Metabolomic Data Analysis with MetaboAnalyst 6.0

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1 Background

The Pathway Analysis module combines results from powerful pathway enrichment analysis with pathway topology analysis to help researchers identify the most relevant pathways involved in the conditions under study.

There are many commercial pathway analysis software tools such as Pathway Studio, MetaCore, or Ingenuity Pathway Analysis (IPA), etc. Compared to these commercial tools, the pathway analysis module was specifically developed for metabolomics studies. It uses high-quality KEGG metabolic pathways as the backend knowledgebase. This module integrates many well-established (i.e. univariate analysis, over-representation analysis) methods, as well as novel algorithms and concepts (i.e. Global Test, GlobalAncova, network topology analysis) into pathway analysis. Another feature is a Google-Map style interactive visualization system to deliver the analysis results in an intuitive manner.

2 Data Input

The Pathway Analysis module accepts either a list of compound labels (common names, HMDB IDs or KEGG IDs) with one compound per row, or a compound concentration table with samples in rows and compounds in columns. The second column must be phenotype labels (binary, multi-group, or continuous). The table is uploaded as comma separated values (.csv).

3 Compound Name Matching

The first step is to standardize the compound labels used in user uploaded data. This is a necessary step since these compounds will be subsequently compared with compounds contained in the pathway library. There are three outcomes from the step - exact match, approximate match (for common names only), and no match. Users should click the textbfView button from the approximate matched results to manually select the correct one. Compounds without match will be excluded from the subsequently pathway analysis.

Table 1 shows the conversion results. Note: *1* indicates exact match, *2* indicates approximate match, and *0* indicates no match. A text file contain the result can be found the downloaded file *name_ map.csv*

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	Query	Match	HMDB	PubChem	KEGG	SMILE
1	(N(1) + N(8))-acetylspermidine	NA	NA	NA	NA	NA
2	1-carboxyethylhistidine	NA	NA	NA	NA	NA
3	1-carboxyethylisoleucine	NA	NA	NA	NA	NA
4	1-carboxyethylleucine	NA	NA	NA	NA	NA
5	1-carboxyethylphenylalanine	NA	NA	NA	NA	NA
6	1-carboxyethyltyrosine	NA	NA	NA	NA	NA
7	1-carboxyethylvaline	NA	NA	NA	NA	NA
8	1-methyl-4-imidazoleacetate	Methylimidazoleacetic acid	HMDB0002820	75810	C05828	CN1C=
9	1-methylhistamine	1-Methylhistamine	HMDB0000898	3614	C05127	CN1C=

