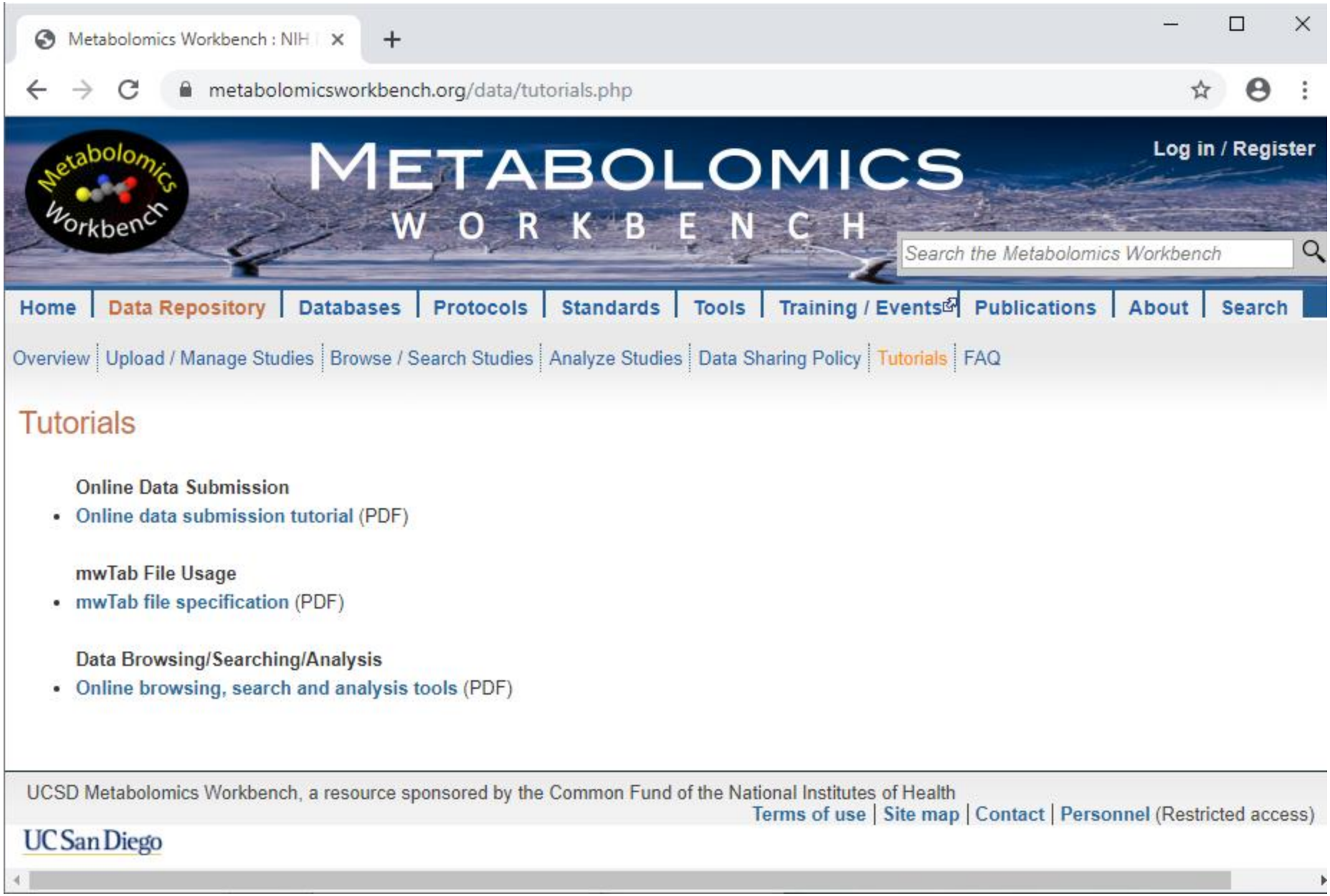
(A total of 95,665 compounds or isobaric mixtures as of 08/22/19)

Download list as text Download list as Excel Convert metabolite names to RefMet Help on RefMet

