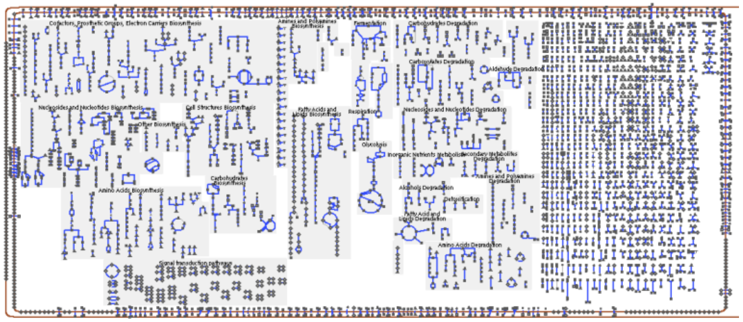
About OMICS Group

OMICS Group International is an amalgamation of Open Access publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology ‘Open Access’, OMICS Group publishes 400 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 300 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

About OMICS Group Conferences

OMICS Group International is a pioneer and leading science event organizer, which publishes around 400 open access journals and conducts over 300 Medical, Clinical, Engineering, Life Sciences, Pharma scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.



Analyzing Metabolomics Data with SmartTables

Peter D. Karp
SRI International

Overview

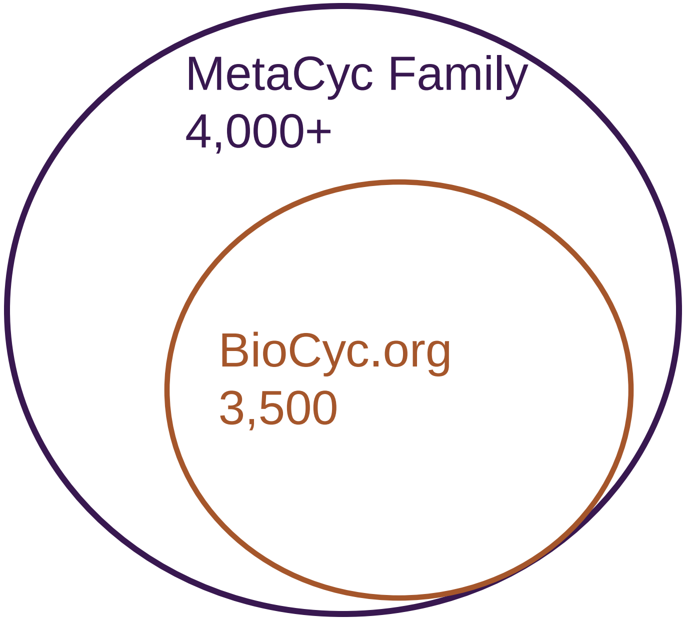
- Overview of MetaCyc family of Pathway/Genome Databases (PGDBs)
- Overview of Pathway Tools software
- SmartTables

MetaCyc Family of Pathway/Genome Databases

- 4,000+ databases from many institutions
- All domains of life with microbial emphasis
- Genomes plus predicted metabolic pathways

- DBs derived from MetaCyc via computational pathway prediction

- Common schema
- **Common controlled vocabularies**
- Managed using Pathway Tools software

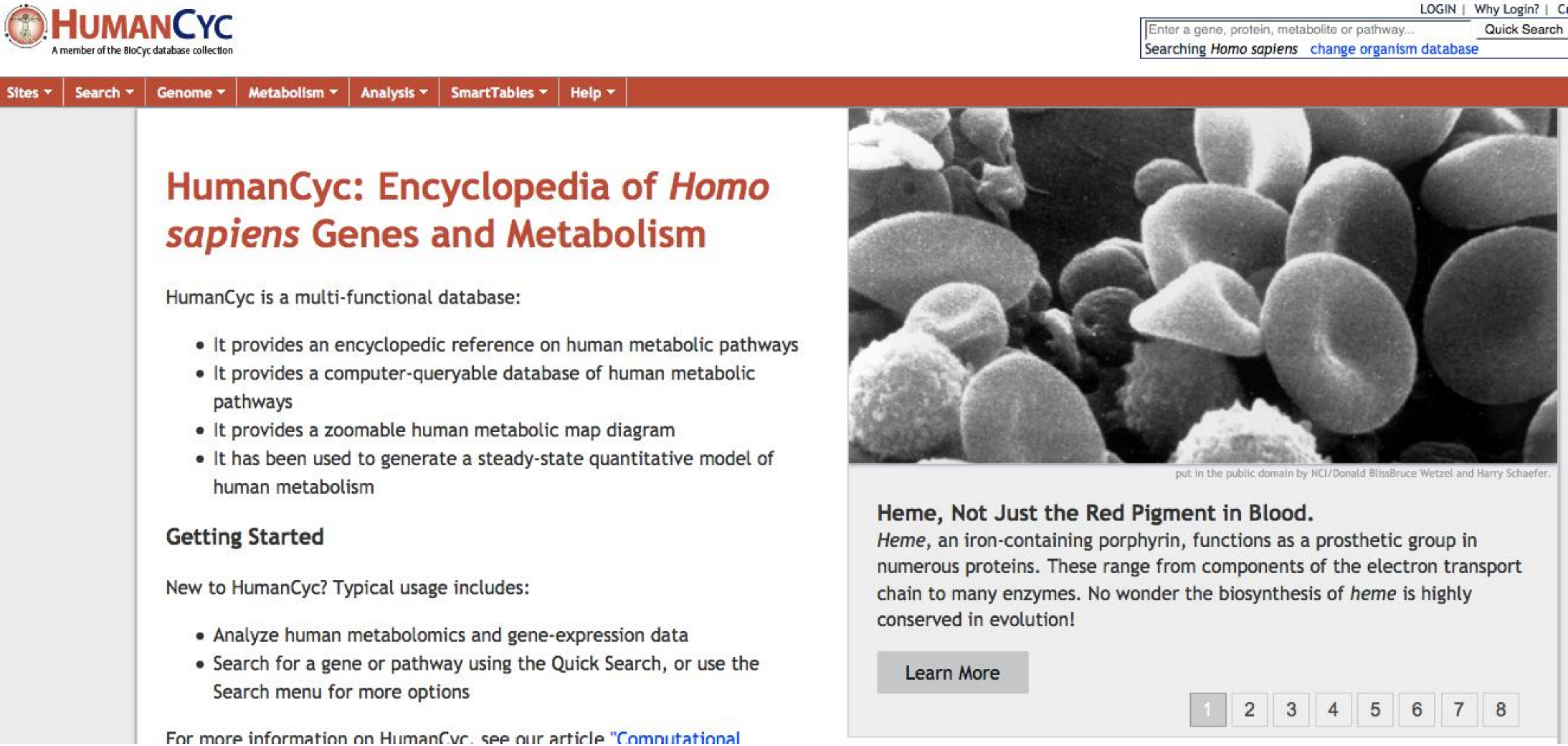


Archives of Toxicology 85:1015 2011

Curated Databases Within the MetaCyc Family

Database	Organism	Organization	Publications Curated From
MetaCyc	Multiorganism	SRI	35,000
EcoCyc	*E. coli*	SRI	25,000
HumanCyc	*H. sapiens*	SRI	
AraCyc	*A. thaliana*	TAIR/Carnegie Institution	2,282
YeastCyc	*S. cerevisiae*	SGD/Stanford/SRI	565
MouseCyc	*M. musculus*	MGD/Jackson Laboratory	

http://biocyc.org/otherpgdbs.shtml



HumanCyc: Encyclopedia of *Homo sapiens* Genes and Metabolism

HumanCyc is a multi-functional database:

- It provides an encyclopedic reference on human metabolic pathways
- It provides a computer-queryable database of human metabolic pathways
- It provides a zoomable human metabolic map diagram
- It has been used to generate a steady-state quantitative model of human metabolism

Getting Started

New to HumanCyc? Typical usage includes:

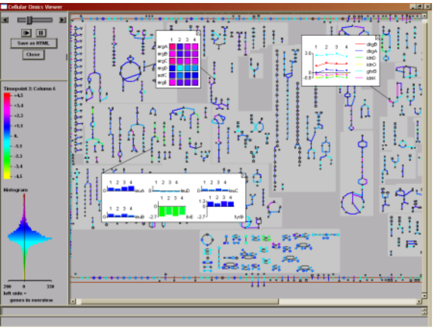
- Analyze human metabolomics and gene-expression data
- Search for a gene or pathway using the Quick Search, or use the Search menu for more options

For more information on HumanCyc, see our article "Computational

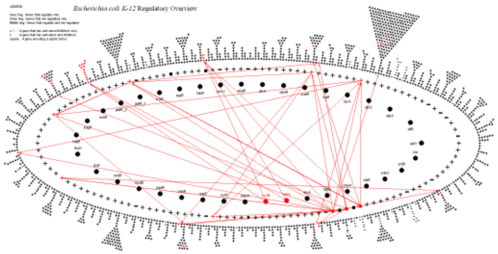
Heme, Not Just the Red Pigment in Blood.
Heme, an iron-containing porphyrin, functions as a prosthetic group in numerous proteins. These range from components of the electron transport chain to many enzymes. No wonder the biosynthesis of *heme* is highly conserved in evolution!

- Human pathways predicted from the human genome in 2004
  - Romero *et al*, *Genome Biology* 6(1):1-17 2004
- 295 pathways, 2600 reactions, 1700 metabolites
- Extensive query and visualization tools linking genome to metabolome
- HumanCyc.org

Pathway Tools Software



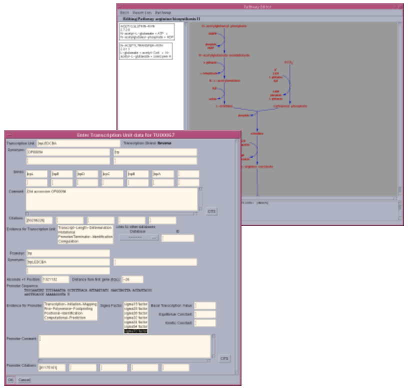
Annotated Genome + PathoLogic

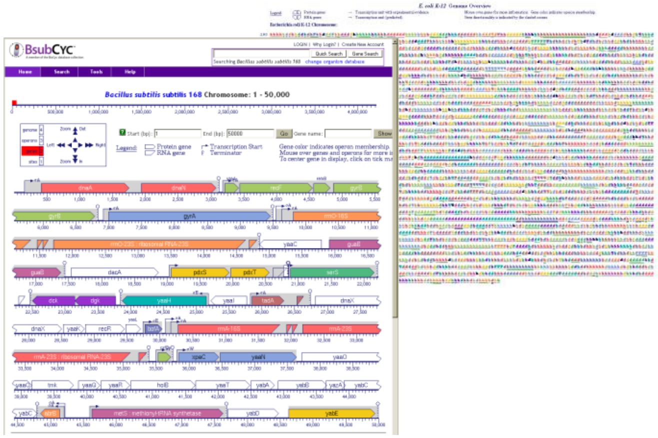


Pathway/Genome Database

MetaFlux

Pathway/Genome Navigator





Pathway/Genome Editors

Briefings in Bioinformatics 11:40-79 2010

Pathway Tools Enables Multi-Use Metabolic Databases

Encyclopedia

humancyc.org/HUMAN/NEW-IMAGE?type=GENE&object=HS04231

HumanCyc
A member of the BioCyc database collection

Searching *Homo sapiens* change organism database

Homo sapiens Enzyme: arginase 1

Gene: ARG1 Accession Number: HS04231 (HumanCyc)

Synonyms: Liver-type arginase, Type I arginase, liver-type arginase

Subunit composition of arginase 1 = $[ARG1]_3$
Arginase-1 = ARG1

Summary:
Arginase catalyzes the hydrolysis of L-arginine to form L-ornithine and urea through a metal-activated hydroxide mechanism [Cox01]. It regulates L-arginine levels and provides L-ornithine for biosynthetic reactions that generate metabolites such as glutamate, glutamine, GABA, agmatine, polyamines, creatine, proline, and nitric oxide [Kim02]. Mammals express two isozymes of arginase, cytosolic arginase 1 highly expressed in liver and erthrocytes, and mitochondrial arginase 2 expressed in other nonhepatic tissue [Iyer98].

