

**Metabolomics Workbench and the National Metabolomics Data Repository**  
**University of California San Diego**  
**and**  
**San Diego Supercomputer Center**

**NMDR browsing and searching tutorial**

**NIH Common Fund's National Metabolomics Data Repository**  
**(supported by NIH grant, U2C-DK119886)**

# Metabolomics Workbench: <https://www.metabolomicsworkbench.org>

## Contains the National Metabolomics Data Repository (NMDR)

The screenshot shows the homepage of the Metabolomics Workbench. At the top, there is a navigation bar with links for Home, Data Repository, Databases, Protocols, Tools, Training / Events, About, and Search. A search bar is located on the right side of the header. Below the navigation bar, a welcome message states: "Welcome to the UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health." The main content area is divided into several sections. On the left, there is a section for the National Metabolomics Data Repository (NMDR) with three columns: "Upload and Manage Studies", "Browse and Search Studies", and "Analyze Studies". Below this, a paragraph states: "As of 02/14/22 a total of 2002 studies have been processed by the National Metabolomics Data Repository (NMDR). There are 1727 publicly available studies and the remainder (275) will be made available subject to their embargo dates." This is followed by a section titled "Recently released studies on NMDR" with three entries: ST002058 - Muscle/Lung/Tumor metabolomics; Mus musculus; University of Colorado Anschutz Medical Campus; ST002059 - 4T1 and SKM cells; Homo sapiens; University of Colorado Anschutz Medical Campus; and ST002067 - Time-Resolved Metabolomics of a Mouse Model of Ovarian High-Grade Serous Carcinoma (LC-MS); Mus musculus; Georgia Institute of Technology. On the right side, there is a "Quick Links - Key Resources" dropdown menu, a "Follow @MetabolomicsWB" button, and a "Tweets by @MetabolomicsWB" section. Below the tweets, there is a section for "NIH Common Fund Stage 2 Metabolomics Consortium Centers" with a list of centers and their coordinators. At the bottom of the main content area, there is a section for the "Metabolite Structure Database" with a sub-section titled "Updates to the Metabolite Structure Database (February 2, 2022)". This section contains a paragraph: "The updated Metabolite structure database of primary and secondary metabolites at the Metabolomics Workbench contains new substructure and text-based searches including by chemical class. Over 164,000 structures have been added including over 10,000 sterols." Below this text is a screenshot of the Metabolite Structure Database interface, showing a search results page with a list of metabolites and their chemical structures. At the bottom of the page, there is a link to "Highlights/News archive".

**Metabolomics Workbench** Log in / Register

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 02/14/22 a total of 2002 studies have been processed by the National Metabolomics Data Repository (NMDR). There are 1727 publicly available studies and the remainder (275) will be made available subject to their embargo dates.

#### Recently released studies on NMDR

**ST002058** - Muscle/Lung/Tumor metabolomics; *Mus musculus*; University of Colorado Anschutz Medical Campus

**ST002059** - 4T1 and SKM cells; *Homo sapiens*; University of Colorado Anschutz Medical Campus

**ST002067** - Time-Resolved Metabolomics of a Mouse Model of Ovarian High-Grade Serous Carcinoma (LC-MS); *Mus musculus*; Georgia Institute of Technology

Quick Links - Key Resources

Follow @MetabolomicsWB

Tweets by @MetabolomicsWB

**Metabolomics Workbench** @MetabolomicsWB

The National Metabolomics Data Repository (NMDR) at @MetabolomicsWB has just processed its 2,000th study! MS/NMR data/metadata on studies covering over 130 species. [Browse/search/download at](#)

### NIH Common Fund Stage 2 Metabolomics Consortium Centers

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

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

**Compound Identification Cores (CIDs)** [Arthur Edison, U. of Georgia](#)  
[Alexey Nesvizhskii, U. of Michigan](#)  
[Oliver Flehn, UC Davis](#)  
[Dean Paul Jones, Emory University](#)  
[Thomas Metz, Pacific Northwest Nat. Lab.](#)

**Data and Tools Cores (DTCs)** [John Weinstein, MD Anderson Cancer C.](#)  
[Jamey Young, Vanderbilt University](#)  
[Xiuxia Du, U. of North Carolina Charlotte](#)  
[Shuzhao Li, Emory University](#)  
[Ala Karnovsky, U. of Michigan](#)  
[Katerina Kechris, U. of Colorado, Denver](#)  
[Gary Patti, Washington U. at St. Louis](#)

### Metabolite Structure Database

#### Updates to the Metabolite Structure Database (February 2, 2022)

The updated Metabolite structure database of primary and secondary metabolites at the [Metabolomics Workbench](#) contains new substructure and text-based searches including by chemical class. Over 164,000 structures have been added including over 10,000 sterols.

[Highlights/News archive](#)

# Metabolomics Workbench Data Portal: Studies



Default sorting order is by most recently released study

## Browse and Search Studies

### • Browse

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

### • Search

- Experimental Projects / Studies
- **MetStat: Perform meta-analysis on named metabolites across all studies:**  
Refine by analysis type, species, sample source, disease association, metabolite classification and biochemi
- Select Studies by species, sample source or disease association
- Search data/metadata in experimental projects/studies
- Search Untargeted MS data by m/z, retention time, instrumentation
- REST service
- Use the Metabolomics Workbench REST service to retrieve different types of data

Summary of all studies

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

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

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

# Metabolomics Workbench Data Portal:Projects

[Home](#) | [Data Repository](#) | [Databases](#) | [Protocols](#) | [Tools](#) | [Training / Events](#) | [About](#) | [Search](#)  
[Overview](#) | [Upload / Manage Data](#) | [Browse / Search Studies](#) | [Analyze Studies](#) | [Tutorials](#) | [FAQ](#)

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

## Browse and Search Studies

### • Browse

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

### Summary of all studies in project PR001288

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

## Summary of all projects

Showing page 2 of 74 Results: [Previous](#) [1](#) [2](#) [3](#) [4](#) [5](#) [Next](#) [Last](#) Showing results 16 to 30 of 1108

(#: Contains untargeted data) Results per page:



Project ID	Project Title	Institute(Experimental)	Institute(Analysis)	Number Of Studies
↑↓	↑↓	↑↓	↑↓	↑↓
PR001291	An observational study of cardiovascular patients in India	Translational Health Science And Technology Institute (THSTI)	Translational Health Science And Technology Institute (THSTI)	1
PR001290	Maternal Hypoxemia and Oxidative Stress	LOMA LINDA UNIVERSITY	LOMA LINDA UNIVERSITY   School of Medicine	1
PR001288	Irradiation causes alterations of polyamine, purine and sulfur metabolism in red blood cells and multiple organs	University of Colorado Anschutz Medical Campus	University of Colorado Anschutz Medical Campus	11
PR001284	A Sentinel Serum Quality Management Program for NMR Metabolomics	University of Michigan	University of Michigan	1
PR001283	MICROMETABOLITE	Aristotle University of Thessaloniki, MICROMETABOLITE project	Aristotle University of Thessaloniki	1
PR001283	MICROMETABOLITE	Aristotle University of Thessaloniki, MICROMETABOLITE project	Aristotle University of Thessaloniki, MICROMETABOLITE project	1
PR001282	TIPs Metabolomics	Vanderbilt University Medical Center	Vanderbilt University Medical Center	2
PR001281	ABO Metabolomics	Vanderbilt University Medical Center	Vanderbilt University Medical Center	2
PR001276	Untargeted primary metabolite profiling in Arabidopsis thaliana	Salk Institute for Biological Studies	Salk Institute for Biological Studies	1
PR001274	Chemoresistant Ovarian Cancer Global Metabolomics	The University of South Australia	The University of South Australia	1
PR001273	Glycine betaine uptake and metabolism in marine microbial communities	University of Washington	University of Washington	1
PR001270	A longitudinal study of the effect of temperature modification in full-scale anaerobic digesters	INRAE	INRAE	1
PR001269	Case-control study on plasma metabolomics analysis in Myalgic encephalomyelitis/chronic fatigue syndrome (ME/CFS)	Columbia University	Columbia University	4
PR001268	Polyamine import and accumulation causes immunomodulation in macrophages engulfing apoptotic cells	University of Colorado Denver	University of Colorado Denver	4
PR001266	Metabolic snapshot of plasma samples to study SARS-CoV-2 pathogenesis	Universidad CEU San Pablo	Universidad CEU San Pablo	1

te classificati

ata

# NMDR:Study-level view contains multiple metadata sections

## Summary of study ST001140

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

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

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

Select appropriate tab below to view additional metadata details:

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

 **View Metadata**

Example: Analysis section

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



# Study-level view : Show named metabolites and measurements

Summary of study ST001140

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

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

Study ID: ST001140  
 Study Title: Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure  
 Study: Glucocorticoids (GCs) are widely used in veterinary and human medicine. Chronic endogenous or iatrogenic GC overexposure impairs metabolic function and can cause Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess (prednisolone and tetraacosactide, respectively) on the plasma lipidome of Beagle dogs. Both, long- and short-term GC resulted in significant changes of the plasma lipidome.   
 University of Zurich  
 Institute of Food Safety and Food Quality, Vetsuisse Faculty, University of Zurich  
 Institute of Food Safety and Food Quality, National University of Singapore

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

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

(Green: p value<=0.05)

Return to study ST001140 main page

Analysis: Phospholipids, Chol. esters and Diacylglycerols

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

Select	Metabolite Name	RefMet Name/Standardized Name*
<input checked="" type="checkbox"/>	CE(16:0)	CE 16:0
<input type="checkbox"/>	CE(16:1)	CE 16:1
<input type="checkbox"/>	CE(17:0)	CE 17:0
<input type="checkbox"/>	CE(17:1)	CE 17:1
<input type="checkbox"/>	CE(18:0)	CE 18:0
<input type="checkbox"/>	CE(18:1)	CE 18:1
<input type="checkbox"/>	CE(18:2)	CE 18:2
<input type="checkbox"/>	CE(18:3)	CE 18:3
<input type="checkbox"/>	CE(20:1)	CE 20:1
<input type="checkbox"/>	CE(20:2)	CE 20:2
<input type="checkbox"/>	CE(20:3)	CE 20:3
<input type="checkbox"/>	CE(20:4)	CE 20:4
<input type="checkbox"/>	CE(20:5)	CE 20:5
<input type="checkbox"/>	CE(22:4)	CE 22:4
<input type="checkbox"/>	CE(22:5)	CE 22:5
<input type="checkbox"/>	CE(22:6)	CE 22:6
<input type="checkbox"/>	CE(24:4)	CE 24:4
<input type="checkbox"/>	DG(16:0_20:4)	DG 16:0_20:4

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

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

Bar graph by sample | 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

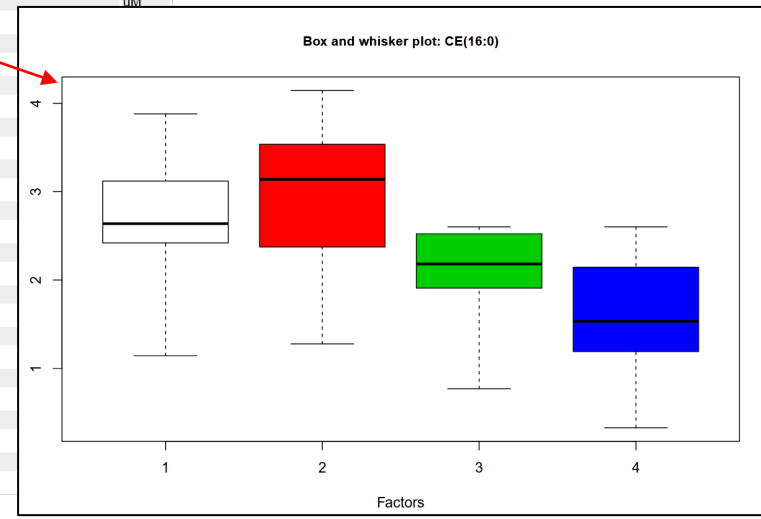
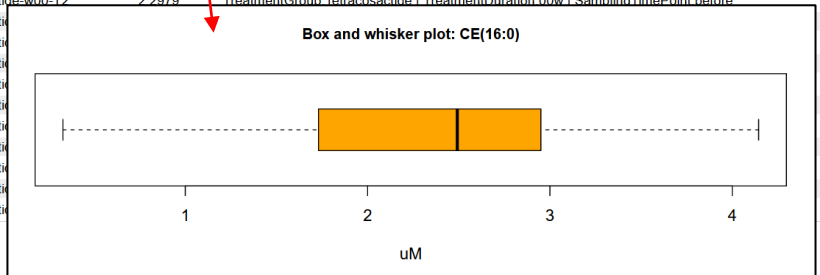
Sample	CE(16:0)	Factors
Prednisolone-d0-P1	2.3688	TreatmentGroup:Prednisolone   TreatmentDuration:0d   SamplingTimePoint:before
Prednisolone-d0-P2	1.1431	TreatmentGroup:Prednisolone   TreatmentDuration:0d   SamplingTimePoint:before
Prednisolone-d0-P3	3.8792	TreatmentGroup:Prednisolone   TreatmentDuration:0d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