10	1-methylhistidine	1-Methylhistidine	HMDB0000001	92105	C01152	CN1C=
11	1-ribosyl-imidazoleacetate	Imidazoleacetic acid riboside	HMDB0002331	440569	C05131	OC[C@
12	11beta-hydroxyandrosterone sulfate	NA	NA	NA	NA	NA
13	17alpha-hydroxypregnanolone glucuronide	NA	NA	NA	NA	NA
14	2-aminoheptanoate	2-Aminoheptanoate	HMDB0094649	5312965		CCCC
15	2-dimethylaminoethanol	Dimethylethanolamine	HMDB0032231	7902	C04308	CN(C)
16	2-furoylcarnitine	NA	NA	NA	NA	NA
17	2-hydroxy-3-methylvalerate	2-Hydroxy-3-methylpentanoic acid	HMDB0000317	10796774		CC[C@
18	2-hydroxyacetaminophen sulfate	2-Hydroxyacetaminophen sulfate	HMDB0062547	86290013		CC(=C
19	2-keto-3-deoxy-gluconate	2-Keto-3-deoxy-D-gluconic acid	HMDB0001353	194024	C01216	OC[C@
20	2-methylhexanoylcarnitine	NA	NA	NA	NA	NA
21	2-methylmalonylcarnitine	NA	NA	NA	NA	NA
22	2-methylserine	NA	NA	NA	NA	NA
23	3-acetylphenol sulfate	NA	NA	NA	NA	NA
24	3-amino-2-piperidone	3-Amino-2-piperidone	HMDB0000323	5200225		NC1CC
25	3-carboxy-4-methyl-5-pentyl-2-furanpropionate	NA	NA	NA	NA	NA
26	3-ethylcatechol sulfate	NA	NA	NA	NA	NA
27	3-hydroxy-2-methylpyridine sulfate	NA	NA	NA	NA	NA
28	3-hydroxyhexanoylcarnitine	3-Hydroxyhexanoylcarnitine	HMDB0013131	53481624		CCC[C
29	3-hydroxyproline	NA	NA	NA	NA	NA
30	3-hydroxypyridine sulfate	NA	NA	NA	NA	NA
31	3-hydroxysebacate	3-Hydroxysebacic acid	HMDB0000350	124350389		O[C@H
32	3-indoleglyoxylic acid	NA	NA	NA	NA	NA
33	3-methyl catechol sulfate	NA	NA	NA	NA	NA
34	3-phosphoglycerate	3-Phosphoglyceric acid	HMDB0000807	724	C00597	OC(CO
35	3-S-cysteinyl-2-methylpropanoate	NA	NA	NA	NA	NA
36	4-acetylcatechol sulfate	NA	NA	NA	NA	NA
37	4-acetylphenyl sulfate	NA	NA	NA	NA	NA
38	4-ethyl-2-methoxyphenol sulfate	NA	NA	NA	NA	NA
39	4-hydroxyglutamate	4-Hydroxy-L-glutamic acid	HMDB0002273	440854	C05947	N[C@@
40	4-hydroxyphenylacetoylcarnitine	NA	NA	NA	NA	NA
41	4-vinylcatechol sulfate	NA	NA	NA	NA	NA
42	4-vinylguaiacol sulfate	NA	NA	NA	NA	NA
43	5-acetylamino-6-amino-3-methyluracil	5-Acetylamino-6-amino-3-methyluracil	HMDB0004400	88299	C16366	CN1C(
44	5-hydroxy-2-methylpyridine sulfate	NA	NA	NA	NA	NA
45	5-hydroxylysine	5-Hydroxylysine	HMDB0000450	3032849	C16741	NC[C@
46	5-hydroxymethyl-2-furoic acid	Sumiki's acid	HMDB0002432	80642	C20448	OCC1=
47	5-hydroxymethyl-2-furoylcarnitine	NA	NA	NA	NA	NA
48	5-hydroxypicolinic acid	NA	NA	NA	NA	NA
49	6-bromotryptophan	NA	NA	NA	NA	NA
50	6'-sialyllactose	6'-Sialyllactose	HMDB0006569	643987		[H][C@
