# Metabolomics Workbench and the National Metabolomics Data Repository

University of California San Diego
and
San Diego Supercomputer Center

## MetStat summary tool

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

# MetStat Summary Statistics for experimental datasets in NMDR

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

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

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

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

Summarize by metabolite **structural class**

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

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

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

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

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

# MetStat: Summary Statistics for experimental datasets in NMDR

## View most frequently encountered metabolites in NMDR studies across all conditions

### 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

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

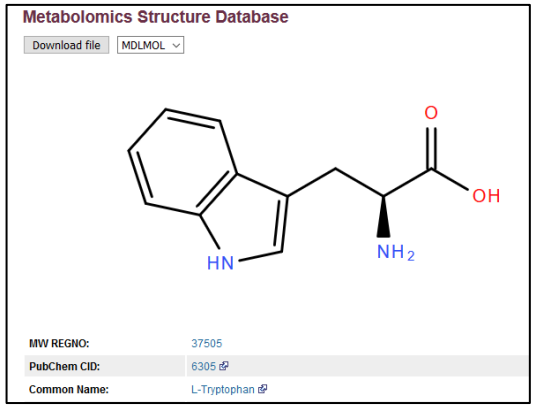
Perform detailed search (All metabolite names were mapped to RefMet nomenclature) Records to display: 200 Submit

| Refmet Name | Studies | Super Class | Main Class | Sub Class |
|---|---|---|---|---|
| Glutamic acid | 452 | Organic acids | Amino acids and peptides | Amino acids |
| Tyrosine | 441 | Organic acids | Amino acids and peptides | Amino acids |
| Phenylalanine | 437 | Organic acids | Amino acids and peptides | Amino acids |
| Glutamine | 435 | Organic acids | Amino acids and peptides | Amino acids |
| Valine | 428 | Organic acids | Amino acids and peptides | Amino acids |
| Aspartic acid | 423 | Organic acids | Amino acids and peptides | Amino acids |
| Proline | 413 | Organic acids | Amino acids and peptides | Amino acids |
| Lysine | 407 | Organic acids | Amino acids and peptides | Amino acids |
| Malic acid | 404 | Organic acids | TCA acids | TCA acids |
| Tryptophan | 395 | Organic acids | Amino acids and peptides | Amino acids |
| Methionine | 394 | Organic acids | Amino acids and peptides | Amino acids |
| Isoleucine | 392 | Organic acids | Amino acids and peptides | Amino acids |
| Alanine | 390 | Organic acids | Amino acids and peptides | Amino acids |
| Serine | 384 | Organic acids | Amino acids and peptides | Amino acids |
| Citric acid | 377 | Organic acids | TCA acids | TCA acids |
| Leucine | 371 | Organic acids | Amino acids and peptides | Amino acids |
| Threonine | 367 | Organic acids | Amino acids and peptides | Amino acids |
| Lactic acid | 365 | Organic acids | Short-chain acids | Short-chain acids |
| Succinic acid | 363 | Organic acids | TCA acids | TCA acids |
| Glycine | 354 | Organic acids | Amino acids and peptides | Amino acids |
| Histidine | 352 | Organic acids | Amino acids and peptides | Amino acids |
| Ornithine | 335 | Organic acids | Amino acids and peptides | Amino acids |
| Asparagine | 328 | Organic acids | Amino acids and peptides | Amino acids |
| Fumaric acid | 324 | Organic acids | TCA acids | TCA acids |
| Stearic acid | 320 | Fatty Acyls | Fatty acids | Saturated FA |
| Oleic acid | 319 | Fatty Acyls | Fatty acids | Unsaturated FA |
| Taurine | 313 | Organic acids | Sulfonic acids | Sulfonic acids |
| Palmitic acid | 310 | Fatty Acyls | Fatty acids | Saturated FA |
| AMP | 305 | Nucleic acids | Purines | Purine ribonucleoside monophosphates |
| Arginine | 295 | Organic acids | Amino acids and peptides | Amino acids |
| Hypoxanthine | 279 | Nucleic acids | Purines | Hypoxanthines |
| Pyroglutamic acid | 273 | Organoheterocyclic compounds | Pyrroline carboxylic acids | Pyrroline carboxylic acids |
| Oxoglutaric acid | 270 | Organic acids | TCA acids | TCA acids |
| Creatinine | 266 | Organoheterocyclic compounds | Azolines | Imidazolines |
| Glucose | 262 | Carbohydrates | Monosaccharides | Monosaccharides |
| Citrulline | 260 | Organic acids | Amino acids and peptides | Amino acids |
| LPC 16:0 | 255 | Glycerophospholipids | Glycerophosphocholines | LPC |
| Pyruvic acid | 254 | Organic acids | Short-chain acids | Short-chain acids |
| Myristic acid | 249 | Fatty Acyls | Fatty acids | Saturated FA |
| Pantothenic acid | 248 | Organic acids | Amino acids and peptides | Amino acids |
| Uric acid | 244 | Nucleic acids | Purines | Xanthines |
| Uridine | 242 | Nucleic acids | Pyrimidines | Pyrimidine ribonucleosides |
| Inosine | 239 | Nucleic acids | Purines | Purine ribonucleosides |
| Carnitine | 238 | Organic nitrogen compounds | Carnitines | Carnitines |
| Palmitoleic acid | 238 | Fatty Acyls | Fatty acids | Unsaturated FA |
| Linoleic acid | 236 | Fatty Acyls | Fatty acids | Unsaturated FA |
| Arachidonic acid | 235 | Fatty Acyls | Fatty acids | Unsaturated FA |
| Xanthine | 232 | Nucleic acids | Purines | Xanthines |

