

# Metabolomics workbench

<https://www.metabolomicsworkbench.org/>

1

The screenshot shows the homepage of the Metabolomics Workbench. At the top, there is a navigation bar with the following links: Home, Data Repository, Databases, Protocols, Tools, Training / Events, About, and Search. The main content area is titled "National Metabolomics Data Repository" and features three columns: "Upload and Manage Studies", "Browse and Search Studies", and "Analyze Studies". A text block states: "As of 03/05/21 a total of 1639 studies have been processed by the the National Metabolomics Data Repository (NMDR). There are 1367 publicly available studies and the remainder (272) will be made available subject to their embargo dates." Below this, there is a section for "Recently released studies on NMDR" with three entries:
 

- ST001218** - Wild type versus TRACK Mice on regular chow and Vitamin A deprived diet; *Mus musculus*; Weill Cornell Medicine
- ST001394** - Metabolomic study of *Escherichia coli* K-12 MG1655 and mutants; *Escherichia coli*; IIT Bombay
- ST001400** - Identification of distinct metabolic perturbations and associated immunomodulatory events during intra-erythrocytic development stage of pediatric *Plasmodium falciparum* malaria; *Homo sapiens*; New York University Abu Dhabi
- ST001421** - Metabolomic study of *Escherichia coli* K-12 MG1655 WT and its transcriptional regulator mutants under anaerobic fermentation conditions; *Escherichia coli*; IIT Bombay

 On the right side, there is a "Quick Links - Key Resources" dropdown menu, a "Follow @MetabolomicsWB" button, and a "Tweets by @MetabolomicsWB" section. The tweet from @MetabolomicsWB says: "Over 1600 studies have been processed by the NMDR to date. Here are the latest releases...". At the bottom right, there is a section for "NIH Common Fund Stage 2 Metabolomics Consortium Centers" listing the "Metabolomics Consortium Coordinating Center (M3C)" led by Richard Yost, U. of Florida, and "Metabolomics Workbench/NMDR" led by Shankar Subramaniam, UC San Diego (this website).

2

**Metabolomics Workbench**

# METABOLOMICS WORKBENCH

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Search the Metabolomics Workbench

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

Welcome to the UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health.

## National Metabolomics Data Repository

Upload and Manage Studies | Browse and Search Studies | Analyze Studies

As of 03/05/21 a total of 1639 studies have been processed by the the National Metabolomics Data Repository (NMDR). There are 1367 publicly available studies and the remainder (272) will be made available subject to their embargo dates.

### Recently released studies on NMDR

**ST001218** - Wild type versus TRACK Mice on regular chow and Vitamin A deprived diet; *Mus musculus*; Weill Cornell Medicine

**ST001394** - Metabolomic study of *Escherichia coli* K-12 MG1655 and mutants; *Escherichia coli*; IIT Bombay.

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**ST001421** - Metabolomic study of *Escherichia coli* K-12 MG1655 WT and its transcriptional regulator mutants under anaerobic fermentation conditions; *Escherichia coli*; IIT Bombay.

Quick Links - Key Resources

Follow @MetabolomicsWB

Tweets by @MetabolomicsWB

**Metabolomics Workbench**  
@MetabolomicsWB

Over 1600 studies have been processed by the NMDR to date. Here are the latest releases...

NIH Common Fund Stage 2 Metabolomics Consortium Centers

Metabolomics Consortium Coordinating Center (M3C) [@M3C](#)  
Richard Yost, U. of Florida

Metabolomics Workbench/NMDR [@MetabolomicsWB](#)  
Shankar Subramaniam, UC San Diego (this website)