Human arginase 1 is an important member of the urea cycle, and functions in the net production of urea for excretion of excess nitrogen. It is abundant in the liver of ureotelic animals [Ikemoto90]. Arginase 1 is also expressed in certain nonhepatic tissues where it can also function in L-arginine homeostasis and influence the outcome of the immune response [Di05]. Arginase 1 is a homotrimeric enzyme that binds two Mn^{2+} per subunit [Orellana02].

Recent work using *in situ* and quantitative PCR studies in mouse, reported that arginase 1 is the predominant isoform expressed during development and in the majority of organs [Cederbaum04].

Gene Citations: [Sparkes86, Haraguchi87, Takiguchi88]

Locations: cytosol

Map Position: [131,741,483 -> 131,752,587] (77.19 centisomes) on Chromosome 6 Length: 11105 bp

Molecular Weight of Polypeptide: 34.735 kD (from nucleotide sequence), 35 kD (experimental)

Molecular Weight of Multimer: 105 kD (experimental)

pI: 10.0 [Nishibe73]

Unification Links: Ensembl:ENSG00000118520 , Entrez-gene:383 , Entrez-Nucleotide:AL121575 , Entrez-Nucleotide:AY074488 , Entrez-Nucleotide:BC005321 , Entrez-Nucleotide:BC020653 , Entrez-Nucleotide:M14502 , Entrez-Nucleotide:X12662 , Entrez:AAA51776 , Entrez:AAH05321 , Entrez:AAH20653 , Entrez:AAL71547 , Entrez:CAA31188 , Entrez:CAB92071 , GeneCards:ARG1 , ModBase:P05089 , MOPED:P05089 , OMIM:207800 , RefSeq:NM_000045 , RefSeq:NP_000036 , Swiss-Model:P05089 , UCSC Human Genome:NM_000045 , UniGene:332405 , UniProt:P05089

Relationship Links: PDB:Structure:1WVA , PDB:Structure:1WVB , PDB:Structure:2AEB

Gene-Reaction Schematic:

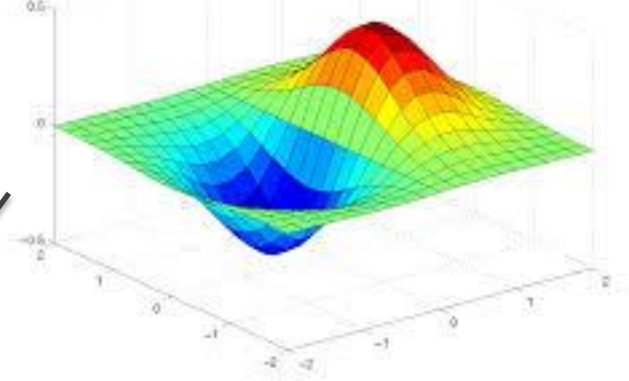
GO Terms:

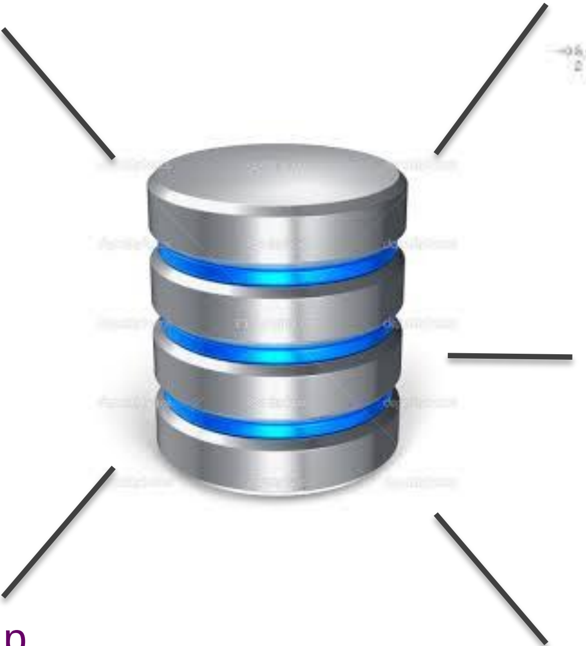
Homo sapiens
Enzyme:
arginase 1

OPERATIONS

Comparison Operations
- Show this gene in another database
- Change organisms/databases for comparison operations
- Search for this gene in other databases
- Show orthologs (with operon diagrams) in multiple databases
- Align in Multi-Genome Browser
- Align gene nucleotide sequence with orthologs
- Align gene product amino acid sequence with orthologs

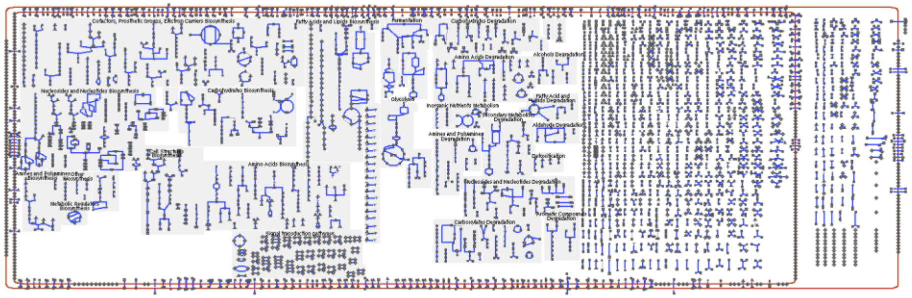
Metabolic Model

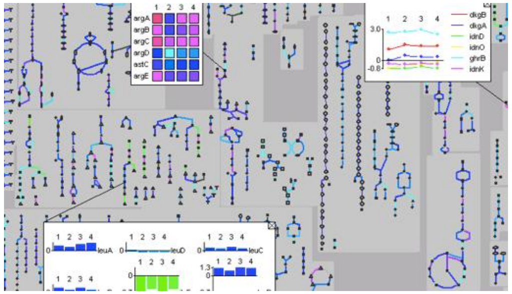




Queryable Database

Zoomable Metabolic Map



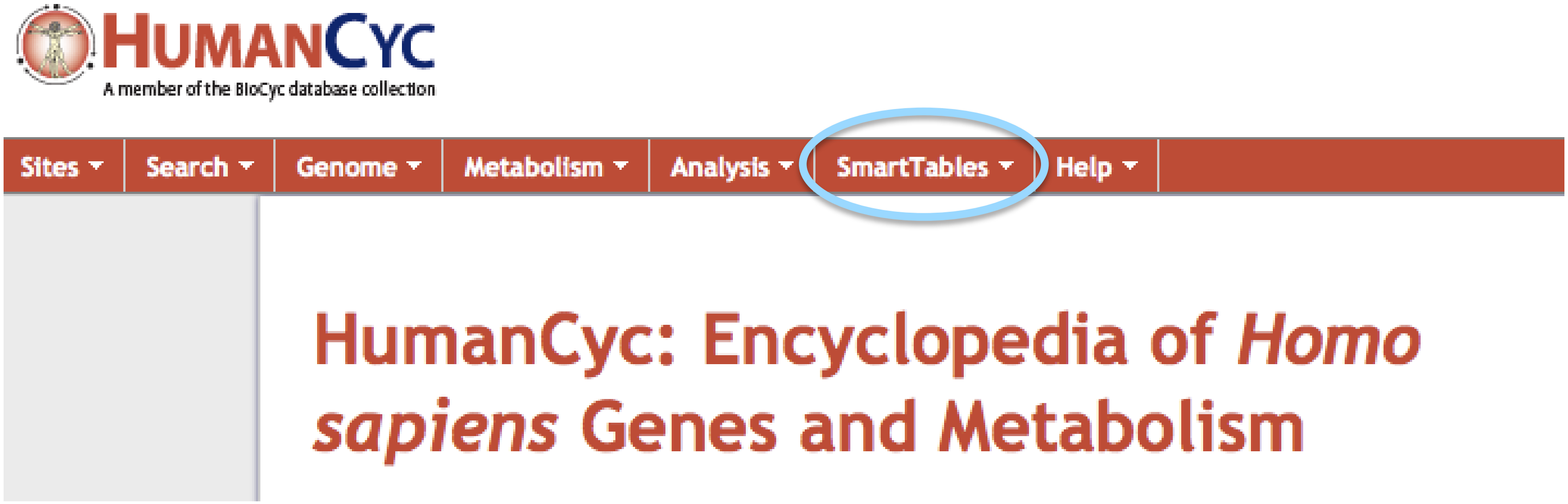


Omics Data Analysis

SmartTables (formerly Web Groups)

- Collect lists of database objects
  - Genes, metabolites, pathways, sequence regions, …
- Transform them into related objects
  (eg: transform list of genes → list of pathways)
- Filter and combine
- Share with public or specific collaborators
- Export to spreadsheet
- Omics analyses

