Metabolomics Workbench and the National Metabolomics Data Repository

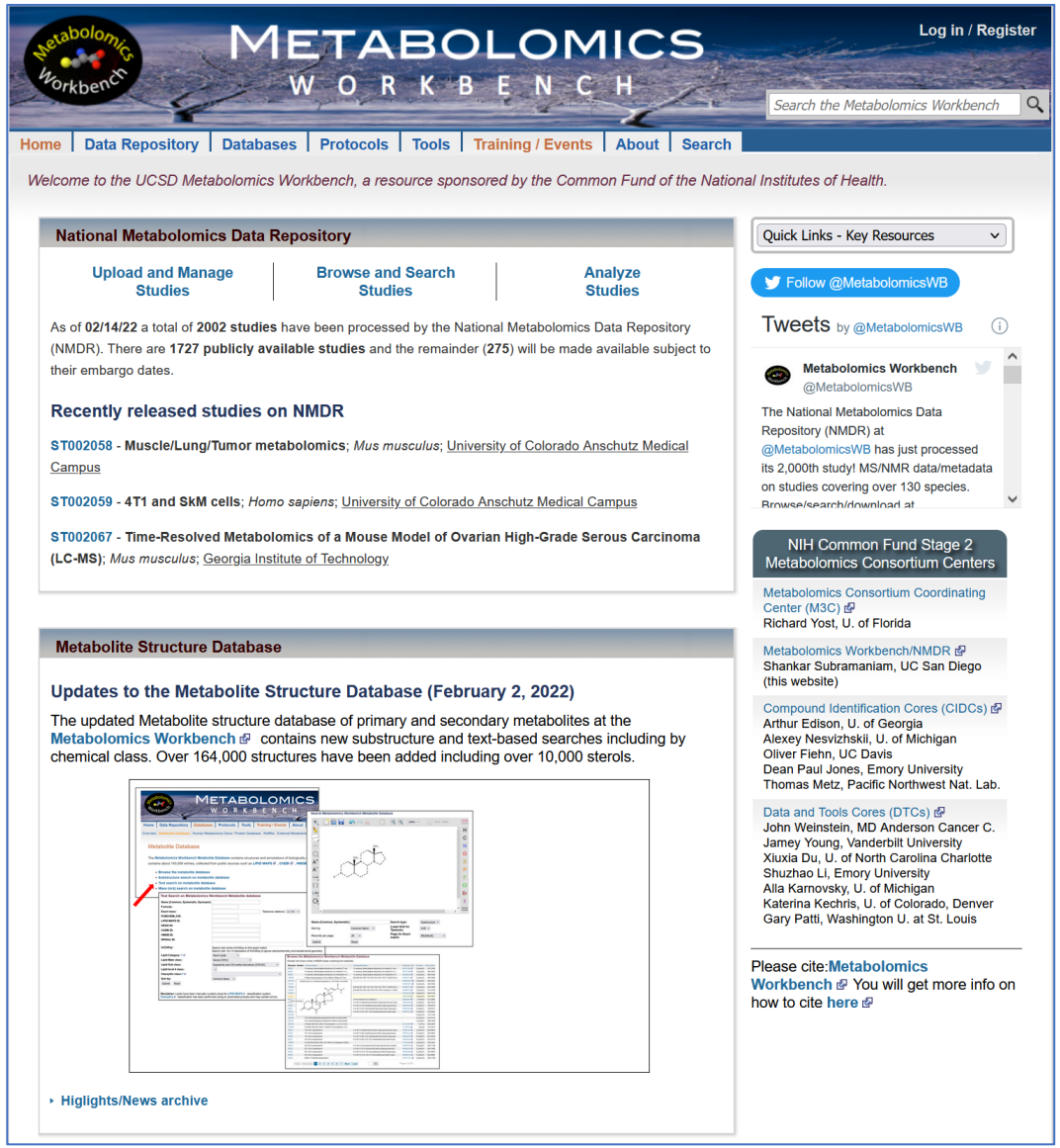
University of California San Diego
and
San Diego Supercomputer Center

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)