Search RefMet: Name: Main class(?): Sub class(?): Submit Reset

Structure	PubChem CID	Metabolite name | *MONA MS spectra*	Main class	Sub class	Formula	Exact mass
78531	100492	Diphyllin	-	-	$C_{21}H_{16}O_7$	380.0896
53321	15402	Nereistoxin	1,2-dithiolanes	1,2-dithiolanes	$C_5H_{11}NS_2$	149.0333
53877	13263	Ametryn | *MS spectra*	1,3,5-triazines	1,3,5-triazines	$C_9H_{17}N_5S$	227.1205
38821	10964	Malondialdehyde	1,3-dicarbonyl compounds	1,3-dicarbonyl compounds	$C_3H_4O_2$	72.0211
50382	26454	Nonane-4,6-dione	1,3-dicarbonyl compounds	Beta-diketones	$C_9H_{16}O_2$	156.1150
42628	38521	Guanadrel Sulfate	1,3-dioxolanes	1,3-dioxolanes	$C_{10}H_{19}N_3O_2$	213.1477
43419	3373	Flumazenil | *MS spectra*	1,4-benzodiazepines	1,4-benzodiazepines	$C_{15}H_{14}FN_3O_3$	303.1019
43583	4506	Nitrazepam | *MS spectra*	1,4-benzodiazepines	1,4-benzodiazepines	$C_{15}H_{11}N_3O_3$	281.0800
52721	2997	Nordazepam | *MS spectra*	1,4-benzodiazepines	1,4-benzodiazepines	$C_{15}H_{11}ClN_2O$	270.0560
43579	4890	Prazepam | *MS spectra*	1,4-benzodiazepines	1,4-benzodiazepines	$C_{19}H_{17}ClN_2O$	324.1029
68111	115208	Tifluadom	1,4-benzodiazepines	1,4-benzodiazepines	$C_{22}H_{20}FN_3OS$	393.1311
70752	6915739	Linderane	1,4-dioxanes	1,4-dioxanes	$C_{15}H_{16}O_4$	260.1049

