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*

Table 1: Result from Com

	Query	Match	HMDB	PubChem	KEGG	SMILES
1	O-Butanoylcarnitine	Butyrylcarnitine	HMDB0002013	213144	C02862	CCCC(=O)O[C@H](CC([O-])
2	Glutaryl-carnitine	Glutarylcarnitine	HMDB0013130	53481699		C[N+](C)(C)C[C@@H](CC(O
3	Arginine-Glutamine	Arginylglutamine	HMDB0028707	7019985		N[C@@H](CCCNC(N)=N)C(
4	Deoxycarnitine	4-Trimethylammoniobutanoic acid	HMDB0001161	725	C01181	C[N+](C)(C)CCCC([O-])=O
5	N-carbomoyl-L-aspartate	Ureidosuccinic acid	HMDB0000828	93072	C00438	NC(=O)N[C@@H](CC(O)=O
6	Deoxyadenosine	Deoxyadenosine	HMDB0000101	13730	C00559	NC1=C2N=CN([C@H]3C[C@
7	5-Methylcytosine	5-Methylcytosine	HMDB0002894	65040	C02376	CC1=C(N)NC(=O)N=C1
8	Raffinose	Raffinose	HMDB0003213	439242	C00492	OC[C@H]1O[C@@](CO)(O[C
9	Glucose	D-Glucose	HMDB0000122	5793	C00031	OC[C@H]1O[C@@H](O)[C@H

10	L-Octanoylcarnitine	Octanoylcarnitine	HMDB0000791	11953814	C02838	CCCCCCCC(=O)O[C@H](C
11	Malate	Malic acid	HMDB0000156	222656	C00149	O[C@@H](CC(O)=O)C(O)=O
12	Creatinine	Creatinine	HMDB0000562	588	C00791	CN1CC(=O)NC1=N
13	Lysine-Glutamine	Lysylglutamine	HMDB0028949	196305		NCCCC[C@H](N)C(=O)N[C@
14	Serine	Serine	HMDB0000187	5951	C00065	N[C@@H](CO)C(O)=O
15	Arginine-Valine	Arginylvaline	HMDB0028722	6992654		CC(C)[C@H](NC(=O)[C@@H
16	Guanidinoacetate	Guanidoacetic acid	HMDB0000128	763	C00581	NC(=N)NCC(O)=O
17	Uric acid	Uric acid	HMDB0000289	1175	C00366	O=C1NC2=C(N1)C(=O)NC(
18	AMP	Adenosine monophosphate	HMDB0000045	6083	C00020	NC1=C2N=CN([C@@H]3O[C
19	Hypotaurine	Hypotaurine	HMDB0000965	107812	C00519	NCCS(O)=O
20	Guanine	Guanine	HMDB0000132	764	C00242	NC1=NC(=O)C2=C(N1)N=C
21	Asparagine	L-Asparagine	HMDB0000168	6267	C00152	N[C@@H](CC(N)=O)C(O)=O
22	Phenethylamine	Phenylethylamine	HMDB0012275	1001	C05332	NCCC1=CC=CC=C1
23	Thiamine	Thiamine	HMDB0000235	1130	C00378	CC1=C(CCO)SC=[N+]1CC1
24	Histidine	Histidine	HMDB0000177	6274	C00135	N[C@@H](CC1=CN=CN1)C(
25	Cyclic AMP	Cyclic AMP	HMDB0000058	6076	C00575	[H][C@@]12COP(O)(=O)O[C
