THE UNIVERSITY OF ALABAMA AT BIRMINGHAM

Knowledge that will change your world

Pathway analysis with Metaboanalyst

Stephen Barnes, PhD

Professor of Pharmacology & Toxicology

sbarnes@uab.edu

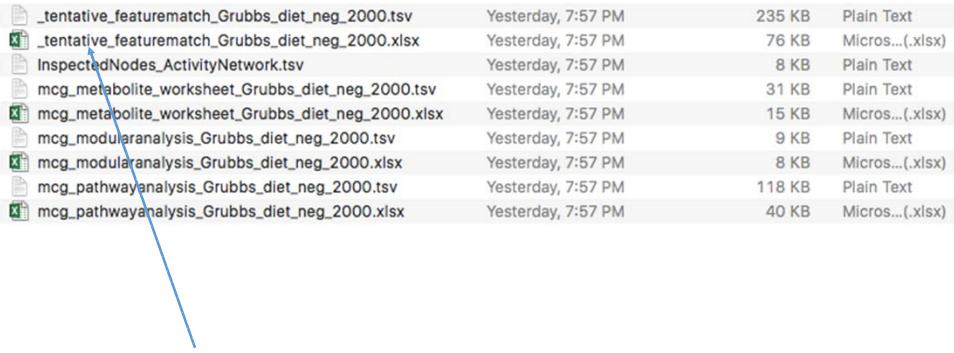
Targeted Metabolomics & Proteomics Laboratory

Find the data in the mummichog file

Mac users: **mummichog-1.0.7 is in the Applications folder**
Open it to locate 1467593683.63.Grubbs_diet_neg_2000

Open the tsv folder

Files in mummichog results folder



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mcg_pathwayanalysis_Grubbs_diet_neg_2000.xlsx	Yesterday, 7:57 PM	40 KB	Micros...(.xlsx)

Identification of each observed ion

A	B	C	D	E
m/z	id	match_form	mz_differe	name
59.014	C00033	M-H[-]	-0.0002	Acetate; Acetic acid; Ethanoic acid; Glacial acetic acid
59.014	C00084	M-H+O[-]	-0.0002	Acetaldehyde; Ethanal
59.014	C00266	M-H[-]	-0.0002	Glycolaldehyde; Hydroxyacetaldehyde
59.014	C02045	M-2H[2-]	-0.0003	
59.014	C06548	M-H+O[-]	-0.0002	Ethylene oxide
59.014	CE5985	M-2H[2-]	-0.0003	
75.010	C00385	M-2H[2-]	0.0005	Xanthine
80.966	C00094	M-H[-]	0.0008	Sulfite
93.035	C00146	M-H[-]	0.0002	Phenol; Benzenol; Hydroxybenzene; Phenic acid; Phenylic acid
93.035	C04221	M-H2O-H[-]	0.0003	trans-1,2-Dihydrobenzene-1,2-diol
93.035	C15584	M-H[-]	0.0002	Phenol
103.004	C00022	M-H+O[-]	0	Pyruvate; Pyruvic acid; 2-Oxopropanoate; 2-Oxopropanoic acid; Pyroracemic acid
103.004	C00168	M-H[-]	-0.0001	Hydroxypyruvate; Hydroxypyruvic acid; 3-Hydroxypyruvate; 3-Hydroxypyruvic ac
103.004	C00222	M-H+O[-]	0	3-Oxopropanoate; Malonate semialdehyde
103.004	C01146	M-H[-]	-0.0001	2-Hydroxy-3-oxopropanoate; Tartronate semialdehyde
111.009	C00490	M-H2O-H[-]	-0.0001	Itaconate; Itaconic acid; Methylenesuccinic acid
111.009	C01732	M-H2O-H[-]	-0.0001	Mesaconate; 2-Methylfumarate; Mesaconic acid; Methylfumaric acid
115.004	C00122	M-H[-]	0.0002	Fumarate; Fumaric acid; trans-Butenedioic acid
115.004	C00149	M-H2O-H[-]	0.0003	(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid
115.004	C00804	M+HCOO[-]	0.0008	Propynoate; Propiolic acid; Acetylenecarboxylic acid; Acetylenemonocarboxylate
115.004	C00122	M-H[-]	0.0005	Fumarate; Fumaric acid; trans-Butenedioic acid
115.004	C00149	M-H2O-H[-]	0.0006	(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid
115.004	C00804	M+HCOO[-]	0.0011	Propynoate; Propiolic acid; Acetylenecarboxylic acid; Acetylenemonocarboxylate
115.004	C00122	M-H[-]	0.0007	Fumarate; Fumaric acid; trans-Butenedioic acid
115.004	C00149	M-H2O-H[-]	0.0008	(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid
116.051	C00148	M(S34)-H[-]	-0.0007	L-Proline; 2-Pyrrolidinecarboxylic acid
116.051	C00763	M(S34)-H[-]	-0.0007	D-Proline
116.051	C02505	M-H2O-H[-]	0.0006	2-Phenylacetamide

