THE UNIVERSITY OF ALABAMA AT BIRMINGHAM

Knowledge that will change your world

Pathway analysis with Metaboanalyst

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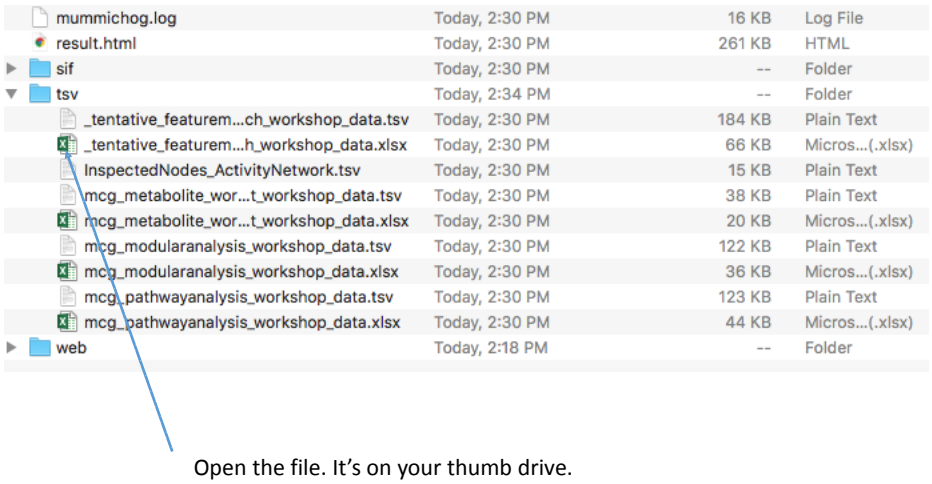
Targeted Metabolomics & Proteomics Laboratory

Files in mummichog results folder



Open the file. It's on your thumb drive.

Identification of each observed ion

	A	B	C	D	E	F	G	H	I
1	m/z	id	match_form	mz_difference	name	pathway			
2	121.0519	C12455	M+Na-2H[-]	0.0004	5-Aminopentanal				
3	125.0972	C06423	M-H2O-H[-]	0.0001	Octanoic acid; Caprylic acid; Octylic acid	Fatty acid activation			
4	131.0653	C00300	M(C13)-H[-]	-0.0003	Creatine; alpha-Methylguanidino acetic acid; M	Glycine, serine, alanine and threonine metabol			
5	135.0461	C00601	M-H+O[-]	0.001	Phenylacetaldehyde; alpha-Tolualdehyde	Ascorbate (Vitamin C) and Aldarate Metabolisr			
6	135.0461	C01801	M(S34)-H[-]	-0.0003	Deoxyribose; 2-Deoxy-D-erythro-pentose; Thyr	Pyrimidine metabolism$Pentose phosphate pa			
7	135.0461	C03765	M-H[-]	0.001	4-Hydroxyphenylacetaldehyde; 2-(4-Hydroxyph	Tyrosine metabolism			
8	135.0461	C07086	M-H[-]	0.001	Phenylacetic acid; Benzylformic acid; Phenylace	Tyrosine metabolism			
9	135.0461	CE0520	M(S34)-H[-]	-0.0003	(R)-glycerol 1-acetate	Glycerophospholipid metabolism			
10	135.0464	C00601	M-H+O[-]	0.0013	Phenylacetaldehyde; alpha-Tolualdehyde	Ascorbate (Vitamin C) and Aldarate Metabolisr			
11	135.0464	C01801	M(S34)-H[-]	0	Deoxyribose; 2-Deoxy-D-erythro-pentose; Thyr	Pyrimidine metabolism$Pentose phosphate pa			
12	135.0464	C03765	M-H[-]	0.0013	4-Hydroxyphenylacetaldehyde; 2-(4-Hydroxyph	Tyrosine metabolism			
13	135.0464	C05649	M(S34)-H[-]	-0.0013	Dihydropteridine; 6,7-Dihydropteridine				
14	135.0464	C07086	M-H[-]	0.0013	Phenylacetic acid; Benzylformic acid; Phenylace	Tyrosine metabolism			
15	135.0464	CE0520	M(S34)-H[-]	0	(R)-glycerol 1-acetate	Glycerophospholipid metabolism			
16	136.0588	C02505	M(Cl37)-H[-]	0.0005	2-Phenylacetamide	Tyrosine metabolism			
17	136.0588	C02558	M(Cl37)-H[-]	0.0005	N-Acetylarylamine				
18	137.0251	C00156	M-H[-]	0.0007	4-Hydroxybenzoate; Hydroxybenzoic acid; 4-Hy	Ubiquinone Biosynthesis			
19	137.0251	C00180	M-H+O[-]	0.0007	Benzoate; Benzoic acid; Benzenecarboxylic acid	Alkaloid biosynthesis II			
20	137.0251	C00633	M-H+O[-]	0.0007	4-Hydroxybenzaldehyde; p-Hydroxybenzaldehyde				
21	137.0251	C01620	M(S34)-H[-]	-0.0006		Ascorbate (Vitamin C) and Aldarate Metabolisr			
22	137.0251	C05585	M-H[-]	0.0007	Gentisate aldehyde				
23	137.0251	C12455	M+K-2H[-]	0.0001	5-Aminopentanal				
24	145.0518	C00233	M-H+O[-]	0.0012	4-Methyl-2-oxopentanoate; 2-Oxoisocaproate	Valine, leucine and isoleucine degradation			
25	145.0518	C00671	M-H+O[-]	0.0012	(S)-3-Methyl-2-oxopentanoic acid; (S)-3-Methyl	Valine, leucine and isoleucine degradation			