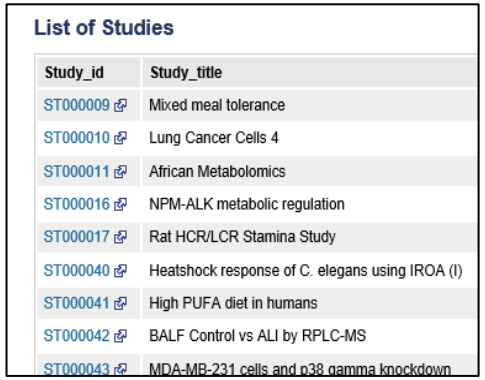
# Links to MW structure database and list of studies containing each metabolite

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

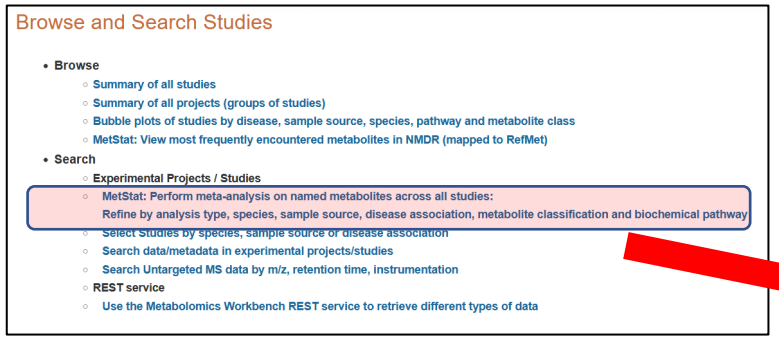
## Structure (MW database)