Accessing SmartTables



HumanCyc: Encyclopedia of *Homo sapiens* Genes and Metabolism

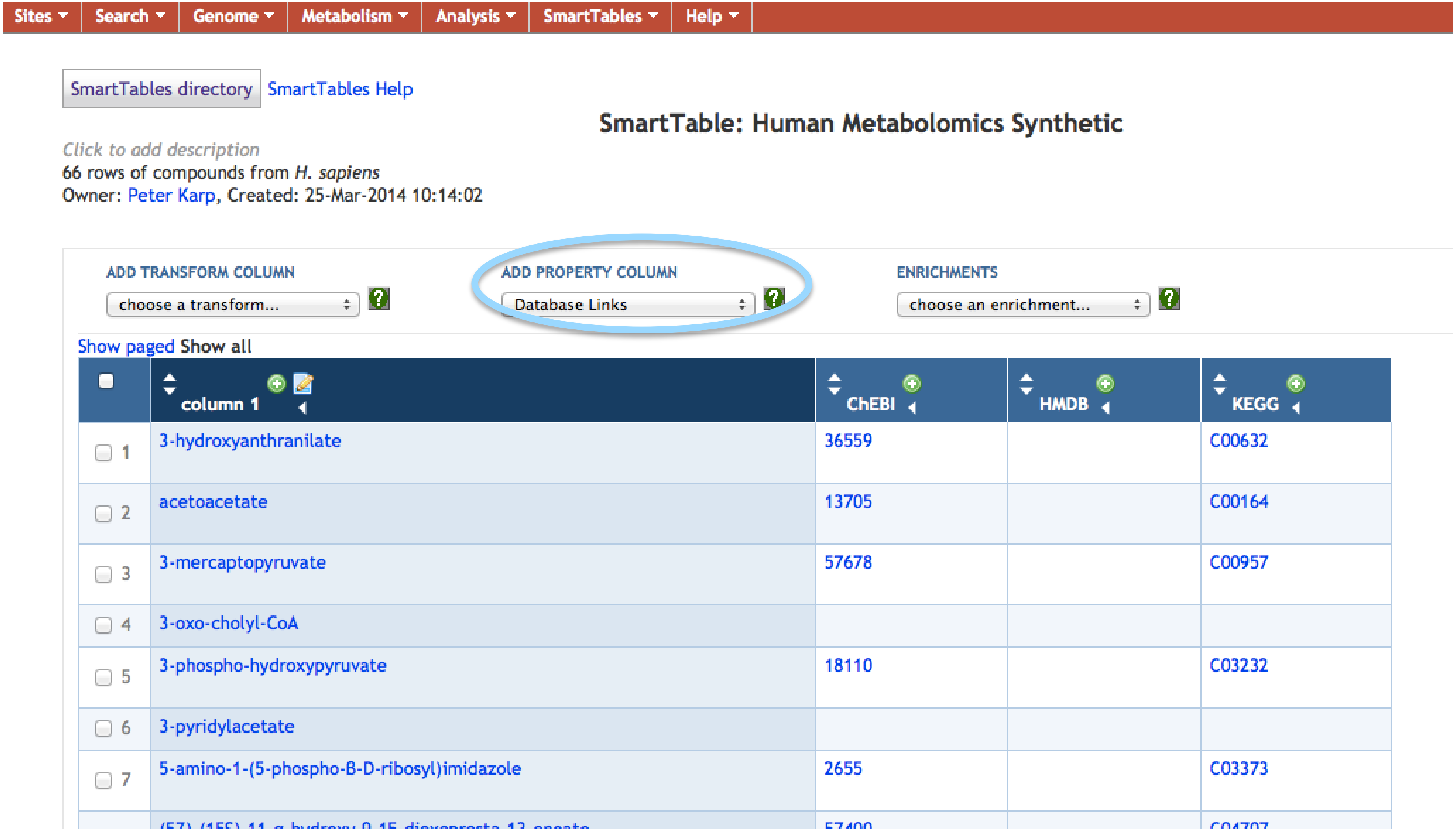
- BioCyc.org, HumanCyc.org, EcoCyc.org…
- To create saved SmartTables, create a (free) BioCyc account for yourself
- From the web menu:
- SmartTables->My SmartTables

Creating SmartTables: User-Defined SmartTables

- Create a SmartTable
  - Type in metabolite names
  - From search results
  - Upload a tab-delimited text file

☐	column 1
☐ 1	a 2-(2-hydroxyacyl)sphingosine
☐ 2	3-hydroxyanthranilate
☐ 3	acetoacetate
☐ 4	3-mercaptopyruvate
☐ 5	3-oxo-cholyl-CoA
☐ 6	3-phospho-hydroxypyruvate
☐ 7	3-pyridylacetate
☐ 8	5-amino-1-(5-phospho-β-D-ribosyl)imidazole
☐ 9	(5Z)-(15S)-11-α-hydroxy-9,15-dioxoprosta-13-enoate
☐ 10	prostaglandin E_2
☐ 11	acetol
☐ 12	β-D-galactosyl-1,3-(*N*-acetyl-β-D-glucosaminyl-1,6)-*N*-acetyl-D-galactosaminyl-R
☐ 13	betaine aldehyde
☐ 14	citrate

Using SmartTables: Browsing Attributes



SmartTables directory SmartTables Help

SmartTable: Human Metabolomics Synthetic

Click to add description
66 rows of compounds from *H. sapiens*
Owner: Peter Karp, Created: 25-Mar-2014 10:14:02

ADD TRANSFORM COLUMN: choose a transform...

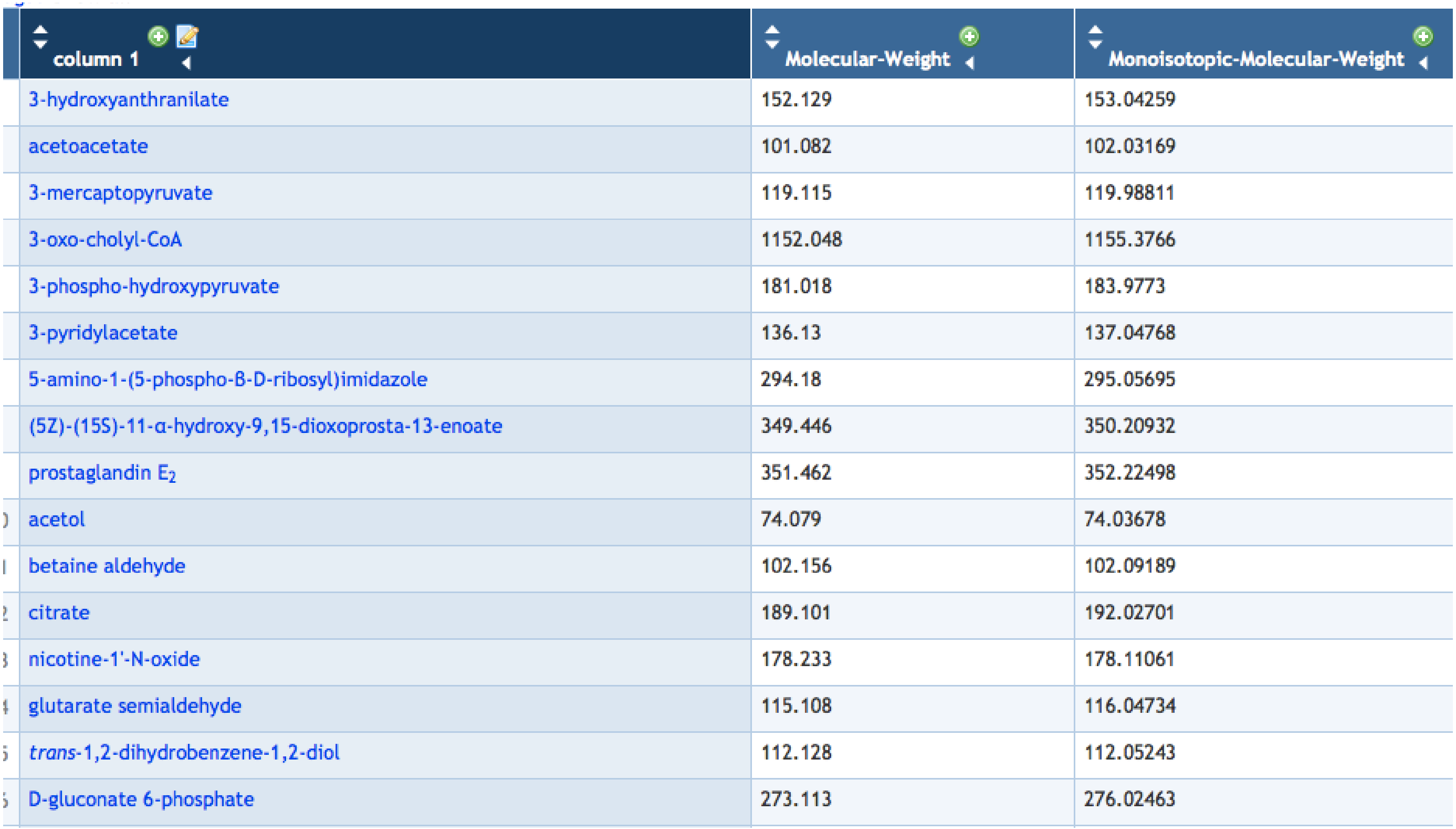
ADD PROPERTY COLUMN: Database Links

ENRICHMENTS: choose an enrichment...

Show paged **Show all**

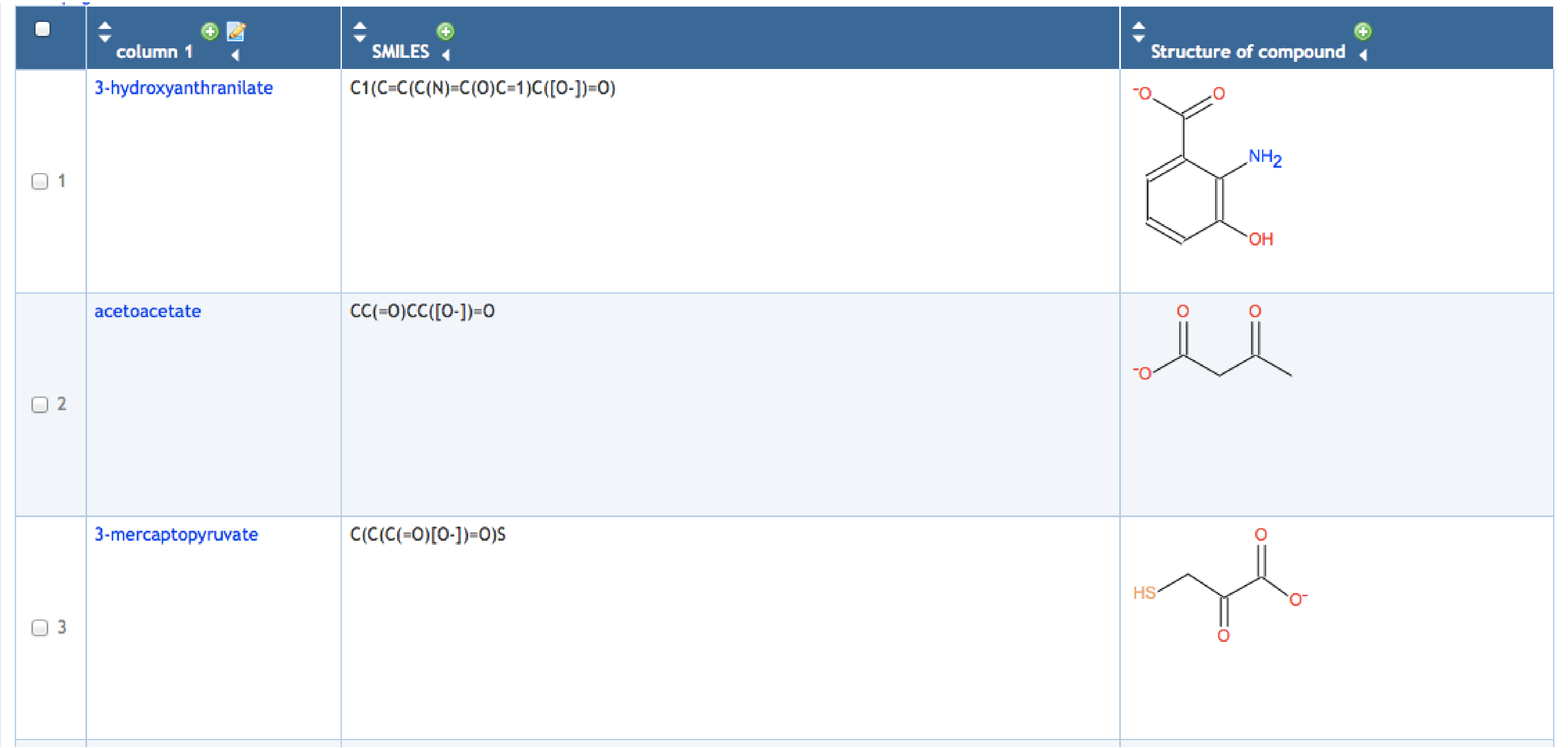
☐	column 1	ChEBI	HMDB	KEGG
☐ 1	3-hydroxyanthranilate	36559		C00632
☐ 2	acetoacetate	13705		C00164
☐ 3	3-mercaptopyruvate	57678		C00957
☐ 4	3-oxo-cholyl-CoA			
☐ 5	3-phospho-hydroxypyruvate	18110		C03232
☐ 6	3-pyridylacetate			
☐ 7	5-amino-1-(5-phospho-β-D-ribosyl)imidazole	2655		C03373
	(5Z)-(15S)-11-α-hydroxy-9,15-dioxoprosta-13-enoate	57400		C04707