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

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

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

Green: p-value <= 0.05



Select a metabolite (checkbox)

# NMDR:Study-level view/download options

## Summary of study ST001140

This data is available at the NIH Common Fund's National Metabolomics Data Repository (NMDR) website, the Metabolomics Workbench, <https://www.metabolomicsworkbench.org>, where it has been assigned Project ID PR000761. The data can be accessed directly via it's Project DOI: [10.21228/M89Q32](https://doi.org/10.21228/M89Q32)

This work is supported by NIH grant, U2C- DK119886. See: <https://www.metabolomicsworkbench.org/about/howtocite.php>

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

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

Select appropriate tab below to view additional metadata details:

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

View Metadata

Sample ID	Subject Name	Sample Name	TreatmentGroup	TreatmentDuration	SamplingTimePoint	Sample Date	Age	Weight
SL019001	P1	Prednisolone-d0-P1	Prednisolone	0d	before	F	12	14.7
SL019002	P2	Prednisolone-d0-P2	Prednisolone	0d	before	F	72	14
SL019003	P4	Prednisolone-d0-P4	Prednisolone	0d	before	F	71	15.4
SL019004	P4	Prednisolone-d0-P4	Prednisolone	0d	before	M	23	16.9
SL019005	P4	Prednisolone-d0-P4	Prednisolone	0d	before	M	32	16.0
SL019006	P8	Prednisolone-d0-P8	Prednisolone	0d	before	M	88	16.3
SL019007	P7	Prednisolone-d0-P7	Prednisolone	0d	before	M	82	12.6
SL019008	P8	Prednisolone-d0-P8	Prednisolone	0d	before	M	80	12.6
SL019009	P2	Prednisolone-d4-P2	Prednisolone	4d	after	F	78	11.8
SL019010	P2	Prednisolone-d4-P2	Prednisolone	4d	after	F	77	12.0
SL019011	P4	Prednisolone-d4-P4	Prednisolone	4d	after	M	29	14.1
SL019012	P5	Prednisolone-d4-P5	Prednisolone	4d	after	M	29	16.5
SL019013	P8	Prednisolone-d4-P8	Prednisolone	4d	after	M	84	11.9
SL019014	P7	Prednisolone-d4-P7	Prednisolone	4d	after	M	81	13
SL019015	P8	Prednisolone-d4-P8	Prednisolone	4d	after	M	43	14
SL019016	T1	Tetraacosaide-d0-T1	Tetraacosaide	0d	before	M	35	14
SL019017	T2	Tetraacosaide-d0-T2	Tetraacosaide	0d	before	F	43	15
SL019018	T3	Tetraacosaide-d0-T3	Tetraacosaide	0d	before	F	6	16
SL019019	T4	Tetraacosaide-d0-T4	Tetraacosaide	0d	before	M	7	17
SL019020	T5	Tetraacosaide-d0-T5	Tetraacosaide	0d	before	M	7	18
SL019021	T8	Tetraacosaide-d0-T8	Tetraacosaide	0d	before	M	8	18
SL019022	T1	Tetraacosaide-d20-T1	Tetraacosaide	20w	after	M	38	15
SL019023	T2	Tetraacosaide-d20-T2	Tetraacosaide	20w	after	F	41	16
SL019024	T3	Tetraacosaide-d20-T3	Tetraacosaide	20w	after	F	6	17
SL019025	T4	Tetraacosaide-d20-T4	Tetraacosaide	20w	after	F	7	18
SL019026	T5	Tetraacosaide-d20-T5	Tetraacosaide	20w	after	M	7	18
SL019027	T8	Tetraacosaide-d20-T8	Tetraacosaide	20w	after	M	8	20

Samples/study design

Select	Metabolite Name	RefMet Name/Standardized Name	Workbench Metabolite ID	PubChem
<input type="checkbox"/>	CE(16:0)	CE 16:0	ME271966	-
<input type="checkbox"/>	CE(16:1)	CE 16:1	ME271967	-
<input type="checkbox"/>	CE(17:0)	CE 17:0	ME271968	-
<input type="checkbox"/>	CE(17:1)	CE 17:1	ME271969	-
<input type="checkbox"/>	CE(18:0)	CE 18:0	ME271970	-
<input type="checkbox"/>	CE(18:1)	CE 18:1	ME271971	-
<input type="checkbox"/>	CE(18:2)	CE 18:2	ME271972	-
<input type="checkbox"/>	CE(18:3)	CE 18:3	ME271973	-
<input type="checkbox"/>	CE(20:1)	CE 20:1	ME271974	-
<input type="checkbox"/>	CE(20:2)	CE 20:2	ME271975	-
<input type="checkbox"/>	CE(20:3)	CE 20:3	ME271976	-

Named metabolites

Sample	Prednisolone-d0-P1	Prednisolone-d0-P2	Prednisolone-d0-P3
Factors	TreatmentGroup	Prednisolone	TreatmentDuration
CE(16:0)	2.3688	1.1431	3.8792
CE(16:1)	0.3856	0.2044	0.6614
CE(17:0)	0.0454	0.0329	0.0822
CE(17:1)	0.0484	0.0269	0.0587
CE(18:0)	0.5856	0.2893	0.6917
CE(18:1)	23.5327	15.5174	28.8094
CE(18:2)	83.6104	39.1071	112.5607
CE(18:3)	0.5341	0.1733	0.9862
CE(20:1)	0.0188	0.0168	0.0247
CE(20:2)	0.1193	0.1270	0.1486
CE(20:3)	1.1965	0.9504	2.6171
CE(20:4)	73.0032	29.3993	79.7335
CE(22:4)	0.0064	0.0055	0.0052
DG(16:0_20:4)	15.9508	50.2891	7