Select and copy the KEGG IDs

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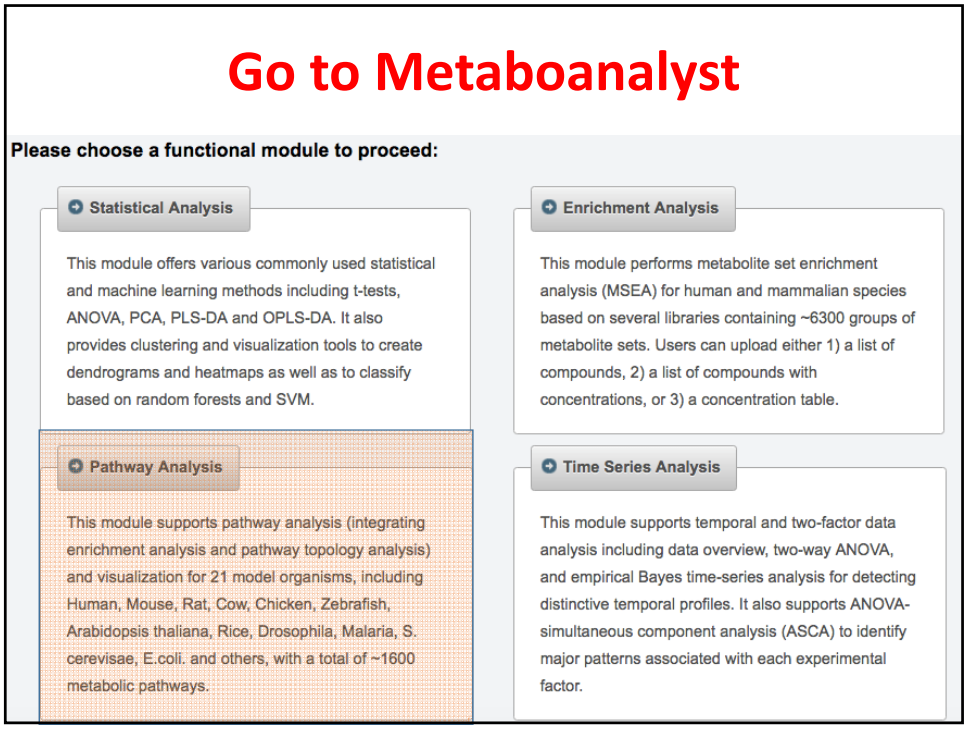
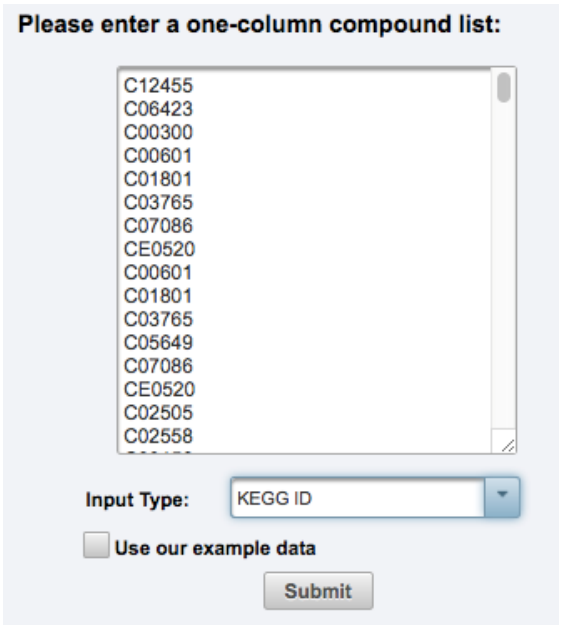
Go to Metaboanalyst