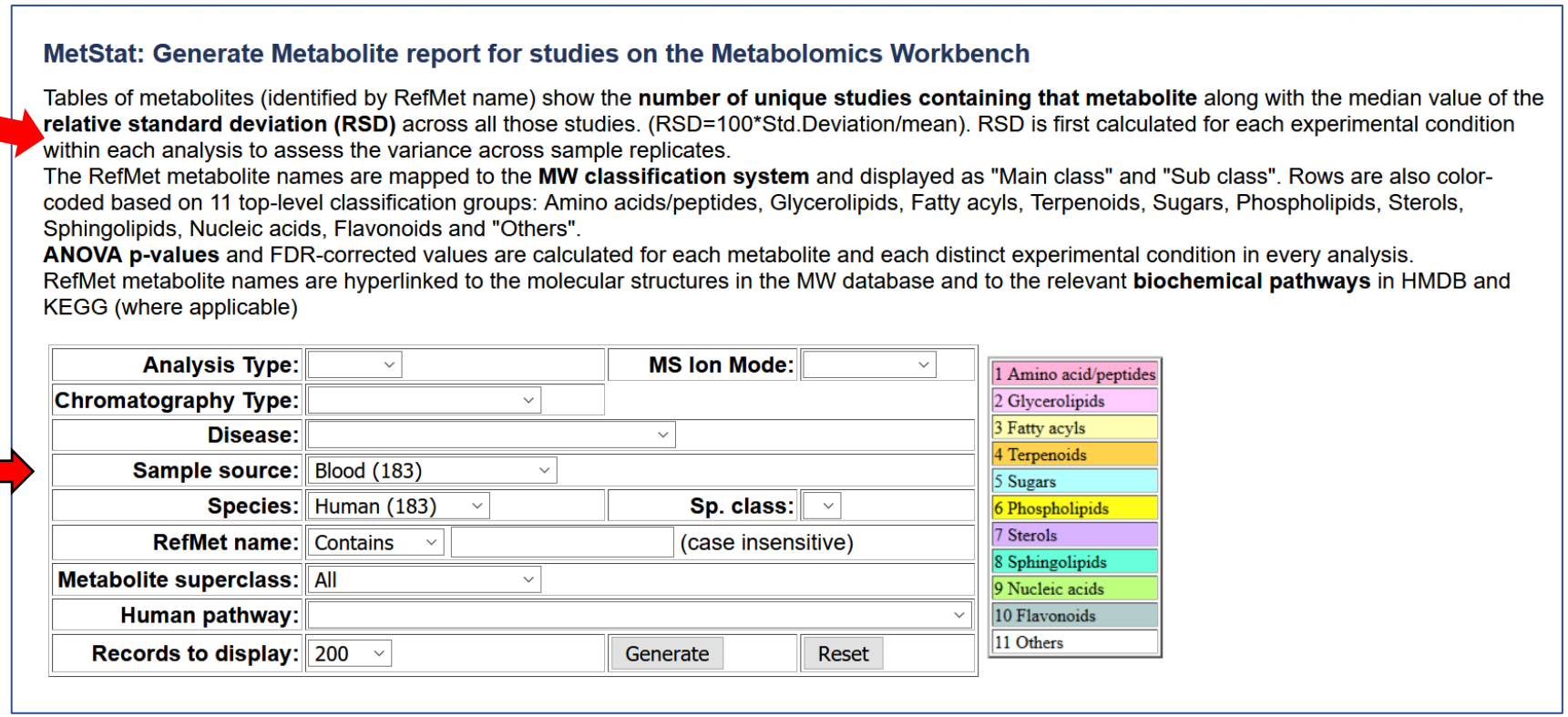



## List of Studies



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




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

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

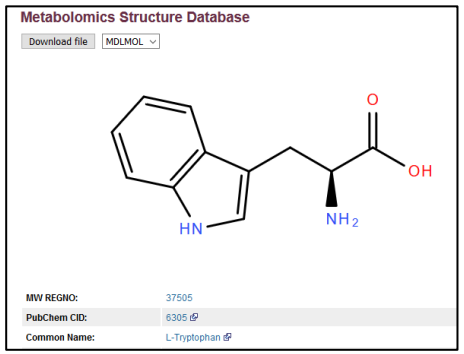
# MetStat summary table of human metabolites detected in blood

