

Metabolomic Data Analysis with MetaboAnalyst 3.0

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1 Background

MESA or Metabolite Set Enrichment Analysis is a way to identify biologically meaningful patterns that are significantly enriched in quantitative metabolomic data. In conventional approaches, metabolites are evaluated individually for their significance under conditions of study. Those compounds that have passed certain significance level are then combined to see if any meaningful patterns can be discerned. In contrast, MSEA directly investigates if a set of functionally related metabolites without the need to preselect compounds based on some arbitrary cut-off threshold. It has the potential to identify subtle but consistent changes among a group of related compounds, which may go undetected with the conventional approaches.

Essentially, MSEA is a metabolomic version of the popular GSEA (Gene Set Enrichment Analysis) software with its own collection of metabolite set libraries as well as an implementation of user-friendly web-interfaces. GSEA is widely used in genomics data analysis and has proven to be a powerful alternative to conventional approaches. For more information, please refer to the original paper by Subramanian A, and a nice review paper by Nam D, Kim SY.

2 MSEA Overview

Metabolite set enrichment analysis consists of four steps - data input, data processing, data analysis, and results download. Different analysis procedures are performed based on different input types. In addition, users can also browse and search the metabolite set libraries as well as upload their self-defined metabolite sets for enrichment analysis. Users can also perform metabolite name mapping between a variety of compound names, synonyms, and major database identifiers.

3 Data Input

There are three enrichment analysis algorithms offered by MSEA. Accordingly, three different types of data inputs are required by these three approaches:

- A list of important compound names - entered as a one column data (*Over Representation Analysis (ORA)*);
- A single measured biofluid (urine, blood, CSF) sample- entered as tab separated two-column data with the first column for compound name, and the second for concentration values (*Single Sample Profiling (SSP)*);
- A compound concentration table - entered as a comma separated (.csv) file with the each sample per row and each metabolite concentration per column. The first column is sample names and the second column for sample phenotype labels (*Quantitative Enrichment Analysis (QEA)*)

You selected Quantitative Enrichment Analysis (QEA) which requires a concentration table. This is the most common data format generated from quantitative metabolomics studies. The phenotype label can be discrete (binary or multi-class) or continuous.

4 Data Process

The first step is to standardize the compound labels. It is an essential step since the compound labels will be subsequently compared with compounds contained in the metabolite set library. MSEA has a built-in tool to convert between compound common names, synonyms, identifiers used in HMDB ID, PubChem, ChEBI, BiGG, METLIN, KEGG, or Reactome. **Table 1** shows the conversion results. Note: *1* indicates exact match, *2* indicates approximate match, and *0* indicates no match. A text file containing the result can be found in the downloaded file *name_map.csv*

Table 1: Result from Compound Name Mapping

Query	Match
1 1,2-dilinoeoyl-GPC	NA
2 1,2-dioeoyl-GPC	NA
3 1,2-dioeoyl-GPE	NA
4 1,2-dipalmitoyl-GPC	NA
5 1,2-distearoyl-GPC	NA
6 1,5-anhydroglucitol	1,5-Anhydrosorbitol
7 1-(1-enyl-oleoyl)-GPE	NA
8 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC	NA
9 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE	NA
10 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC	NA
11 1-(1-enyl-palmitoyl)-2-linoleoyl-GPE	NA
12 1-(1-enyl-palmitoyl)-2-oleoyl-GPC	NA
13 1-(1-enyl-palmitoyl)-2-oleoyl-GPE	NA
14 1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC	NA
15 1-(1-enyl-palmitoyl)-2-palmitoyl-GPC	NA
16 1-(1-enyl-palmitoyl)-GPC	NA
17 1-(1-enyl-palmitoyl)-GPE	NA
18 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE	NA
19 1-(1-enyl-stearoyl)-2-linoleoyl-GPE	NA
20 1-(1-enyl-stearoyl)-2-oleoyl-GPE	NA
21 1-(1-enyl-stearoyl)-GPE	NA
22 1-(3-aminopropyl)-2-pyrrolidone	NA
23 1-arachidonoyl-GPC	NA
24 1-arachidonoyl-GPE	NA
25 1-arachidonoyl-GPI	NA
26 1-lignoceroyl-GPC	NA
27 1-linolenoyl-GPC	NA
28 1-linoleoyl-2-arachidonoyl-GPC	NA
29 1-linoleoyl-GPC	NA
30 1-linoleoyl-GPE	NA
31 1-linoleoyl-GPI	NA
32 1-linoleoylglycerol	NA
33 1-methylguanidine	Methylguanidine
34 1-methylhistidine	1-Methylhistidine
35 1-methylimidazoleacetate	NA
36 1-methylnicotinamide	1-Methylnicotinamide
37 1-oleoyl-2-linoleoyl-glycerol	NA
38 1-oleoyl-2-linoleoyl-GPC	NA
39 1-oleoyl-2-linoleoyl-GPE	NA
40 1-oleoyl-3-linoleoyl-glycerol	NA
41 1-oleoyl-GPC	NA
42 1-oleoyl-GPE	NA
43 1-oleoyl-GPI	NA
44 1-oleoyl-GPS	NA
45 1-oleoylglycerol	NA
46 1-palmitoleoyl-2-linoleoyl-GPC	NA
47 1-palmitoleoyl-2-oleoyl-glycerol	NA
48 1-palmitoleoyl-3-oleoyl-glycerol	NA
49 1-palmitoleoyl-GPC	NA
50 1-palmitoleoylglycerol	NA
51 1-palmitoyl-2-arachidonoyl-GPC	NA
52 1-palmitoyl-2-arachidonoyl-GPE	NA
53 1-palmitoyl-2-linoleoyl-glycerol	NA
54 1-palmitoyl-2-linoleoyl-GPC	NA
55 1-palmitoyl-2-linoleoyl-GPE	NA
56 1-palmitoyl-2-oleoyl-GPC	NA
57 1-palmitoyl-2-oleoyl-GPE	NA
58 1-palmitoyl-2-oleoyl-GPG	NA
59 1-palmitoyl-2-palmitoleoyl-GPC	NA
60 1-palmitoyl-2-stearoyl-GPC	NA
61 1-palmitoyl-3-linoleoyl-glycerol	NA
62 1-palmitoyl-GPC	NA

63	1-palmitoyl-GPE	NA
64	1-palmitoyl-GPG	NA
65	1-palmitoyl-GPI	NA
66	1-stearoyl-2-arachidonoyl-GPC	NA
67	1-stearoyl-2-arachidonoyl-GPE	NA
68	1-stearoyl-2-arachidonoyl-GPI	NA
69	1-stearoyl-2-arachidonoyl-GPS	NA
70	1-stearoyl-2-linoleoyl-GPC	NA
71	1-stearoyl-2-linoleoyl-GPE	NA
72	1-stearoyl-2-oleoyl-GPC	NA
73	1-stearoyl-2-oleoyl-GPE	NA
74	1-stearoyl-2-oleoyl-GPS	NA
75	1-stearoyl-GPC	NA
76	1-stearoyl-GPE	NA
77	1-stearoyl-GPI	NA
78	1-stearoyl-GPS	NA
79	10-heptadecenoate	NA
80	10-nonadecenoate	NA
81	12,13-DiHOME	12,13-DHOME
82	12-HETE	12-HETE
83	15-HETE	15(S)-HETE
84	15-methylpalmitate	NA
85	16-hydroxypalmitate	NA
86	17-methylstearate	NA
87	2'-deoxycytidine	Deoxycytidine
88	2'-deoxyguanosine	Deoxyguanosine
89	2'-deoxyinosine	Deoxyinosine
90	2'-deoxyuridine	Deoxyuridine
91	2-aminoadipate	Aminoadipic acid
92	2-aminoheptanoate	NA
93	2-aminooctanoate	DL-2-Aminooctanoic acid
94	2-hydroxy-3-methylvalerate	2-Hydroxy-3-methylpentanoic acid
95	2-hydroxyadipate	2-Hydroxyadipic acid
96	2-hydroxybutyrate/2-hydroxyisobutyrate	NA
97	2-hydroxyglutarate	2-Hydroxyglutarate
98	2-hydroxystearate	NA
99	2-linoleoylglycerol	NA
100	2-methylbutyrylcarnitine	NA
101	2-methylbutyrylglycine	2-Methylbutyrylglycine
102	2-methylcitrate/homocitrate	NA
103	2-methylmalonyl carnitine	NA
104	2-oleoylglycerol	NA
105	2-palmitoleoyl-GPC	NA
106	2-palmitoyl-GPC	NA
107	2-stearoyl-GPE	NA
108	3-(4-hydroxyphenyl)lactate	3-(4-Hydroxyphenyl)lactate
109	3-aminoisobutyrate	3-Aminoisobutanoic acid
110	3-hydroxy-3-methylglutarate	3-Hydroxymethylglutaric acid
111	3-hydroxybutyrate	3-Hydroxybutyric acid
112	3-hydroxybutyrylcarnitine	NA
113	3-hydroxyisobutyrate	(S)-3-Hydroxyisobutyric acid
114	3-indoxyl	NA
115	3-methylcytidine	NA
116	3-methylhistidine	3-Methylhistidine
117	3-phosphoglycerate	3-Phosphoglyceric acid
118	3-ureidopropionate	Ureidopropionic acid
119	4-cholesten-3-one	Cholestenone
120	4-ethylphenylsulfate	NA
121	4-guanidinobutanoate	4-Guanidinobutanoic acid
122	4-hydroxy-nonenal-glutathione	NA
123	4-hydroxybutyrate	4-Hydroxybutyric acid
124	4-imidazoleacetate	Imidazoleacetic acid
125	4-vinylphenol sulfate	NA
126	5-aminovalerate	5-Aminopentanoic acid
127	5-dodecenoate	5-Dodecenoic acid
128	5-hydroxylysine	5-Hydroxylysine
129	5-methylthioadenosine	5'-Methylthioadenosine
130	5-oxoproline	Pyroglutamic acid
131	6-oxopiperidine-2-carboxylic acid	NA
132	6-phosphogluconate	6-Phosphogluconic acid
133	7-hydroxycholesterol	7b-Hydroxycholesterol
134	7-methylguanine	7-Methylguanine
135	9,10-DiHOME	9,10-DHOME
136	acetylcarnitine	L-Acetylcarnitine
137	acetylphosphate	Acetylphosphate
138	aconitate	NA
139	adenine	Adenine
140	adenosine	Adenosine
141	adenosine 2'-monophosphate	NA
142	adenosine 3',5'-diphosphate	Adenosine 3',5'-diphosphate
143	adenosine 3'-monophosphate	NA
144	adenosine 5'-diphosphoribose	Adenosine diphosphate ribose
145	adenosine 5'-monophosphate	Adenosine monophosphate
146	adrenate	Adrenic acid
147	alanine	Alanine
148	allantoin	Allantoin
149	alpha-hydroxyisocaproate	Leucinic acid