Tutorials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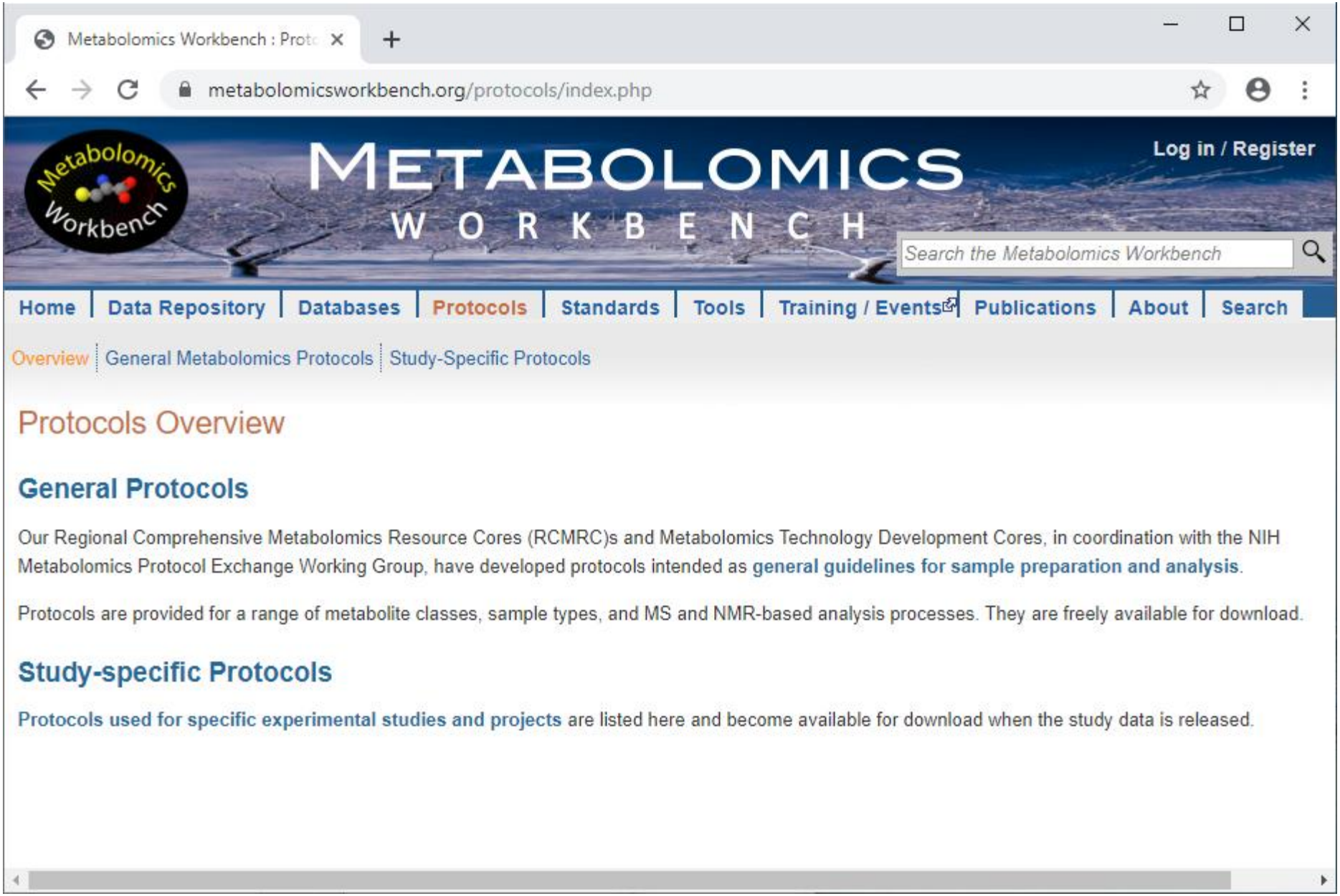
Overview

- Metabolomics workbench
- **Data Repository**
  - Browse/Search Studies
  - Analyze Studies
  - Upload/Manage Studies
- Databases
- **Protocols**
- Standards