51	8-methoxykynurenate	8-Methoxykynurenate	HMDB0060426	76230	C05830	COC1=
52	adenosine 3	Cyclic AMP	HMDB0000058	6076	C00575	[H][C@
53	adipoylcarnitine	NA	NA	NA	NA	NA
54	alpha-CEHC sulfate	NA	NA	NA	NA	NA
55	alpha-ketoglutarate	Oxoglutaric acid	HMDB0000208	51	C00026	OC(=C
56	azeloylcarnitine	NA	NA	NA	NA	NA
57	betaine	Betaine	HMDB0000043	247	C00719	C[N+](
58	butyrylputrescine/isobutyrylputrescine	NA	NA	NA	NA	NA
59	C-glycosyltryptophan	NA	NA	NA	NA	NA
60	carboxy-methyl-arginine	NA	NA	NA	NA	NA
61	carnitine of C10H14O2	NA	NA	NA	NA	NA
62	cis-3	NA	NA	NA	NA	NA
63	cortolone glucuronide	NA	NA	NA	NA	NA
64	cyclo(gly-pro)	NA	NA	NA	NA	NA
65	cyclo(his-pro)	NA	NA	NA	NA	NA
66	cyclo(pro-sulfo-tyr)	NA	NA	NA	NA	NA
67	cystathionine	L-Cystathionine	HMDB0000099	439258	C02291	N[C@@
68	cytosine	Cytosine	HMDB0000630	597	C00380	NC1=C
69	delta-CEHC sulfate	NA	NA	NA	NA	NA
70	dimethylglycine	Dimethylglycine	HMDB0000092	673	C01026	CN(C)
71	dopamine 4-sulfate	Dopamine 4-sulfate	HMDB0004148	123932	C13691	NCCC
72	enterolactone sulfate	NA	NA	NA	NA	NA
73	epiandrosterone glucuronide	NA	NA	NA	NA	NA
74	etiocholanolone glucuronide	Etiocholanolone glucuronide	HMDB0004484	443078	C11136	[H][C@
75	ferulic acid 4-sulfate	Ferulic acid 4-O-sulfate	HMDB0029200	6305574		COC1=
76	formiminoglutamate	Formiminoglutamic acid	HMDB0000854	439233	C00439	OC(=C
77	gamma-carboxyglutamate	gamma-Carboxyglutamic acid	HMDB0041900	40772		NC(CC
78	gamma-CEHC glucuronide	NA	NA	NA	NA	NA
79	gamma-CEHC sulfate	NA	NA	NA	NA	NA
80	gamma-glutamylhistidine	gamma-Glutamylhistidine	HMDB0029151	7017195		N[C@@
81	glucuronide of C10H18O2 (11)	NA	NA	NA	NA	NA
82	glucuronide of C10H18O2 (12)	NA	NA	NA	NA	NA
83	glucuronide of C12H20O3 (4)	NA	NA	NA	NA	NA
84	glucuronide of C8H14O2 (3)	NA	NA	NA	NA	NA
85	glutamine conjugate of C10H16O2 (2)	NA	NA	NA	NA	NA
86	glutamine conjugate of C8H12O2 (1)	NA	NA	NA	NA	NA
87	glycerate	Glyceric acid	HMDB0000139	439194	C00258	OC[C@
88	glycine conjugate of C10H14O2 (1)	NA	NA	NA	NA	NA
89	glycine conjugate of C10H14O2 (2)	NA	NA	NA	NA	NA
90	glycocholate glucuronide (1)	NA	NA	NA	NA	NA
91	glycolithocholate sulfate	Sulfolithocholylglycine	HMDB0002639	72222	C11301	[H][C@
92	glycoursodeoxycholic acid sulfate	NA	NA	NA	NA	NA
93	guanidinoacetate	Guanidoacetic acid	HMDB0000128	763	C00581	NC(=N
94	guanosine-3	NA	NA	NA	NA	NA
95	heptanoylglutamine	N-Heptanoylglycine	HMDB0013010	10932172		CCCC
96	homoarginine	Homo-L-arginine	HMDB0000670	9085	C01924	N[C@@