Select and copy the KEGG IDs

A	B	C	D	E
m/z	id	match_form	mz_differe	name
59.014	C00033	M-H[-]	-0.0002	Acetate; Acetic acid; Ethanoic acid; Glacial acetic acid
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59.014	C06548	M-H+O[-]	-0.0002	Ethylene oxide
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93.035	C04221	M-H2O-H[-]	0.0003	trans-1,2-Dihydrobenzene-1,2-diol
93.035	C15584	M-H[-]	0.0002	Phenol
103.004	C00022	M-H+O[-]	0	Pyruvate; Pyruvic acid; 2-Oxopropanoate; 2-Oxopropanoic acid; Pyroracemic acic
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111.009	C01732	M-H2O-H[-]	-0.0001	Mesaconate; 2-Methylfumarate; Mesaconic acid; Methylfumaric acid
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115.004	C00149	M-H2O-H[-]	0.0003	(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid
115.004	C00804	M+HCOO[-]	0.0008	Propynoate; Propiolic acid; Acetylenecarboxylic acid; Acetylenemonocarboxylate
115.004	C00122	M-H[-]	0.0005	Fumarate; Fumaric acid; trans-Butenedioic acid
115.004	C00149	M-H2O-H[-]	0.0006	(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid
115.004	C00804	M+HCOO[-]	0.0011	Propynoate; Propiolic acid; Acetylenecarboxylic acid; Acetylenemonocarboxylate
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115.004	C00149	M-H2O-H[-]	0.0008	(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid
116.051	C00148	M(S34)-H[-]	-0.0007	L-Proline; 2-Pyrrolidinecarboxylic acid
116.051	C00763	M(S34)-H[-]	-0.0007	D-Proline
116.051	C02505	M-H2O-H[-]	0.0006	2-Phenylacetamide

Go to Metaboanalyst

Please choose a functional module to proceed:

Statistical Analysis

This module offers various commonly used statistical and machine learning methods including t-tests, ANOVA, PCA, PLS-DA and OPLS-DA. It also provides clustering and visualization tools to create dendrograms and heatmaps as well as to classify based on random forests and SVM.

Enrichment Analysis

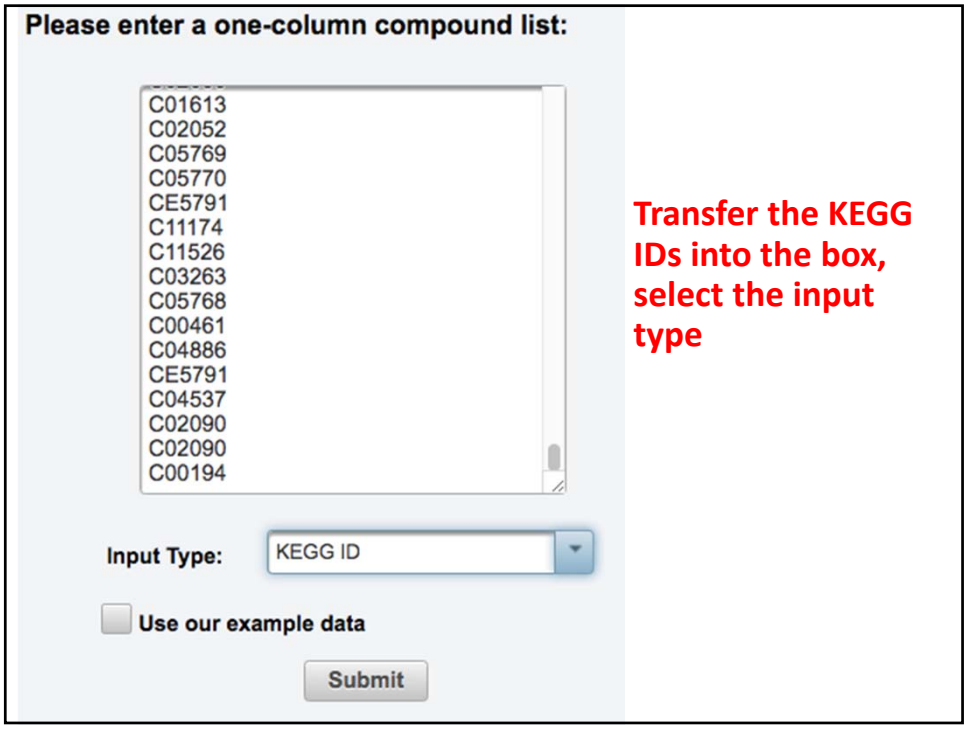
This module performs metabolite set enrichment analysis (MSEA) for human and mammalian species based on several libraries containing ~6300 groups of metabolite sets. Users can upload either 1) a list of compounds, 2) a list of compounds with concentrations, or 3) a concentration table.