Protocols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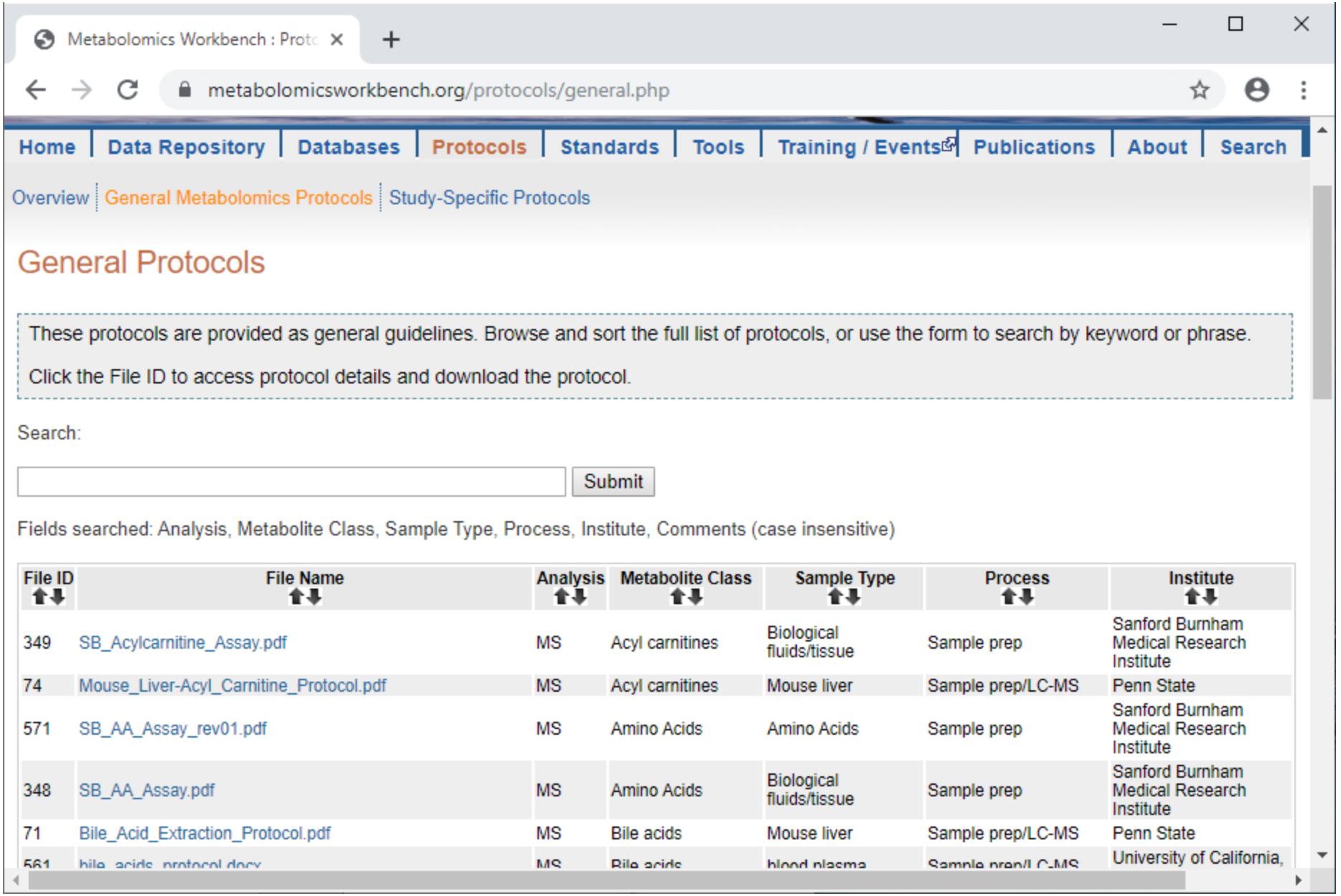
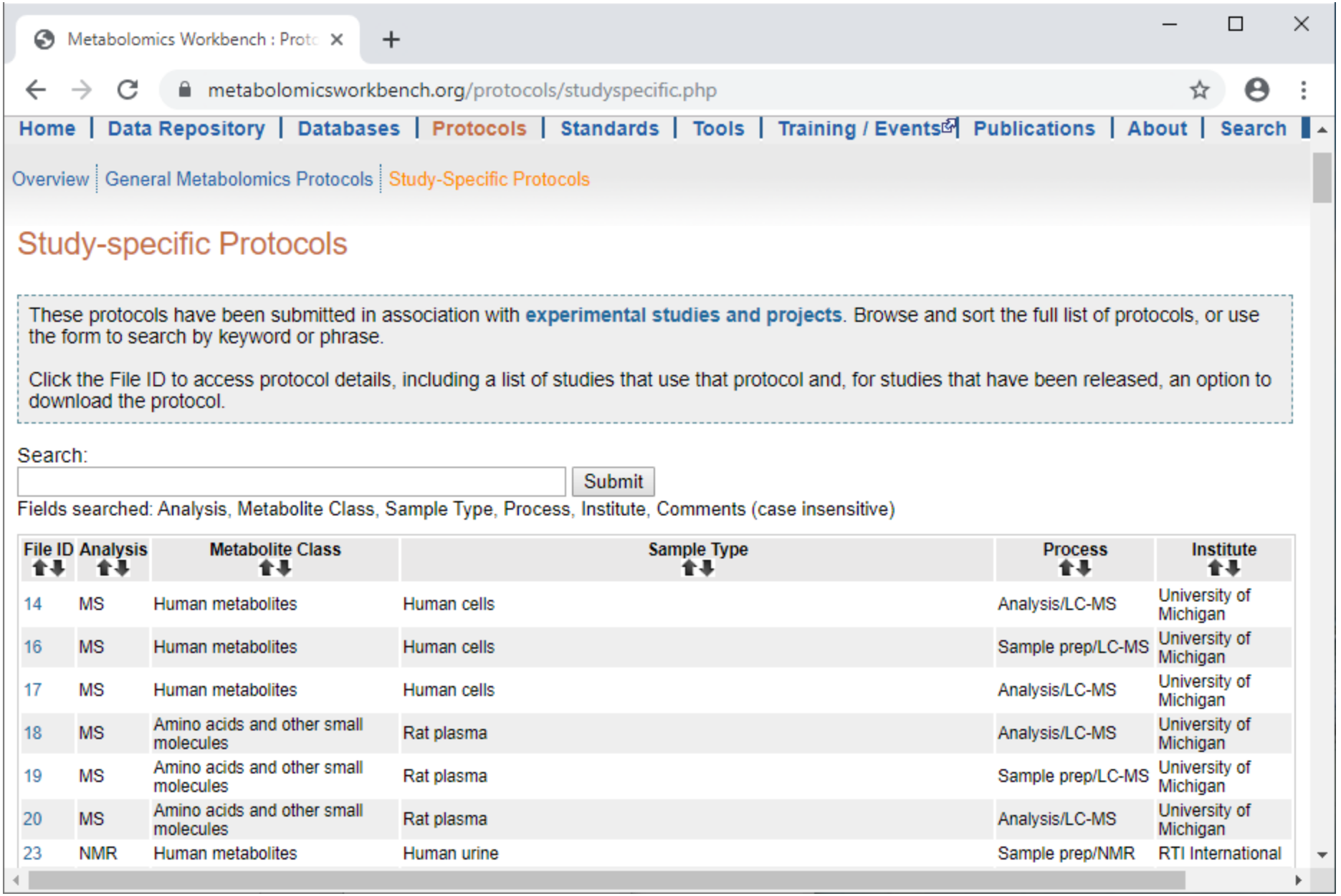
Study-Specific Protocols
Protocols Overview
General Protocols
Our Regional Comprehensive Metabolomics Resource Cores (RCMRC)s and Metabolomics Technology Development Cores, in coordination with the NIH Metabolomics Protocol Exchange Working Group, have developed protocols intended as general guidelines for sample preparation and analysis.
Protocols are provided for a range of metabolite classes, sample types, and MS and NMR-based analysis processes. They are freely available for download.
Study-specific Protocols
Protocols used for specific experimental studies and projects are listed here and become available for download when the study data is released.