97	hydroxy-N6	NA	NA	NA	NA	NA
98	hydroxyasparagine	Hydroxylated lecithin	HMDB0032332	44237312	C03124	N[C@@
99	hydroxyproline	4-Hydroxyproline	HMDB0000725	5810	C01157	O[C@H
100	indoleacetate	Indoleacetic acid	HMDB0000197	802	C00954	OC(=O
101	isocitric lactone	NA	NA	NA	NA	NA
102	lanthionine	Lanthionine	HMDB0240656	98504		N[C@@
103	levulinoylcarnitine	NA	NA	NA	NA	NA
104	m-tyramine	m-Tyramine	HMDB0004989	11492		NCCC
105	methyl-4-hydroxybenzoate sulfate	Methyl-4-hydroxybenzoate sulfate	HMDB0168668	122164837		COC(=
106	N-acetyl-cadaverine	N-Acetylcadaverine	HMDB0002284	189087		CC(=O
107	N-acetylglutamate	N-Acetyl-L-glutamic acid	HMDB0001138	70914	C00624	CC(=O
108	N-acetylhistamine	N-Acetylhistamine	HMDB0013253	69602	C05135	CC(=O
109	N-acetylhistidine	N-Acetylhistidine	HMDB0032055	75619	C02997	CC(=O
110	N-acetylisoleucine	N-Acetylisoleucine	HMDB0061684	7036275		CC[C@
111	N-acetylleucine	N-Acetyl-Leu	HMDB0011756	70912	C02710	CC(C)(
112	N-acetylputrescine	N-Acetylputrescine	HMDB0002064	122356	C02714	CC(=O
113	N-acetyltryptophan	N-Acetyltryptophan	HMDB0013713	700653		CC(=O
114	N-acetylvaline	N-Acetylvaline	HMDB0011757	66789		CC(C)
115	N-succinyl-isoleucine	NA	NA	NA	NA	NA
116	N6-methyladenosine	N6-Methyladenosine	HMDB0004044	102175		CNC1=
117	norvaline	Norvaline	HMDB0013716	439575	C01799	CCC[C
118	orotidine	Orotidine	HMDB0000788	92751	C01103	OC[C@
119	paraxanthine	Paraxanthine	HMDB0001860	4687	C13747	CN1C=
120	phenethylamine	Phenylethylamine	HMDB0012275	1001	C05332	NCCC
121	phenylacetylleucine	NA	NA	NA	NA	NA
122	phenylalanine	Phenylalanine	HMDB0000159	6140	C00079	N[C@@
123	phenyllactate	D-Phenyllactic acid	HMDB0000563	444718	C05607	[H][C@
124	phosphate	Phosphate	HMDB0001429	1004	C00009	OP(O)
125	phosphocholine	Phosphorylcholine	HMDB0001565	1014	C00588	C[N+]((
126	phosphoethanolamine	O-Phosphoethanolamine	HMDB0000224	1015	C00346	NCCO
127	prolylglycine	Prolylglycine	HMDB0011178	6426709		OC(=O
128	pyridoxal	Pyridoxal	HMDB0001545	1050	C00250	CC1=N
129	quinolinate	Quinolinic acid	HMDB0000232	1066	C03722	OC(=O
130	S-adenosylmethionine	S-Adenosylmethionine	HMDB0001185	34756	C00019	C[S+]((
131	S-carboxymethyl-L-cysteine	S-Carboxymethyl-L-cysteine	HMDB0029415	1080		NC(CS
132	sarcosine	Sarcosine	HMDB0000271	1088	C00213	CNCC(
133	suberoylcarnitine	NA	NA	NA	NA	NA
134	succinimide	NA	NA	NA	NA	NA
135	succinylcarnitine	Succinylcarnitine	HMDB0061717	131802075		C[N+]((
136	taurine	Taurine	HMDB0000251	1123	C00245	NCCS(
137	taurolithocholate 3-sulfate	Taurolithocholic acid 3-sulfate	HMDB0002580	440071	C03642	[H][C@
138	tetrahydrocortisol glucuronide	NA	NA	NA	NA	NA
139	tetrahydrocortisone	Tetrahydrocortisone	HMDB0000903	12444617	C05470	[H][C@
140	tetrahydrocortisone glucuronide	NA	NA	NA	NA	NA
141	tiglyl carnitine	Tiglylcarnitine	HMDB0002366	91825636		C\C=C
142	trans-3	NA	NA	NA	NA	NA
143	trans-aconitate	trans-Aconitic acid	HMDB0000958	444212	C02341	OC(=O
144	trans-urocanate	Trans-urocanate	HMDB0062562	1178		OC(=O
145	triethanolamine	Triethanolamine	HMDB0032538	7618	C06771	OCCN
146	tryptamine	Tryptamine	HMDB0000303	1150	C00398	NCCC
147	tryptophan	L-Tryptophan	HMDB0000929	6305	C00078	N[C@@
148	tyramine	Tyramine	HMDB0000306	5610	C00483	NCCC
149	umbelliferone sulfate	4-Methylumbelliferone sulfate	HMDB0240465		C11585	CC1=C
150	ursocholate	Ursocholic acid	HMDB0000917	122340	C17644	[H][C@