26	Hypoxanthine	Hypoxanthine	HMDB0000157	790	C00262	OC1=NC=NC2=C1NC=N2
27	2-Hydroxyglutarate	2-Hydroxyglutarate	HMDB0059655	43	C02630	OC(CCC(O)=O)C(O)=O
28	Nicotinamide riboside	Nicotinamide riboside	HMDB0000855	439924	C03150	NC(=O)C1=C[N+](=CC=C1
29	Glutamine	Glutamine	HMDB0000641	5961	C00064	N[C@@H](CCC(N)=O)C(O)=
30	N-acetyl-L-ornithine	N2-Acetylornithine	HMDB0003357	439232	C00437	CC(=O)N[C@@H](CCCN)C(
31	NADH	NADH	HMDB0001487	439153	C00004	NC(=O)C1=CN(C=CC1)[C@
32	Cellobiose	Cellobiose	HMDB0000055	10712	C00185	OC[C@H]1O[C@@H](O[C@H]
33	Norvaline	Norvaline	HMDB0013716	439575	C01799	CCC[C@@H](N)C(O)=O
34	Indole	Indole	HMDB0000738	798	C00463	N1C=CC2=C1C=CC=C2
35	Orotate	Orotic acid	HMDB0000226	967	C00295	OC(=O)C1=CC(=O)NC(=O
36	Fructose	D-Fructose	HMDB0000660	439709	C00095	OC[C@H]1O[C@](O)(CO)[C@
37	Nicotinate	Nicotinic acid	HMDB0001488	938	C00253	OC(=O)C1=CN=CC=C1
38	5- Methylthioadenosine	5'-Methylthioadenosine	HMDB0001173	439176	C00170	CSC[C@H]1O[C@H]([C@H](C
39	Ornithine	Ornithine	HMDB0000214	6262	C00077	NCCC[C@H](N)C(O)=O
40	Uridine	Uridine	HMDB0000296	6029	C00299	OC[C@H]1O[C@H]([C@H](O)
41	Phosphocholine	Phosphorylcholine	HMDB0001565	1014	C00588	C[N+](C)(C)CCOP(O)(O)=O
42	Cytosine	Cytosine	HMDB0000630	597	C00380	NC1=CC=NC(=O)N1
43	L-Palmitoylcarnitine	L-Palmitoylcarnitine	HMDB0240774	16902		[H][C@](CC([O-])=O)(C[N+](
44	UMP	Uridine 5'-monophosphate	HMDB0000288	6030	C00105	O[C@H]1[C@@H](O)[C@@H](
45	Glucuronic acid	D-Glucuronic acid	HMDB0000127	444791	C00191	O[C@H]1O[C@@H]([C@@H](O
46	Carnitine	L-Carnitine	HMDB0000062	10917	C00487	C[N+](C)(C)C[C@H](O)CC(O
47	ADP-D-Glucose	ADP-glucose	HMDB0006557	16500	C00498	NC1=C2N=CN([C@@H]3O[C
48	Montiporic Acid C	NA	NA	NA	NA	NA
49	Montiporic Acid D	NA	NA	NA	NA	NA
50	Dihydroxyacetone phosphate	Dihydroxyacetone phosphate	HMDB0001473	668	C00111	OCC(=O)COP(O)(O)=O
51	Montiporic Acid A	NA	NA	NA	NA	NA
52	Nicotinamide ribotide	Nicotinamide ribotide	HMDB0000229	14181	C00455	NC(=O)C1=C[N+](=CC=C1
53	Montiporic Acid B	NA	NA	NA	NA	NA
54	Porphobilinogen	Porphobilinogen	HMDB0000245	1021	C00931	NCC1=C(CC(O)=O)C(CCC(