Protocols



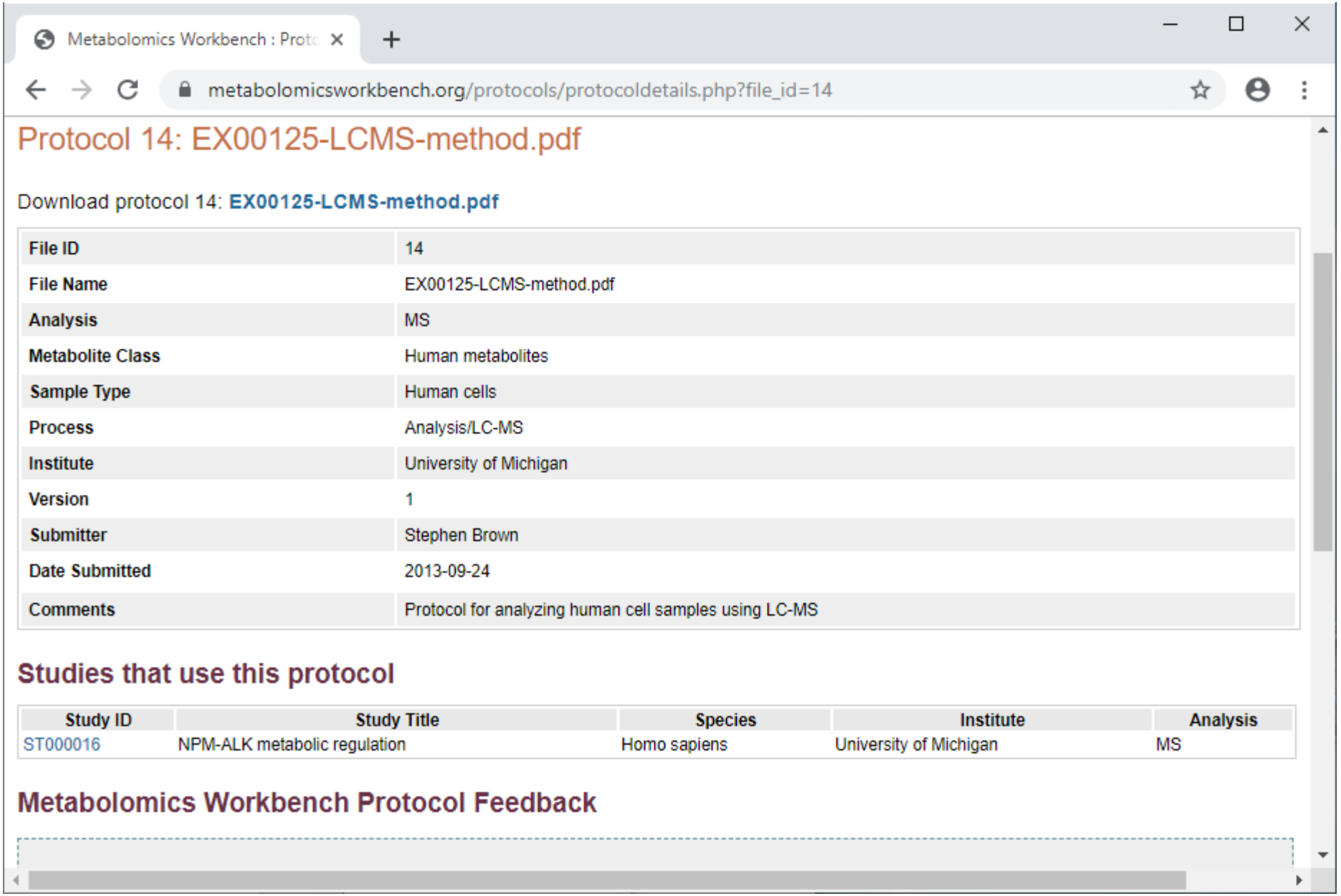
File ID	File Name	Analysis	Metabolite Class	Sample Type	Process	Institute
349	SB_Acylcarnitine_Assay.pdf	MS	Acyl carnitines	Biological fluids/tissue	Sample prep	Sanford Burnham Medical Research Institute
74	Mouse_Liver-Acyl_Carnitine_Protocol.pdf	MS	Acyl carnitines	Mouse liver	Sample prep/LC-MS	Penn State
571	SB_AA_Assay_rev01.pdf	MS	Amino Acids	Amino Acids	Sample prep	Sanford Burnham Medical Research Institute
348	SB_AA_Assay.pdf	MS	Amino Acids	Biological fluids/tissue	Sample prep	Sanford Burnham Medical Research Institute
71	Bile_Acid_Extraction_Protocol.pdf	MS	Bile acids	Mouse liver	Sample prep/LC-MS	Penn State
561	bile_acids_protocol.docx	MS	Bile acids	blood plasma	Sample prep/LC-MS	University of California,

Protocols



File ID	Analysis	Metabolite Class	Sample Type	Process	Institute
14	MS	Human metabolites	Human cells	Analysis/LC-MS	University of Michigan
16	MS	Human metabolites	Human cells	Sample prep/LC-MS	University of Michigan
17	MS	Human metabolites	Human cells	Analysis/LC-MS	University of Michigan
18	MS	Amino acids and other small molecules	Rat plasma	Analysis/LC-MS	University of Michigan
19	MS	Amino acids and other small molecules	Rat plasma	Sample prep/LC-MS	University of Michigan
20	MS	Amino acids and other small molecules	Rat plasma	Analysis/LC-MS	University of Michigan
23	NMR	Human metabolites	Human urine	Sample prep/NMR	RTI International