Download dataset

```

METABOLOMICS WORKBENCH borlab_20190119_202009 DATATRACK_ID:1609 STUDY_ID:ST001140 ANALYSIS_ID:AN001070 PROJECT_ID:PR000761
VERSION 2
CREATED ON February 21, 2019, 4:41 pm
PROJECT
PROJECT TITLE Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess
PROJECT SUMMARY Glucocorticoid (GC) are widely used in veterinary and human medicine. Chronic endogenous or iatrogenic GC overexposure impairs metabolic function and can result in diverse side-effects, including Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess (induced by prednisolone and tetraacosaide, respectively) on the plasma lipidome of Beagle dogs. Both, long- and short-term GC resulted in significant changes of the plasma lipidome.
PROJECT TITLE National University of Singapore and University of Zurich
DEPARTMENT Multiple
PRELIMINARY NAME Singapore Lipidomics Incubator (SLING)
ADDRESS 80
CITY 28 Medical Drive, Singapore 117645, Singapore
PHONE +6565146683
PROJECT
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14.7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14.7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","11.8"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","12.0"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14.1"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","16.5"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","11.9"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","13"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","15"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","16"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","17"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","18"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","38"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","41"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","6"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","8"],
}

```

Download mwTab (text)

```

METABOLOMICS WORKBENCH borlab_20190119_202009 DATATRACK_ID:1609 STUDY_ID:ST001140 ANALYSIS_ID:AN001070 PROJECT_ID:PR000761
VERSION 2
CREATED ON February 21, 2019, 4:41 pm
PROJECT
PROJECT TITLE Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess
PROJECT SUMMARY Glucocorticoid (GC) are widely used in veterinary and human medicine. Chronic endogenous or iatrogenic GC overexposure impairs metabolic function and can result in diverse side-effects, including Cushing's syndrome. This study examines the effects of experimentally induced short-term and long-term GC excess (induced by prednisolone and tetraacosaide, respectively) on the plasma lipidome of Beagle dogs. Both, long- and short-term GC resulted in significant changes of the plasma lipidome.
PROJECT TITLE National University of Singapore and University of Zurich
DEPARTMENT Multiple
PRELIMINARY NAME Singapore Lipidomics Incubator (SLING)
ADDRESS 80
CITY 28 Medical Drive, Singapore 117645, Singapore
PHONE +6565146683
PROJECT
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14.7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14.7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","11.8"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","12.0"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14.1"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","16.5"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","11.9"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","13"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Prednisolone","TreatmentDuration","4d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","14"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","15"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","16"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","17"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","0d","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","18"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","38"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","41"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","6"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","7"],
}
STUDY_ID:"ST001140",
STUDY_TITLE:"Changes in the Canine Plasma Lipidome after Short- and Long-Term Excess Glucocorticoid Exposure",
FACTORS:["TreatmentGroup","Tetraacosaide","TreatmentDuration","20w","SamplingTimePoint"],
ADDITIONAL_SAMPLE_DATA:["Sex","Age_months","Weight_kg","8"],
}

```

Download mwTab (json)

# NMDR: raw data view/download

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

## Download data

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

- [View archive contents](#)
- [Download individual raw files](#)
- [ST001738\\_File\\_Naming\\_AdipoAtlas.xlsx \(16.4K\)](#)
- [ST001738\\_ccms\\_peak\\_identification.zip \(4.6G\)](#)
- [ST001738\\_ccms\\_peak\\_quantification.zip \(2.1G\)](#)

} [Download compressed raw files](#)

### ST001738: Archive File:ST001738\_ccms\_peak\_identification.zip

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

### ST001738: Archive File:ST001738\_ccms\_peak\_identification.zip

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



# Collaboration with Global Natural Product Social Molecular Networking (GNPS)

**Metabolomics Workbench**

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

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

ST001709: Archive File:ST001709\_data.zip

Download Individual Sample File	Size(bytes)	GNPS Dashboard Link
Data/mzXML/Sample_01__neg.mzXML	8407713	Display in GNPS
Data/mzXML/Sample_01__pos.mzXML	8903745	Display in GNPS
Data/mzXML/Sample_02__neg.mzXML	8369519	Display in GNPS
Data/mzXML/Sample_02__pos.mzXML	8649071	Display in GNPS
Data/mzXML/Sample_03__neg.mzXML	8213569	Display in GNPS
Data/mzXML/Sample_03__pos.mzXML	8604720	Display in GNPS
Data/mzXML/Sample_04__neg.mzXML		Display in GNPS
Data/mzXML/Sample_04__pos.mzXML		Display in GNPS
Data/mzXML/Sample_05__neg.mzXML		Display in GNPS
Data/mzXML/Sample_05__pos.mzXML		Display in GNPS
Data/mzXML/Sample_06__neg.mzXML		Display in GNPS
Data/mzXML/Sample_06__pos.mzXML		Display in GNPS
Data/mzXML/Sample_07__neg.mzXML		Display in GNPS
Data/mzXML/Sample_07__pos.mzXML		Display in GNPS
Data/mzXML/Sample_08__neg.mzXML		Display in GNPS

Opening Sample\_01\_\_neg.mzXML

You have chosen to open:

Sample\_01\_\_neg.mzXML  
which is: MZXML file  
from: https://www.metabolomicsworkbench.org

What should Firefox do with this file?

Open with

Save File

Do this automatically for files like this from now on.