3

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Log in / Register

Search the Metabolomics Workbench

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

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

## Browse and Search Studies

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

UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health

Terms of use | Site map | Contact | NMDR Personnel

4





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Study ID	Study Title	Species	Institute
ST000002	Intestinal Samples II pre/post transplantation	Human	University of California, Davis
ST000004	Lipidomics studies on NIDDK / NIST human plasma samples	Human	LIPID MAPS
ST000009	Mixed meal tolerance	Human	University of Michigan
ST000010	Lung Cancer Cells 4	Human	University of Michigan
ST000011	African Metabolomics	Human	University of Michigan
ST000016	NPM-ALK metabolic regulation	Human	University of Michigan
ST000020	Biomarker Discovery in Knee Osteoarthritis (I)	Human	University of North Carolina
ST000022	Biomarker Discovery in Knee Osteoarthritis (II)	Human	University of North Carolina
ST000041	High PUFA diet in humans	Human	University of Michigan
ST000042	BALF Control vs ALI by RPLC-MS	Human	University of Michigan
ST000043	MDA-MB-231 cells and p38 gamma knockdown	Human	University of Michigan
ST000044	Pilot experiment looking for the existence of certain molecules in pancreatic cancer cells	Human	University of Michigan
ST000045	Plasma metabolomics: Comparison of non-diabetic controls with T1D patients	Human	Mayo Clinic
ST000046	Identification of altered metabolic pathways in Alzheimer's disease, mild cognitive impairment and cognitively normals using Metabolomics (plasma)	Human	Mayo Clinic
ST000047	Identification of altered metabolic pathways in Alzheimer's disease, mild cognitive impairment and cognitively normals using Metabolomics (CSF)	Human	Mayo Clinic
ST000050	Preterm Neonatal Urinary Renal Developmental and acute kidney injury Metabolic Profiling	Human	University of North Carolina
ST000051	Fetal metabolomic signature of exposure to IAs during pregnancy	Human	University of North Carolina
ST000054	Metabolic Microenvironments in Normal Breast and Breast Cancer (MS analysis)	Human	University of North Carolina
ST000058	Metabolite changes associated with methionine stress sensitivity of cancer (GC TOF MS analysis)	Human	University of California, Davis
ST000061	Metabolic Profiling of Visceral and Subcutaneous Adipose Tissue from Colorectal Cancer Patients: GC-TOF MS analysis of subcutaneous and visceral adipose tissue samples	Human	University of California, Davis
ST000062	Biomarkers for Depression in Human Plasma in a Population Sample	Human	University of California, Davis
ST000063	Biomarkers for Depression in Human Cerebrospinal Fluid in a Population Sample	Human	University of California, Davis
ST000065	Metabolic Profiling of Visceral and Subcutaneous Adipose Tissue from Colorectal Cancer Patients: GC-TOF MS analysis of serum samples	Human	University of California, Davis
ST000076	A549 Cell Study	Human	University of Kentucky
ST000077	Metabolite changes associated with methionine stress sensitivity of cancer (CSH QTOF MS analysis)	Human	University of California, Davis
ST000081	Metabolic Profiling of Visceral and Subcutaneous Adipose Tissue from Colorectal Cancer Patients: UHPLC-QTOF MS analysis of subcutaneous and visceral adipose tissue samples	Human	University of California, Davis
ST000082	Metabolic Profiling of Visceral and Subcutaneous Adipose Tissue from Colorectal Cancer Patients: UHPLC-QTOF MS analysis of serum samples	Human	University of California, Davis

7



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## Experimental projects/studies search results

### Studies on diabetes – clinical and pre-clinical

Modify Search

Showing results 1 to 18 of 18 (†: Contains untargeted data) Results per page: 50

Project ID	Project Title	Institute (Experimental)	Institute (Analysis)	Number Of Studies
PR001050	Parallel multi-omics in high-risk subjects for the identification of integrated biomarker signatures of 4 type 1 diabetes	University of Miami	University of Miami	1
PR000987	Gut microbiota mediates the interplay between immunity and glucose metabolism	Oregon State University	Oregon State University	1
PR000840	Phenotyping blood metabolites in day and night in type 2 diabetes	Indiana University School of Medicine	Indiana University School of Medicine	1
PR000630	Metabolomics Linking Air Pollution, Obesity and Type 2 Diabetes	Emory University	Emory University	1
PR000581	Diabetes and Chronic Kidney Disease progression	University of Michigan	University of Michigan	1
PR000458	Biomarkers of diabetes risk in children: role of obesity and exercise	Mayo Clinic	Mayo Clinic	2
PR000416	Metabolomic study on a schizophrenia and type 2 diabetes susceptibility gene Nos1AP-rs12742393	Shanghai Jiao Tong University Affiliated Sixth People's Hospital	Shanghai Jiao Tong University Affiliated Sixth People's Hospital	1
PR000410	Urine metabolomic profiling of diabetic nephropathy in the steptozotocin induced type-1 diabetes mouse model.	North Carolina A&T State University	RTI International	1
PR000409	Plasma metabolomic profiling of diabetic nephropathy in the steptozotocin induced type-1 diabetes mouse model	North Carolina A&T State University	RTI International	1
PR000396	Utility of canine diabetes as a model for human type 1 diabetes	University of Florida	University of Florida	1
PR000395	Kidney tissue metabolomic profiling of diabetic nephropathy in the steptozotocin induced type-1 diabetes mouse model.	North Carolina A&T State University	RTI International	1
PR000389	Effects of herb DG and KK01 on Type 2 Diabetes Mellitus (T2DM)	RTI International	University of North Carolina	1
PR000359	Metabolomics of Saliva Samples Obtained from Subjects with Diabetes	University of North Carolina at Chapel Hill	University of North Carolina	1
PR000330	Impact of Long-Term Poor and Good Glycemic Control on Metabolomics Alterations in Type 1 Diabetic People.	Mayo Clinic	Mayo Clinic	2
PR000311	Urine metabolomics for the study of Gestational Diabetes Mellitus	University of Aveiro	University of Aveiro	1
PR000083	Quantitative metabolomics by H-NMR and LC-MS/MS confirms altered metabolic pathways in diabetes	Mayo Clinic	Mayo Clinic	1
PR000054	Combined Metabolomics and Lipidomics of Type 1 Diabetes	University of California, Davis	University of California, Davis	2
PR000044	Concordance of changes in metabolic pathways based on plasma metabolomics and skeletal muscle transcriptomics in type 1 diabetes.	Mayo Clinic	Mayo Clinic	1

Download results CSV

8



## Link to the first diabetes study

<https://www.metabolomicsworkbench.org/data/DRCCMetadata.php?Mode=Project&ProjectID=PR001050>

9

### Summary of project PR001050

Data from proteomics, metabolomics, lipidomics and transcriptomics

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 PR001050. The data can be accessed directly via it's Project DOI: [10.21228/M8ZX18](https://doi.org/10.21228/M8ZX18)  This work is supported by NIH grant, U2C- DK119886.