150	alpha-hydroxyisovalerate	2-Hydroxy-3-methylbutyric acid
151	alpha-ketoglutarate	NA
152	alpha-tocopherol	Alpha-Tocopherol
153	anserine	Anserine
154	arabitol/xylitol	NA
155	arabonate/xylonate	NA
156	arachidate	Arachidic acid
157	arachidonate	NA
158	arachidonoyl ethanolamide	NA
159	arginine	L-Arginine
160	argininosuccinate	Argininosuccinic acid
161	ascorbate	Ascorbic acid
162	asparagine	L-Asparagine
163	aspartate	L-Aspartic acid
164	azelate	Azelaic acid
165	behenoyl sphingomyelin	NA
166	beta-alanine	Beta-Alanine
167	beta-guanidinopropanoate	NA
168	beta-hydroxyisovaleroylcarnitine	NA
169	beta-muricholate	NA
170	betaine	Betaine
171	betaine aldehyde	Betaine aldehyde
172	butyrylcarnitine	Butyrylcarnitine
173	C-glycosyltryptophan	NA
174	campesterol	Campesterol
175	carboxyethyl-GABA	N-Carboxyethyl-g-aminobutyric acid
176	carnitine	Carnitine
177	carnosine	Carnosine
178	catechol sulfate	NA
179	cholesterol	Cholesterol
180	choline	Choline
181	choline phosphate	Phosphorylcholine
182	citrate	Citric acid
183	citrulline	Citrulline
184	corticosterone	Corticosterone
185	creatine	Creatine
186	creatine phosphate	Phosphocreatine
187	creatinine	Creatinine
188	cystathionine	L-Cystathionine
189	cysteine	Cysteine
190	cysteine s-sulfate	NA
191	cysteine sulfinic acid	3-Sulfinioalanine
192	cystine	L-Cystine
193	cytidine	Cytidine
194	cytidine 3'-monophosphate	NA
195	cytidine 5'-diphosphocholine	Citicoline
196	cytidine 5'-monophosphate	Cytidine monophosphate
197	cytidine 5'-monophospho-N-acetylneuraminic acid	NA
198	cytidine-5'-diphosphoethanolamine	NA
199	cytosine	Cytosine
200	decanoylcarnitine	Decanoylcarnitine
201	dehydroascorbate	Dehydroascorbate
202	deoxycarnitine	4-Trimethylammoniobutanoic acid
203	dihomo-linoleate	NA
204	dihomo-linolenate	NA
205	dihydroxyphenylalanine	NA
206	dihydroxyacetone	Dihydroxyacetone
207	dimethyl	NA
208	dimethylarginine	NA
209	dimethylglycine	Dimethylglycine
210	docosadienoate	NA
211	docosaehxaenoate	Docosaehxaenoic acid
212	docosapentaenoate	Docosapentaenoic acid
213	dopamine sulfate	NA
214	eicosapentaenoate	Eicosapentaenoic acid
215	eicosenoate	Eicosenoic acid
216	equol sulfate	NA
217	ergothioneine	Ergothioneine
218	erucate	NA
219	erythronate*	NA
220	ethylmalonate	Ethylmalonic acid
221	flavin adenine dinucleotide	FAD
222	fructose	D-Fructose
223	fumarate	Fumaric acid
224	galactitol	Galactitol
225	galactonate	Galactonic acid
226	gamma-aminobutyrate	Gamma-Aminobutyric acid
227	gamma-carboxyglutamate	NA
228	gamma-glutamyl-epsilon-lysine	NA
229	gamma-glutamylalanine	5-L-Glutamyl-L-alanine
230	gamma-glutamylglutamate	Gamma Glutamylglutamic acid
231	gamma-glutamylglutamine	Gamma-Glutamyl Glutamine
232	gamma-glutamylglycine	NA
233	gamma-glutamylhistidine	NA
234	gamma-glutamylisoleucine*	NA
235	gamma-glutamylleucine	L-gamma-glutamyl-L-leucine
236	gamma-glutamylphenylalanine	Glutamylphenylalanine

237	gamma-glutamylvaline	L-gamma-glutamyl-L-valine
238	gamma-tocopherol/beta-tocopherol	NA
239	gluconate	Gluconic acid
240	glucose	D-Glucose
241	glucuronate	D-Glucuronic acid
242	glutamate	D-Glutamic acid
243	glutamate, gamma-methyl ester	NA
244	glutamine	L-Glutamine
245	glutarate	Glutaric acid
246	glutarylcarntine	Glutarylcarntine
247	glutathione, oxidized (GSSG)	NA
248	glutathione, reduced (GSH)	NA
249	glycerate	Glyceric acid
250	glycerol	Glycerol
251	glycerol 3-phosphate	Glycerol 3-phosphate
252	glycerophosphoethanolamine	Glycerylphosphorylethanolamine
253	glycerophosphoglycerol	NA
254	glycerophosphoinositol*	NA
255	glycerophosphorylcholine	Glycerophosphocholine
256	glycine	Glycine
257	glycosyl-N-palmitoyl-sphingosine	NA
258	glycosyl-N-stearoyl-sphingosine	NA
259	glycylleucine	Glycyl-L-leucine
260	glycylvaline	NA
261	guanidinoacetate	Guanidoacetic acid
262	guanidinossuccinate	Guanidinossuccinic acid
263	guanine	Guanine
264	guanosine	Guanosine
265	guanosine 5'- monophosphate	NA
266	gulonic acid*	NA
267	heme	Heme
268	hexadecanedioate	Hexadecanedioic acid
269	hexanoylcarntine	Hexanoylcarntine
270	hexanoylglycine	Hexanoylglycine
271	hippurate	Hippuric acid
272	histamine	Histamine
273	histidine	L-Histidine
274	homoarginine	Homo-L-arginine
275	homocitrulline	Homocitrulline
276	homostachydrine*	NA
277	hypotaurine	Hypotaurine
278	hypoxanthine	Hypoxanthine
279	imidazole lactate	Imidazole lactate
280	imidazole propionate	NA
281	indolelactate	Indolelactic acid
282	inosine	Inosine
283	inosine 5'-monophosphate (IMP)	NA
284	Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate	NA
285	isobutyrylcarntine	NA
286	isocitrate	Isocitric acid
287	isoleucine	(+/-)-erythro-Isoleucine
288	isoleucylglycine	NA
289	isovalerylcarntine	Isovalerylcarntine
290	isovalerylglycine	Isovalerylglycine
291	kynurenate	Kynurenic acid
292	kynurenine	L-Kynurenine
293	lactate	L-Lactic acid
294	laurylcarntine	NA
295	leucine	L-Leucine
296	leucylglycine	NA
297	linoleate	Linoleic acid
298	linolenate	Alpha-Linolenic acid
299	linoleoylcarntine*	NA
300	lysine	L-Lysine
301	malate	NA
302	malonylcarntine	Malonylcarntine
303	maltose	D-Maltose
304	maltotriose	Maltotriose
305	mannitol/sorbitol	NA
306	mannose	D-Mannose
307	margarate	Heptadecanoic acid
308	mead acid	5,8,11-Eicosatrienoic acid
309	methionine	NA
310	methionine sulfoxide	Methionine sulfoxide
311	methyl glucopyranoside	NA
312	methylmalonate	Methylmalonic acid
313	methylphosphate	NA
314	methylsuccinate	Methylsuccinic acid
315	myo-inositol	Myoinositol
316	myristate	Myristic acid
317	myristoleate	Myristoleic acid
318	myristoylcarntine	Tetradecanoylcarntine
319	N-acetyl-aspartyl-glutamate	NA
320	N-acetyl-beta-alanine	N-Acetyl-beta-alanine
321	N-acetyl-glucosamine 1-phosphate	N-Acetyl-glucosamine 1-phosphate
322	N-acetylalanine	N-Acetyl-L-alanine
323	N-acetylarginine	NA