Metabolomics Workbench Data Portal: Studies

Default sorting order is by most recently released study

Browse and Search Studies

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

Summary of all studies

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

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

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

Metabolomics Workbench Data Portal:Projects

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

Browse and Search Studies

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  - MetStat: View most frequently encountered metabolites in NMDR (mapped to RefMet)

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: 15

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

Summary of all studies in project PR001288

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

NMDR:Study-level view contains multiple metadata sections

Summary of study ST001140

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

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

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

Select appropriate tab below to view additional metadata details:

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

← View Metadata

Example: Analysis section

Combined analysis:

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

Study-level view : Show named metabolites and measurements

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	rsity of Zurich
	G);Vetsuisse Faculty, University of Zurich

Return to study ST001140 main page

Analysis: Phospholipids, Chol. esters and Diacylglycerols

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

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

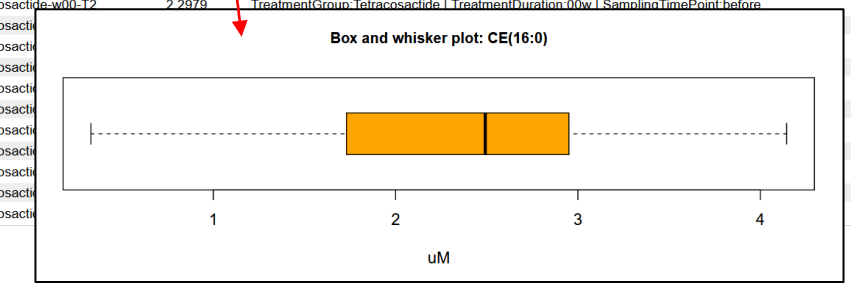
Select a metabolite (checkbox)

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

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

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

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



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

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

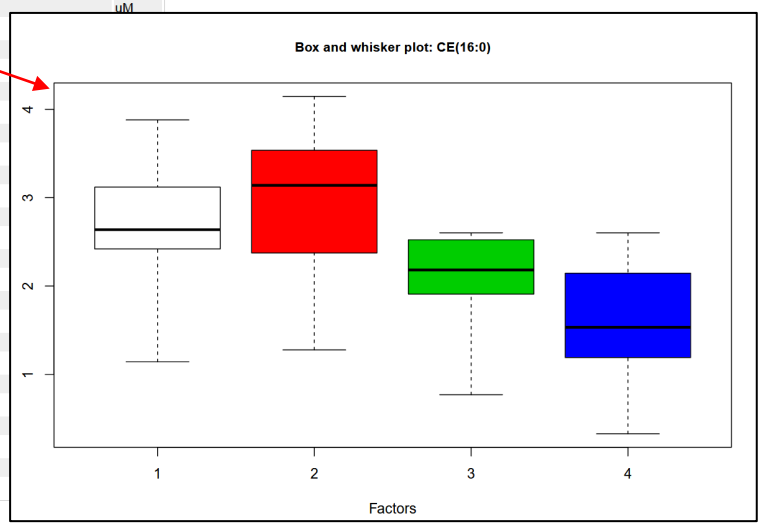
(Green: p value<=0.05)

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

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

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

Green: p-value <= 0.05



NMDR:Study-level view/download options

Summary of study ST001140

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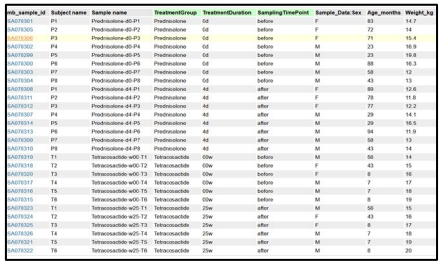
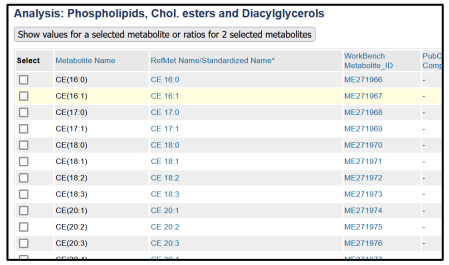
Select appropriate tab below to view additional metadata details:

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

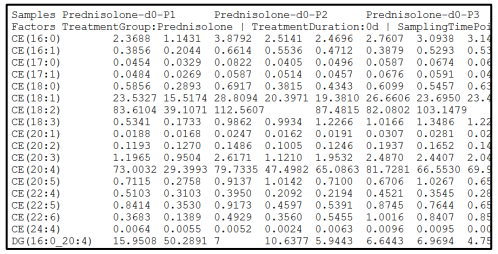
View Metadata



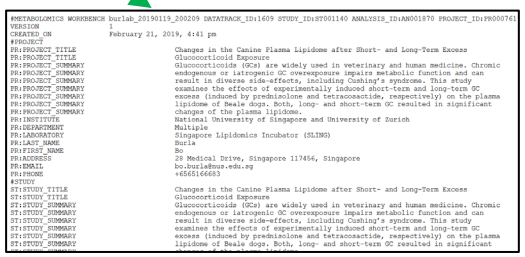
Samples/study design



Named metabolites



Download dataset



Download mwTab (text)

Download mwTab (json)

NMDR: raw data view/download

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

Download data

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

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

} Download compressed raw files

ST001738: Archive File:ST001738_ccms_peak_identification.zip

Archive: .test/Studies/ST001738_ccms_peak_identification.zip

Length	Date	Time	Name
135568928	04-12-2021	16:42	Polar_Fusion_NEG_SAT_ob_1.mzML
134904804	04-12-2021	16:42	Polar_Fusion_NEG_SAT_ob_2.mzML
134393660	04-12-2021	16:43	Polar_Fusion_NEG_SAT_ob_3.mzML
134892339	04-12-2021	16:43	Polar_Fusion_NEG_SAT_ob_4.mzML
135015899	04-12-2021	16:43	Polar_Fusion_NEG_SAT_ob_5.mzML
134443440	04-12-2021	16:43	Polar_Fusion_NEG_SAT_ob_6.mzML
135875506	04-12-2021	16:43	Polar_Fusion_NEG_VAT_ob_1.mzML
134398714	04-12-2021	16:43	Polar_Fusion_NEG_VAT_ob_2.mzML
134824391	04-12-2021	16:44	Polar_Fusion_NEG_VAT_ob_3.mzML
135063431	04-12-2021	16:44	Polar_Fusion_NEG_VAT_ob_4.mzML
134428351	04-12-2021	16:44	Polar_Fusion_NEG_VAT_ob_5.mzML
134646218	04-12-2021	16:44	Polar_Fusion_NEG_VAT_ob_6.mzML
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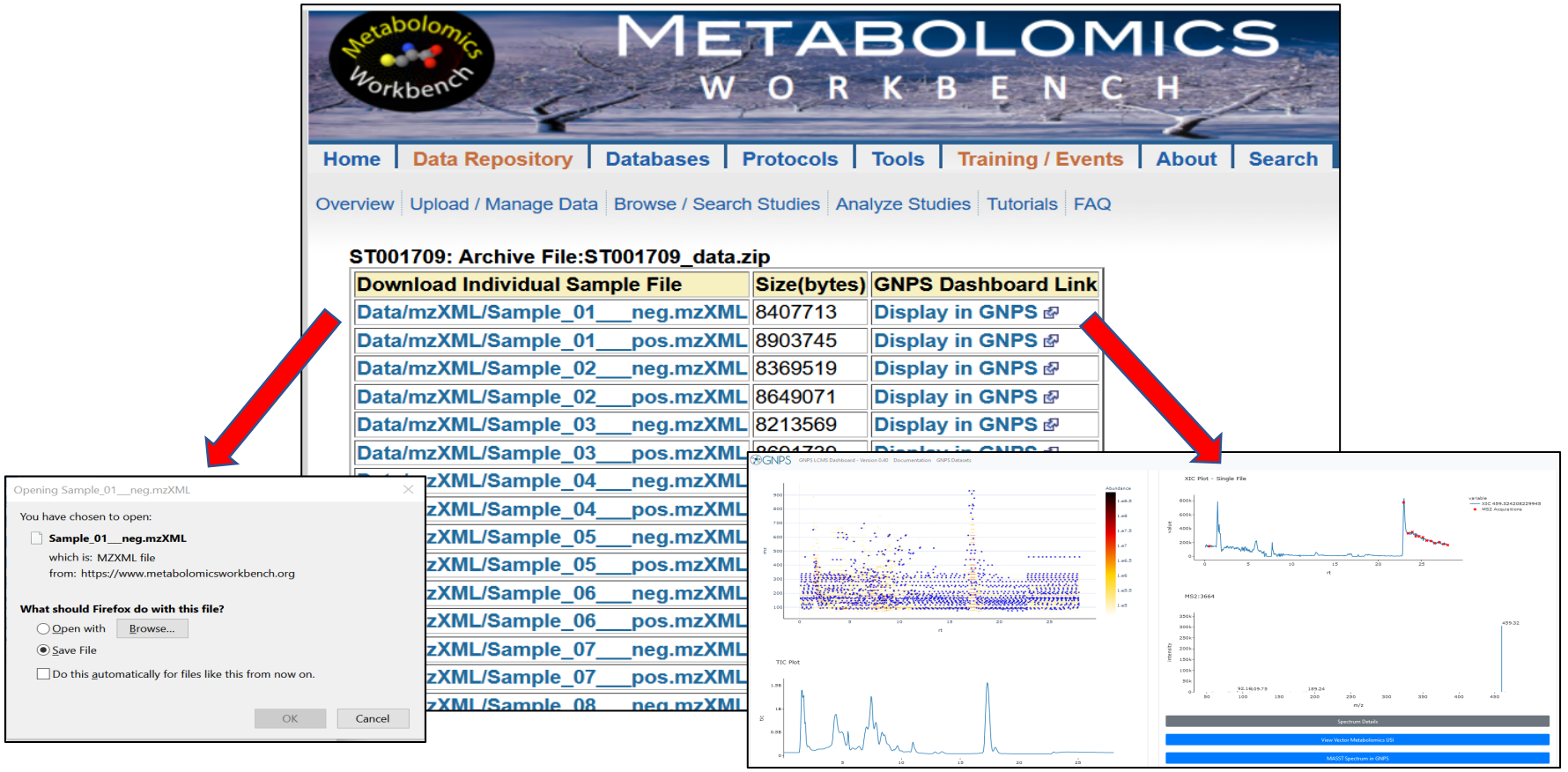
152479314	04-12-2021	16:46	Polar_Fusion_POS_VAT_ob_1.mzML
149743624	04-12-2021	16:46	Polar_Fusion_POS_VAT_ob_2.mzML