Using SmartTables: Browsing Attributes



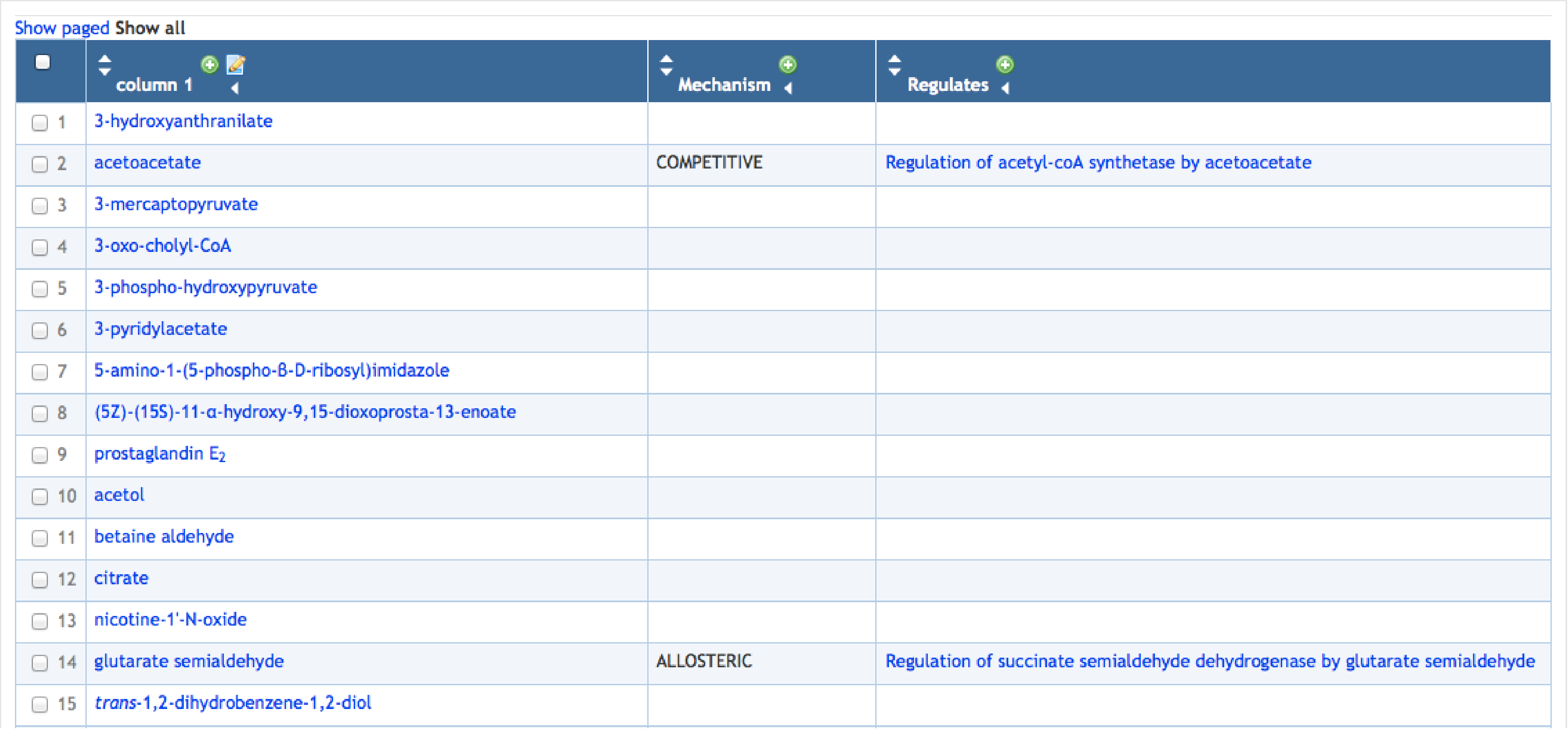
column 1	Molecular-Weight	Monoisotopic-Molecular-Weight
3-hydroxyanthranilate	152.129	153.04259
acetoacetate	101.082	102.03169
3-mercaptopyruvate	119.115	119.98811
3-oxo-cholyl-CoA	1152.048	1155.3766
3-phospho-hydroxypyruvate	181.018	183.9773
3-pyridylacetate	136.13	137.04768
5-amino-1-(5-phospho-β-D-ribosyl)imidazole	294.18	295.05695
(5Z)-(15S)-11-α-hydroxy-9,15-dioxoprosta-13-enoate	349.446	350.20932
prostaglandin E_2	351.462	352.22498
acetol	74.079	74.03678
betaine aldehyde	102.156	102.09189
citrate	189.101	192.02701
nicotine-1'-N-oxide	178.233	178.11061
glutarate semialdehyde	115.108	116.04734
trans-1,2-dihydrobenzene-1,2-diol	112.128	112.05243
D-gluconate 6-phosphate	273.113	276.02463

Using SmartTables: Browsing Attributes



☐	column 1	SMILES	Structure of compound
☐ 1	3-hydroxyanthranilate	C1(C=C(C(N)=C(O)C=1)C([O-])=O)	
☐ 2	acetoacetate	CC(=O)CC([O-])=O	
☐ 3	3-mercaptopyruvate	C(C(C(=O)[O-])=O)S	

Using SmartTables: Browsing Attributes



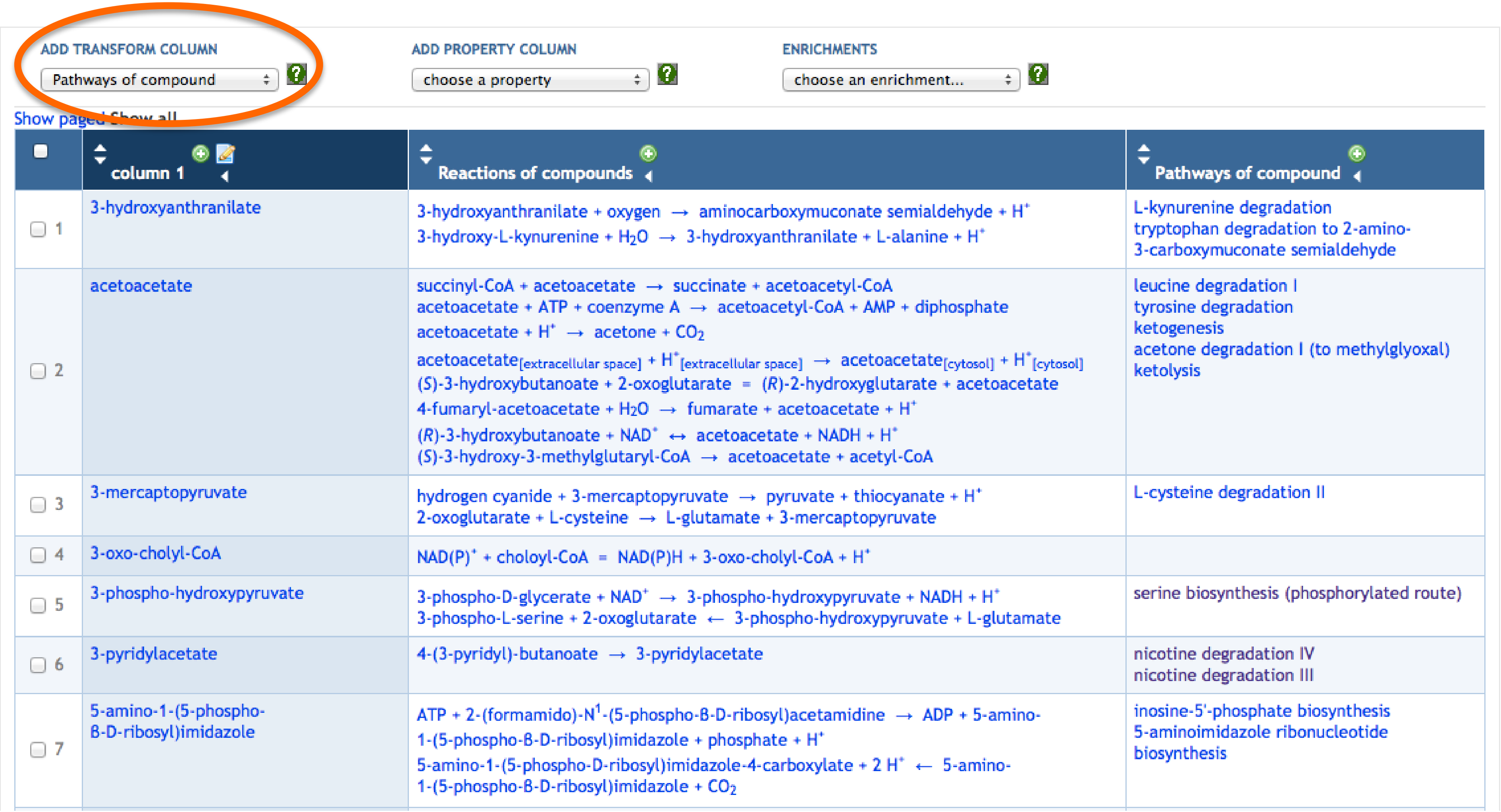
Show paged **Show all**

☐	column 1	Mechanism	Regulates
☐ 1	3-hydroxyanthranilate		
☐ 2	acetoacetate	COMPETITIVE	Regulation of acetyl-coA synthetase by acetoacetate
☐ 3	3-mercaptopyruvate		
☐ 4	3-oxo-cholyl-CoA		
☐ 5	3-phospho-hydroxypyruvate		
☐ 6	3-pyridylacetate		
☐ 7	5-amino-1-(5-phospho-β-D-ribosyl)imidazole		
☐ 8	(5Z)-(15S)-11-α-hydroxy-9,15-dioxoprosta-13-enoate		
☐ 9	prostaglandin E_2		
☐ 10	acetol		
☐ 11	betaine aldehyde		
☐ 12	citrate		
☐ 13	nicotine-1'-N-oxide		
☐ 14	glutarate semialdehyde	ALLOSTERIC	Regulation of succinate semialdehyde dehydrogenase by glutarate semialdehyde
☐ 15	*trans*-1,2-dihydrobenzene-1,2-diol		