324	N-acetylasparagine	N-Acetylasparagine
325	N-acetylaspartate	N-Acetyl-L-aspartic acid
326	N-acetylglucosamine 6-phosphate	N-Acetylglucosamine 6-phosphate
327	N-acetylglutamate	N-Acetylglutamic acid
328	N-acetylglutamine	N-Acetylglutamine
329	N-acetylglycine	Acetylglycine
330	N-acetylhistidine	N-Acetylhistidine
331	N-acetylleucine	N-Acetylleucine
332	N-acetylmethionine	N-Acetyl-L-methionine
333	N-acetylneuraminate	NA
334	N-acetylphenylalanine	N-Acetyl-L-phenylalanine
335	N-acetylputrescine	N-Acetylputrescine
336	N-acetylserine	N-Acetylserine
337	N-acetyltaurine	NA
338	N-acetylthreonine	NA
339	N-alpha-acetylornithine	NA
340	N-carbamoylaspartate	Ureidosuccinic acid
341	N-delta-acetylornithine	NA
342	N-formylmethionine	NA
343	N-formylphenylalanine	NA
344	N-glycolylneuraminate	N-Glycolylneuraminic acid
345	N-methyl-4-aminobutyric acid	NA
346	N-monomethylarginine	NA
347	N-palmitoyl-sphinganine	NA
348	N-palmitoyl-sphingosine	NA
349	N-palmitoyltaurine	NA
350	N-stearoyltaurine	NA
351	N1-Methyl-2-pyridone-5-carboxamide	N1-Methyl-2-pyridone-5-carboxamide
352	N1-methyladenosine	1-Methyladenosine
353	N2-acetyllysine/N6-acetyllysine	NA
354	N6,N6,N6-trimethyllysine	NA
355	N6-carboxymethyllysine	NA
356	N6-succinyladenosine	NA
357	nicotinamide	Niacinamide
358	nicotinamide adenine dinucleotide	NAD
359	nicotinamide riboside	Nicotinamide riboside
360	nonadecanoate	Nonadecanoic acid
361	O-sulfo-L-tyrosine	NA
362	octanoylcarnitine	L-Octanoylcarnitine
363	oleamide	Oleamide
364	oleate/vaccenate	NA
365	oleoyl ethanolamide	NA
366	oleoylcarnitine	Oleoylcarnitine
367	ornithine	Ornithine
368	orotate	Orotic acid
369	orotidine	Orotidine
370	oxalate	Oxalic acid
371	p-cresol sulfate	p-Cresol sulfate
372	p-cresol-glucuronide*	NA
373	palmitate	Palmitic acid
374	palmitoleate	Palmitoleic acid
375	palmitoyl dihydrosphingomyelin	NA
376	palmitoyl ethanolamide	Palmitoylethanolamide
377	palmitoyl sphingomyelin	NA
378	palmitoylcarnitine	NA
379	pantothenate	Pantothenic acid
380	phenol sulfate	NA
381	phenylacetyl glycine	Phenylacetyl glycine
382	phenylalanine	L-Phenylalanine
383	phenylalanyl glycine	NA
384	phenyllactate	Phenyllactic acid
385	phosphate	Phosphate
386	phosphoenolpyruvate	Phosphoenolpyruvic acid
387	phosphoethanolamine	O-Phosphoethanolamine
388	phosphopantetheine	Pantetheine 4'-phosphate
389	pipecolate	Pipecolic acid
390	pro-hydroxy-pro	NA
391	proline	L-Proline
392	prolylglycine	L-prolyl-L-glycine
393	propionylcarnitine	Propionylcarnitine
394	pseudouridine	Pseudouridine
395	putrescine	Putrescine
396	pyridoxal	Pyridoxal
397	pyridoxamine	Pyridoxamine
398	pyridoxamine phosphate	NA
399	pyridoxate	NA
400	pyroglutamine*	NA
401	quinolinate	Quinolinic acid
402	retinol	Vitamin A
403	ribitol	Ribitol
404	riboflavin	Riboflavin
405	ribonate	Ribonic acid
406	ribose	D-Ribose
407	ribulose	L-Ribulose
408	S-adenosylhomocysteine	S-Adenosylhomocysteine
409	S-adenosylmethionine	S-Adenosylmethionine
410	saccharopine	Saccharopine

411	salicylate	Salicylic acid
412	sarcosine	Sarcosine
413	sebacate	Sebacic acid
414	sedoheptulose-7-phosphate	D-Sedoheptulose 7-phosphate
415	serine	L-Serine
416	spermidine	Spermidine
417	sphinganine	Sphinganine
418	sphingomyelin	SM(d18:1/18:0)
419	sphingosine	Sphingosine
420	stachydrine	Proline betaine
421	stearate	Stearic acid
422	stearidonate	NA
423	stearoyl ethanolamide	Stearoylethanolamide
424	stearoyl sphingomyelin	NA
425	stearoylcarnitine	Stearoylcarnitine
426	succinate	Succinic acid
427	succinylcarnitine	NA
428	sucrose	Sucrose
429	sulfate*	NA
430	tartronate	NA
431	taurine	Taurine
432	tauro-beta-muricholate	Tauro-b-muricholic acid
433	taurochenodeoxycholate	Taurochenodesoxycholic acid
434	taurocholate	Taurocholic acid
435	taurocyamine	Taurocyamine
436	taurodeoxycholate	NA
437	tauroursodeoxycholate	Tauroursodeoxycholic acid
438	tetradecanedioate	Tetradecanedioic acid
439	thiamin	Thiamine
440	thiamin monophosphate	Thiamine monophosphate
441	threonate	Threonic acid
442	threonine	L-Threonine
443	thymidine	Thymidine
444	tiglylcarnitine	Tiglylcarnitine
445	trans-4-hydroxyproline	4-Hydroxyproline
446	trans-uocanate	NA
447	tricosanoyl	NA
448	trigonelline	Trigonelline
449	trimethylamine N-oxide	Trimethylamine N-oxide
450	tryptophan	D-Tryptophan
451	tyrosine	L-Tyrosine
452	tyrosylglycine	NA
453	UDP-galactose	Uridine diphosphategalactose
454	UDP-glucose	Uridine diphosphate glucose
455	UDP-glucuronate	Uridine diphosphate glucuronic acid
456	UDP-N-acetylgalactosamine	Uridine diphosphate-N-acetylgalactosamine
457	UDP-N-acetylglucosamine	Uridine diphosphate-N-acetylglucosamine
458	uracil	Uracil
459	urate	Uric acid
460	urea	Urea
461	uridine	Uridine
462	uridine 5'-diphosphate	Uridine 5'-diphosphate
463	uridine 5'-monophosphate	Uridine 5'-monophosphate
464	valine	L-Valine
465	valylglycine	NA
466	xanthine	Xanthine
467	xanthosine	Xanthosine

The second step is to check concentration values. For SSP analysis, the concentration must be measured in *umol* for blood and CSF samples. The urinary concentrations must be first converted to *umol/mmol_creatinine* in order to compare with reported concentrations in literature. No missing or negative values are allowed in SSP analysis. The concentration data for QEA analysis is more flexible. Users can upload either the original concentration data or normalized data. Missing or negative values are allowed (coded as *NA*) for QEA. Please note, MSEA does not perform data normalization. If normalization is important, you should first normalize your data before upload. You can use our companion website **MetaboAnalyst** www.metaboanalyst.ca for a variety of data processing and normalization methods.

5 Selection of Metabolite Set Library

Before proceeding to enrichment analysis, a metabolite set library has to be chosen. There are seven built-in libraries offered by MSEA:

- Metabolic pathway associated metabolite sets (*currently contains 88 entries*);
- Disease associated metabolite sets (reported in blood) (*currently contains 416 entries*);
- Disease associated metabolite sets (reported in urine) (*currently contains 346 entries*);
- Disease associated metabolite sets (reported in CSF) (*currently contains 124 entries*);
- Metabolite sets associated with SNPs (*currently contains 4500 entries*);
- Predicted metabolite sets based on computational enzyme knockout model (*currently contains 912 entries*);
- Metabolite sets based on locations (*currently contains 57 entries*);

In addition, MSEA also allows user-defined metabolite sets to be uploaded to perform enrichment analysis on arbitrary groups of compounds which researchers want to test. The metabolite set library is simply a two-column comma separated text file with the first column for metabolite set names and the second column for its compound names (**must use HMDB compound name**) separated by "; ". Please note, the built-in libraries are mainly from human studies. The functional grouping of metabolites may not be valid. Therefore, for data from subjects other than human being, users are suggested to upload their self-defined metabolite set libraries for enrichment analysis.

6 Enrichment Analysis

Quantitative enrichment analysis (QEA) will be performed when the user uploads a concentration table. The enrichment analysis is performed using package **globaltest**¹. It uses a generalized linear model to estimate a *Q-statistic* for each metabolite set, which describes the correlation between compound concentration profiles, X, and clinical outcomes, Y. The *Q statistic* for a metabolite set is the average of the *Q* statistics for each metabolite in the set. **Figure 2** below summarizes the result.

¹Jelle J. Goeman, Sara A. van de Geer, Floor de Kort and Hans C. van Houwelingen. *A global test for groups of genes: testing association with a clinical outcome*, Bioinformatics Vol. 20 no. 1 2004, pages 93-99

Enrichment Overview (top 50)

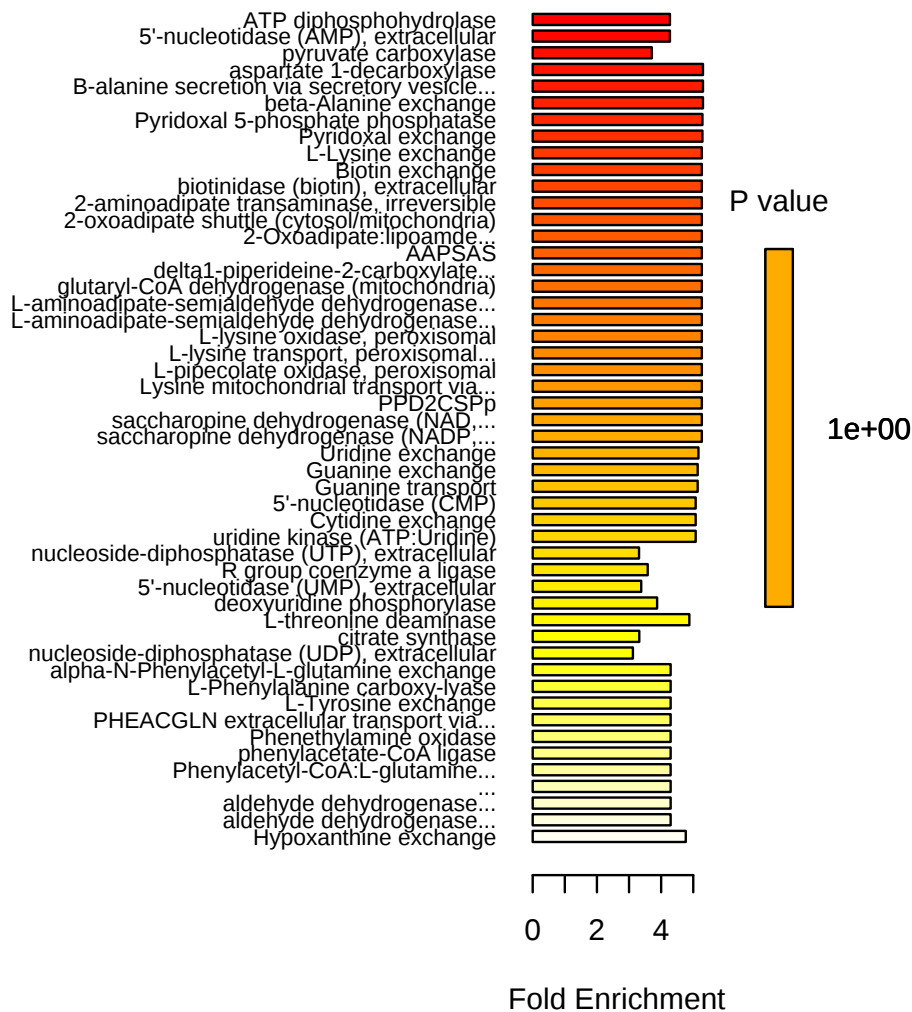


Figure 1: Summary Plot for Quantitative Enrichment Analysis (QEA)