Pathway Analysis

This module supports pathway analysis (integrating enrichment analysis and pathway topology analysis) and visualization for 21 model organisms, including Human, Mouse, Rat, Cow, Chicken, Zebrafish, Arabidopsis thaliana, Rice, Drosophila, Malaria, S. cerevisae, E.coli. and others, with a total of ~1600 metabolic pathways.

Time Series Analysis

This module supports temporal and two-factor data analysis including data overview, two-way ANOVA, and empirical Bayes time-series analysis for detecting distinctive temporal profiles. It also supports ANOVA-simultaneous component analysis (ASCA) to identify major patterns associated with each experimental factor.

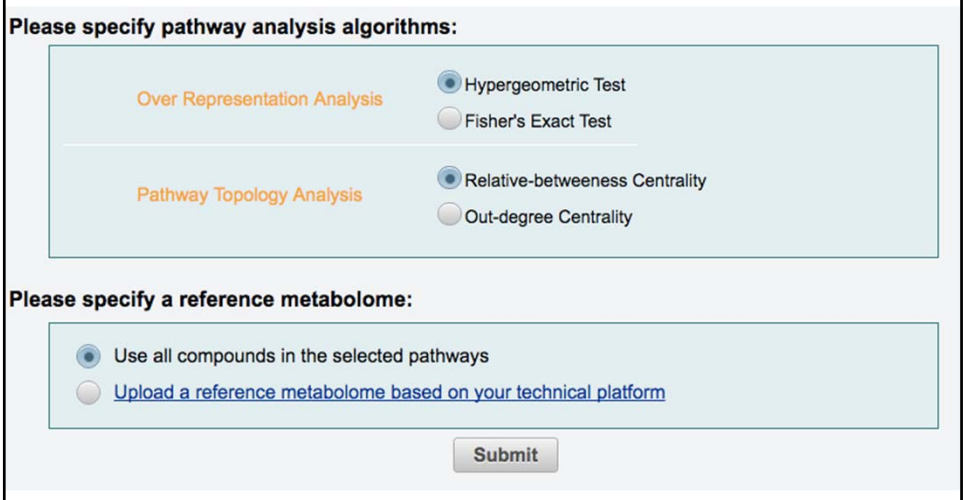


Listed metabolites

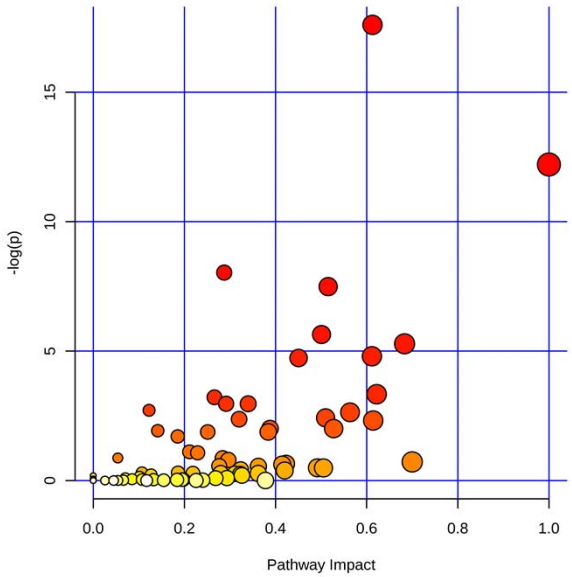
Query	Hit	HMDB	PubChem	KEGG	Details
id		-	-	-	View
C00033	Acetic acid	HMDB00042	176	C00033	
C00084	Acetaldehyde	HMDB00990	177	C00084	
C00266	Glycolaldehyde	HMDB03344	756	C00266	
C02045	L-Erythrulose	HMDB06293	5460032	C02045	
C06548		-	-	-	View
CE5985		-	-	-	View
C00385	Xanthine	HMDB00292	1188	C00385	
C00094		-	-	-	View
C00146	Phenol	HMDB00228	996	C00146	
C04221	trans-1,2-Dihydrobenzene-1,2-diol	HMDB01164	149186	C04221	
C15584		-	-	-	View
C00022	Pyruvic acid	HMDB00243	1060	C00022	
C00168	Hydroxypyruvic acid	HMDB01352	964	C00168	
C00222	Malonic semialdehyde	HMDB11111	868	C00222	
C01146	Tartronate semialdehyde	HMDB06938	1122	C01146	