55	Tryptophan	L-Tryptophan	HMDB0000929	6305	C00078	N[C@@H](CC1=CNC2=C1C=
56	a-ketoglutarate	Oxoglutaric acid	HMDB0000208	51	C00026	OC(=O)CCC(=O)C(O)=O
57	Citrate	Citric acid	HMDB0000094	311	C00158	OC(=O)CC(O)(CC(O)=O)C
58	ADP	ADP	HMDB0001341	6022	C00008	NC1=NC=NC2=C1N=CN2[C
59	Thymidine	Thymidine	HMDB0000273	5789	C00214	CC1=CN([C@H]2C[C@H](O)
60	N-octanoylglycine	Capryloylglycine	HMDB0000832	84290		CCCCCCCC(=O)NCC(O)=O
61	ADP-ribose	Adenosine diphosphate ribose	HMDB0001178	192	C00301	NC1=C2N=CN(C3OC(COP(
62	1-Methylimidazole acetic acid	Methylimidazoleacetic acid	HMDB0002820	75810	C05828	CN1C=NC(CC(O)=O)=C1
63	GMP	Guanosine monophosphate	HMDB0001397	6804	C00144	NC1=NC2=C(N=CN2[C@@H
64	Cresol	p-Cresol	HMDB0001858	2879	C01468	CC1=CC=C(O)C=C1
65	Itaconic acid	Itaconic acid	HMDB0002092	811	C00490	OC(=O)CC(=C)C(O)=O
66	Carbamoyl phosphate	Carbamoyl phosphate	HMDB0001096	278	C00169	NC(=O)OP(O)(O)=O
67	Phenylalanine	Phenylalanine	HMDB0000159	6140	C00079	N[C@@H](CC1=CC=CC=C1
68	5-methylthioadenosine	5'-Methylthioadenosine	HMDB0001173	439176	C00170	CSC[C@H]1O[C@H]([C@H](C
69	Isoleucine	Isoleucine	HMDB0000172	6306	C00407	CC[C@H](C)[C@H](N)C(O)=
70	4-Aminobutyrate	gamma-Aminobutyric acid	HMDB0000112	119	C00334	NCCCC(O)=O
71	GTP	Guanosine triphosphate	HMDB0001273	6830	C00044	NC1=NC2=C(N=CN2[C@@H
72	Glutamate	Glutamic acid	HMDB0000148	33032	C00025	N[C@@H](CCC(O)=O)C(O)=
73	ATP	Adenosine triphosphate	HMDB0000538	5957	C00002	NC1=NC=NC2=C1N=CN2[C
74	Hippuric acid	Hippuric acid	HMDB0000714	464	C01586	OC(=O)CNC(=O)C1=CC=C
75	Methionine	Methionine	HMDB0000696	6137	C00073	CSCC[C@H](N)C(O)=O
76	Pterin	Pterin	HMDB0000802	73000	C00715	NC1=NC2=NC=CN=C2C(=
77	Glucose-6-phosphate	Glucose 6-phosphate	HMDB0001401	5958	C00092	OC1O[C@H](COP(O)(O)=O)
78	Lumichrome	NA	NA	NA	NA	NA
79	Succinate	Succinic acid	HMDB0000254	1110	C00042	OC(=O)CCC(O)=O
80	Coenzyme A	Coenzyme A	HMDB0001423	87642	C00010	CC(C)(COP(O)(=O)OP(O)(

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 **cel** (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