GNPS Dashboard - version 0.8 - Documentation - GNPS Default

XIC Plot - Single File

MS2: 3664

Spectrum Details

View Metabolomics ID

MS/MS Spectrum in GNPS

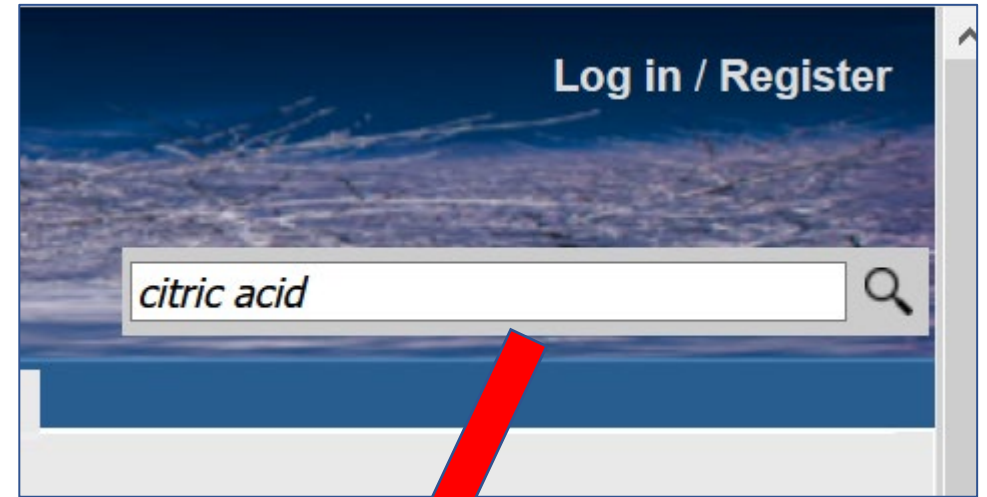
View spectral details of MS raw data files deposited in NMDR via the GNPS dashboard

GNPS Dashboard: Collaborative Analysis of Mass Spectrometry Data in the Web Browser  
D. Petras et al, Nature Methods (2021) <https://doi.org/10.1038/s41592-021-01339-5>

# Metabolomics Workbench Quick search

## What is searched?

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



Search the Metabolomics V [Study-specific Protocols](#)

**Database search results for "CITRIC ACID"**

Metabolomics Workbench [RefMet](#) Database: Exact name search  
**1 matches**

Metabolomics Workbench [RefMet](#) Database: Partial name search  
**5 matches**

Metabolomics Workbench [Metabolite](#) Database: Name search  
**18 matches**

Metabolomics Workbench NMDR MS Studies: Name search on reported metabolites (RefMet name)  
**661 matches**

# Regular expression search

## What is searched?

- Metabolite common names and systematic names in MW metabolite database

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

Structure	Studies	Common Name	Systematic Name	PubChem CID	Formula
<a href="#">1479</a>	<a href="#">1</a>	2-oxo-4-hydroxy-hexanoic acid	2-oxo-4-hydroxy-hexanoic acid	<a href="#">441164</a>	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>
<a href="#">1525</a>	<a href="#">3</a>	2-oxo capric acid	2-oxo-decanoic acid	<a href="#">259794</a>	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>
<a href="#">1526</a>	<a href="#">46</a>	3-methyl pyruvic acid	2-oxo-butanoic acid	<a href="#">58</a>	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>
<a href="#">1528</a>	-	2-keto valeric acid	2-oxo-pentanoic acid	<a href="#">74563</a>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>
<a href="#">1531</a>	<a href="#">6</a>	2-keto-n-caproic acid	2-oxo-hexanoic acid	<a href="#">159664</a>	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>
<a href="#">1535</a>	-	2-Keto-n-heptylic acid	2-oxo-heptanoic acid	<a href="#">5282977</a>	C <sub>7</sub> H <sub>12</sub> O <sub>3</sub>
<a href="#">1540</a>	-	2-keto-n-caprylic acid	2-oxo-octanoic acid	<a href="#">67600</a>	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>
<a href="#">1546</a>	-	n-heptanoyl acetic acid	2-oxo-nonanoic acid	<a href="#">259793</a>	C <sub>9</sub> H <sub>16</sub> O <sub>3</sub>
<a href="#">1564</a>	-	2-keto tridecanoic acid	2-oxo-tridecanoic acid	<a href="#">5282989</a>	C <sub>13</sub> H <sub>24</sub> O <sub>3</sub>
<a href="#">1573</a>	-	2-keto palmitic acid	2-oxo-hexadecanoic acid	<a href="#">5282996</a>	C <sub>16</sub> H <sub>30</sub> O <sub>3</sub>
<a href="#">1584</a>	<a href="#">254</a>	Pyruvic acid	2-oxo-propionic acid	<a href="#">1060</a>	C <sub>3</sub> H <sub>4</sub> O <sub>3</sub>
<a href="#">1594</a>	-	2-oxo-undecanoic acid	2-oxo-undecanoic acid	<a href="#">5312886</a>	C <sub>11</sub> H <sub>20</sub> O <sub>3</sub>
<a href="#">1597</a>	-	2-oxo-dodecanoic acid	2-oxo-dodecanoic acid	<a href="#">5312887</a>	C <sub>12</sub> H <sub>22</sub> O <sub>3</sub>
<a href="#">1605</a>	-	2-oxo-tetradecanoic acid	2-oxo-tetradecanoic acid	<a href="#">5312894</a>	C <sub>14</sub> H <sub>26</sub> O <sub>3</sub>
<a href="#">1609</a>	-	2-oxo-pentadecanoic acid	2-oxo-pentadecanoic acid	<a href="#">5312896</a>	C <sub>15</sub> H <sub>28</sub> O <sub>3</sub>
<a href="#">1614</a>	-	2-oxo-heptadecanoic acid	2-oxo-heptadecanoic acid	<a href="#">5312901</a>	C <sub>17</sub> H <sub>32</sub> O <sub>3</sub>
<a href="#">1619</a>	-	2-oxo-nonadecanoic acid	2-oxo-nonadecanoic acid	<a href="#">5312918</a>	C <sub>19</sub> H <sub>36</sub> O <sub>3</sub>
<a href="#">1622</a>	-	2-oxo-eicosanoic acid	2-oxo-eicosanoic acid	<a href="#">5312921</a>	C <sub>20</sub> H <sub>38</sub> O <sub>3</sub>
<a href="#">1624</a>	-	2-oxo-heneicosanoic acid	2-oxo-heneicosanoic acid	<a href="#">5312923</a>	C <sub>21</sub> H <sub>40</sub> O <sub>3</sub>
<a href="#">1629</a>	-	2-oxo-docosanoic acid	2-oxo-docosanoic acid	<a href="#">5312928</a>	C <sub>22</sub> H <sub>42</sub> O <sub>3</sub>
<a href="#">1633</a>	-	2-oxo-tricosanoic acid	2-oxo-tricosanoic acid	<a href="#">5312932</a>	C <sub>23</sub> H <sub>44</sub> O <sub>3</sub>
<a href="#">1651</a>	<a href="#">1</a>	5-Amino-2-oxopentanoic acid	2-oxo-5-amino-pentanoic acid	<a href="#">439402</a>	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>
<a href="#">1652</a>	<a href="#">15</a>	2-Oxo-4-methylthiobutanoic acid	2-oxo-4-methylthio-butanoic acid	<a href="#">473</a>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> S
<a href="#">1656</a>	<a href="#">4</a>	2-Oxo-4E-hexenoic acid	2-Oxo-4E-hexenoic acid	<a href="#">5280996</a>	C <sub>6</sub> H <sub>9</sub> O <sub>3</sub>
<a href="#">1673</a>	-	Dihydroxy-fumaric acid	2-oxo-3,4,4-trihydroxy-3E-butenoic acid	<a href="#">54678503</a>	C <sub>4</sub> H <sub>4</sub> O <sub>6</sub>
<a href="#">2032</a>	<a href="#">67</a>	Oxaloacetic acid	2-oxo-butanedioic acid	<a href="#">970</a>	C <sub>4</sub> H <sub>4</sub> O <sub>5</sub>
<a href="#">2033</a>	<a href="#">43</a>	Oxoadipic acid	2-oxo-hexanedioic acid	<a href="#">71</a>	C <sub>6</sub> H <sub>8</sub> O <sub>5</sub>
<a href="#">2298</a>	<a href="#">7</a>	2-oxo-octadecanoic acid	2-oxo-octadecanoic acid	<a href="#">439332</a>	C <sub>18</sub> H <sub>34</sub> O <sub>3</sub>
<a href="#">37082</a>	<a href="#">38</a>	Glyoxylic acid	2-oxoacetic acid	<a href="#">760</a>	C <sub>2</sub> H <sub>2</sub> O <sub>3</sub>
<a href="#">37133</a>	<a href="#">69</a>	Phenylpyruvic acid	2-oxo-3-phenylpropanoic acid	<a href="#">997</a>	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>