## Sorted by number of studies in which that metabolite is reported

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

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

## Structure (MW db)

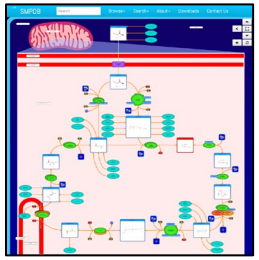


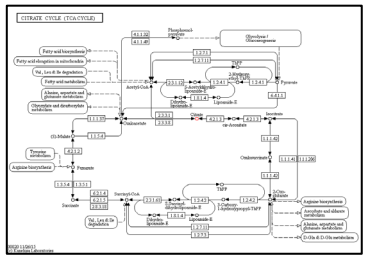

## List of Studies

**List of Studies**

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

## [P]:Human Pathways (SMP/KEGG)






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

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

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

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

| Refmet Name [Pathways] | Studies [Data Details] | RSD | Main Class | Sub Class |
|---|---|---|---|---|
| Proline [P] | 111 [Data] | 32.29 | Amino acids and peptides | Amino acids |
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| Glutamic acid [P] | 101 [Data] | 43.28 | Amino acids and peptides | Amino acids |
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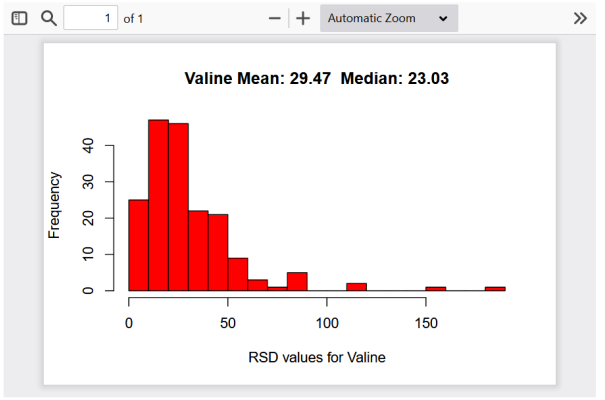
| LPC 16:0 [P] | 74 [Data] | 35.90 | Glycerophosphocholines | LPC |
| Carnitine [P] | 73 [Data] | 23.34 | Carnitines | Carnitines |

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




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

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

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

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

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

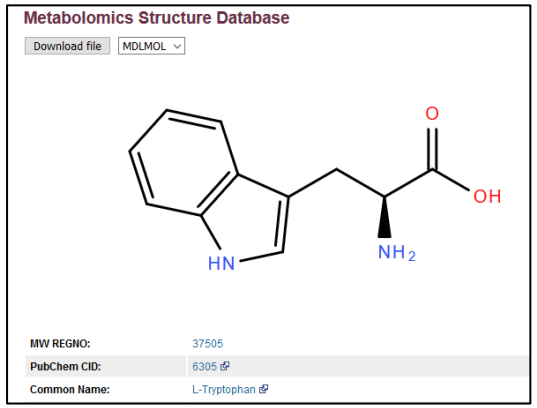
# Search summary showing metabolite name, median RSD and classification

**Search parameters: Source:Diabetes | Most significant ANOVA measurements**

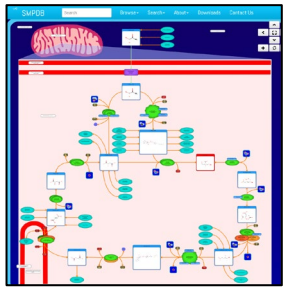
| Refmet Name [Pathways] | Studies [Data Details] | RSD | Main Class | Sub Class |
|---|---|---|---|---|
| Valine [P] | 28 [Data] | 24.34 | Amino acids and peptides | Amino acids |
| Isoleucine [P] | 27 [Data] | 28.22 | Amino acids and peptides | Amino acids |
| Tyrosine [P] | 26 [Data] | 22.18 | Amino acids and peptides | Amino acids |
| Glutamic acid [P] | 26 [Data] | 29.46 | Amino acids and peptides | Amino acids |
| Tryptophan [P] | 25 [Data] | 23.41 | Amino acids and peptides | Amino acids |
| Proline [P] | 25 [Data] | 39.10 | Amino acids and peptides | Amino acids |
| Lysine [P] | 24 [Data] | 25.48 | Amino acids and peptides | Amino acids |
| Methionine [P] | 24 [Data] | 27.08 | Amino acids and peptides | Amino acids |