ST001738: Archive File:ST001738_ccms_peak_identification.zip

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

Collaboration with Global Natural Product Social Molecular Networking (GNPS)



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

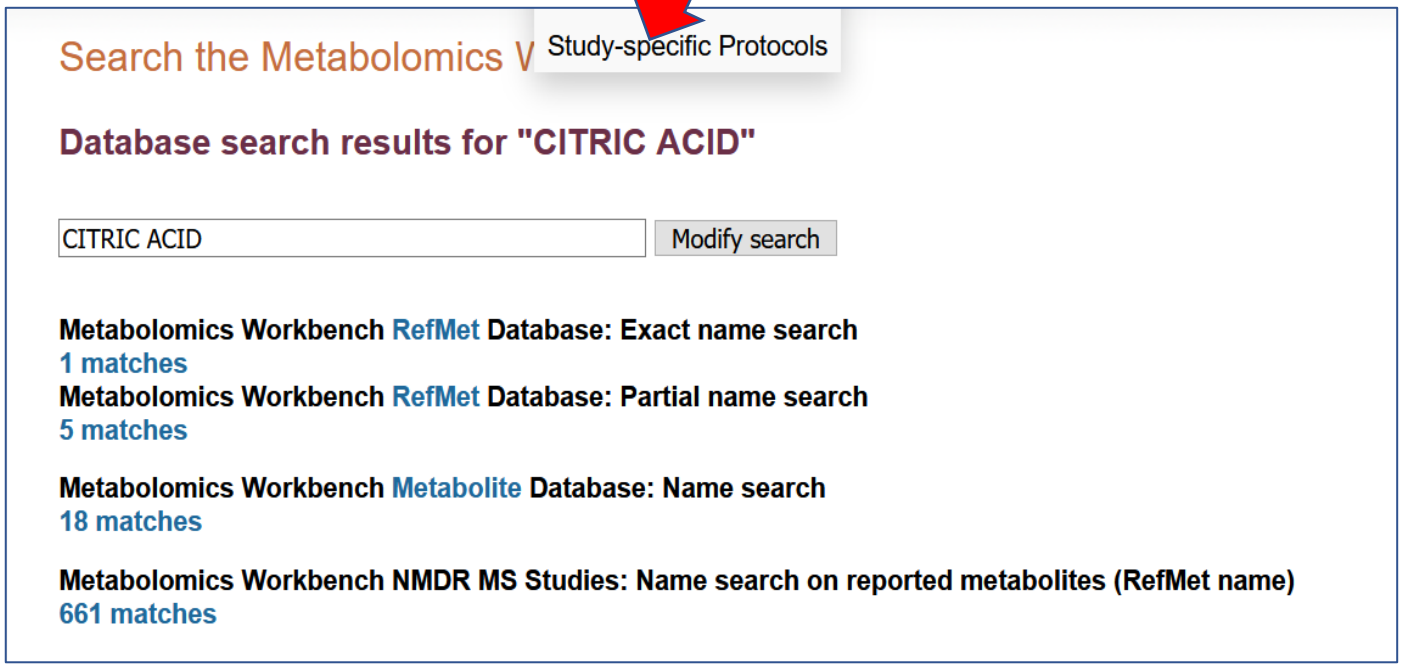
GNPS Dashboard: Collaborative Analysis of Mass Spectrometry Data in the Web Browser