Table 2: Result from Quantitative Enrichment Analysis

	Total Cmpd	Hits	Statistic Q	Expected Q	Raw p	Holm p	FDR
ATP diphosphohydrolase	7	2	61.06	14.29	4.31E-03	1.00E+00	6.26E-02
5'-nucleotidase (AMP), extracellular	5	2	61.06	14.29	4.31E-03	1.00E+00	6.26E-02
pyruvate carboxylase	9	7	53.01	14.29	4.71E-03	1.00E+00	6.26E-02
aspartate 1-decarboxylase	1	1	75.75	14.29	4.93E-03	1.00E+00	6.26E-02
B-alanine secretion via secretory vesicle (ATP driven)	1	1	75.75	14.29	4.93E-03	1.00E+00	6.26E-02
beta-Alanine exchange	1	1	75.75	14.29	4.93E-03	1.00E+00	6.26E-02
Pyridoxal 5-phosphate phosphatase	2	1	75.52	14.29	5.08E-03	1.00E+00	6.26E-02
Pyridoxal exchange	1	1	75.52	14.29	5.08E-03	1.00E+00	6.26E-02
L-Lysine exchange	2	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
Biotin exchange	3	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
biotinidase (biotin), extracellular	3	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
2-aminoadipate transaminase, irreversible	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
2-oxoadipate shuttle (cytosol/mitochondria)	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
2-Oxoadipate:lipoamide 2-oxidoreductase(decarboxylating and acceptor-succinylating) (mitochondria)	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
AAPSAS	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
delta1-piperidine-2-carboxylate reductase, peroxisomal	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
glutaryl-CoA dehydrogenase (mitochondria)	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
L-aminoadipate-semialdehyde dehydrogenase (NADH)	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
L-aminoadipate-semialdehyde dehydrogenase (NADH), mitochondrial	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
L-lysine oxidase, peroxisomal	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
L-lysine transport, peroxisomal (irreversible)	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
L-pipecolate oxidase, peroxisomal	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
Lysine mitochondrial transport via ornithine carrier	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
PPD2CSPp	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
saccharopine dehydrogenase (NAD, L-glutamate forming), mitochondrial	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
saccharopine dehydrogenase (NADP, L-lysine forming), mitochondrial	1	1	75.25	14.29	5.26E-03	1.00E+00	6.26E-02
Uridine exchange	1	1	73.74	14.29	6.32E-03	1.00E+00	6.26E-02
Guanine exchange	1	1	73.40	14.29	6.58E-03	1.00E+00	6.26E-02
Guanine transport	1	1	73.40	14.29	6.58E-03	1.00E+00	6.26E-02
5'-nucleotidase (CMP)	1	1	72.51	14.29	7.30E-03	1.00E+00	6.26E-02
Cytidine exchange	1	1	72.51	14.29	7.30E-03	1.00E+00	6.26E-02
uridine kinase (ATP:Uridine)	1	1	72.51	14.29	7.30E-03	1.00E+00	6.26E-02
nucleoside-diphosphatase (UTP), extracellular	7	3	47.32	14.29	8.04E-03	1.00E+00	6.26E-02
R group coenzyme a ligase	11	2	51.18	14.29	9.21E-03	1.00E+00	6.26E-02
5'-nucleotidase (UMP), extracellular	12	7	48.28	14.29	9.44E-03	1.00E+00	6.26E-02
deoxyuridine phosphorylase	3	3	55.35	14.29	9.85E-03	1.00E+00	6.26E-02
L-threonine deaminase	3	1	69.70	14.29	9.91E-03	1.00E+00	6.26E-02
citrate synthase	7	5	47.42	14.29	1.03E-02	1.00E+00	6.26E-02
nucleoside-diphosphatase (UDP), extracellular	12	8	44.59	14.29	1.04E-02	1.00E+00	6.26E-02
alpha-N-Phenylacetyl-L-glutamine exchange	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
L-Phenylalanine carboxy-lyase	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
L-Tyrosine exchange	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
PHEACGLN extracellular transport via diffusion	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
Phenethylamine oxidase	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
phenylacetate-CoA ligase	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
Phenylacetyl-CoA:L-glutamine	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
alpha-N-phenylacetyltransferase	3	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
L-Phenylalanine,tetrahydrobiopterin:indoxigen oxidoreductase (4-hydroxylating)	2	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
aldehyde dehydrogenase (phenylacetaldehyde, NAD)	2	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
aldehyde dehydrogenase (phenylacetaldehyde, NADP)	2	2	61.37	14.29	1.14E-02	1.00E+00	6.26E-02
Hypoxanthine exchange	1	1	68.10	14.29	1.17E-02	1.00E+00	6.26E-02
Hypoxanthine transport	1	1	68.10	14.29	1.17E-02	1.00E+00	6.26E-02
ADPribose diphosphatase	8	3	53.02	14.29	1.30E-02	1.00E+00	6.26E-02

L-phenylalanine transport via diffusion (extracellular to cytosol)	1	1	66.37	14.29	1.38E-02	1.00E+00	6.26E-02
AMP exchange	1	1	66.00	14.29	1.43E-02	1.00E+00	6.26E-02
ADPribose transport	6	2	44.73	14.29	1.47E-02	1.00E+00	6.26E-02
aspartate carbamoyltransferase (reversible)	7	5	43.13	14.29	1.59E-02	1.00E+00	6.26E-02
carbamoyl-phosphate synthase (glutamine-hydrolysing)	7	5	43.13	14.29	1.59E-02	1.00E+00	6.26E-02
dihydroorotic acid dehydrogenase (quinone10)	7	5	43.13	14.29	1.59E-02	1.00E+00	6.26E-02
orotidine-5'-phosphate decarboxylase	7	5	43.13	14.29	1.59E-02	1.00E+00	6.26E-02
ubiquinol-6 cytochrome c reductase, Complex III	7	5	43.13	14.29	1.59E-02	1.00E+00	6.26E-02
O2 transport (diffusion)	6	5	43.13	14.29	1.59E-02	1.00E+00	6.26E-02
pyridoxamine 5'-phosphate oxidase	4	2	46.83	14.29	1.60E-02	1.00E+00	6.26E-02
pyridoxamine kinase	4	2	46.83	14.29	1.60E-02	1.00E+00	6.26E-02
pyridoxamine transport via diffusion	4	2	46.83	14.29	1.60E-02	1.00E+00	6.26E-02
pyridoxine 5'-phosphate oxidase	4	2	46.83	14.29	1.60E-02	1.00E+00	6.26E-02
pyridoxine kinase	4	2	46.83	14.29	1.60E-02	1.00E+00	6.26E-02
pyridoxine transport via diffusion	4	2	46.83	14.29	1.60E-02	1.00E+00	6.26E-02
R total 2 position exchange	7	1	63.98	14.29	1.71E-02	1.00E+00	6.26E-02
beta-Carotene dioxygenase	6	1	63.98	14.29	1.71E-02	1.00E+00	6.26E-02
beta-carotene transport via diffusion	6	1	63.98	14.29	1.71E-02	1.00E+00	6.26E-02
Retinol transport via facilitated diffusion	5	1	63.98	14.29	1.71E-02	1.00E+00	6.26E-02
retinyl ester hydrolase, extracellular	5	1	63.98	14.29	1.71E-02	1.00E+00	6.26E-02
fatty acid retinol efflux	1	1	63.98	14.29	1.71E-02	1.00E+00	6.26E-02
L-Phenylalanine exchange	73	11	45.02	14.29	1.82E-02	1.00E+00	6.26E-02
glyceraldehyde-3-phosphate dehydrogenase	19	11	50.31	14.29	1.83E-02	1.00E+00	6.26E-02
asparagine synthase (glutamine-hydrolysing)	1	1	62.73	14.29	1.91E-02	1.00E+00	6.26E-02
L-asparaginase (mitochondrial)	1	1	62.73	14.29	1.91E-02	1.00E+00	6.26E-02
L-Asparagine exchange	1	1	62.73	14.29	1.91E-02	1.00E+00	6.26E-02
L-asparagine transport, mitochondrial	1	1	62.73	14.29	1.91E-02	1.00E+00	6.26E-02
L-Glutamine exchange	1	1	62.62	14.29	1.93E-02	1.00E+00	6.26E-02
cytochrome c oxidase, mitochondrial Complex IV	12	6	43.95	14.29	1.94E-02	1.00E+00	6.26E-02
carboxylic acid dissociation	22	8	45.34	14.29	2.06E-02	1.00E+00	6.26E-02
R total flux	2	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
fatty acyl-CoA synthase (n-C8:0CoA), lumped reaction	4	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
fatty acyl-CoA synthase (n-C10:0CoA)	5	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
fatty-acyl-CoA synthase (n-C12:0CoA)	5	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
fatty-acyl-CoA synthase (n-C14:0CoA)	5	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
dephospho-CoA kinase	1	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
pantetheine-phosphate adenylyltransferase	1	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
pantothenate kinase	1	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
Pantothenate sodium symporter II	1	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
phosphopantothenate-cysteine ligase	1	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
phosphopantothenoylcysteine decarboxylase	1	1	61.75	14.29	2.08E-02	1.00E+00	6.26E-02
UMP exchange	2	2	45.52	14.29	2.12E-02	1.00E+00	6.26E-02
phosphoribosylpyrophosphate synthetase	23	16	43.91	14.29	2.13E-02	1.00E+00	6.26E-02
Trehalose exchange	100	27	42.16	14.29	2.13E-02	1.00E+00	6.26E-02
Arginine/Lysine exchanger (Argin)	1	1	61.05	14.29	2.20E-02	1.00E+00	6.26E-02
L-arginine transport in via sodium symport	1	1	61.05	14.29	2.20E-02	1.00E+00	6.26E-02
L-arginine transport via diffusion (extracellular to cytosol)	1	1	61.05	14.29	2.20E-02	1.00E+00	6.26E-02
lipid, flip-flop intracellular transport	98	19	41.95	14.29	2.20E-02	1.00E+00	6.26E-02
NAD nucleosidase	2	1	60.97	14.29	2.22E-02	1.00E+00	6.26E-02
NAD synthase (glutamine-hydrolysing)	2	1	60.97	14.29	2.22E-02	1.00E+00	6.26E-02
Nicotinic acid uptake	2	1	60.97	14.29	2.22E-02	1.00E+00	6.26E-02
NICRNS	2	1	60.97	14.29	2.22E-02	1.00E+00	6.26E-02
nucleotide phosphatase	2	1	60.97	14.29	2.22E-02	1.00E+00	6.26E-02
Glutamate transport via Na, H symport and K antiport	21	14	45.98	14.29	2.26E-02	1.00E+00	6.26E-02