4 Pathway Analysis

In this step, users are asked to select a pathway library, as well as specify the algorithms for pathway enrichment analysis and pathway topology analysis.

4.1 Pathway Library

There are 15 pathway libraries currently supported, with a total of 1173 pathways :

- Homo sapiens (human) [80]
- Mus musculus (mouse) [82]
- Rattus norvegicus (rat) [81]
- Bos taurus (cow) [81]
- Danio rerio (zebrafish) [81]
- Drosophila melanogaster (fruit fly) [79]
- Caenorhabditis elegans (nematode) [78]
- Saccharomyces cerevisiae (yeast) [65]
- Oryza sativa japonica (Japanese rice) [83]
- Arabidopsis thaliana (thale cress) [87]
- Escherichia coli K-12 MG1655 [87]
- Bacillus subtilis [80]
- Pseudomonas putida KT2440 [89]
- Staphylococcus aureus N315 (MRSA/VSSA)[73]
- Thermotoga maritima [57]

Your selected pathway library code is **hsa** (KEGG organisms abbreviation).

4.2 Over Representation Analysis

Over-representation analysis tests if a particular group of compounds is represented more than expected by chance within the user uploaded compound list. In the context of pathway analysis, we are testing if compounds involved in a particular pathway are enriched compared to random hits. MetPA offers two of the most commonly used methods for over-representation analysis:

- Fishers'Exact test
- Hypergeometric Test

Please note, MetPA uses one-tailed Fisher's exact test which will give essentially the same result as the result calculated by the hypergeometric test.

The selected over-representation analysis method is 'Hypergeometric test'.