Protocol detail view



Protocol 14: EX00125-LCMS-method.pdf

Download protocol 14: **EX00125-LCMS-method.pdf**

File ID	14
File Name	EX00125-LCMS-method.pdf
Analysis	MS
Metabolite Class	Human metabolites
Sample Type	Human cells
Process	Analysis/LC-MS
Institute	University of Michigan
Version	1
Submitter	Stephen Brown
Date Submitted	2013-09-24
Comments	Protocol for analyzing human cell samples using LC-MS

Studies that use this protocol

Study ID	Study Title	Species	Institute	Analysis
ST000016	NPM-ALK metabolic regulation	Homo sapiens	University of Michigan	MS

Metabolomics Workbench Protocol Feedback

Overview

- Metabolomics workbench
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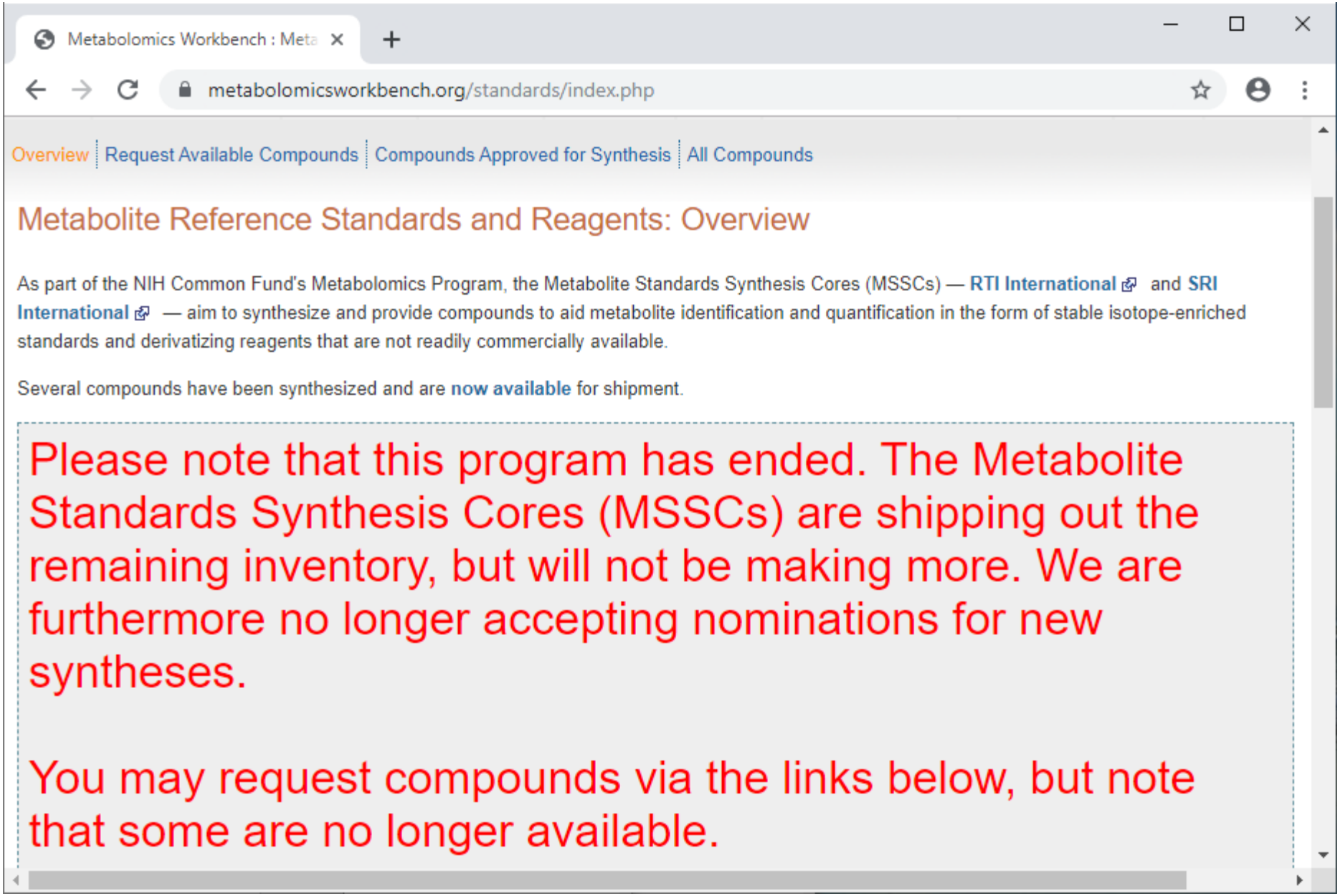
Standards