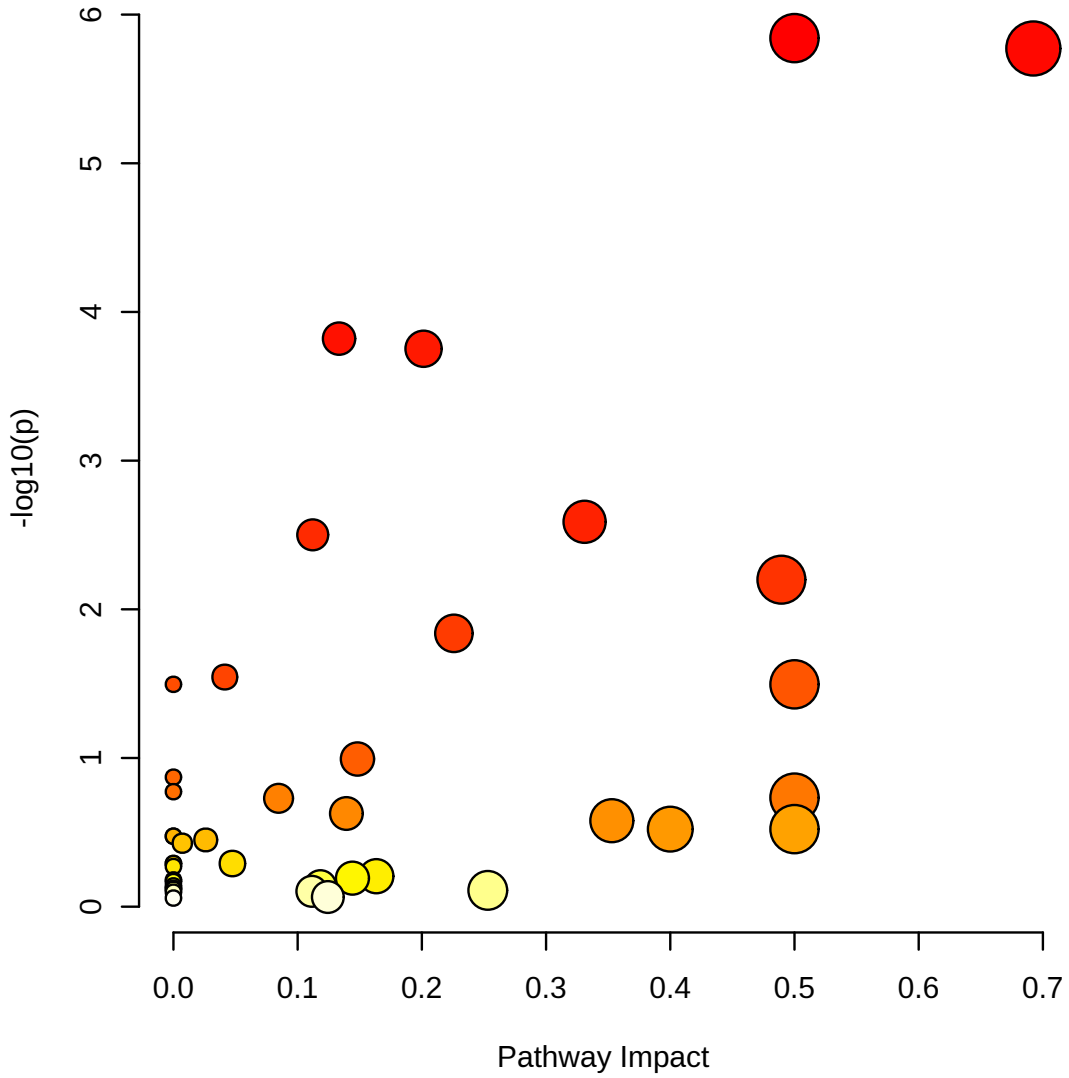

Figure 1: Summary of Pathway Analysis

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
Arginine biosynthesis	6	0.30	5	1.44E-06	5.84E+00	1.09E-04	6.42E-05	0.50
Alanine, aspartate and glutamate metabolism	20	0.99	8	1.69E-06	5.77E+00	1.27E-04	6.42E-05	0.69
Butanoate metabolism	12	0.60	5	1.51E-04	3.82E+00	1.12E-02	3.36E-03	0.13
Purine metabolism	65	3.23	11	1.77E-04	3.75E+00	1.29E-02	3.36E-03	0.20
Pyrimidine metabolism	40	1.99	7	2.58E-03	2.59E+00	1.86E-01	3.92E-02	0.33
Glyoxylate and dicarboxylate metabolism	31	1.54	6	3.16E-03	2.50E+00	2.24E-01	4.00E-02	0.11
Starch and sucrose metabolism	16	0.80	4	6.32E-03	2.20E+00	4.42E-01	6.86E-02	0.49
Citrate cycle (TCA cycle)	20	0.99	4	1.45E-02	1.84E+00	1.00E+00	1.38E-01	0.23
Nicotinate and nicotinamide metabolism	14	0.70	3	2.85E-02	1.54E+00	1.00E+00	2.21E-01	0.04
Nitrogen metabolism	6	0.30	2	3.20E-02	1.50E+00	1.00E+00	2.21E-01	0.00
Phenylalanine metabolism	6	0.30	2	3.20E-02	1.50E+00	1.00E+00	2.21E-01	0.50
Arginine and proline metabolism	23	1.14	3	1.02E-01	9.93E-01	1.00E+00	6.43E-01	0.15
Inositol phosphate metabolism	26	1.29	3	1.35E-01	8.71E-01	1.00E+00	7.87E-01	0.00
Galactose metabolism	15	0.75	2	1.69E-01	7.73E-01	1.00E+00	8.87E-01	0.00
Phenylalanine, tyrosine and tryptophan biosynthesis	4	0.20	1	1.85E-01	7.33E-01	1.00E+00	8.87E-01	0.50
Fructose and mannose metabolism	16	0.80	2	1.87E-01	7.29E-01	1.00E+00	8.87E-01	0.08
Cysteine and methionine metabolism	34	1.69	3	2.36E-01	6.27E-01	1.00E+00	1.00E+00	0.14
Taurine and hypotaurine metabolism	6	0.30	1	2.64E-01	5.78E-01	1.00E+00	1.00E+00	0.35
Thiamine metabolism	7	0.35	1	3.01E-01	5.22E-01	1.00E+00	1.00E+00	0.40
Ascorbate and aldarate metabolism	7	0.35	1	3.01E-01	5.22E-01	1.00E+00	1.00E+00	0.50
Valine, leucine and isoleucine biosynthesis	8	0.40	1	3.36E-01	4.74E-01	1.00E+00	1.00E+00	0.00
Histidine metabolism	8	0.40	1	3.36E-01	4.74E-01	1.00E+00	1.00E+00	0.00
Glutathione metabolism	25	1.24	2	3.56E-01	4.49E-01	1.00E+00	1.00E+00	0.03