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

Metabolomics Workbench Quick search

What is searched?

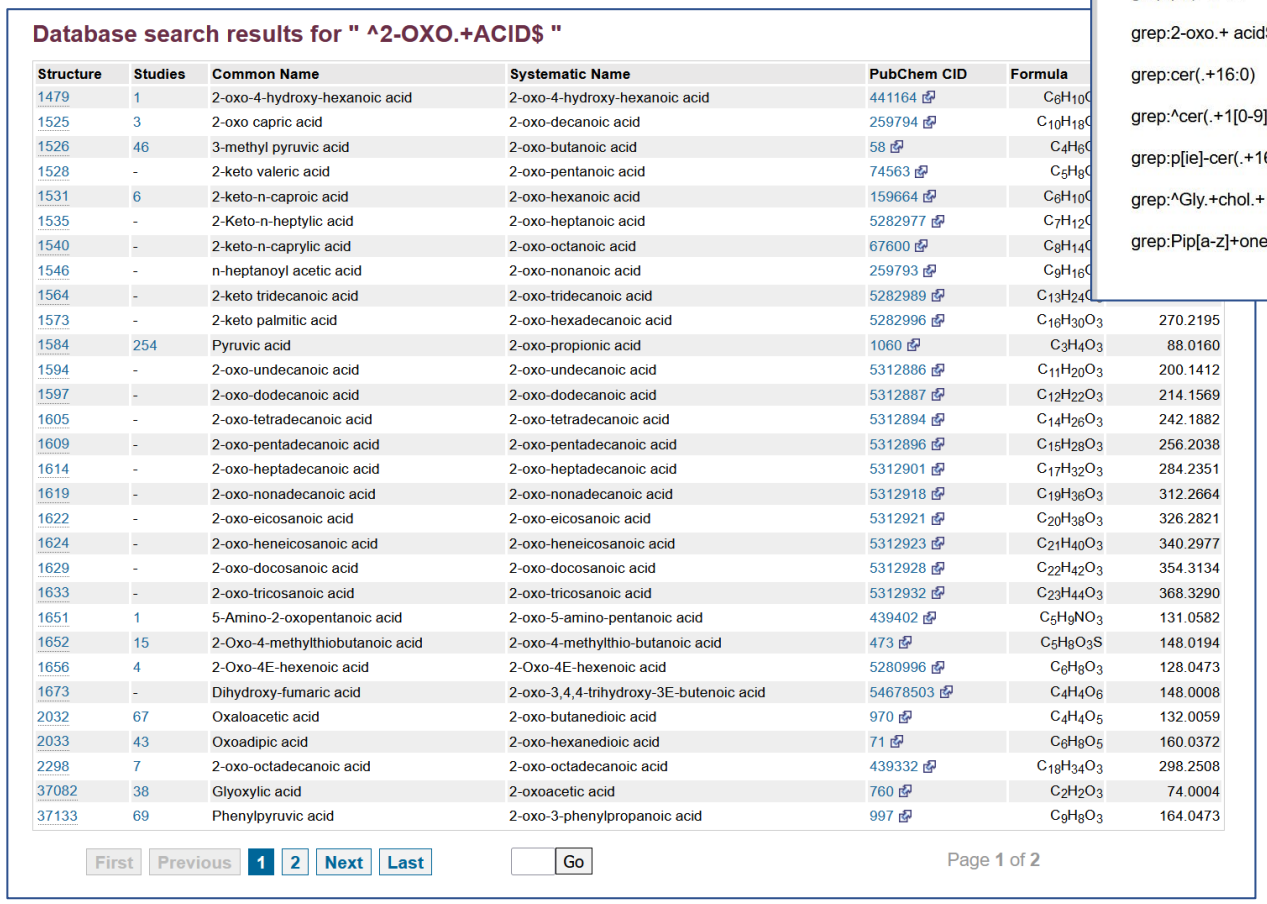
- Metabolite name
- Metabolite InChIKey
- PubChem Compound ID
- Molecular formula
- Metabolite mass (+/- 0.5 daltons)
- Metabolite class
- Study title
- NMDR Study ID
- NMDR Project ID
- NMDR studies containing that metabolite