Transfer the KEGG IDs into the box, select the input type and submit

Listed metabolites

Compound Name/ID Standardization:

PLease note:

- Greek alphabets are not recognized, they should be replaced by English names (i.e. alpha, beta)
- Query names in normal white indicate exact match - marked by "1" in the download file;
- Query names highlighted indicate **no exact or unique match** - marked by "0" in the downloaded file;
- For **compound name**, you should click the **View** link to perform **approximate search** and manually select the correct match if found;
- For **KEGG ID**, it is possible to have multiple hits, you should click the **View** link to manually select the correct match if found;

Query	Hit	HMDB	PubChem	KEGG	Details
C12455	5-Aminopentanal	HMDB12815	443849	C12455	
C06423	Caprylic acid	HMDB00482	379	C06423	
C00300	Creatine	HMDB00064	586	C00300	
C00601	Phenylacetaldehyde	HMDB06236	998	C00601	
C01801	Deoxyribose	HMDB03224	22833604	C01801	
C03765	4-Hydroxyphenylacetaldehyde	HMDB03767	440113	C03765	
C07086	Phenylacetic acid	HMDB00209	999	C07086	
CE0520		-	-	-	View

No records?

Query name: CE0520

	Matched Name	HMDB	PubChem	KEGG
No records found.				