Lysine degradation	26	1.29	2	3.74E-01	4.27E-01	1.00E+00	1.00E+00	0.01
D-Amino acid metabolism	14	0.70	1	5.13E-01	2.90E-01	1.00E+00	1.00E+00	0.00
Glycerolipid metabolism	14	0.70	1	5.13E-01	2.90E-01	1.00E+00	1.00E+00	0.00
Glycerophospholipid metabolism	34	1.69	2	5.13E-01	2.90E-01	1.00E+00	1.00E+00	0.05
Pentose and glucuronate interconversions	15	0.75	1	5.37E-01	2.70E-01	1.00E+00	1.00E+00	0.00
Pantothenate and CoA biosynthesis	19	0.94	1	6.24E-01	2.05E-01	1.00E+00	1.00E+00	0.16
Pyruvate metabolism	20	0.99	1	6.43E-01	1.92E-01	1.00E+00	1.00E+00	0.14
Porphyrin metabolism	21	1.04	1	6.61E-01	1.80E-01	1.00E+00	1.00E+00	0.00
Propanoate metabolism	22	1.09	1	6.78E-01	1.69E-01	1.00E+00	1.00E+00	0.00
Glycolysis / Gluconeogenesis	25	1.24	1	7.25E-01	1.40E-01	1.00E+00	1.00E+00	0.00
Folate biosynthesis	25	1.24	1	7.25E-01	1.40E-01	1.00E+00	1.00E+00	0.12
Lipoic acid metabolism	27	1.34	1	7.52E-01	1.24E-01	1.00E+00	1.00E+00	0.00
Sphingolipid metabolism	28	1.39	1	7.65E-01	1.16E-01	1.00E+00	1.00E+00	0.00
Glycine, serine and threonine metabolism	29	1.44	1	7.77E-01	1.10E-01	1.00E+00	1.00E+00	0.25
Tryptophan metabolism	30	1.49	1	7.88E-01	1.03E-01	1.00E+00	1.00E+00	0.11
Amino sugar and nucleotide sugar metabolism	31	1.54	1	7.99E-01	9.74E-02	1.00E+00	1.00E+00	0.00
Fatty acid degradation	38	1.89	1	8.61E-01	6.49E-02	1.00E+00	1.00E+00	0.12
Valine, leucine and isoleucine degradation	40	1.99	1	8.75E-01	5.79E-02	1.00E+00	1.00E+00	0.00

6 Appendix: R Command History

```
 [1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
 [2] "cmpd.vec<-c(\"O-Butanoylcarnitine\",\"Glutaryl-carnitine\",\"Arginine-Glutamine\",\"Deoxycarni
 [3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
 [4] "mSet<-CrossReferencing(mSet, \"name\");"
 [5] "mSet<-CreateMappingResultTable(mSet)"
 [6] "mSet<-PerformDetailMatch(mSet, \"Glutaryl-carnitine\");"
 [7] "mSet<-GetCandidateList(mSet);"
 [8] "mSet<-SetCandidate(mSet, \"Glutaryl-carnitine\", \"Glutarylcarnitine\");"
 [9] "mSet<-PerformDetailMatch(mSet, \"Arginine-Glutamine\");"
[10] "mSet<-GetCandidateList(mSet);"