Regular expression search

What is searched?

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



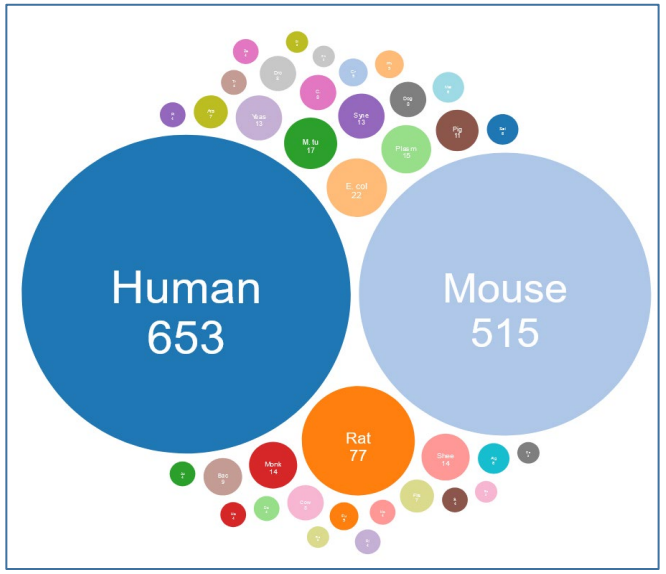
Database search results for " ^2-OXO.+ACID$ "

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

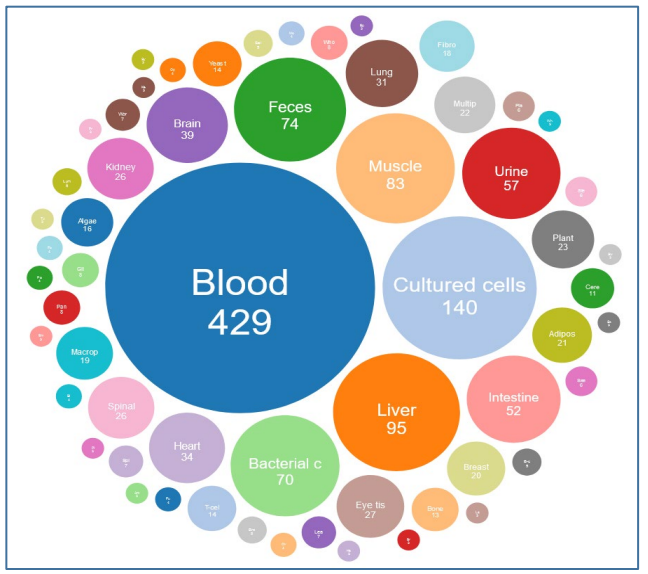
First Previous 1 2 Next Last Go Page 1 of 2