methenyltetrahydrofolate cyclohydrolase	4	3	59.03	14.29	2.28E-02	1.00E+00	6.26E-02
glycine hydroxymethyltransferase, reversible	18	10	48.16	14.29	2.29E-02	1.00E+00	6.26E-02
succinate transport, mitochondrial	1	1	60.26	14.29	2.35E-02	1.00E+00	6.26E-02
protoporphyrinogen oxidase, mitochondrial	53	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
alpha-methylacyl-CoA racemase	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
alpha-methylacyl-CoA racemase (reductase)	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Chenodeoxyglycocholate exchange	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
FADH2 transporter, peroxisomal	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
glycocholate exchange	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Taurocholic acid exchange	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
acyl-Coenzyme A oxidase 2, branched chain	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
hydroxysteroid (17-beta) dehydrogenase 4	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
5-beta-cholestane-3-alpha,7-alpha,12-alpha-triol 27-hydroxylase	44	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
C-14 sterol reductase	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
C-3 sterol keto reductase (zymosterol)	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
C-4 sterol methyl oxidase (4,4-dimethylzymosterol)	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
cholesterol precursor intracellular transport	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
cytochrome P450 lanosterol 14-alpha-demethylase	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
FAD transporter, endoplasmic reticulum	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
FADH2 transporter, endoplasmic reticulum	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
lanosterol synthase	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Previtamin D3 formation	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Squalene epoxidase, endoplasmic reticular (NADP)	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Squalene synthase	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Vitamin D3 exchange	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Vitamin D3 formation	49	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
dimethylallyltranstransferase	39	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
geranyltranstransferase	39	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
isopentenyl-diphosphate D-isomerase	39	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
glycochenodeoxycholate exchange	41	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
7-dehydrocholesterol reductase	50	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
Beta oxidation of long chain fatty acid	52	14	37.79	14.29	2.39E-02	1.00E+00	6.26E-02
phosphoglycerate dehydrogenase	23	11	47.35	14.29	2.41E-02	1.00E+00	6.26E-02
phosphoserine phosphatase (L-serine)	23	11	47.35	14.29	2.41E-02	1.00E+00	6.26E-02
phosphoserine transaminase	23	11	47.35	14.29	2.41E-02	1.00E+00	6.26E-02
FAD transporter, peroxisomal	70	6	44.33	14.29	2.50E-02	1.00E+00	6.26E-02
sterol 12-alpha-hydroxylase	42	13	38.74	14.29	2.52E-02	1.00E+00	6.26E-02
sterol 12-alpha-hydroxylase (nadh)	42	13	38.74	14.29	2.52E-02	1.00E+00	6.26E-02
CO2 exchange	8	3	55.50	14.29	2.52E-02	1.00E+00	6.26E-02
Inosine exchange	1	1	59.27	14.29	2.54E-02	1.00E+00	6.26E-02
purine-nucleoside phosphorylase (Inosine)	1	1	59.27	14.29	2.54E-02	1.00E+00	6.26E-02
glutamine synthetase	34	24	42.99	14.29	2.57E-02	1.00E+00	6.26E-02
dehydroascorbate transport (uniport)	27	8	35.88	14.29	2.57E-02	1.00E+00	6.26E-02
peroxisomal thiolase 2	45	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
bile acid intracellular transport	45	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
carnitine O-acyltransferase, mitochondrial	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
carnitine O-acyltransferase, peroxisomal	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
carnitine-propcarnitine carrier, peroxisomal	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
cytochrome P450, family 7, subfamily A, polypeptide 1	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
taurine transport (sodium symport) (cytosol to peroxisome)	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
taurochenodeoxycholate exchange	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
transport into the mitochondria from cytosol (carnitine)	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
Cytochrome P450 27	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02

aldo-keto reductase family 1, member C4 (chlordecone reductase; 3-alpha hydroxysteroid dehydrogenase, type I; dihydrodiol dehydrogenase 4)	45	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
aldo-keto reductase family 1, member D1 (delta 4-3-ketosteroid-5-beta-reductase)	45	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
Very-long-chain-fatty-acid-CoA ligase	45	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
5-beta-cytochrome P450, family 27, subfamily A, polypeptide 1	42	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
bile acid Coenzyme A: amino acid N-acyltransferase	45	15	38.62	14.29	2.61E-02	1.00E+00	6.26E-02
3-beta-hydroxysteroid-delta(8),delta(7)-isomerase	44	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
C-3 sterol dehydrogenase (4-methylzymosterol)	44	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
C-4 methyl sterol oxidase	44	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Carbon monoxide exchange	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
CO transporter via diffusion	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
coproporphyrinogen oxidase (O2 required)	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Ferrochelatase, mitochondrial	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Heme oxygenase 1	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Heme transport to cytosol	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
hydroxymethylbilan synthase	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
iron (II) transport	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Nad(p)h biliverdin reductase	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
protoporphyrinogen IX mitochondrial transport	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
uroporphyrinogen decarboxylase (uroporphyrinogen III)	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
uroporphyrinogen-III synthase	39	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
24-dehydrocholesterol reductase [Precursor]	46	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Lathosterol oxidase	46	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
hydrogen peroxide transport via diffusion	35	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
o2 transport (diffusion)	35	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
fatty acid intracellular transport	42	13	36.65	14.29	2.68E-02	1.00E+00	6.26E-02
Vitamin D-25-hydroxylase (D3)	7	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
sterol O-acyltransferase (acyl-Coenzyme A: cholesterol acyltransferase) 1	5	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
25-Hydroxyvitamin D3 exchange	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
cholesterol efflux (ATP dependent)	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
cholesterol ester exchange	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
Cholesterol exchange	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
cholesterol intracellular transport	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
diphosphomevalonate decarboxylase	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
Hydroxymethylglutaryl CoA reductase (ir)	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
Hydroxymethylglutaryl-CoA reversible peroxisomal transport	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
mevalonate kinase (atp)	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
phosphomevalonate kinase	6	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
7-alpha,24(S)-Dihydroxycholesterol exchange	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
7-alpha,25-Dihydroxycholesterol exchange	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
7-alpha,27-Dihydroxycholesterol exchange	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
cholesterol 25-hydroxylase	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
cytochrome P450, family 46, subfamily A, polypeptide 1	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
oxysterol 7-alpha-hydroxylase	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
24 trihydroxy cholesterol transport	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
25 trihydroxy cholesterol transport	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
27 trihydroxy cholesterol transport	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
oxysterol 7alpha-hydroxylase	8	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
cholesterol ester (from FULLR2) exchange	2	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
Lecithin-cholesterol acyltransferase	2	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
lysophosphatidylcholine (homo sapiens) exchange	2	1	58.48	14.29	2.71E-02	1.00E+00	6.26E-02
hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 7	37	14	39.53	14.29	2.71E-02	1.00E+00	6.26E-02