4.3 Pathway Topology Analysis

The structure of biological pathways represent our knowledge about the complex relationships among molecules within a cell or a living organism. However, most pathway analysis algorithms fail to take structural information into consideration when estimating which pathways are significantly changed under conditions of study. It is well-known that changes in more important positions of a network will trigger a more severe impact on the pathway than changes occurred in marginal or relatively isolated positions.

The pathway topology analysis uses two well-established node centrality measures to estimate node importance - **degree centrality** and **betweenness centrality**. Degree centrality is defined as the number of links occurred upon a node. For a directed graph there are two types of degree: in-degree for links come from other nodes, and out-degree for links initiated from the current node. Metabolic networks are directed graph. Here we only consider the out-degree for node importance measure. It is assumed that nodes upstream will have regulatory roles for the downstream nodes, not vice versa. The betweenness centrality measures the number of shortest paths going through the node. Since the metabolic network is directed, we use the relative betweenness centrality for a metabolite as the importance measure. The degree centrality measure focuses more on local connectivities, while the betweenness centrality measure focuses more on global network topology. For more detailed discussions on various graph-based methods for analyzing biological networks, please refer to the article by Tero Aittokallio, T. et al. [1]

Please note, for comparison among different pathways, the node importance values calculated from centrality measures are further normalized by the sum of the importance of the pathway. Therefore, the total/maximum importance of each pathway is 1; the importance measure of each metabolite node is actually the percentage w.r.t the total pathway importance, and the pathway impact value is the cumulative percentage from the matched metabolite nodes.

Your selected node importance measure for topological analysis is 'relative betweenness centrality'.

5 Pathway Analysis Result

The results from pathway analysis are presented graphically as well as in a detailed table.

A Google-map style interactive visualization system was implemented to facilitate data exploration. The graphical output contains three levels of view: **metabolome view**, **pathway view**, and **compound view**. Only the metabolome view is shown below. Pathway views and compound views are generated dynamically based on your interactions with the visualization system. They are available in your downloaded files.

[1] Tero Aittokallio and Benno Schwikowski. *Graph-based methods for analyzing networks in cell biology*, Briefings in Bioinformatics 2006 7(3):243-255