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

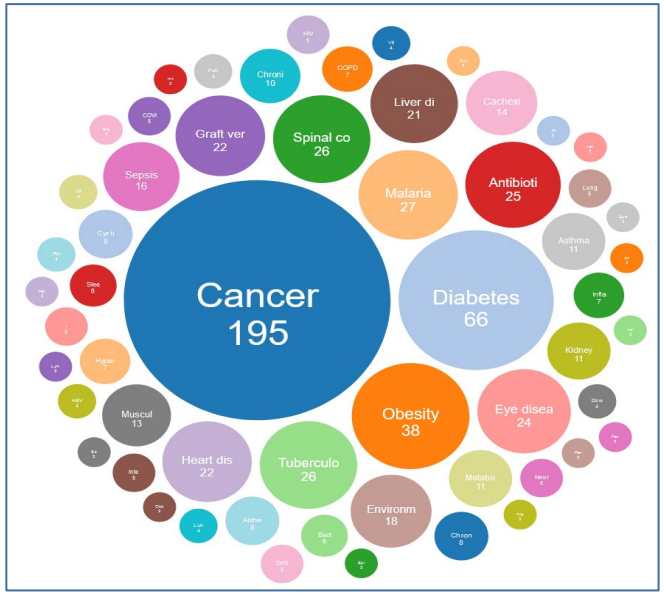
Species



Sample source



Disease



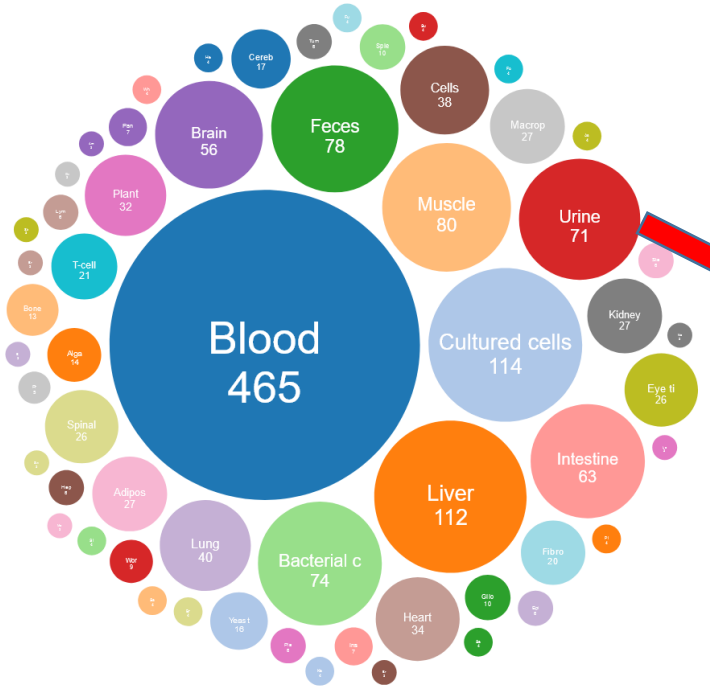
Metabolite class

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

Select Sample source link

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

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



Sample source data (All studies)

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

Browse and Search Studies

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

Click on "Urine" bubble

Click on "Urine" link

Studies involving sample source:Urine

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

List of all studies with urine as a sample source

Text search on NMDR studies/projects

Data/metadata in experimental projects/studies

Search specific data fields

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

Additional MS parameters:

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

Display by: Study

Search Reset

Browse and Search Studies

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

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

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

Text search on NMDR metadata (all sections)

Data/metadata in experimental projects/studies

Search specific data fields

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

Display by: Study

Search Reset

Search all experimental metadata fields

Text query NAFLD

Search Reset

Browse and Search Studies

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  - Select Studies by species, sample source or disease association
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  - 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

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  - Select Studies by species, sample source or disease association
  - Search data/metadata in experimental projects/studies
  - Search Untargeted MS data by m/z, retention time, instrumentation
  - REST service
  - Use the Metabolomics Workbench REST service to retrieve different types of data

Search untargeted MS data on the Metabolomics Workbench

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

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

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

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

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

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