taurine transport (sodium sym- port) (2:1)	40	14	39.53	14.29	2.71E-02	1.00E+00	6.26E-02
GMP reductase	6	4	50.52	14.29	2.77E-02	1.00E+00	6.26E-02
guanine phosphoribosyltrans- ferase	6	4	50.52	14.29	2.77E-02	1.00E+00	6.26E-02
adenosine kinase	3	2	55.21	14.29	2.79E-02	1.00E+00	6.26E-02
Phosphatidylserine synthase	3	2	55.21	14.29	2.79E-02	1.00E+00	6.26E-02
homo sapiens							
Phosphatidylserine decarboxy- lase	5	2	55.21	14.29	2.79E-02	1.00E+00	6.26E-02
phosphatidylserine flippase	6	2	55.21	14.29	2.79E-02	1.00E+00	6.26E-02
glycine passive transport to mi- tochondria	4	2	55.21	14.29	2.79E-02	1.00E+00	6.26E-02
triose-phosphate isomerase	6	2	55.21	14.29	2.79E-02	1.00E+00	6.26E-02
Fatty acid omega-hydroxylase	2	1	58.09	14.29	2.79E-02	1.00E+00	6.26E-02
fatty-acid-CoA ligase (tetradec- anoate)	2	1	58.09	14.29	2.79E-02	1.00E+00	6.26E-02
omega hydroxy tetradecanoate (n-C14:0) exchange	2	1	58.09	14.29	2.79E-02	1.00E+00	6.26E-02
Tetradecanoate (n-C14:0) trans- port in via uniport	2	1	58.09	14.29	2.79E-02	1.00E+00	6.26E-02
GMP synthase	4	2	49.01	14.29	2.82E-02	1.00E+00	6.26E-02
purine-nucleoside phosphorylase (Guanosine)	3	2	49.01	14.29	2.82E-02	1.00E+00	6.26E-02
Proline dehydrogenase	34	12	37.59	14.29	2.83E-02	1.00E+00	6.26E-02
dihydroceramide desaturase	38	12	37.59	14.29	2.83E-02	1.00E+00	6.26E-02
Vitamin D3 uptake	12	2	39.60	14.29	2.84E-02	1.00E+00	6.26E-02
NADP transporter, peroxisome	9	2	39.60	14.29	2.84E-02	1.00E+00	6.26E-02
NADPH transporter, peroxisome	9	2	39.60	14.29	2.84E-02	1.00E+00	6.26E-02
Betaine transport (sodium sym- port) (2:1)	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
betaine-aldehyde dehydrogenase, mitochondrial	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
betaine-homocysteine S- methyltransferase	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
choline dehydrogenase (FAD ac- ceptor), mitochondrial	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
choline transport via diffusion (cytosol to mitochondria)	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
dimethylglycine dehydrogenase, mitochondrial	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
dimethylglycine transport via diffusion (cytosol to mitochon- dria)	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
formaldehyde transport via diffu- sion (mitochondrial)	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
Glycine betaine exchange	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
Glycine betaine transport via diffusion (mitochondria to cy- tosol)	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
phosphatidylethanolamine N- methyltransferase	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
S-Adenosyl-L-methionine intra- cellular diffusion	1	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
phosphatidylethanolamine scramblase	2	1	57.74	14.29	2.87E-02	1.00E+00	6.26E-02
ADPribose 2'-phosphate ex- change	4	2	56.97	14.29	2.92E-02	1.00E+00	6.26E-02
Nicotinamide acid uptake	2	2	56.97	14.29	2.92E-02	1.00E+00	6.26E-02
1-Methylnicotinamide exchange	3	2	56.97	14.29	2.92E-02	1.00E+00	6.26E-02
N1-Methylnicotinamide trans- port	3	2	56.97	14.29	2.92E-02	1.00E+00	6.26E-02
Nicotinamide N- methyltransferase	3	2	56.97	14.29	2.92E-02	1.00E+00	6.26E-02
Histidine transport (Na, H cou- pled)	1	1	57.31	14.29	2.96E-02	1.00E+00	6.32E-02
adenosylhomocysteinase	16	3	45.32	14.29	3.12E-02	1.00E+00	6.46E-02
methionine adenosyltransferase	16	3	45.32	14.29	3.12E-02	1.00E+00	6.46E-02
Succinate exchange	3	3	45.42	14.29	3.17E-02	1.00E+00	6.46E-02
4-Aminobutanoate exchange	1	1	56.27	14.29	3.21E-02	1.00E+00	6.46E-02
4-aminobutanoate mitochondrial transport via diffusion	1	1	56.27	14.29	3.21E-02	1.00E+00	6.46E-02
4-aminobutyrate transaminase, reversible (mitochondrial)	1	1	56.27	14.29	3.21E-02	1.00E+00	6.46E-02
Glutamate Decarboxylase	1	1	56.27	14.29	3.21E-02	1.00E+00	6.46E-02
succinate-semialdehyde dehydro- genase (NAD) reversible (mito- chondrial)	1	1	56.27	14.29	3.21E-02	1.00E+00	6.46E-02
fatty-acid-CoA ligase (oc- tanoate)	1	1	56.25	14.29	3.21E-02	1.00E+00	6.46E-02
Octanoate transport via diffu- sion	1	1	56.25	14.29	3.21E-02	1.00E+00	6.46E-02
glutamine phosphoribo- syldiphosphate amidotransferase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
phosphoribosylaminoimidazole carboxylase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02

phosphoribosylaminoimidazole synthase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
phosphoribosylaminoimidazolecarboxamide formyltransferase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
phosphoribosylaminoimidazolesuccinylcarboxamide synthase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
phosphoribosylformylglycinamide synthase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
phosphoribosylglycinamide formyltransferase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
phosphoribosylglycinamide synthase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
adenylosuccinate lyase	14	9	40.77	14.29	3.26E-02	1.00E+00	6.46E-02
ATP transporter, peroxisomal	12	3	43.41	14.29	3.36E-02	1.00E+00	6.61E-02
O2 transport, endoplasmic reticulum	13	3	43.41	14.29	3.36E-02	1.00E+00	6.61E-02
ATP synthase (four protons for one ATP)	22	13	40.68	14.29	3.45E-02	1.00E+00	6.72E-02
L-Ascorbate exchange	18	5	31.24	14.29	3.55E-02	1.00E+00	6.72E-02
R group artificial flux	14	3	48.76	14.29	3.72E-02	1.00E+00	6.72E-02
IMP dehydrogenase	5	3	43.31	14.29	3.73E-02	1.00E+00	6.72E-02
thiamin pyrophosphatase	1	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
Thiamin exchange	2	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
Thiamin monophosphate exchange	2	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
thiamin phosphatase	3	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
Thiamin triphosphate exchange	3	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
thiamine diphosphokinase	3	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
Thiamine monophosphate transport in via anion antiport	3	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
Thiamine transport in via proton antiport	3	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
Thiamine triphosphate transport in via anion antiport	3	1	54.07	14.29	3.76E-02	1.00E+00	6.72E-02
NAD nucleosidase,extracellular	4	4	42.00	14.29	3.98E-02	1.00E+00	6.72E-02
glutamate 5-kinase (m)	1	1	53.26	14.29	3.99E-02	1.00E+00	6.72E-02
glutamate-5-semialdehyde dehydrogenase (m)	1	1	53.26	14.29	3.99E-02	1.00E+00	6.72E-02
L-glutamate 5-semialdehyde dehydratase, reversible, mitochondrial	1	1	53.26	14.29	3.99E-02	1.00E+00	6.72E-02
L-Proline exchange	1	1	53.26	14.29	3.99E-02	1.00E+00	6.72E-02
L-proline transport, mitochondrial	1	1	53.26	14.29	3.99E-02	1.00E+00	6.72E-02
methionine synthase	7	3	43.11	14.29	3.99E-02	1.00E+00	6.72E-02
5,10-methylenetetrahydrofolatereductase (NADPH)	9	3	43.11	14.29	3.99E-02	1.00E+00	6.72E-02
3,4-Dihydroxy-L-phenylalanine exchange	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Tetrahydrobiopterin-4a-carbinolamine dehydratase	11	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Iodide:hydrogen-peroxide oxidoreductase 3	10	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Triiodothyronine exchange	10	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
4-Hydroxyphenylpyruvate:oxygen oxidoreductase	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
fumarylacetoacetase	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Homogentisate:oxygen 1,2-oxidoreductase (deacylizing)	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
L-tyrosine transport	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
maleylacetoacetate isomerase	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
tyrosine 3-monooxygenase	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
tyrosine transaminase	1	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Tyramine O-sulfate exchange	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Tyramine O-sulfate transport (diffusion)	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Tyramine Sulfotransferase	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Iodide:hydrogen-peroxide oxidoreductase	5	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Iodide:hydrogen-peroxide oxidoreductase 2	5	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
4-Hydroxyphenylacetaldehyde:NAD+ oxidoreductase	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
4-Hydroxyphenylacetate exchange	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
hydroxyphenylacetate transport via diffusion	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Tyramine:oxygen oxidoreductase(deaminating)(flavin-containing) (cytosol)	2	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
L-Tyrosine carboxy-lyase	3	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
Tyrosine:dopa oxidase	3	1	53.14	14.29	4.02E-02	1.00E+00	6.72E-02
R group artificial flux (C18:3, n-3)	1	1	52.78	14.29	4.12E-02	1.00E+00	6.72E-02
stearidonic acid exchange	1	1	52.78	14.29	4.12E-02	1.00E+00	6.72E-02