Metabolomics Workbench : Meta
metabolomicsworkbench.org/standards/index.php
Overview | Request Available Compounds | Compounds Approved for Synthesis | All Compounds
Metabolite Reference Standards and Reagents: Overview
As part of the NIH Common Fund's Metabolomics Program, the Metabolite Standards Synthesis Cores (MSSCs) — RTI International and SRI International — aim to synthesize and provide compounds to aid metabolite identification and quantification in the form of stable isotope-enriched standards and derivatizing reagents that are not readily commercially available.
Several compounds have been synthesized and are now available for shipment.
Please note that this program has ended. The Metabolite Standards Synthesis Cores (MSSCs) are shipping out the remaining inventory, but will not be making more. We are furthermore no longer accepting nominations for new syntheses.
You may request compounds via the links below, but note that some are no longer available.

Standards

Metabolomics Workbench : Meta

metabolomicsworkbench.org/standards/index.php

Request Available Compounds

- Browse **compounds that have been synthesized and are available for shipment**.
- Search by Common name, InChiKey, IUPAC name, Synonyms, PubChem CID, and Status
- Download synthesis reports.
- Request aliquots of **available compounds**.

Browse / Search Compounds

- Browse all **compounds approved for synthesis** plus the **complete list of compounds**, including all nominations.
- Search by Common name, InChiKey, IUPAC name, Synonyms, PubChem CID, and Status
- Link to compound structure and detailed annotations.

Metabolomics Workbench Standards Feedback

Search standards

Metabolomics Workbench : Meta

metabolomicsworkbench.org/standards/browse.php

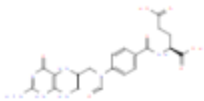
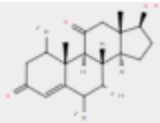
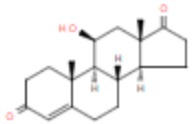
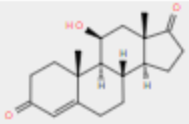
Search:

Submit

Fields searched:
Common name, InChiKey, IUPAC name, Synonyms, PubChem CID, Pathway Cassette, Status (case insensitive)

Browse by Pathway Cassette

- Folates/1C metabolism
- Epigenetics
- Pentose phosphate
- Krebs cycle
- Miscellaneous/drugs
- Steroids/bioactive lipids
- Glycolysis
- Nucleotide pathways
- Reagents
- Redox/coenzymes
- Branched-chain amino acid oxidation

Structure	Common Name	InChiKey	Isotopic Label Type	Isotopic Label Position	Pathway Cassette	MSSC	Status	Request this compound
	10-Formyl-tetrahydrofolic acid	AUFGTPPARQZWDO-YUZLPWPTSA-N			Folates/1C metabolism	RTI	completed	REQUEST
	11-keto-1,6,7-trideuterotestosterone	WTPMRQZHJLJSBO-FLDABYKKSA-N			Steroids/bioactive lipids	RTI	completed	REQUEST
	11β-Hydroxyandrostenedione	WSCUHXPGYUMQEX-KCZNZURUSA-N	unlabelled parent *		Steroids/bioactive lipids	RTI	completed *	REQUEST
	11β-Hydroxyandrostenedione-d3		^{2}H	carbons 1,6,7	Steroids/bioactive lipids	RTI	completed ‡	REQUEST

The End