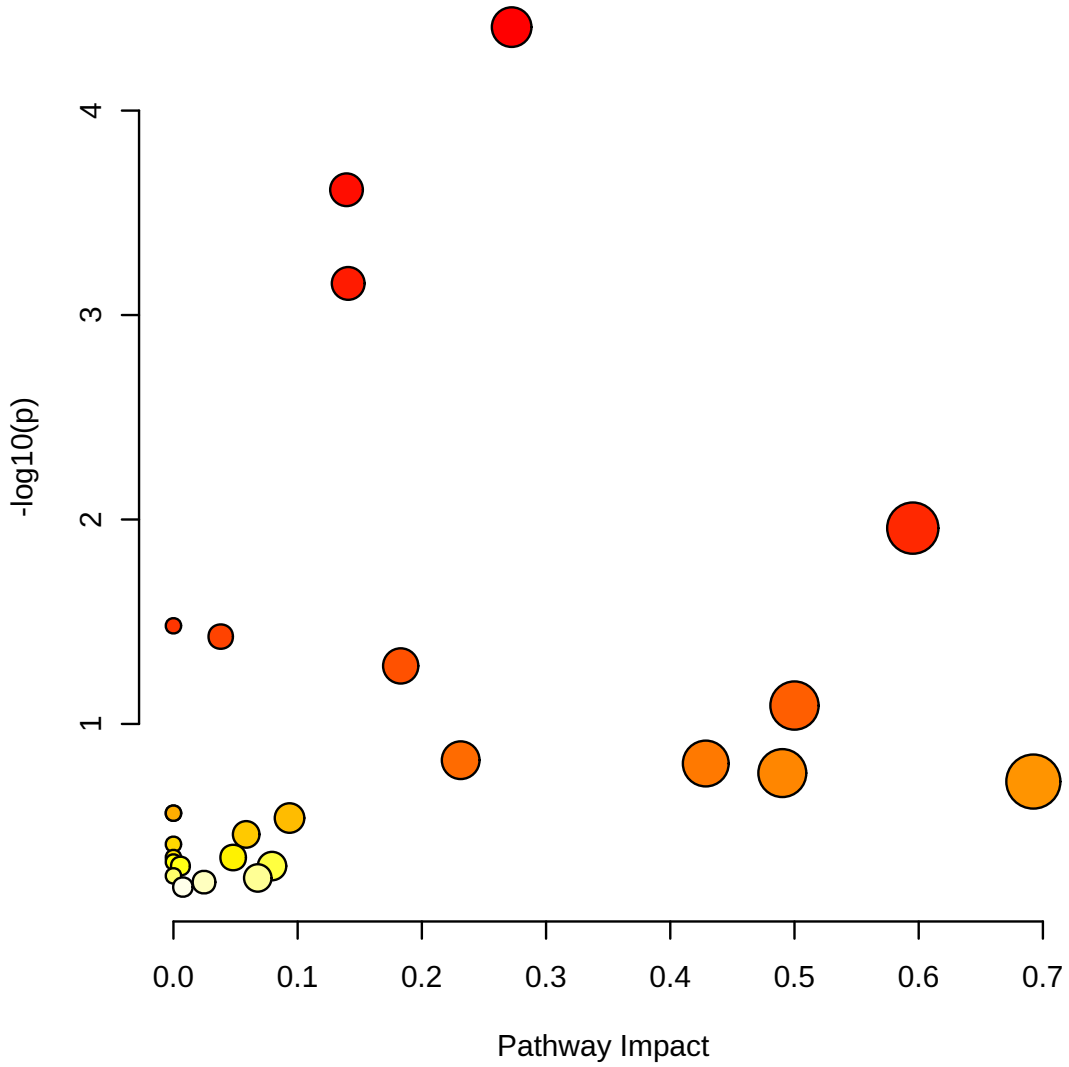

Figure 1: Summary of Pathway Analysis

The table below shows the detailed results from the pathway analysis. Since we are testing many pathways at the same time, the statistical p values from enrichment analysis are further adjusted for multiple testings. In particular, the **Total** is the total number of compounds in the pathway; the **Hits** is the actually matched number from the user uploaded data; the **Raw p** is the original p value calculated from the enrichment analysis; the **Holm p** is the p value adjusted by Holm-Bonferroni method; the **FDR p** is the p value adjusted using False Discovery Rate; the **Impact** is the pathway impact value calculated from pathway topology analysis.

Table 2: Result from Pathway Analysis

	Total	Expected	Hits	Raw p	-log10(p)	Holm adjust	FDR	Impact
Glycine, serine and threonine metabolism	33	0.69	6	3.91E-05	4.41E+00	3.12E-03	3.12E-03	0.27
Histidine metabolism	16	0.34	4	2.44E-04	3.61E+00	1.93E-02	9.76E-03	0.14
Arginine and proline metabolism	36	0.75	5	7.00E-04	3.15E+00	5.46E-02	1.87E-02	0.14
Phenylalanine metabolism	8	0.17	2	1.10E-02	1.96E+00	8.49E-01	2.20E-01	0.60
Arginine biosynthesis	14	0.29	2	3.31E-02	1.48E+00	1.00E+00	4.99E-01	0.00
Glycerophospholipid metabolism	36	0.75	3	3.74E-02	1.43E+00	1.00E+00	4.99E-01	0.04
Tryptophan metabolism	41	0.86	3	5.20E-02	1.28E+00	1.00E+00	5.95E-01	0.18
Phenylalanine, tyrosine and tryptophan biosynthesis	4	0.08	1	8.13E-02	1.09E+00	1.00E+00	8.13E-01	0.50
Cysteine and methionine metabolism	33	0.69	2	1.50E-01	8.23E-01	1.00E+00	1.00E+00	0.23
Taurine and hypotaurine metabolism	8	0.17	1	1.56E-01	8.06E-01	1.00E+00	1.00E+00	0.43
Vitamin B6 metabolism	9	0.19	1	1.74E-01	7.60E-01	1.00E+00	1.00E+00	0.49
Caffeine metabolism	10	0.21	1	1.91E-01	7.18E-01	1.00E+00	1.00E+00	0.69
Butanoate metabolism	15	0.31	1	2.73E-01	5.64E-01	1.00E+00	1.00E+00	0.00
Nicotinate and nicotinamide metabolism	15	0.31	1	2.73E-01	5.64E-01	1.00E+00	1.00E+00	0.00
Glycerolipid metabolism	16	0.34	1	2.89E-01	5.40E-01	1.00E+00	1.00E+00	0.09
Citrate cycle (TCA cycle)	20	0.42	1	3.47E-01	4.60E-01	1.00E+00	1.00E+00	0.06
Pentose phosphate pathway	23	0.48	1	3.88E-01	4.12E-01	1.00E+00	1.00E+00	0.00
Lipoic acid metabolism	28	0.59	1	4.50E-01	3.47E-01	1.00E+00	1.00E+00	0.00
Alanine, aspartate and glutamate metabolism	28	0.59	1	4.50E-01	3.47E-01	1.00E+00	1.00E+00	0.05
Lysine degradation	30	0.63	1	4.73E-01	3.25E-01	1.00E+00	1.00E+00	0.00
Sphingolipid metabolism	32	0.67	1	4.96E-01	3.05E-01	1.00E+00	1.00E+00	0.01
Glyoxylate and dicarboxylate metabolism	32	0.67	1	4.96E-01	3.05E-01	1.00E+00	1.00E+00	0.08
Steroid hormone biosynthesis	87	1.82	2	5.53E-01	2.57E-01	1.00E+00	1.00E+00	0.00
Pyrimidine metabolism	39	0.82	1	5.67E-01	2.47E-01	1.00E+00	1.00E+00	0.07
Tyrosine metabolism	42	0.88	1	5.94E-01	2.26E-01	1.00E+00	1.00E+00	0.02
Primary bile acid biosynthesis	46	0.96	1	6.28E-01	2.02E-01	1.00E+00	1.00E+00	0.01