nucleoside-triphosphatase (GTP)	7	1	52.73	14.29	4.14E-02	1.00E+00	6.72E-02
5'-nucleotidase (GMP), extracellular	5	1	52.73	14.29	4.14E-02	1.00E+00	6.72E-02
nucleoside-diphosphatase (GDP), extracellular	7	1	52.73	14.29	4.14E-02	1.00E+00	6.72E-02
formimidoyltransferase cyclodeaminase	2	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
Glutamate formimidoyltransferase	2	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
Histamine exchange	2	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
histidase	2	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
imidazolonepropionase	2	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
urocanase	2	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
histidine decarboxylase	3	2	36.58	14.29	4.16E-02	1.00E+00	6.72E-02
acetyl-CoA carboxylase	17	4	39.64	14.29	4.19E-02	1.00E+00	6.72E-02
3-Hydroxy-L-kynurenine hydrolase	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
3-hydroxyanthranilate 3,4-dioxygenase	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
5-hydroxy-L-tryptophan secretion via secretory vesicle (ATP driven)	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
kynurenine 3-monooxygenase	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
L-Tryptophan:oxygen 2,3-oxidoreductase (decyclizing)	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
N-Formyl-L-kynurenine amidohydrolase	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
nicotinate-nucleotide diphosphorylase (carboxylating)	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
Quinolinate Synthase (Eukaryotic)	21	5	38.88	14.29	4.23E-02	1.00E+00	6.72E-02
NADP nucleosidase,extracellular	3	1	52.20	14.29	4.29E-02	1.00E+00	6.78E-02
Nicotinamide exchange	1	1	52.20	14.29	4.29E-02	1.00E+00	6.78E-02
timnodonic acid exchange	1	1	51.98	14.29	4.36E-02	1.00E+00	6.87E-02
pyridoxal transport via diffusion	19	6	35.16	14.29	4.41E-02	1.00E+00	6.93E-02
Glycine exchange	1	1	50.90	14.29	4.69E-02	1.00E+00	7.33E-02
Choline exchange	1	1	50.88	14.29	4.70E-02	1.00E+00	7.33E-02
Citrate exchange	1	1	50.81	14.29	4.72E-02	1.00E+00	7.33E-02
H+ exchange	2	1	50.81	14.29	4.72E-02	1.00E+00	7.33E-02
L-Lactate exchange	1	1	50.30	14.29	4.88E-02	1.00E+00	7.54E-02
Glutathione dehydrogenase (dehydroascorbate reductase)	29	7	35.43	14.29	4.92E-02	1.00E+00	7.54E-02
1-acylglycerol-3-phosphate O-acyltransferase 1	4	1	50.05	14.29	4.97E-02	1.00E+00	7.54E-02
glycerol-3-phosphate acyltransferase	4	1	50.05	14.29	4.97E-02	1.00E+00	7.54E-02
Glycerol exchange	1	1	50.05	14.29	4.97E-02	1.00E+00	7.54E-02
glycerol kinase	1	1	50.05	14.29	4.97E-02	1.00E+00	7.54E-02
glycerol transport via channel	1	1	50.05	14.29	4.97E-02	1.00E+00	7.54E-02
lipase	3	1	50.05	14.29	4.97E-02	1.00E+00	7.54E-02
transport into the mitochondria (carnitine)	4	3	46.43	14.29	5.28E-02	1.00E+00	7.97E-02
carnitine transferase	4	3	46.43	14.29	5.28E-02	1.00E+00	7.97E-02
Nitric Oxide Synthase (NO forming)	28	8	31.65	14.29	5.61E-02	1.00E+00	8.34E-02
Steryl-sulfatase	5	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
3',5'-bisphosphate nucleotidase	7	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
adenylyl-sulfate kinase	7	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
sulfate adenylyltransferase	7	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
2-Aminoacrylate sulfotransferase	1	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
3-Sulfoalanine carboxy-lyase	1	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
L-Serine hydro-lyase	1	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Taurine exchange	1	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
sulfite oxidase	4	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Cyanide sulfurtransferase, mitochondrial	3	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Cyanide transport via diffusion (mitochondrial)	3	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Thiocyanate transport via diffusion (mitochondrial)	3	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
thiosulfate transport via sodium symport	3	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Cyanide transport via diffusion (extracellular to cytosol)	4	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Thiocyanate exchange	4	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Thiocyanate transport via diffusion (cytosol to extracellular)	4	1	47.68	14.29	5.80E-02	1.00E+00	8.34E-02
Arachidic acid exchange	19	5	32.80	14.29	5.81E-02	1.00E+00	8.34E-02
fatty acyl-CoA desaturase (n-C18:2CoA -> n-C18:3CoA)	5	2	47.12	14.29	5.90E-02	1.00E+00	8.39E-02
carnitine O-palmitoyltransferase	3	2	47.12	14.29	5.90E-02	1.00E+00	8.39E-02
Beta oxidation of fatty acid	3	2	47.12	14.29	5.90E-02	1.00E+00	8.39E-02
Iodide:hydrogen-peroxide oxidoreductase 4	25	5	33.08	14.29	6.07E-02	1.00E+00	8.60E-02
L-Thyroxine exchange	25	5	33.08	14.29	6.07E-02	1.00E+00	8.60E-02
Adenine exchange	1	1	46.23	14.29	6.35E-02	1.00E+00	8.95E-02

adenine reversible transport, cytosol	1	1	46.23	14.29	6.35E-02	1.00E+00	8.95E-02
fatty acid transport via diffusion	22	7	36.84	14.29	6.52E-02	1.00E+00	9.00E-02
carnitine O-acetyltransferase, reverse direction, peroxisomal	8	4	34.39	14.29	6.65E-02	1.00E+00	9.00E-02
carnitine-acetylcarnitine carrier, peroxisomal	8	4	34.39	14.29	6.65E-02	1.00E+00	9.00E-02
2-oxoisovalerate dehydrogenase (acylating; 3-methyl-2-oxobutanoate), mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
3-amino-isobutyrate transport	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
3-amino-isobutyrate transport, mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
3-hydroxyacyl-CoA dehydratase (3-hydroxyisobutyryl-CoA) (mitochondria)	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
3-hydroxyisobutyrate dehydrogenase, mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
3-hydroxyisobutyryl-CoA hydrolase, mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
acyl-CoA dehydrogenase (isobutyryl-CoA), mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
L-3-Amino-isobutanoate exchange	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
L-3-aminoisobutyrate transaminase, mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
malonate-semialdehyde dehydrogenase (acylating), mitochondrial	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
methylmalonate-semialdehyde dehydrogenase	2	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
L-valine transport via diffusion (extracellular to cytosol)	1	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
Valine reversible mitochondrial transport	1	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
valine transaminase, mitochondrial	1	1	45.43	14.29	6.68E-02	1.00E+00	9.00E-02
fatty-acid-CoA ligase (hexadecenoate)	1	1	45.05	14.29	6.84E-02	1.00E+00	9.15E-02
hexadecenoate (n-C16:1) exchange	1	1	45.05	14.29	6.84E-02	1.00E+00	9.15E-02
palmitoyl-CoA desaturase (n-C16:0CoA -> n-C16:1CoA)	1	1	45.05	14.29	6.84E-02	1.00E+00	9.15E-02
fatty-acid-CoA ligase (n-C26:0)	3	1	44.95	14.29	6.88E-02	1.00E+00	9.16E-02
lignoceric acid exchange	3	1	44.95	14.29	6.88E-02	1.00E+00	9.16E-02
fatty-acid-CoA ligase	24	7	36.46	14.29	7.00E-02	1.00E+00	9.29E-02
O2 transport, peroxisomal	5	3	30.95	14.29	8.14E-02	1.00E+00	1.08E-01
Linoleic acid (n-C18:2) transport in via diffusion	3	1	41.89	14.29	8.28E-02	1.00E+00	1.09E-01
gamma-linolenic acid exchange	2	1	41.89	14.29	8.28E-02	1.00E+00	1.09E-01
glucosamine-6-phosphate deaminase	6	6	30.52	14.29	8.38E-02	1.00E+00	1.10E-01
Maltodextrin glucosidase (maltotriose), extracellular	2	2	39.88	14.29	8.40E-02	1.00E+00	1.10E-01
methenyltetrahydrifkate cyclohydrolase, mitochondrial	8	2	31.52	14.29	8.48E-02	1.00E+00	1.11E-01
enolase	6	2	32.67	14.29	8.94E-02	1.00E+00	1.16E-01
pyruvate kinase	6	2	32.67	14.29	8.94E-02	1.00E+00	1.16E-01
C180 fatty acid activation	1	1	39.72	14.29	9.39E-02	1.00E+00	1.21E-01
2-aminomuconate reductase	20	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
aminomuconate-semialdehyde dehydrogenase	20	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
picolinic acid decarboxylase	20	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
Reduced glutathione exchange	18	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
cysteinesulfinic acid oxidase	17	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
Hypotaurine oxidase	17	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
Glutathione:cystine oxidoreductase	20	4	28.70	14.29	9.49E-02	1.00E+00	1.21E-01
Cytosine deaminase	1	1	39.12	14.29	9.72E-02	1.00E+00	1.23E-01
cytosine transport via facilitated diffusion	1	1	39.12	14.29	9.72E-02	1.00E+00	1.23E-01
sucrose hydrolyzing enzyme, extracellular	1	1	39.01	14.29	9.78E-02	1.00E+00	1.24E-01
alpha-Tocopherol (Vit. E) transport	1	1	38.54	14.29	1.00E-01	1.00E+00	1.27E-01
alpha-Tocopherol demand	1	1	38.54	14.29	1.00E-01	1.00E+00	1.27E-01
Dehydroascorbate exchange	2	1	38.17	14.29	1.03E-01	1.00E+00	1.29E-01
L-Serine exchange	1	1	37.24	14.29	1.08E-01	1.00E+00	1.36E-01
adenylosuccinate synthase	4	2	32.88	14.29	1.11E-01	1.00E+00	1.39E-01
N-acetyl-glucosamine lysosomal efflux	8	6	27.74	14.29	1.14E-01	1.00E+00	1.42E-01
N-acetylglucosamine kinase	8	6	27.74	14.29	1.14E-01	1.00E+00	1.42E-01
D-Mannose exchange	1	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
hexokinase (D-mannose:ATP)	1	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
beta-galactosidase, lysosomal	3	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
galactose efflux from lysosome	3	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01