SmartTable Transformations

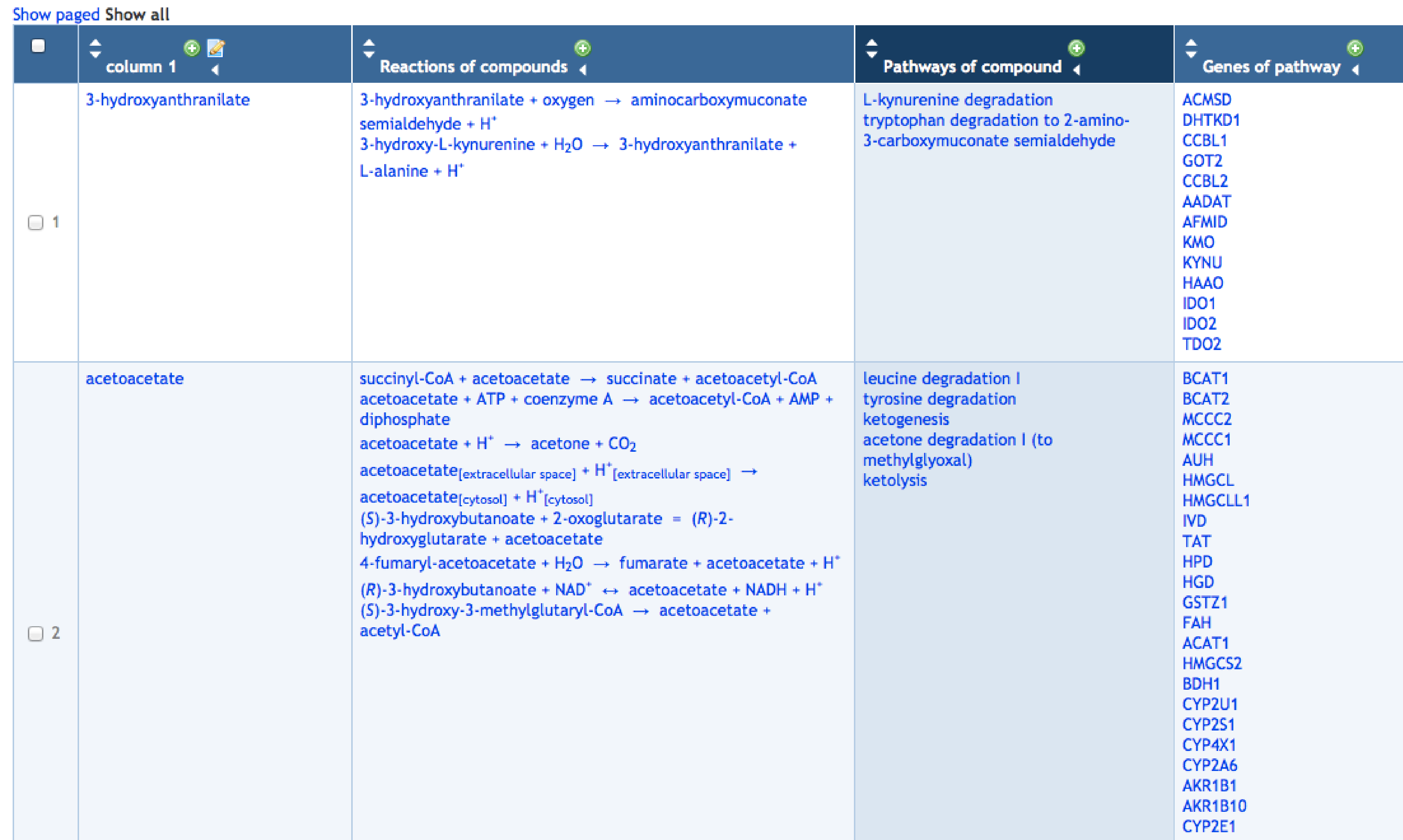
- Create new columns that are computed from existing columns

Transformations: Reactions and Pathways of Metabolite



☐	column 1	Reactions of compounds	Pathways of compound
☐ 1	3-hydroxyanthranilate	3-hydroxyanthranilate + oxygen → aminocarboxymuconate semialdehyde + H^+ 3-hydroxy-L-kynurenine + H_2O → 3-hydroxyanthranilate + L-alanine + H^+	L-kynurenine degradation tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde
☐ 2	acetoacetate	succinyl-CoA + acetoacetate → succinate + acetoacetyl-CoA acetoacetate + ATP + coenzyme A → acetoacetyl-CoA + AMP + diphosphate acetoacetate + H^+ → acetone + CO_2 acetoacetate$_{\text{[extracellular space]}}$ + $H^+_{\text{[extracellular space]}}$ → acetoacetate$_{\text{[cytosol]}}$ + $H^+_{\text{[cytosol]}}$ (*S*)-3-hydroxybutanoate + 2-oxoglutarate = (*R*)-2-hydroxyglutarate + acetoacetate 4-fumaryl-acetoacetate + H_2O → fumarate + acetoacetate + H^+ (*R*)-3-hydroxybutanoate + NAD^+ ↔ acetoacetate + NADH + H^+ (*S*)-3-hydroxy-3-methylglutaryl-CoA → acetoacetate + acetyl-CoA	leucine degradation I tyrosine degradation ketogenesis acetone degradation I (to methylglyoxal) ketolysis
☐ 3	3-mercaptopyruvate	hydrogen cyanide + 3-mercaptopyruvate → pyruvate + thiocyanate + H^+ 2-oxoglutarate + L-cysteine → L-glutamate + 3-mercaptopyruvate	L-cysteine degradation II
☐ 4	3-oxo-cholyl-CoA	$NAD(P)^+$ + choloyl-CoA = NAD(P)H + 3-oxo-cholyl-CoA + H^+	
☐ 5	3-phospho-hydroxypyruvate	3-phospho-D-glycerate + NAD^+ → 3-phospho-hydroxypyruvate + NADH + H^+ 3-phospho-L-serine + 2-oxoglutarate ← 3-phospho-hydroxypyruvate + L-glutamate	serine biosynthesis (phosphorylated route)
☐ 6	3-pyridylacetate	4-(3-pyridyl)-butanoate → 3-pyridylacetate	nicotine degradation IV nicotine degradation III
☐ 7	5-amino-1-(5-phospho-β-D-ribosyl)imidazole	ATP + 2-(formamido)-N^1-(5-phospho-β-D-ribosyl)acetamidine → ADP + 5-amino-1-(5-phospho-β-D-ribosyl)imidazole + phosphate + H^+ 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate + 2 H^+ ← 5-amino-1-(5-phospho-β-D-ribosyl)imidazole + CO_2	inosine-5'-phosphate biosynthesis 5-aminoimidazole ribonucleotide biosynthesis