Choose a species

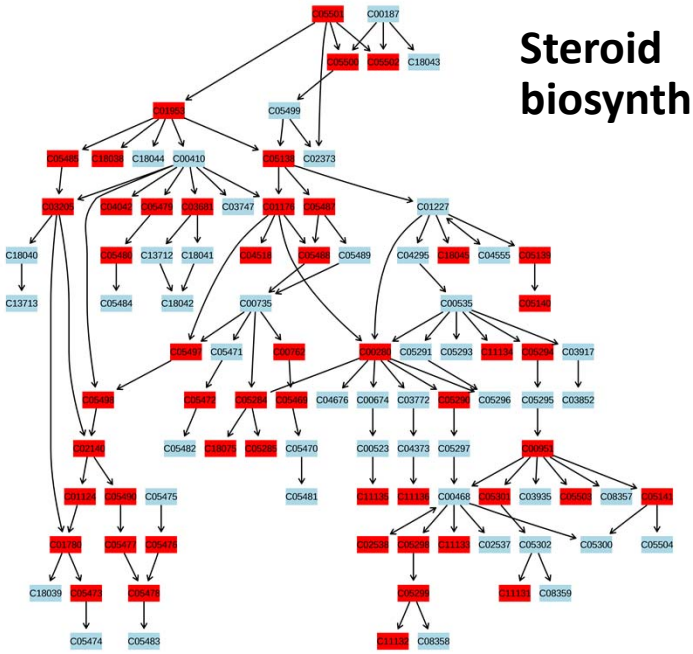
Statistical analysis selection



Significant pathways

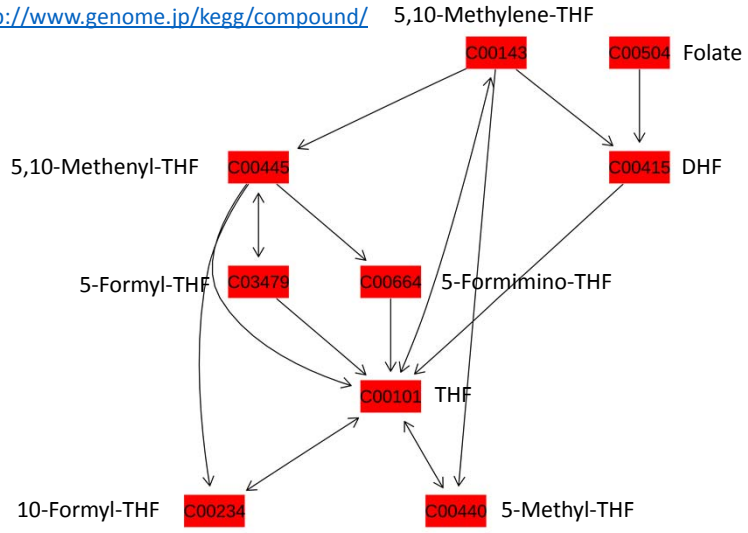


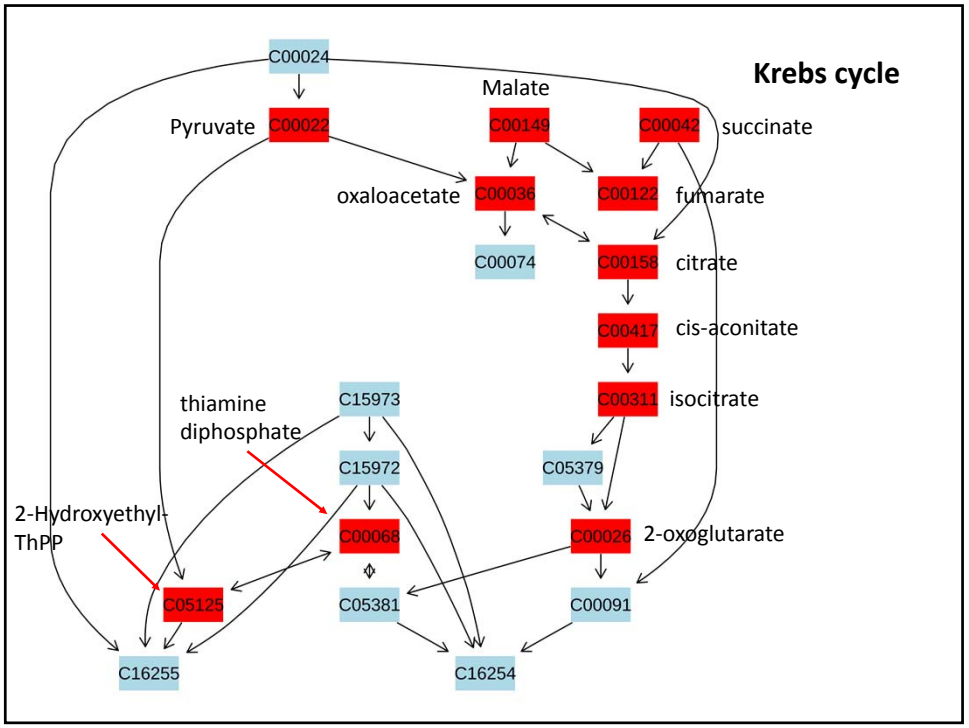
Steroid biosynthesis



One carbon metabolism

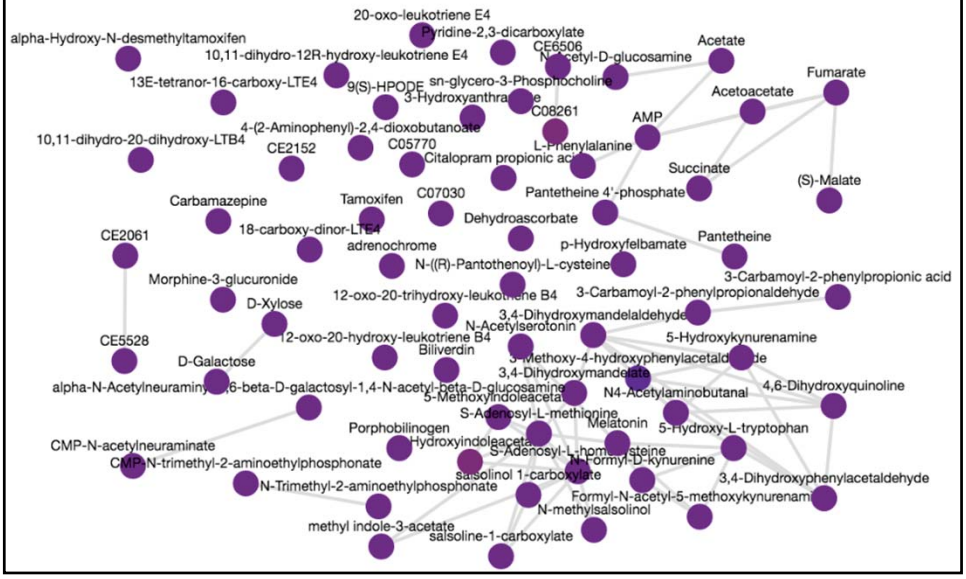
http://www.genome.jp/kegg/compound/





Mummichog "view" of metabolism

Grubbs_diet_neg



Mummichog pathways

Grubbs_diet_neg

Pathways	overlap_size	pathway_size	p-value (raw)	p-value
Sialic acid metabolism	16	18	0.00189	0.00172
Tryptophan metabolism	37	53	0.01277	0.00186
Drug metabolism - cytochrome P450	26	37	0.03198	0.00224
Linoleate metabolism	15	19	0.02282	0.00225
Porphyrin metabolism	12	15	0.03614	0.00272
Glycerophospholipid metabolism	16	22	0.05896	0.00307
Tyrosine metabolism	40	66	0.17048	0.00519
N-Glycan Degradation	6	7	0.09438	0.00701
Leukotriene metabolism	19	31	0.26898	0.01149
Pyruvate Metabolism	7	10	0.24864	0.0177
Phytanic acid peroxisomal oxidation	3	3	0.15901	0.02704
Heparan sulfate degradation	3	3	0.15901	0.02704
Omega-3 fatty acid metabolism	3	3	0.15901	0.02704
Chondroitin sulfate degradation	3	3	0.15901	0.02704
Vitamin B5 - CoA biosynthesis from pantothenate	5	7	0.30078	0.03145
Keratan sulfate degradation	5	7	0.30078	0.03145
Aminosugars metabolism	14	25	0.51141	0.04728

Questions?