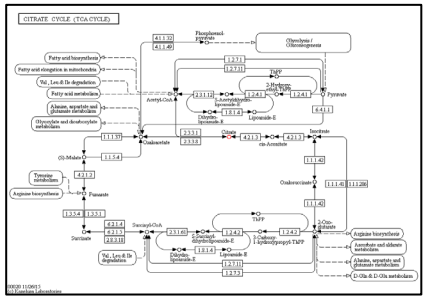
Relative standard deviation (RSD) =100*Standard deviation/mean
The RSD is calculated separately for each experimental condition within each study.
It is a measure of the variance across sample replicates

**Structure (MW db)**




**Human Pathways (SMP/KEGG)**





**List of Studies**

List of Studies

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

# List of human studies on blood that report Proline

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

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

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

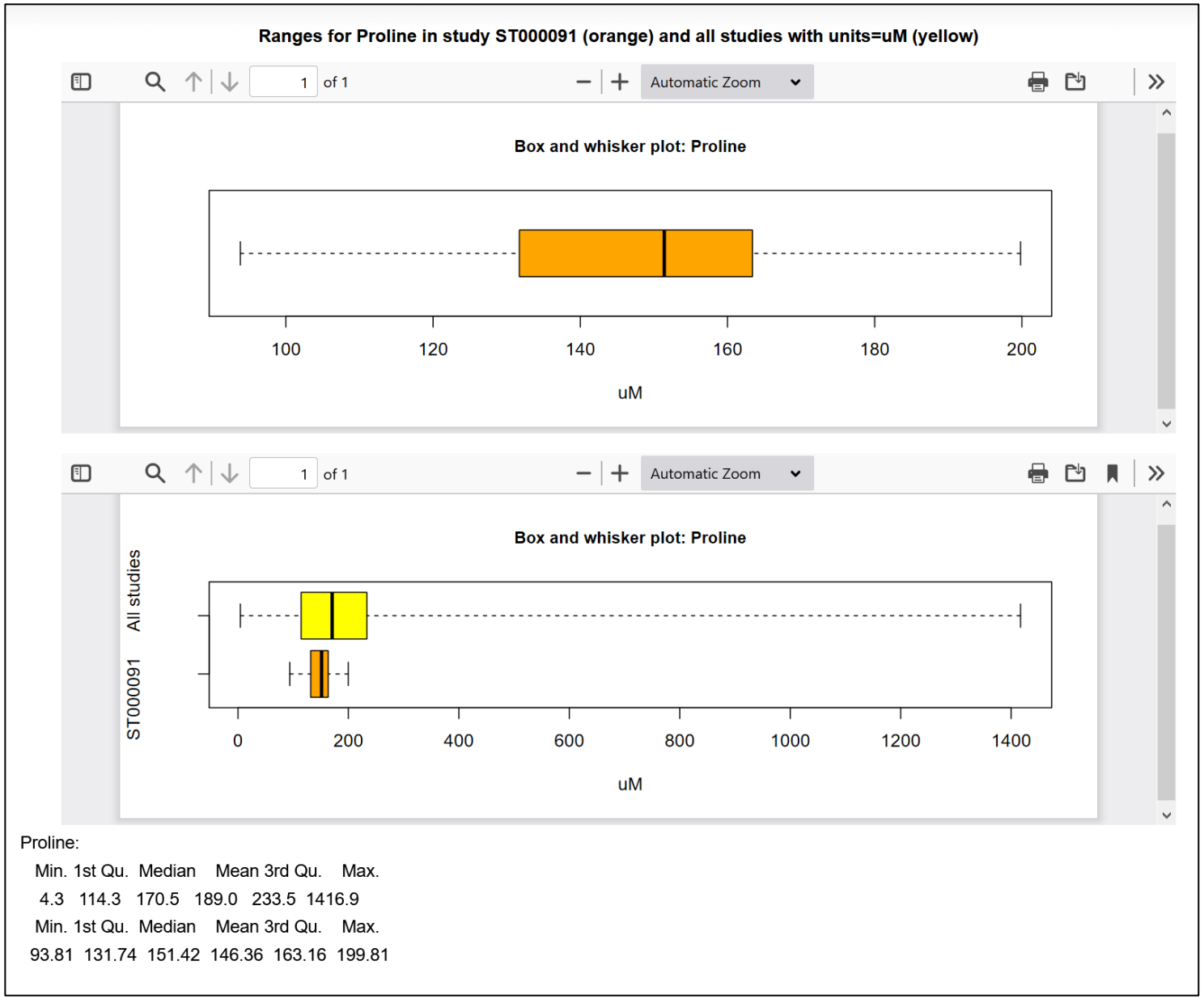
Click on a study link in the “Units(range) column