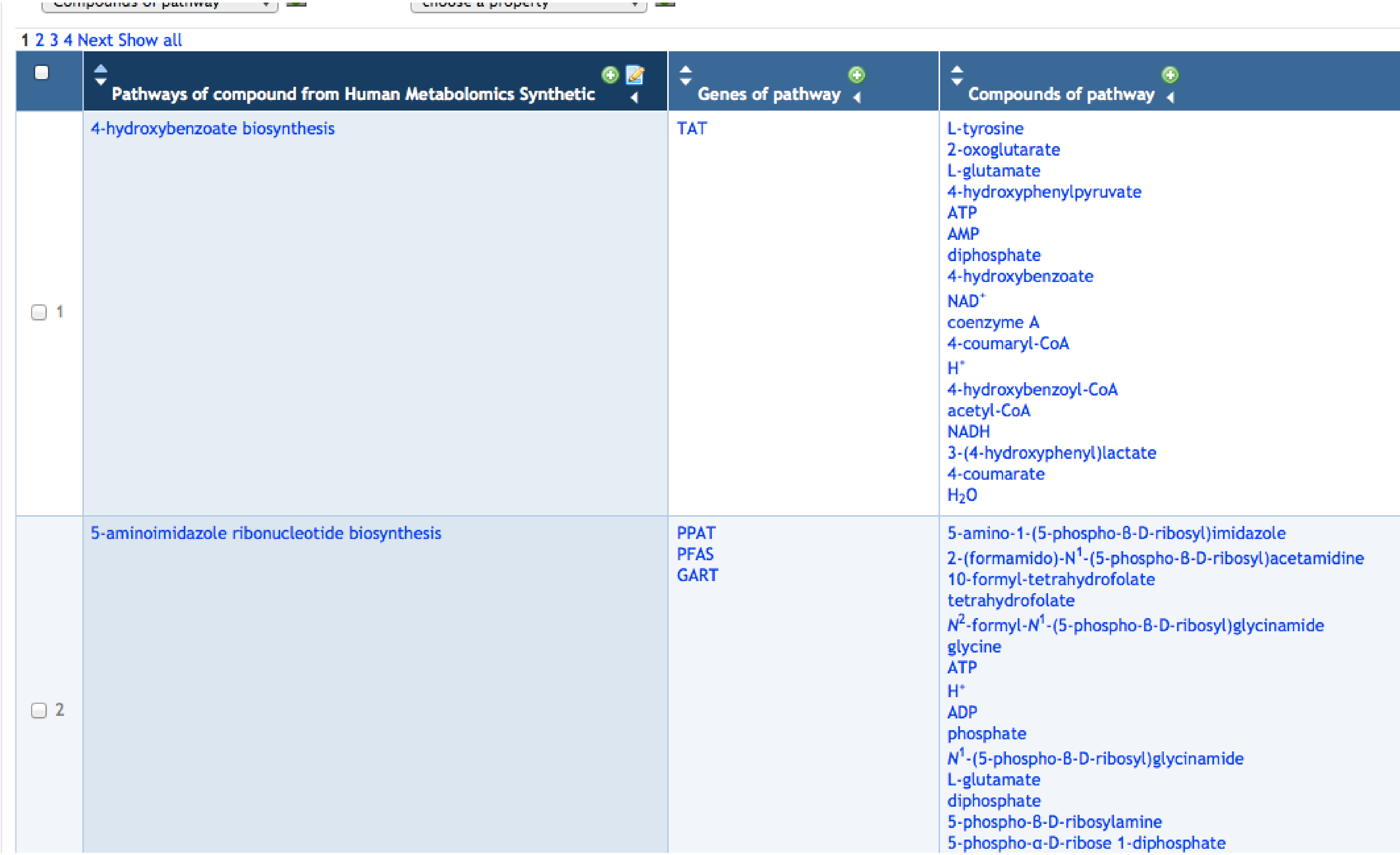
Transformations: Genes of Pathway



Show paged Show all

☐	column 1	Reactions of compounds	Pathways of compound	Genes of pathway
☐ 1	3-hydroxyanthranilate	3-hydroxyanthranilate + oxygen → aminocarboxymuconate semialdehyde + H^+ 3-hydroxy-L-kynurenine + H_2O → 3-hydroxyanthranilate + L-alanine + H^+	L-kynurenine degradation tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde	ACMSD DHTKD1 CCBL1 GOT2 CCBL2 AADAT AFMID KMO KYNU HAAO IDO1 IDO2 TDO2
☐ 2	acetoacetate	succinyl-CoA + acetoacetate → succinate + acetoacetyl-CoA acetoacetate + ATP + coenzyme A → acetoacetyl-CoA + AMP + diphosphate acetoacetate + H^+ → acetone + CO_2 acetoacetate$_{\text{[extracellular space]}}$ + $H^+_{\text{[extracellular space]}}$ → acetoacetate$_{\text{[cytosol]}}$ + $H^+_{\text{[cytosol]}}$ (*S*)-3-hydroxybutanoate + 2-oxoglutarate = (*R*)-2-hydroxyglutarate + acetoacetate 4-fumaryl-acetoacetate + H_2O → fumarate + acetoacetate + H^+ (*R*)-3-hydroxybutanoate + NAD^+ ↔ acetoacetate + NADH + H^+ (*S*)-3-hydroxy-3-methylglutaryl-CoA → acetoacetate + acetyl-CoA	leucine degradation I tyrosine degradation ketogenesis acetone degradation I (to methylglyoxal) ketolysis	BCAT1 BCAT2 MCCC2 MCCC1 AUH HMGCL HMGCLL1 IVD TAT HPD HGD GSTZ1 FAH ACAT1 HMGCS2 BDH1 CYP2U1 CYP2S1 CYP4X1 CYP2A6 AKR1B1 AKR1B10 CYP2E1

Transformations: New SmartTable from Column



☐	Pathways of compound from Human Metabolomics Synthetic	Genes of pathway	Compounds of pathway
☐ 1	4-hydroxybenzoate biosynthesis	TAT	L-tyrosine 2-oxoglutarate L-glutamate 4-hydroxyphenylpyruvate ATP AMP diphosphate 4-hydroxybenzoate NAD$^+$ coenzyme A 4-coumaryl-CoA H$^+$ 4-hydroxybenzoyl-CoA acetyl-CoA NADH 3-(4-hydroxyphenyl)lactate 4-coumarate H$_2$O
☐ 2	5-aminoimidazole ribonucleotide biosynthesis	PPAT PFAS GART	5-amino-1-(5-phospho-β-D-ribosyl)imidazole 2-(formamido)-N^1-(5-phospho-β-D-ribosyl)acetamidine 10-formyl-tetrahydrofolate tetrahydrofolate N^2-formyl-N^1-(5-phospho-β-D-ribosyl)glycinamide glycine ATP H$^+$ ADP phosphate N^1-(5-phospho-β-D-ribosyl)glycinamide L-glutamate diphosphate 5-phospho-β-D-ribosylamine 5-phospho-α-D-ribose 1-diphosphate

Other Operations on SmartTables

- Set union, intersection, difference among two SmartTables
- Filter SmartTable rows to keep/reject all rows containing specified value or substring or regular expression
- Share SmartTable with public or specified users
- Freeze SmartTable for publication

Enrichment Analysis

- Statistical method to find classes of objects that have more or less objects than would be expected by chance

* Based on the Hypergeometric Distribution

- Can perform enrichment, depletion, or both

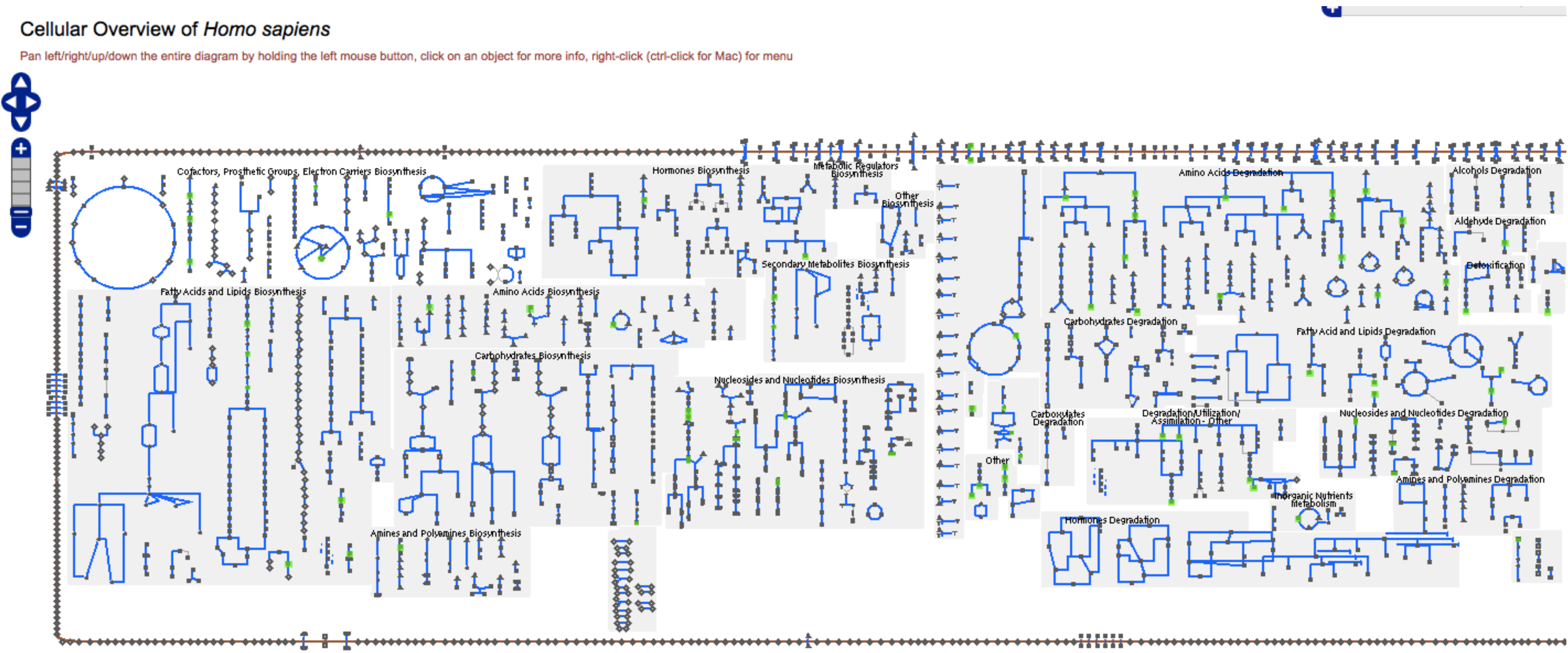
- Multiple ontologies can be used in Pathway Tools

* Multiple testing correction optional

Enrichment Analysis

☐ 1	NAD *de novo* biosynthesis	0.01065204	nicotinate adenine dinucleotide formate *N*-formylkynurenine 3-hydroxyanthranilate
☐ 2	tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde	0.010885004	formate *N*-formylkynurenine 3-hydroxyanthranilate
☐ 3	NAD Biosynthesis	0.014184234	nicotinate adenine dinucleotide formate *N*-formylkynurenine 3-hydroxyanthranilate
☐ 4	NAD Metabolism	0.01838762	nicotinate adenine dinucleotide formate *N*-formylkynurenine 3-hydroxyanthranilate
☐ 5	tryptophan utilization II	0.030494805	formate *N*-formylkynurenine 3-hydroxyanthranilate serotonin nicotinate adenine dinucleotide
☐ 6	tryptophan degradation	0.04628297	formate *N*-formylkynurenine 3-hydroxyanthranilate
	tryptophan utilization I	0.050800793	formate *N*-formylkynurenine 3-hydroxyanthranilate

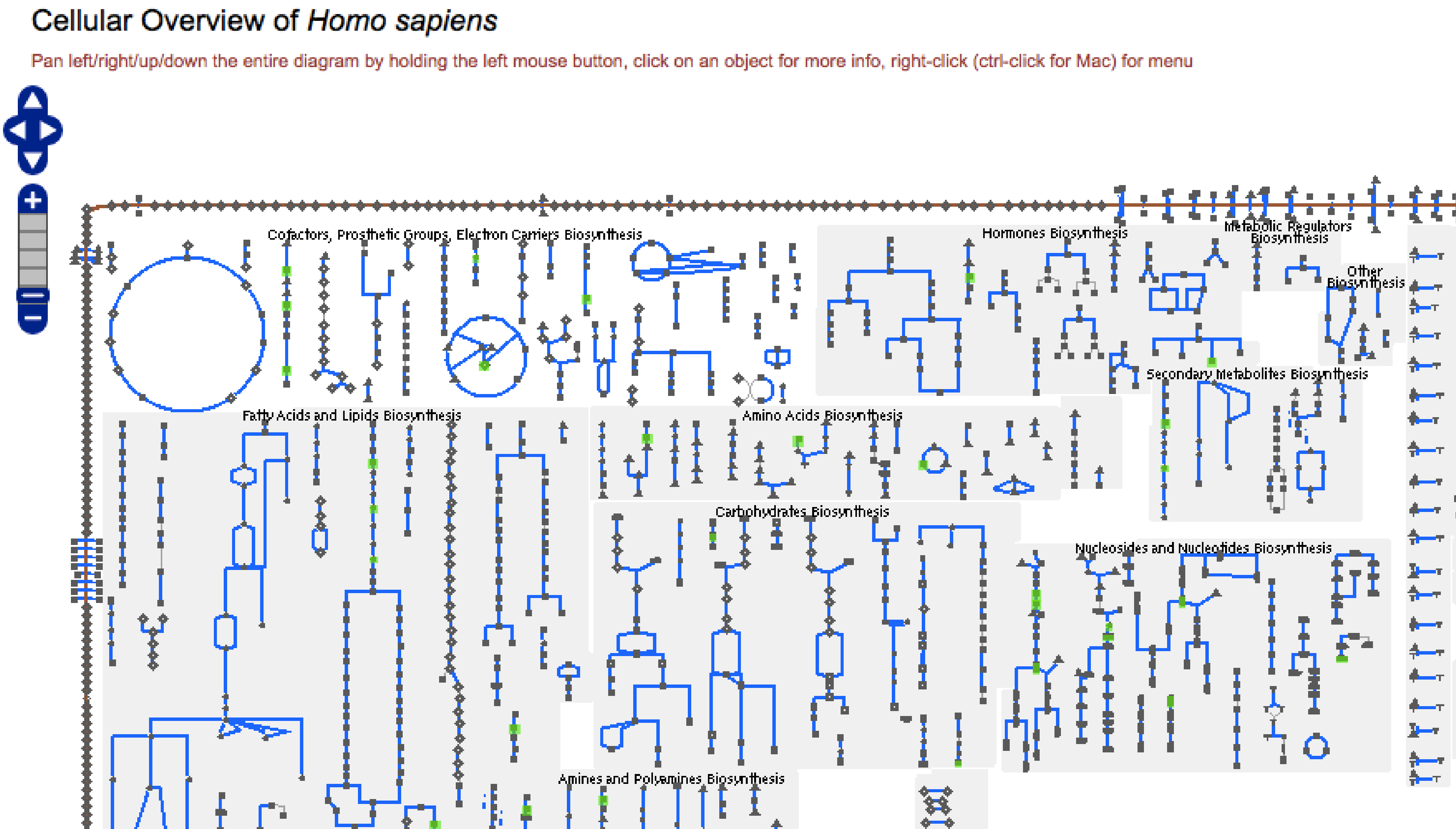
Paint Metabolomics Data onto Cellular Overview – Boolean Data