Page 1 of 2

Log in / Register

grep:^2-oxo.+ acid\$

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

Keyword Search | Advanced Searches | Regular expression Searches

### Regular Expression Searches

Use the 'grep:' prefix to perform a regular expression (grep) search

Both common name and systematic name will be searched in the metabolite database (case insensitive)

#### Examples

grep:pc(+/.+:1

grep:2-oxo.+ acid\$

grep:cer(+16:0)

grep:^cer(+1[0-9]:0)

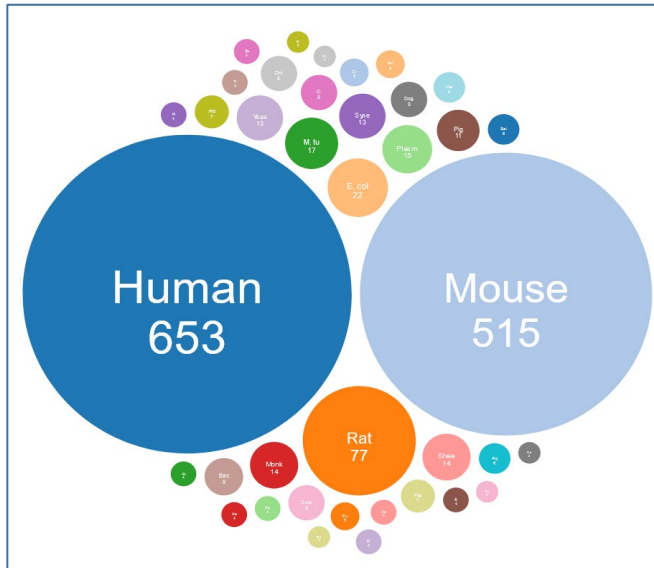
grep:p[ie]-cer(+16:0)