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

<b>Project ID:</b>	PR001050
<b>Project DOI:</b>	doi: 10.21228/M8ZX18
<b>Project Title:</b>	Parallel multi-omics in high-risk subjects for the identification of integrated biomarker signatures of 4 type 1 diabetes
<b>Project Summary:</b>	Biomarkers are of paramount importance for early disease detection and are particularly valuable in type 1 diabetes (T1D) to prevent significant $\beta$ cell loss before the onset of clinical symptoms. Thus far, single-omics studies have failed to identify such T1D biomarkers. Here, we present proof-of-concept studies to demonstrate the potential for identifying integrated biomarker signature(s) of T1D using parallel multi-omics. Blood from human subjects at high risk for T1D (and healthy controls; n=4 each) were subjected to parallel unlabeled proteomics, metabolomics, lipidomics, and transcriptomics. The integrated dataset was analyzed using Ingenuity Pathway Analysis (IPA) software for disturbances in the at-risk subjects compared to the controls.
<b>Institute:</b>	University of Miami
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<b>First Name:</b>	Sanjoy
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<b>Email:</b>	sbhattacharya@med.miami.edu
<b>Phone:</b>	305-482-4103

10

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

<b>Study ID</b>	ST001642
<b>Study Title</b>	Lipidomics in high-risk subjects for the identification of integrated biomarker signatures of type 1 diabetes
<b>Study Summary</b>	We present the lipidome of plasma collected from high-risk type 1 diabetes subjects. The methyl tert-butyl ether (MTBE) method was used for lipid extraction, followed by high performance liquid chromatography (HPLC) tandem mass spectrometry (LC-MS/MS) using a Q Exactive Orbitrap mass spectrometer and an Accela 600 HPLC. Lipid species were identified and quantified by analyzing the raw files in LipidSearch 4.2. Further analysis was conducted using Graphpad Prism and Ingenuity Pathway Analysis (IPA).
<b>Institute</b>	University of Miami
<b>Last Name</b>	Bhattacharya
<b>First Name</b>	Sanjoy
<b>Address</b>	1638 NW 10th Avenue, Room 706-A, Miami, FL 33136
<b>Email</b>	sbhattacharya@med.miami.edu
<b>Phone</b>	305-482-4103
<b>Submit Date</b>	2021-01-06
<b>Raw Data Available</b>	Yes
<b>Raw Data File Type(s)</b>	.raw
<b>Analysis Type Detail</b>	LC-MS
<b>Release Date</b>	2021-01-25
<b>Release Version</b>	1

11

## Statistics Toolbox for Study: ST001642

**Title: Lipidomics in high-risk subjects for the identification of integrated biomarker signatures of type 1 diabetes**

Select a dataset:

Reversed phase POSITIVE ION MODE ▼

Run analyses on data in Study ST001642 Dataset: Reversed phase POSITIVE ION MODE

Metabolite classes (all analyses combined)

- [Pie chart of metabolite super classes](#)
- [Pie chart of metabolite main classes](#)
- [Pie chart of metabolite sub classes](#)

Normalization and averaging


- [Show Metabolite averages per experimental factor](#)
- [Perform normalization on data](#)
- [Create Relative log abundance plots](#)

Univariate analysis

- [Perform multi-condition dot plot analysis New!](#)
- [Perform Volcano plot analysis](#)
- [Perform ANOVA analysis](#)

12

**MetENP: Metabolite enrichment and species-specific pathway annotation New!**

- [MetENPWeb analysis](#)
- [MetENP R package](#) 
- [MetENP tutorial](#)

**Clustering and correlation**

- [Perform hierarchical or heatmap cluster analysis](#)
- [Perform Clustered correlation analysis](#)
- [Perform Network analysis on correlated metabolites](#)

**Multivariate analysis**

- [Perform Principal component analysis](#)
- [Perform Linear discriminant analysis](#)
- [Perform Partial least-squares discriminant analysis \(PLS-DA\)](#)

**Classification and feature analysis**

- [Perform OPLS-DA and VIP projection](#)
- [Random Forest and VIP projection](#)

**Mapping metabolites to human biochemical pathways**

- [Map study metabolites to HMDB and KEGG pathways](#)
- [Map study metabolites to pathways with ratio/t-test data](#)