[11] "mSet<-SetCandidate(mSet, \"Arginine-Glutamine\", \"Arginylglutamine\");"
[12] "mSet<-PerformDetailMatch(mSet, \"N-carbomoyl-L-aspartate\");"
[13] "mSet<-GetCandidateList(mSet);"
[14] "mSet<-SetCandidate(mSet, \"N-carbomoyl-L-aspartate\", \"Ureidosuccinic acid\");"
[15] "mSet<-PerformDetailMatch(mSet, \"Lysine-Glutamine\");"
[16] "mSet<-GetCandidateList(mSet);"
[17] "mSet<-SetCandidate(mSet, \"Lysine-Glutamine\", \"Lysylglutamine\");"
[18] "mSet<-PerformDetailMatch(mSet, \"Arginine-Valine\");"
[19] "mSet<-GetCandidateList(mSet);"
[20] "mSet<-SetCandidate(mSet, \"Arginine-Valine\", \"Arginylvaline\");"
[21] "mSet<-PerformDetailMatch(mSet, \"5- Methylthioadenosine\");"
[22] "mSet<-GetCandidateList(mSet);"
[23] "mSet<-SetCandidate(mSet, \"5- Methylthioadenosine\", \"5'-Methylthioadenosine\");"
[24] "mSet<-PerformDetailMatch(mSet, \"1-Methylimidazole acetic acid\");"
[25] "mSet<-GetCandidateList(mSet);"
[26] "mSet<-SetCandidate(mSet, \"1-Methylimidazole acetic acid\", \"Methylimidazoleacetic acid\");"
[27] "mSet<-PerformDetailMatch(mSet, \"Cresol\");"
[28] "mSet<-GetCandidateList(mSet);"
[29] "mSet<-SetCandidate(mSet, \"Cresol\", \"p-Cresol\");"
[30] "mSet<-SetKEGG.PathLib(mSet, \"cel\", \"current\")"
[31] "mSet<-SetMetabolomeFilter(mSet, F);"
[32] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[33] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA, NA, NA )"
[34] "mSet<-PlotKEGGPath(mSet, \"Alanine, aspartate and glutamate metabolism\",576, 480, \"png\", NU
[35] "mSet<-RerenderMetPAGraph(mSet, \"zoom1716238155533.png\",576.0, 480.0, 100.0)"
[36] "mSet<-PlotKEGGPath(mSet, \"Arginine biosynthesis\",576, 480, \"png\", NULL)"
[37] "mSet<-PlotKEGGPath(mSet, \"Alanine, aspartate and glutamate metabolism\",576, 480, \"png\", NU
[38] "mSet<-SaveTransformedData(mSet)"
[39] "mSet<-PreparePDFReport(mSet, \"guest16942010429013006125\")\n"
```

The report was generated on Mon May 20 16:49:30 2024 with R version 4.3.2 (2023-10-31), OS system: Linux, version: -Ubuntu SMP Tue Mar 5 20:16:58 UTC 2024 .