N-Acetylneuraminate lyase (reversible)	3	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
s2l2n2m2masn transport, extracellular to lysosome	3	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
sialidase, lysosomal	3	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
n2m2nmasn transport, extracellular to lysosome	2	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
endo-beta-N-acetylglucosaminidase, lysosomal	4	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
glycosylasparaginase, lysosomal	4	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
beta-N-acetylhexosaminidase, lysosomal	4	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
L-Fucose exchange	4	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
alpha-fucosidase, extracellular	4	1	35.53	14.29	1.19E-01	1.00E+00	1.44E-01
L-aspartate transport via Na, H symport and K antiport	1	1	34.92	14.29	1.23E-01	1.00E+00	1.48E-01
N-acetylglucosamine-6-phosphate deacetylase	5	5	26.07	14.29	1.25E-01	1.00E+00	1.51E-01
5'-nucleotidase (CMP), extracellular	1	1	33.86	14.29	1.30E-01	1.00E+00	1.56E-01
Urate exchange	1	1	32.02	14.29	1.44E-01	1.00E+00	1.71E-01
urate export from cytosol	1	1	32.02	14.29	1.44E-01	1.00E+00	1.71E-01
urate export from peroxisome	1	1	32.02	14.29	1.44E-01	1.00E+00	1.71E-01
xanthine diffusion in peroxisome	1	1	32.02	14.29	1.44E-01	1.00E+00	1.71E-01
xanthine oxidase, peroxisomal	1	1	32.02	14.29	1.44E-01	1.00E+00	1.71E-01
D-Glucose exchange	1	1	31.52	14.29	1.48E-01	1.00E+00	1.75E-01
pyridoxal kinase	17	5	23.74	14.29	1.61E-01	1.00E+00	1.90E-01
5'-nucleotidase (dCMP)	1	1	29.79	14.29	1.62E-01	1.00E+00	1.90E-01
Deoxycytidine exchange	1	1	29.79	14.29	1.62E-01	1.00E+00	1.90E-01
deoxycytidine transport via diffusion	1	1	29.79	14.29	1.62E-01	1.00E+00	1.90E-01
2-oxoisovalerate dehydrogenase (acylating; 4-methyl-2-oxopentaoate), mitochondrial	1	1	27.01	14.29	1.87E-01	1.00E+00	2.16E-01
acyl-CoA dehydrogenase (isovaleryl-CoA), mitochondrial	1	1	27.01	14.29	1.87E-01	1.00E+00	2.16E-01
leucine mitochondrial transport	1	1	27.01	14.29	1.87E-01	1.00E+00	2.16E-01
leucine transaminase, mitochondrial	1	1	27.01	14.29	1.87E-01	1.00E+00	2.16E-01
methylcrotonoyl-CoA carboxylase, mitochondrial	1	1	27.01	14.29	1.87E-01	1.00E+00	2.16E-01
methylglutaconyl-CoA hydratase (reversible), mitochondrial	1	1	27.01	14.29	1.87E-01	1.00E+00	2.16E-01
thioredoxin reductase (NADPH)	9	2	24.18	14.29	1.87E-01	1.00E+00	2.16E-01
Guanosine exchange	1	1	26.98	14.29	1.87E-01	1.00E+00	2.16E-01
alpha-mannosidase, lysosomal	7	4	22.63	14.29	1.93E-01	1.00E+00	2.21E-01
beta-mannosidase, lysosomal	7	4	22.63	14.29	1.93E-01	1.00E+00	2.21E-01
DM Asn-X-Ser/Thr(ly)	7	4	22.63	14.29	1.93E-01	1.00E+00	2.21E-01
mannose efflux from lysosome	7	4	22.63	14.29	1.93E-01	1.00E+00	2.21E-01
arginase	1	1	25.63	14.29	2.01E-01	1.00E+00	2.28E-01
arginase (m)	1	1	25.63	14.29	2.01E-01	1.00E+00	2.28E-01
arginine mitochondrial transport via ornithine carrier	1	1	25.63	14.29	2.01E-01	1.00E+00	2.28E-01
H2O transport, lysosomal	5	3	22.55	14.29	2.03E-01	1.00E+00	2.30E-01
alpha-amylase, extracellular (glygn2 -> glygn4)	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
alpha-amylase, extracellular (strch1 -> strch2)	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
glucoamylase, extracellular (glygn5 -> malt)	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
Maltose exchange	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
oligo-1,6-glucosidase (glygn4 -> glygn5), extracellular	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
oligo-1,6-glucosidase (strch2 -> strch3), extracellular	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
Tyr-194 of apo-glycogenin protein (primer for glycogen synthesis) exchange	1	1	24.57	14.29	2.12E-01	1.00E+00	2.37E-01
adrenic acid exchange	1	1	23.98	14.29	2.18E-01	1.00E+00	2.40E-01
fatty acyl-CoA desaturase (n-C20:3CoA -> n-C20:4CoA)	3	1	23.98	14.29	2.18E-01	1.00E+00	2.40E-01
fatty-acyl-CoA elongation (n-C20:4CoA)	3	1	23.98	14.29	2.18E-01	1.00E+00	2.40E-01
argininosuccinate lyase	3	2	22.10	14.29	2.19E-01	1.00E+00	2.40E-01
argininosuccinate synthase	3	2	22.10	14.29	2.19E-01	1.00E+00	2.40E-01
carbamoyl-phosphate synthase (ammonia) (mitochondria)	2	2	22.10	14.29	2.19E-01	1.00E+00	2.40E-01
Creatine transport (sodium symport) (2:1)	2	2	22.10	14.29	2.19E-01	1.00E+00	2.40E-01
ornithine carbamoyltransferase, irreversible	2	2	22.10	14.29	2.19E-01	1.00E+00	2.40E-01
Urea exchange	2	2	22.10	14.29	2.19E-01	1.00E+00	2.40E-01
inositol oxygenase	1	1	22.81	14.29	2.31E-01	1.00E+00	2.52E-01
myo-inositol 1-phosphatase	1	1	22.81	14.29	2.31E-01	1.00E+00	2.52E-01
myo-Inositol exchange	1	1	22.81	14.29	2.31E-01	1.00E+00	2.52E-01

myo-Inositol-1-phosphate synthase	1	1	22.81	14.29	2.31E-01	1.00E+00	2.52E-01
Adenosine exchange	1	1	19.91	14.29	2.68E-01	1.00E+00	2.91E-01
Deoxyuridine exchange	1	1	18.81	14.29	2.83E-01	1.00E+00	3.06E-01
deoxyuridine transport via diffusion	1	1	18.81	14.29	2.83E-01	1.00E+00	3.06E-01
Creatine exchange	1	1	18.67	14.29	2.85E-01	1.00E+00	3.06E-01
glycine amidinotransferase (c)	1	1	18.67	14.29	2.85E-01	1.00E+00	3.06E-01
guanidinoacetate N-methyltransferase (c)	1	1	18.67	14.29	2.85E-01	1.00E+00	3.06E-01
heptadecanoate transport into the mitochondria	1	1	17.44	14.29	3.03E-01	1.00E+00	3.24E-01
Beta oxidation of long chain fatty acid (odd chain)	2	1	17.44	14.29	3.03E-01	1.00E+00	3.24E-01
carnitine fatty-acyl transferase	2	1	17.44	14.29	3.03E-01	1.00E+00	3.24E-01
L-carnitine transport out of mitochondria via diffusion	7	2	18.33	14.29	3.10E-01	1.00E+00	3.29E-01
methylmalonyl-CoA mutase	8	2	18.33	14.29	3.10E-01	1.00E+00	3.29E-01
Propionyl-CoA carboxylase, mitochondrial	8	2	18.33	14.29	3.10E-01	1.00E+00	3.29E-01
ADPribose exchange	2	2	17.69	14.29	3.29E-01	1.00E+00	3.48E-01
3-Methylimidazole acetaldehyde:NAD+ oxidoreductase	2	1	11.20	14.29	4.18E-01	1.00E+00	4.38E-01
3-Methylimidazoleacetic acid exchange	2	1	11.20	14.29	4.18E-01	1.00E+00	4.38E-01
3MLDA extracellular transport via diffusion	2	1	11.20	14.29	4.18E-01	1.00E+00	4.38E-01
Histamine uniport	2	1	11.20	14.29	4.18E-01	1.00E+00	4.38E-01
N-Methylhistamine:oxygen oxidoreductase (deaminating)	2	1	11.20	14.29	4.18E-01	1.00E+00	4.38E-01
S-Adenosyl-L-methionine:histamine N-tele-methyltransferase	2	1	11.20	14.29	4.18E-01	1.00E+00	4.38E-01
glyoxylate oxidase	1	1	6.65	14.29	5.37E-01	1.00E+00	5.61E-01
Oxalate exchange	1	1	6.65	14.29	5.37E-01	1.00E+00	5.61E-01
Sarcosine dehydrogenase (m)	1	1	4.69	14.29	6.07E-01	1.00E+00	6.29E-01
Sarcosine transport (extracellular to cytosol)	1	1	4.69	14.29	6.07E-01	1.00E+00	6.29E-01
Sarcosine transport (mitochondrial)	1	1	4.69	14.29	6.07E-01	1.00E+00	6.29E-01
5-L-Glutamyl-L-alanine exchange	1	1	1.89	14.29	7.45E-01	1.00E+00	7.64E-01
5-Oxoproline amidohydrolase (ATP-hydrolysing) (ir)	1	1	1.89	14.29	7.45E-01	1.00E+00	7.64E-01
gamma-glutamylcyclotransferase	1	1	1.89	14.29	7.45E-01	1.00E+00	7.64E-01
g-glutamyltransferase (e)	2	1	1.89	14.29	7.45E-01	1.00E+00	7.64E-01
gamma-glutamylcysteine synthetase	3	1	1.89	14.29	7.45E-01	1.00E+00	7.64E-01
glutathione synthetase	3	1	1.89	14.29	7.45E-01	1.00E+00	7.64E-01
UDP exchange	2	1	1.27	14.29	7.90E-01	1.00E+00	8.08E-01
D-Fructose exchange	1	1	1.03	14.29	8.11E-01	1.00E+00	8.25E-01
D-sorbitol dehydrogenase (D-fructose producing)	1	1	1.03	14.29	8.11E-01	1.00E+00	8.25E-01
D-sorbitol reductase	1	1	1.03	14.29	8.11E-01	1.00E+00	8.25E-01
ornithine transport via diffusion (extracellular to cytosol)	1	1	0.57	14.29	8.60E-01	1.00E+00	8.73E-01
thymd transport	1	1	0.49	14.29	8.69E-01	1.00E+00	8.77E-01
thymidine transport (1:2 Na/Thymd cotransport)	1	1	0.49	14.29	8.69E-01	1.00E+00	8.77E-01
thymidine transport in via sodium symport	1	1	0.49	14.29	8.69E-01	1.00E+00	8.77E-01
hypothetical enyme	1	1	0.22	14.29	9.13E-01	1.00E+00	9.18E-01
Pyridoxamine exchange	1	1	0.22	14.29	9.13E-01	1.00E+00	9.18E-01
fatty-acyl-CoA elongation (n-C20:5CoA)	2	1	0.08	14.29	9.46E-01	1.00E+00	9.46E-01
fatty acyl-CoA desaturase (n-C22:5CoA -> n-C22:6CoA)	1	1	0.08	14.29	9.46E-01	1.00E+00	9.46E-01
nC22:6 exchange	1	1	0.08	14.29	9.46E-01	1.00E+00	9.46E-01

The report was generated on Fri Sep 25 03:51:37 2015 with R version 3.2.0 (2015-04-16). Thank you for using MetaboAnalyst! For suggestions and feedback please contact Jeff Xia (jeff.xia@mcgill.ca).