OK Cancel

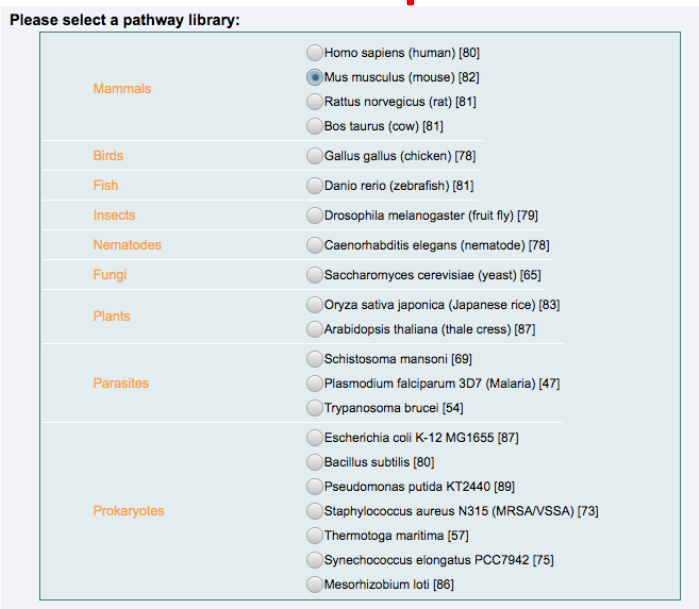
Proceed to bottom of the table

CE2635		-	-	-	View
CE2635		-	-	-	View
C01051	Uroporphyrinogen III	HMDB01086	1179	C01051	
C05766	Uroporphyrinogen I	HMDB02211	440775	C05766	
C05774	Cobinamide	HMDB06902	11528127	C05774	
CE5800		-	-	-	View
C05774	Cobinamide	HMDB06902	11528127	C05774	