Cellular Overview of *Homo sapiens*

Pan left/right/up/down the entire diagram by holding the left mouse button, click on an object for more info, right-click (ctrl-click for Mac) for menu

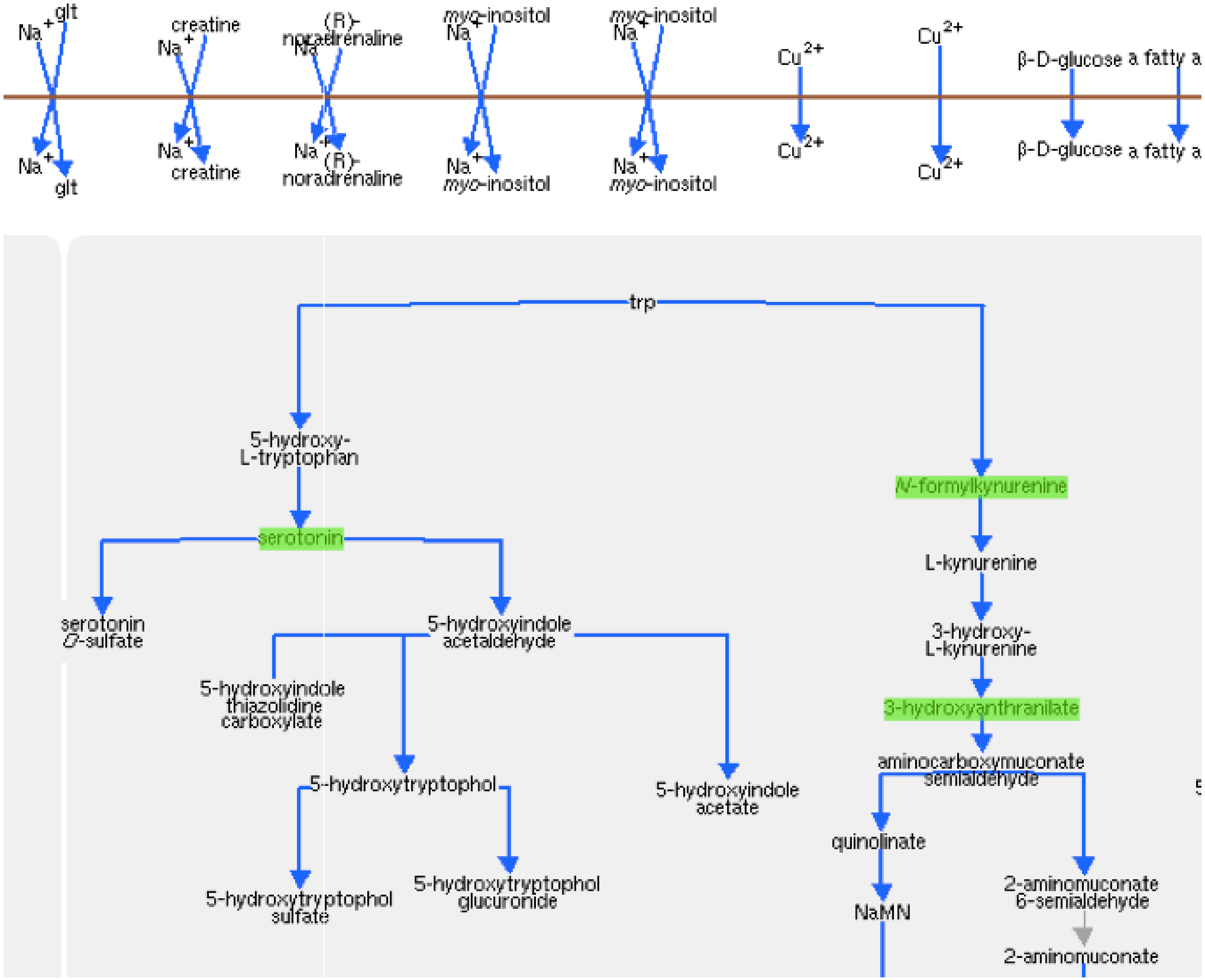
Paint Metabolomics Data onto Cellular Overview



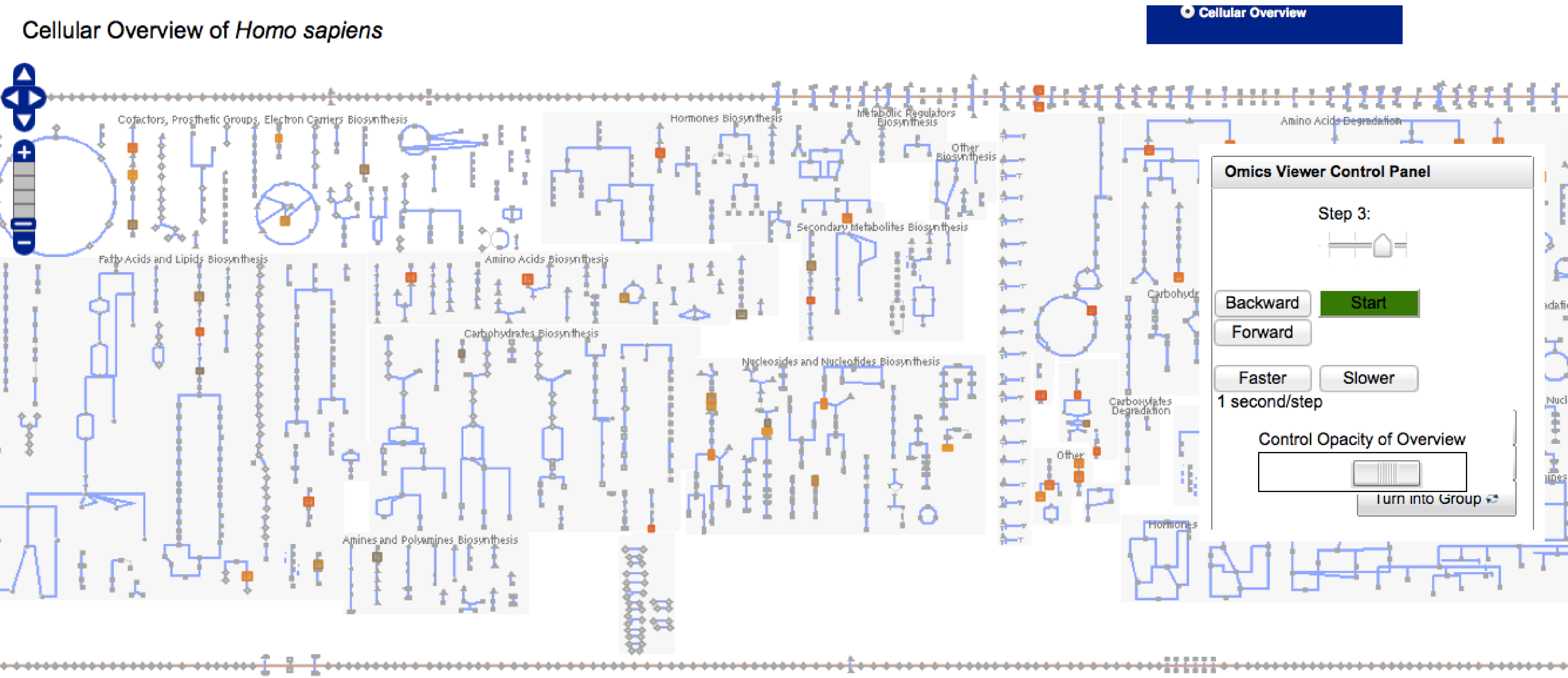
Cellular Overview of *Homo sapiens*

Pan left/right/up/down the entire diagram by holding the left mouse button, click on an object for more info, right-click (ctrl-click for Mac) for menu