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

# Boxplot for Proline in human blood

Study ST000091

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

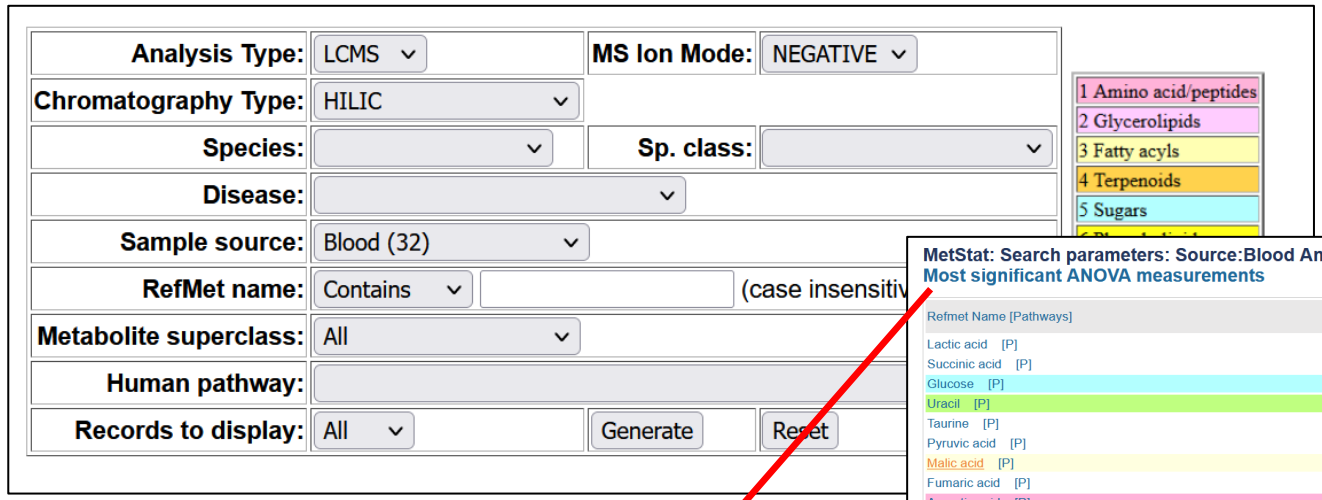


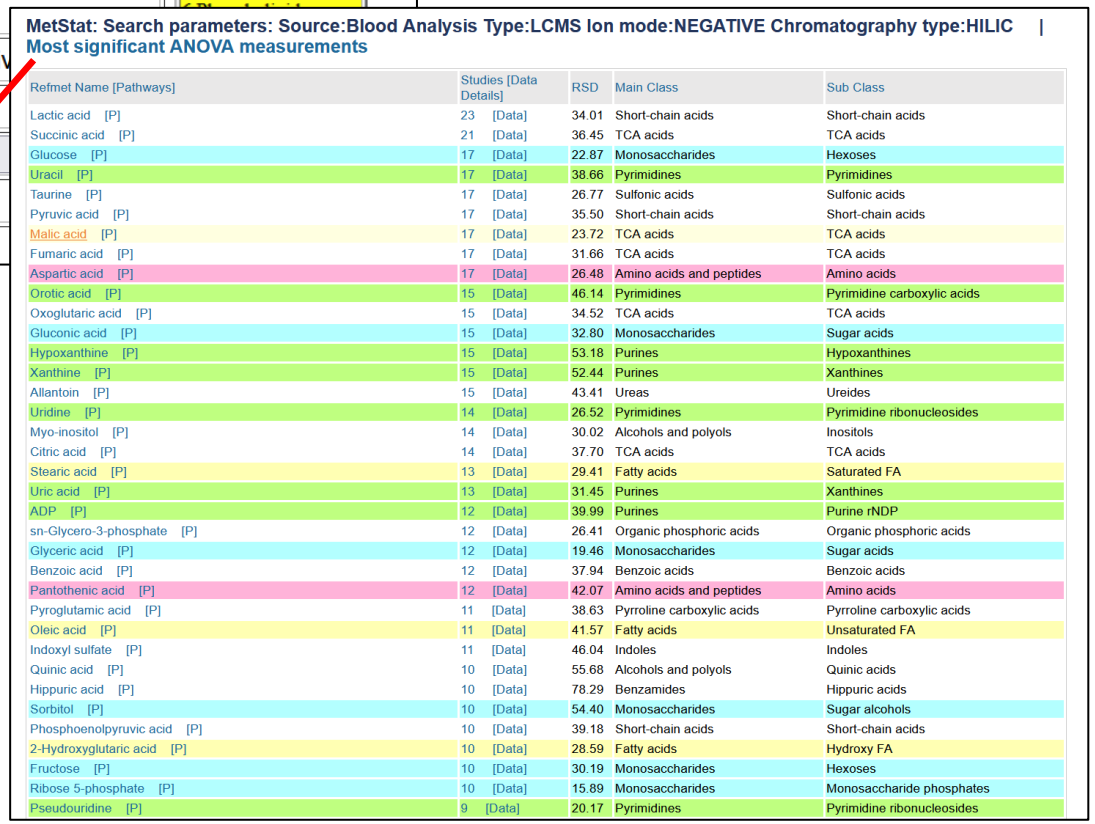

Proline:

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

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

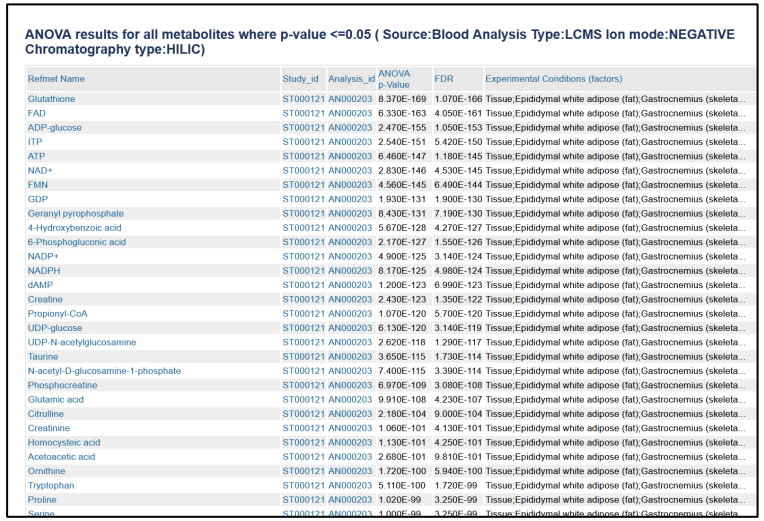
**MetStat query buider: Select criteria, e.g. species, sample source, analysis type, ion mode, disease association, metabolite class.**