6 Appendix: R Command History

```
 [1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
 [2] "cmpd.vec<-c(\"(N(1) + N(8))-acetylspermidine\",\"1-carboxyethylhistidine\",\"1-carboxyethyliso
 [3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
 [4] "mSet<-CrossReferencing(mSet, \"name\");"
 [5] "mSet<-CreateMappingResultTable(mSet)"
 [6] "mSet<-PerformDetailMatch(mSet, \"(N(1) + N(8))-acetylspermidine\");"
 [7] "mSet<-GetCandidateList(mSet);"
 [8] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylhistidine\");"
 [9] "mSet<-GetCandidateList(mSet);"
[10] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylisoleucine\");"
[11] "mSet<-GetCandidateList(mSet);"
[12] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylleucine\");"
[13] "mSet<-GetCandidateList(mSet);"
[14] "mSet<-PerformDetailMatch(mSet, \"1-ribosyl-imidazoleacetate\");"
[15] "mSet<-GetCandidateList(mSet);"
[16] "mSet<-SetCandidate(mSet, \"1-ribosyl-imidazoleacetate\", \"Imidazoleacetic acid riboside\");"
[17] "mSet<-PerformDetailMatch(mSet, \"11beta-hydroxyandrosterone sulfate\");"
[18] "mSet<-GetCandidateList(mSet);"
[19] "mSet<-PerformDetailMatch(mSet, \"2-furoylcarnitine\");"
[20] "mSet<-GetCandidateList(mSet);"
[21] "mSet<-PerformDetailMatch(mSet, \"2-keto-3-deoxy-gluconate\");"
[22] "mSet<-GetCandidateList(mSet);"
[23] "mSet<-SetCandidate(mSet, \"2-keto-3-deoxy-gluconate\", \"2-Keto-3-deoxy-D-gluconic acid\");"
[24] "mSet<-PerformDetailMatch(mSet, \"2-methylhexanoylcarnitine\");"
[25] "mSet<-GetCandidateList(mSet);"
[26] "mSet<-PerformDetailMatch(mSet, \"2-methylmalonylcarnitine\");"
[27] "mSet<-GetCandidateList(mSet);"
[28] "mSet<-PerformDetailMatch(mSet, \"2-methylserine\");"
[29] "mSet<-GetCandidateList(mSet);"
[30] "mSet<-PerformDetailMatch(mSet, \"3-acetylphenol sulfate\");"
[31] "mSet<-GetCandidateList(mSet);"
[32] "mSet<-PerformDetailMatch(mSet, \"3-carboxy-4-methyl-5-pentyl-2-furanpropionate\");"
[33] "mSet<-GetCandidateList(mSet);"
[34] "mSet<-PerformDetailMatch(mSet, \"3-ethylcatechol sulfate\");"
[35] "mSet<-GetCandidateList(mSet);"
[36] "mSet<-PerformDetailMatch(mSet, \"3-hydroxy-2-methylpyridine sulfate\");"
[37] "mSet<-GetCandidateList(mSet);"
[38] "mSet<-PerformDetailMatch(mSet, \"3-indoleglyoxylic acid\");"
[39] "mSet<-GetCandidateList(mSet);"
[40] "mSet<-PerformDetailMatch(mSet, \"3-methyl catechol sulfate\");"
[41] "mSet<-GetCandidateList(mSet);"
[42] "mSet<-PerformDetailMatch(mSet, \"3-S-cysteinyl-2-methylpropanoate\");"
[43] "mSet<-GetCandidateList(mSet);"
[44] "mSet<-PerformDetailMatch(mSet, \"4-vinylcatechol sulfate\");"
[45] "mSet<-GetCandidateList(mSet);"
[46] "mSet<-PerformDetailMatch(mSet, \"5-hydroxypicolinic acid\");"
[47] "mSet<-GetCandidateList(mSet);"
[48] "mSet<-PerformDetailMatch(mSet, \"6-bromotryptophan\");"
[49] "mSet<-GetCandidateList(mSet);"
[50] "mSet<-PerformDetailMatch(mSet, \"adenosine 3\");"
[51] "mSet<-GetCandidateList(mSet);"
[52] "mSet<-SetCandidate(mSet, \"adenosine 3\", \"Cyclic AMP\");"
[53] "mSet<-PerformDetailMatch(mSet, \"adipoylcarnitine\");"
[54] "mSet<-GetCandidateList(mSet);"
[55] "mSet<-PerformDetailMatch(mSet, \"alpha-CEHC sulfate\");"
[56] "mSet<-GetCandidateList(mSet);"
```

```
[57] "mSet<-PerformDetailMatch(mSet, \"azeloylcarnitine\");"
[58] "mSet<-GetCandidateList(mSet);"
[59] "mSet<-PerformDetailMatch(mSet, \"C-glycosyltryptophan\");"
[60] "mSet<-GetCandidateList(mSet);"
[61] "mSet<-PerformDetailMatch(mSet, \"heptanoylglutamine\");"
[62] "mSet<-GetCandidateList(mSet);"
[63] "mSet<-SetCandidate(mSet, \"heptanoylglutamine\", \"N-Heptanoylglycine\");"
[64] "mSet<-PerformDetailMatch(mSet, \"hydroxyasparagine\");"
[65] "mSet<-GetCandidateList(mSet);"
[66] "mSet<-SetCandidate(mSet, \"hydroxyasparagine\", \"Hydroxylated lecithin\");"
[67] "mSet<-PerformDetailMatch(mSet, \"guanosine-3\");"
[68] "mSet<-GetCandidateList(mSet);"
[69] "mSet<-PerformDetailMatch(mSet, \"isocitric lactone\");"
[70] "mSet<-GetCandidateList(mSet);"
[71] "mSet<-PerformDetailMatch(mSet, \"N-acetyl-cadaverine\");"
[72] "mSet<-GetCandidateList(mSet);"
[73] "mSet<-SetCandidate(mSet, \"N-acetyl-cadaverine\", \"N-Acetylcadaverine\");"
[74] "mSet<-PerformDetailMatch(mSet, \"N-succinyl-isoleucine\");"
[75] "mSet<-GetCandidateList(mSet);"
[76] "mSet<-PerformDetailMatch(mSet, \"phenylacetylleucine\");"
[77] "mSet<-GetCandidateList(mSet);"
[78] "mSet<-PerformDetailMatch(mSet, \"succinimide\");"
[79] "mSet<-GetCandidateList(mSet);"
[80] "mSet<-PerformDetailMatch(mSet, \"tetrahydrocortisol glucuronide\");"
[81] "mSet<-GetCandidateList(mSet);"
[82] "mSet<-PerformDetailMatch(mSet, \"tetrahydrocortisone glucuronide\");"
[83] "mSet<-GetCandidateList(mSet);"
[84] "mSet<-PerformDetailMatch(mSet, \"umbelliferone sulfate\");"
[85] "mSet<-GetCandidateList(mSet);"
[86] "mSet<-SetCandidate(mSet, \"umbelliferone sulfate\", \"4-Methylumbelliferone sulfate\");"
[87] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[88] "mSet<-SetMetabolomeFilter(mSet, F);"
[89] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[90] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA, NA, NA )"
[91] "mSet<-SaveTransformedData(mSet)"
[92] "mSet<-PreparePDFReport(mSet, \"guest32975221000615112O3\")\n"
```

The report was generated on Mon Oct 7 14:49:02 2024 with R version 4.2.2 (2022-10-31), OS system: Linux.