Paint Metabolomics Data onto Cellular Overview



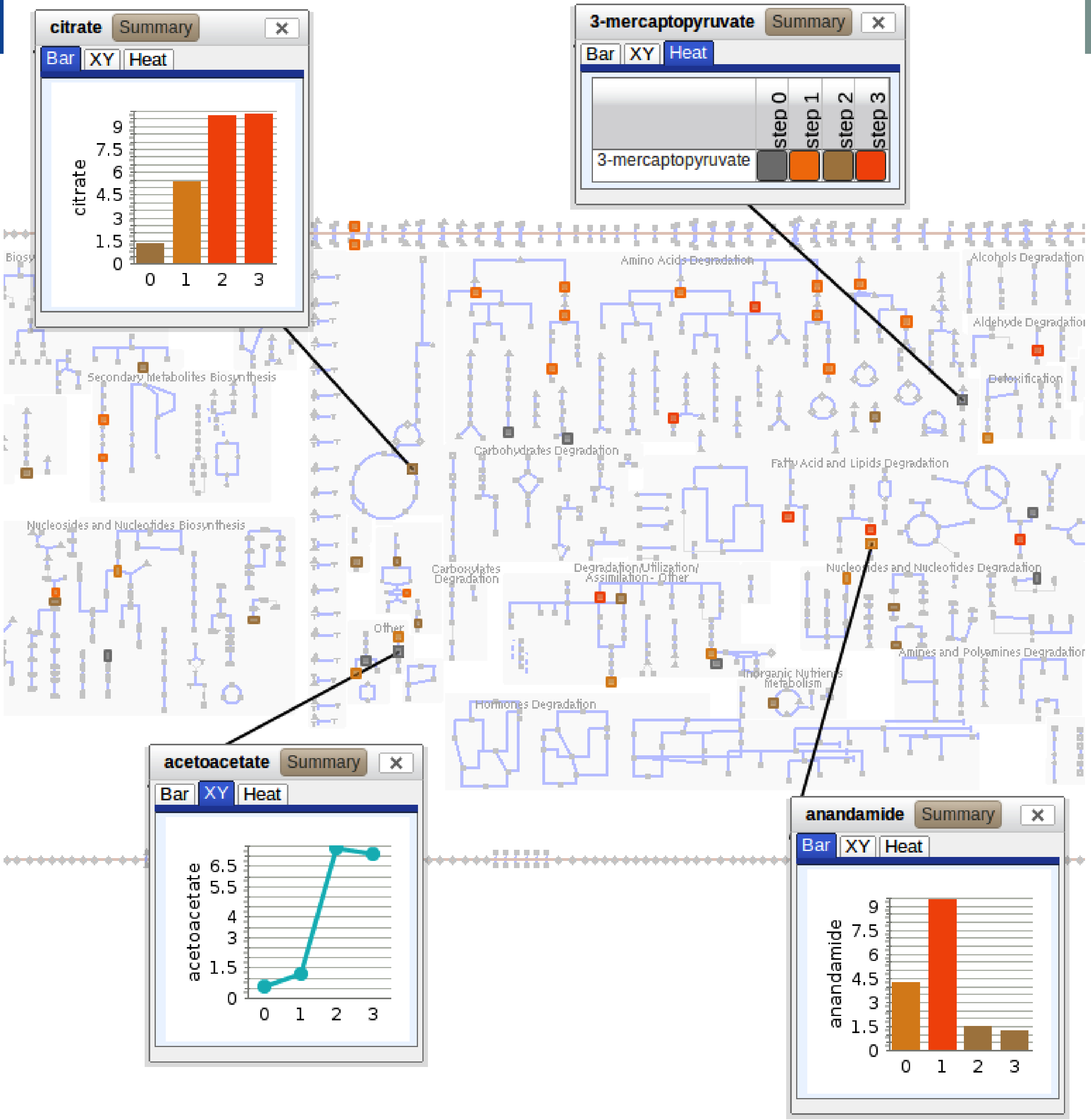
Paint Metabolomics Data onto Cellular Overview – Animation of Numeric Data

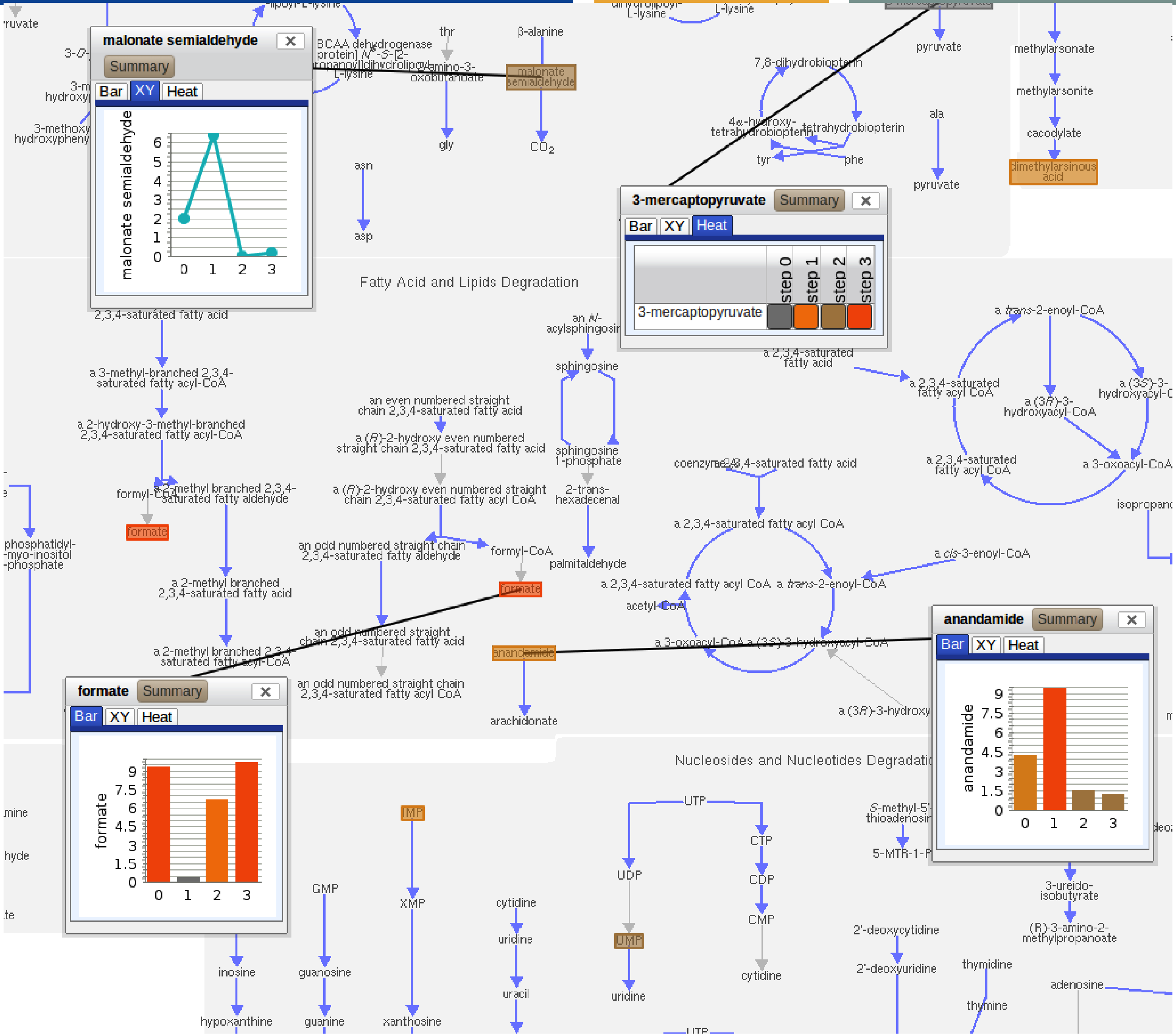

Cellular Overview of *Homo sapiens*

Step 3:

1 second/step

Control Opacity of Overview


citrate
Summary
Bar
XY
Heat
citrate
0
1.5
3
4.5
6
7.5
9
0
1
2
3
3-mercaptopyruvate
Summary
Bar
XY
Heat
step 0
step 1
step 2
step 3
3-mercaptopyruvate
Biosy
Amino Acids Degradation
Alcohols Degradation
Aldehyde Degradatio
Detoxification
Secondary Metabolites Biosynthesis
Carbohydrates Degradation
Fatty Acid and Lipids Degradation
Nucleosides and Nucleotides Biosynthesis
Carboxylates Degradation
Degradation/Utilization/ Assimilation - Other
Nucleosides and Nucleotides Degradation
Other
Amines and Polyamines Degradatio
Inorganic Nutrients Metabolism
Hormones Degradation
acetoacetate
Summary
Bar
XY
Heat
acetoacetate
0
1.5
3
4
5.5
6.5
0
1
2
3
anandamide
Summary
Bar
XY
Heat
anandamide
0
1.5
3
4.5
6
7.5
9
0
1
2
3


malonate semialdehyde
Summary
Bar
XY
Heat
malonate semialdehyde
6
5
4
3
2
1
0
0
1
2
3
3-mercaptopyruvate
Summary
Bar
XY
Heat
step 0
step 1
step 2
step 3
3-mercaptopyruvate
anandamide
Summary
Bar
XY
Heat
anandamide
9
7.5
6
4.5
3
1.5
0
0
1
2
3
formate
Summary
Bar
XY
Heat
formate
9
7.5
6
4.5
3
1.5
0
0
1
2
3
Fatty Acid and Lipids Degradation
Nucleosides and Nucleotides Degradation
BCAA dehydrogenase
thr
β-alanine
2-amino-3-oxobutanoate
malonate semialdehyde
gly
CO2
asn
asp
7,8-dihydrobiopterin
4α-hydroxy-tetrahydrobiopterin
tetrahydrobiopterin
tyr
phe
pyruvate
ala
pyruvate
methylarsonate
methylarsonite
cacodylate
dimethylarsinous acid
2,3,4-saturated fatty acid
a 3-methyl-branched 2,3,4-saturated fatty acyl-CoA
a 2-hydroxy-3-methyl-branched 2,3,4-saturated fatty acyl-CoA
formyl-CoA
a 2-methyl branched 2,3,4-saturated fatty aldehyde
formate
a 2-methyl branched 2,3,4-saturated fatty acid
a 2-methyl branched 2,3,4-saturated fatty acyl-CoA
an even numbered straight chain 2,3,4-saturated fatty acid
a (R)-2-hydroxy even numbered straight chain 2,3,4-saturated fatty acid
a (R)-2-hydroxy even numbered straight chain 2,3,4-saturated fatty acyl CoA
an odd numbered straight chain 2,3,4-saturated fatty aldehyde
formyl-CoA
formate
an odd numbered straight chain 2,3,4-saturated fatty acid
an odd numbered straight chain 2,3,4-saturated fatty acyl CoA
an N-acylsphingosine
sphingosine
sphingosine 1-phosphate
2-trans-hexadecenal
palmitaldehyde
anandamide
arachidonate
a 2,3,4-saturated fatty acid
coenzyme A
a 2,3,4-saturated fatty acid
a 2,3,4-saturated fatty acyl CoA
a 2,3,4-saturated fatty acyl CoA
a trans-2-enoyl-CoA
acetyl-CoA
a 3-oxoacyl-CoA
a (3S)-3-hydroxyacyl-CoA
a cis-3-enoyl-CoA
a (3R)-3-hydroxy
a trans-2-enoyl-CoA
a 2,3,4-saturated fatty acyl CoA
a (3S)-3-hydroxyacyl-C
a (3R)-3-hydroxyacyl-CoA
a 2,3,4-saturated fatty acyl CoA
a 3-oxoacyl-CoA
isopropanol
phosphatidyl-myo-inositol-phosphate
IMP
GMP
XMP
inosine
guanosine
xanthosine
hypoxanthine
guanine
cytidine
uridine
uracil
UTP
UDP
UMP
uridine
CTP
CDP
CMP
cytidine
S-methyl-5'-thioadenosine
5-MTR-1-P
2'-deoxycytidine
2'-deoxyuridine
thymidine
thymine
adenosine
3-ureido-isobutyrate
(R)-3-amino-2-methylpropanoate

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