grep:^Gly.+chol.+ acid\$

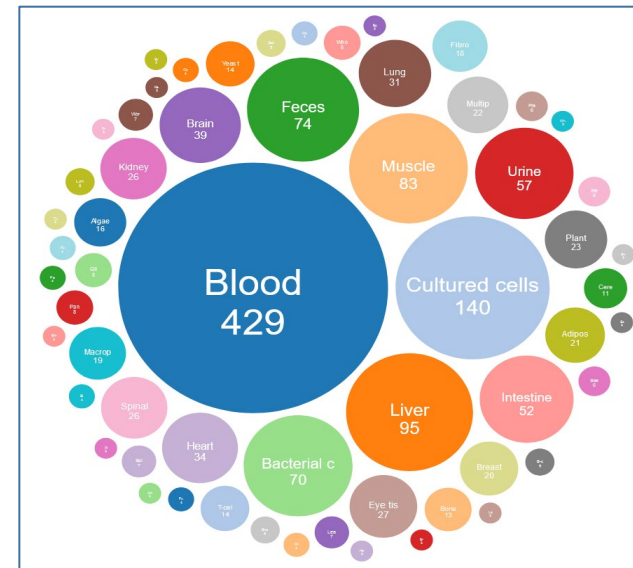
grep:Pip[a-z]+one\$

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

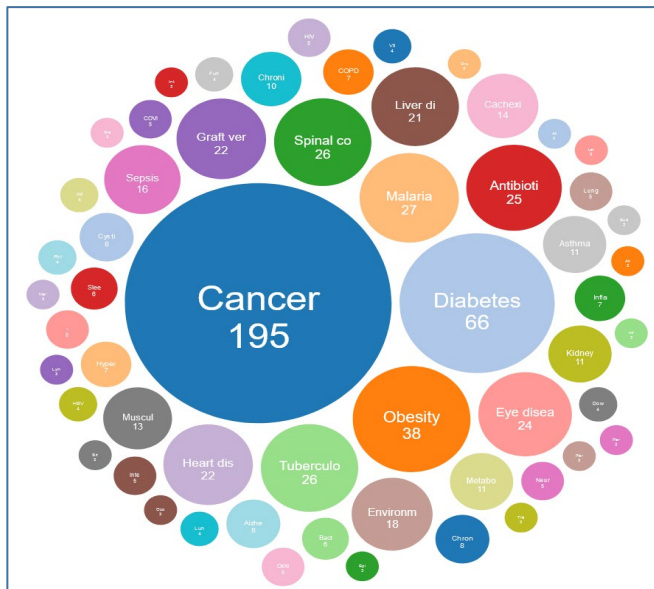
Species



Sample source



Disease



Metabolite class



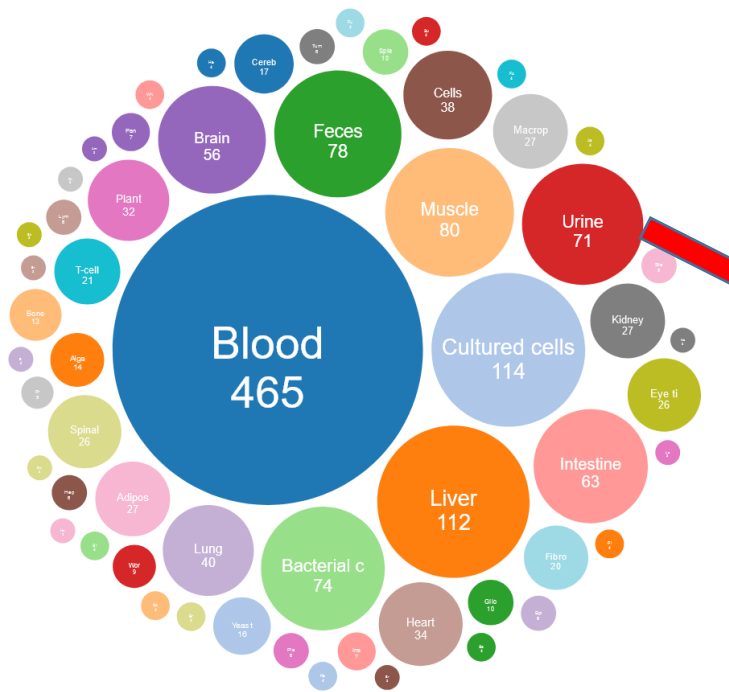


# MW Usability: Bubble chart access to key NMDR study search parameters (Species, disease, sample source, metabolic pathways, metabolite classes)

## Select Sample source link

Sample Source Species class Species Disease Human pathways Metabolite class

Sample source: Minimum studies:  Chart size:  Color scheme:



**Sample source data (All studies)**

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

Click on "Urine" bubble

## 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)

List of all studies with urine as a sample source

Studies involving sample source:Urine

Study ID	Study Title	Species	Institute
ST000020	Biomarker Discovery in Knee Osteoarthritis (I)	Human	University of North Carolina
ST000022	Biomarker Discovery in Knee Osteoarthritis (II)	Human	University of North Carolina
ST000029	Metabolites Involved in Early Life Antibiotic Exposures(DaraSTAT-Urine)	Mouse	University of North Carolina
ST000037	Metabolomics Involved in Early Life Antibiotic Exposures(EstroSTAT-Urine)	Mouse	University of North Carolina
ST000050	Preterm Neonatal Urinary Renal Developmental and acute kidney injury Metabolomic Profiling	Human	University of North Carolina
ST000059	A statistical analysis of the effects of urease pre-treatment on the measurement of the urinary metabolome by gas chromatography/mass spectrometry	Human	Pacific Northwest National Laboratory
ST000231	Quick Comparison of Urine Metabolites in Human and SD Rats of Different Sex by Untargeted UPLC-TOFMS and In-house Software Platform	Human	Beijing Institute of Radiation Medicine
ST000239	Quick Comparison of Urine Metabolites in Human and SD Rats of Different Sex by Untargeted UPLC-TOFMS and In-house Software Platform	Rat	Beijing Institute of Radiation Medicine
ST000259	Signal Intensities Derived from Different NMR Probes and Parameters Contribute to Variations in Quantification of Metabolites	Human	University of Michigan
ST000291	LC-MS Based Approaches to Investigate Metabolic Differences in the Urine of Young Women after Drinking Cranberry Juice or Apple Juice	Human	University of Florida
ST000329	Minimal change disease and focal segmental sclerosis in urine	Human	University of California, Davis
ST000381	Urinary Metabolites in ICPBS Diagnosis (part I)	Human	University of California, Davis
ST000382	Urinary Metabolites in ICPBS Diagnosis (part II)	Human	University of California, Davis
ST000398	Metabolic profiling of maternal urine can aid clinical management of Gestational Diabetes Mellitus (GDM)	Human	University of Aveiro
ST000444	Preconcentration of organic solutes in urine by bubble bursting	Human	V.I. Kulakov Research Center for Obstetrics, Gynecology and Perinatology
ST000559	Urine metabolomic profiling of diabetic nephropathy in the streptozotocin induced type-1 diabetes mouse model	Mouse	RTI International
ST000573	Exploratory research on first and second trimester urinary metabolic profiles and fetal growth restriction	Human	Mayo Clinic
ST000603	Urinary Volatile Compound, Associated with Chronic Inflammation in Interstitial Cystitis	Human	University of California, Davis
ST000611	Relative level of inosine/adenosine and sarcosine	Human	Baylor College of Medicine
ST000615	GC-MS measurement of sarcosine in urine samples	Human	Baylor College of Medicine
ST000628	TCA Cycle Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from 20 Participants of the DASH2 Clinical Trial (part I)	Human	Mayo Clinic
ST000629	Amino Acid Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from 20 Participants of the DASH2 Clinical Trial (part II)	Human	Mayo Clinic
ST000630	Neurotransmitter Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from 20 Participants of the DASH2 Clinical Trial (part III)	Human	Mayo Clinic
ST000631	TCA Cycle Metabolites of Dietary Salt Effects on Blood Pressure in Rat Urine (part IV)	Rat	Mayo Clinic
ST000632	Amino Acid Metabolites of Dietary Salt Effects on Blood Pressure in Rat Urine (part V)	Rat	Mayo Clinic
ST000633	Neurotransmitter Metabolites of Dietary Salt Effects on Blood Pressure in Rat Urine (part VI)	Rat	Mayo Clinic
ST000634	TCA Cycle Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from DASH2 Clinical Trial (part VII)	Human	Mayo Clinic
ST000635	Amino Acid Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from DASH2 Clinical Trial (part VIII)	Human	Mayo Clinic
ST000636	Neurotransmitter Metabolites of Dietary Salt Effects on Blood Pressure in Human Urine from DASH2 Clinical Trial (part IX)	Human	Mayo Clinic
ST000786	N-acetylputrescine-g lactam Identification	Human	Colorado State University
ST000891	NMR comparison of urine samples by 1D NOESY presat and PURGE	Human	University of Georgia
ST000901	Murine vitamin A deficiency results in a hypermetabolic state and alterations in bacterial community structure and metabolism (Urine)	Mouse	Pennsylvania State University
ST000917	Biomarkers of NAFLD progression: a lipidomics approach to an epidemic. Part 3:Urine	Human	LIPID MAPS
ST000922	Crab Urine Study	Crab	Georgia Institute of Technology
ST000934	Metabolome profiles in urogenital schistosomiasis and associated pathologies	Human	University of Ibadan, Nigeria
ST000973	Metabolome profiles in urogenital schistosomiasis and associated pathologies (part II)	Human	University of Ibadan, Nigeria
ST001039	Denver Asthma Panel Study-CHEAR Ancillary Study (part II)	Human	Emory University
ST001047	1H-NMR urinary metabolomic profiling for diagnosis of gastric cancer.	Human	University of Alberta
ST001048	Pediatric Inner-City Environmental Exposures at School and Home and Asthma Study	Human	ICahn School of Medicine at Mount Sinai
ST001069	Evaluation of Seryl-leucine core 1 O-glycosylated peptide (SLC1G) in TB patient urine	Human	Colorado State University