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

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

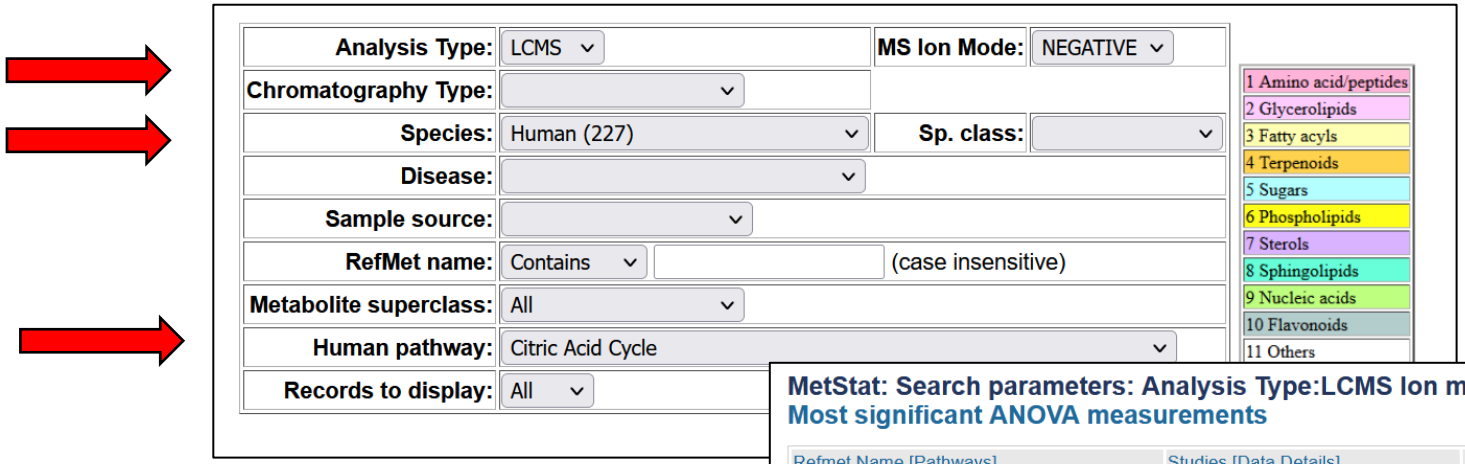


ANOVA results for all metabolites where p-value <=0.05 ( Source:Blood Analysis Type:LCMS Ion mode:NEGATIVE Chromatography type:HILIC)

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

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

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



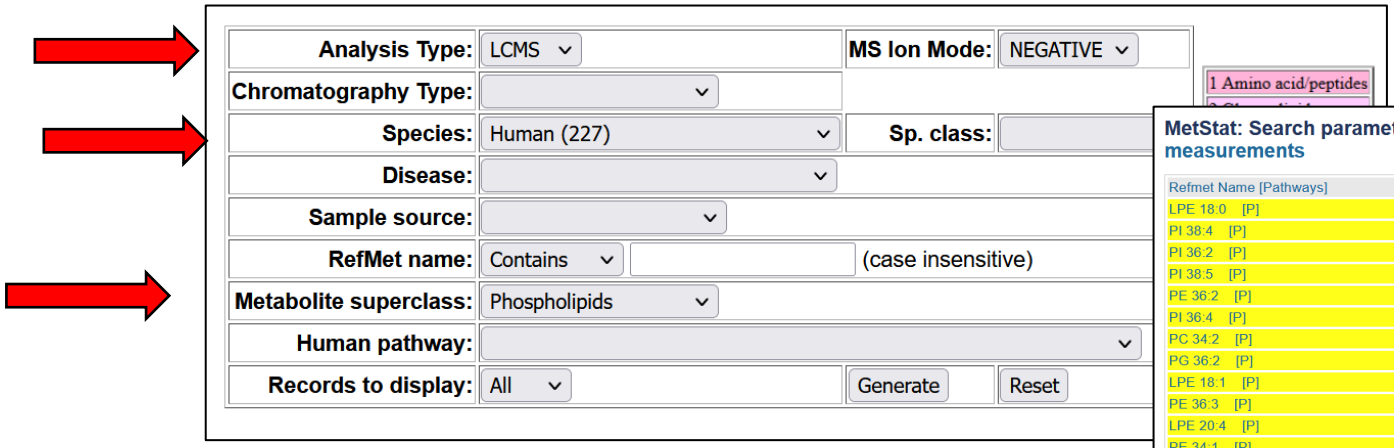

**MetStat: Search parameters: Analysis Type:LCMS Ion mode:NEGATIVE Species:Human Pathway ID:SMP00057**

**Most significant ANOVA measurements**

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

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

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




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

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

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