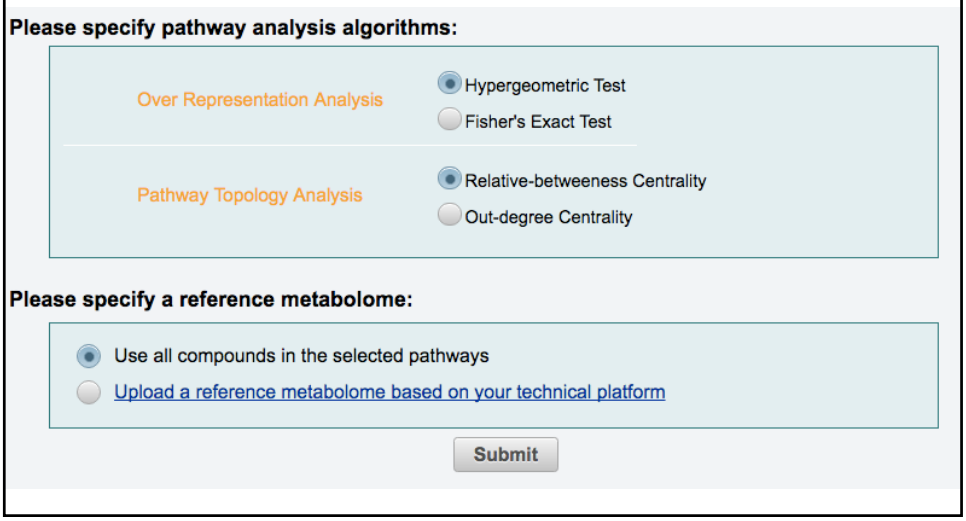
You can download the result here

Submit

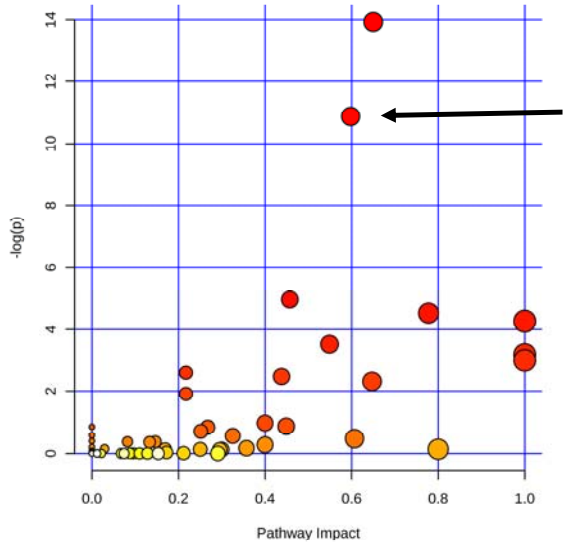
Choose a species



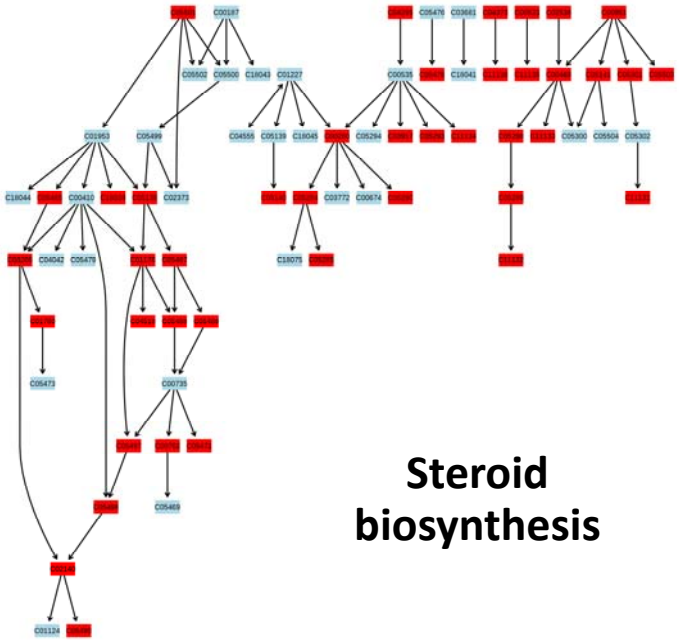
Statistical analysis selection



Significant pathways

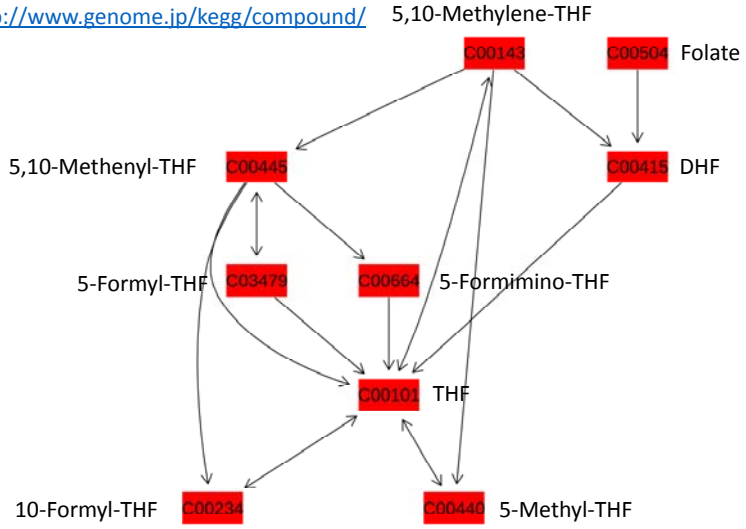


Steroid biosynthesis



One carbon metabolism

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



Mummichog pathways

Workshop study

Pathway Name	Match Status	p	-log(p)	Holm p	FDR	Impact	Details
Drug metabolism - cytochrome P450	37/56	8.9246E-7	13.929	7.3182E-5	7.3182E-5	0.65003	KEGG
Steroid hormone biosynthesis	42/72	1.8919E-5	10.875	0.0015325	7.7569E-4	0.59781	KEGG
Arachidonic acid metabolism	20/36	0.0070611	4.9532	0.56489	0.193	0.45729	KEGG
Phenylalanine metabolism	8/11	0.010871	4.5216	0.85882	0.22286	0.77778	KEGG
Phenylalanine, tyrosine and tryptophan biosynthesis	4/4	0.014069	4.2638	1.0	0.23073	1.0	KEGG
Tryptophan metabolism	20/40	0.029381	3.5274	1.0	0.40153	0.54903	KEGG
Ubiquinone and other terpenoid-quinone biosynthesis	3/3	0.040932	3.1958	1.0	0.47949	1.0	KEGG
One carbon pool by folate	6/9	0.049559	3.0046	1.0	0.50797	1.0	KEGG

Big omission – no records for the isoflavones that were the prominent ions. Isoflavones are in the diet as β-glucosides. They were hydrolyzed by intestinal wall enzymes, sulfated and glucuronidated and excreted into bile. In the colon, they were differentially metabolized in this experiment. The treatment eliminated the sulfatases and allowed the sulfated genistein and daidzein to accumulate.

Questions?