Click on "Urine" link

# Text search on NMDR studies/projects

## Data/metadata in experimental projects/studies

### Search specific data fields

Subject type:

Species:

Project or study title:

Institution:

Year submitted:

Analysis type:

### Additional MS parameters:

MS type:

MS ion mode:

MS instrument type:

MS instrument name:

Display by:

## Browse and Search Studies

### • Browse

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

### • Search

- **Experimental Projects / Studies**
- [MetStat: Perform meta-analysis on named metabolites across all studies: Refine by analysis type, species, sample source, disease association, metabolite classification and biochemical pathway](#)
- [Select Studies by species, sample source or disease association](#)
- [Search data/metadata in experimental projects/studies](#)
- [Search Untargeted MS data by m/z, retention time, instrumentation](#)
- **REST service**
- [Use the Metabolomics Workbench REST service to retrieve different types of data](#)

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

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

# Text search on NMDR metadata (all sections)

Data/metadata in experimental projects/studies

**Search specific data fields**

Subject type:

Species:

Project or study title:

Institution:

Year submitted:

Analysis type:


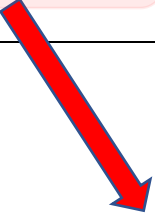
Display by:

**Search all experimental metadata fields**

Text query

## Browse and Search Studies

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



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

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

## Browse and Search Studies

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

**Search untargeted MS data on the Metabolomics Workbench**

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

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

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

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

Results for untargeted MS search on m/z:657.485 (+/-0.01) POSITIVE mode									
Details	Name	m/z	RT	RT_Units	Study	Ion_mode	MS_Instrument	MS_Inst_Type	Chromatography
AN001527		657.4762	1.03	Minutes	ST000932	POSITIVE	Agilent 6220 TOF	TOF	Normal phase
AN001064		657.4765	23.5	Minutes	ST000689	POSITIVE	Agilent 6530 QTOF	QTOF	Reversed phase
AN001532		657.4779	1.02	Minutes	ST000935	POSITIVE	Agilent 6220 TOF	TOF	Normal phase
AN002964		657.4785	22.27	Minutes	ST001828	POSITIVE	Agilent 6445 Q-TOF	QTOF	Reversed phase
AN000806		657.4801	16.34	Minutes	ST000528	POSITIVE	Thermo Orbitrap	Orbitrap	Reversed phase
AN003044		657.48059	2.92	Minutes	ST001882	POSITIVE	Thermo Q Exactive HF hybrid Orbitrap	Orbitrap	Reversed phase
AN000806		657.4806	21.25	Minutes	ST000528	POSITIVE	Thermo Orbitrap	Orbitrap	Reversed phase
AN003049		657.48176	2.16	Minutes	ST001885	POSITIVE	Thermo Orbitrap ID-X tribrid	Orbitrap/ion trap	Reversed phase
AN003049		657.48183	2.48	Minutes	ST001885	POSITIVE	Thermo Orbitrap ID-X tribrid	Orbitrap/ion trap	Reversed phase
AN000627		657.4820	4.4	Minutes	ST000391	POSITIVE	Agilent 6530A QTOF	QTOF	HILIC
AN000741		657.4824	16.31	Minutes	ST000476	POSITIVE	Orbitrap	Orbitrap	Reversed phase
AN000808		657.4836	16.2	Minutes	ST000530	POSITIVE	Thermo Orbitrap	Orbitrap	Reversed phase
AN001776		657.4841	51.5	Seconds	ST001091	POSITIVE	Thermo Fusion Tribrid Orbitrap	Orbitrap/ion trap	HILIC
AN000953		657.4848	46.54	Minutes	ST000621	POSITIVE	Waters Synapt G2 S QTOF	QTOF	Reversed phase
AN000627		657.4850	2.4	Minutes	ST000391	POSITIVE	Agilent 6530A QTOF	QTOF	HILIC
AN001516		657.4850	9.08	Minutes	ST000923	POSITIVE	Thermo Q Exactive Plus Orbitrap	Orbitrap	Reversed phase
AN001436		657.4853	8.87	Minutes	ST000880	POSITIVE	Thermo Q Exactive Plus Orbitrap	Orbitrap	Reversed phase
AN000347		657.4853	20.14	Minutes	ST000232	POSITIVE	Thermo Q Exactive Orbitrap	Orbitrap	Reversed phase
AN001609	DG (36:3) [M+K] <sup>+</sup>	657.4854	6.59	Minutes	ST000983	POSITIVE	Agilent 6530 QTOF	QTOF	Reversed phase
AN001610	DG (36:3) [M+K] <sup>+</sup>	657.4854	6.59	Minutes	ST000984	POSITIVE	Agilent 6530 QTOF	QTOF	Reversed phase
AN001611	DG (36:3) [M+K] <sup>+</sup>	657.4854	6.59	Minutes	ST000985	POSITIVE	Agilent 6550 QTOF	QTOF	Reversed phase
AN001612	DG (36:3) [M+K] <sup>+</sup>	657.4854	6.59	Minutes	ST000986	POSITIVE	Agilent 6560 Ion Mobility	QTOF	Reversed phase
AN001613	DG (36:3) [M+K] <sup>+</sup>	657.4854	6.59	Minutes	ST000987	POSITIVE	Leco Citius LC-HRT	QTOF	Reversed phase