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	SMIL
1	1-carboxyethylhistidine	NA	NA	NA	NA	NA
2	1-carboxyethylisoleucine	NA	NA	NA	NA	NA
3	1-carboxyethylleucine	NA	NA	NA	NA	NA
4	1-carboxyethyltyrosine	NA	NA	NA	NA	NA
5	1-carboxyethylvaline	NA	NA	NA	NA	NA
6	1-methylhistamine	1-Methylhistamine	HMDB0000898	3614	C05127	CN1C
7	1-methylxanthine	1-Methylxanthine	HMDB0010738	80220	C16358	CN1C
8	1-ribosyl-imidazoleacetate	Imidazoleacetic acid riboside	HMDB0002331	440569	C05131	OC[C
9	11beta-hydroxyandrosterone sulfate	NA	NA	NA	NA	NA

10	11beta-hydroxyetiocholanolone glucuronide	NA	NA	NA	NA	NA
11	2-hydroxy-3-methylvalerate	2-Hydroxy-3-methylpentanoic acid	HMDB0000317	10796774		CC[C
12	2-keto-3-deoxy-gluconate	2-Keto-3-deoxy-D-gluconic acid	HMDB0001353	194024	C01216	OC[C
13	2-methoxyhydroquinone glucuronide	NA	NA	NA	NA	NA
14	2-piperidinone	2-Piperidinone	HMDB0011749	12665		O=C
15	3-carboxy-4-methyl-5-pentyl-2-furanpropionate	NA	NA	NA	NA	NA
16	3-hydroxyphenylacetate	3-Hydroxyphenylacetic acid	HMDB0000440	12122	C05593	OC(=
17	3-methoxytyramine sulfate	NA	NA	NA	NA	NA
18	3-S-cysteinyl-2-methylpropanoate	NA	NA	NA	NA	NA
19	3-sulfo-L-alanine	NA	NA	NA	NA	NA
20	4-ethylphenol glucuronide	NA	NA	NA	NA	NA
21	4-hydroxyglutamate	4-Hydroxy-L-glutamic acid	HMDB0002273	440854	C05947	N[C@
22	5-hydroxylysine	5-Hydroxylysine	HMDB0000450	3032849	C16741	NC[C
23	6-bromotryptophan	NA	NA	NA	NA	NA
24	6'-sialyllactose	6'-Sialyllactose	HMDB0006569	643987		[H][C
25	adenosine 3	Cyclic AMP	HMDB0000058	6076	C00575	[H][C
26	alpha-ketoglutarate	Oxoglutaric acid	HMDB0000208	51	C00026	OC(=
27	androsterone glucuronide	Androsterone glucuronide	HMDB0002829	114833	C11135	[H][C
28	anserine	Anserine	HMDB0000194	112072	C01262	CN1C
29	beta-hydroxyisovalerylglycine	NA	NA	NA	NA	NA
30	catechol glucuronide	NA	NA	NA	NA	NA
31	catechol sulfate	Pyrocatechol sulfate	HMDB0059724	3083879		OC1=
32	cholate	Cholic acid	HMDB0000619	221493	C00695	C[C@
33	cinnamoylglycine	Cinnamoylglycine	HMDB0011621	709625		OC(=
34	cortolone glucuronide	NA	NA	NA	NA	NA
35	cystathionine	L-Cystathionine	HMDB0000099	439258	C02291	N[C@
36	daidzein 7-O-glucuronide	Daidzein 7-O-glucuronide	HMDB0041718	11316354		O[C@
37	dehydroandrosterone glucuronide	NA	NA	NA	NA	NA
38	dimethylglycine	Dimethylglycine	HMDB0000092	673	C01026	CN(C
39	dopamine 4-sulfate	Dopamine 4-sulfate	HMDB0004148	123932	C13691	NCC
40	epiandrosterone glucuronide	NA	NA	NA	NA	NA
41	epiandrosterone sulfate	Epiandrosterone sulfate	HMDB0062657	9929317		[H][C
42	ethyl alpha-glucopyranoside	NA	NA	NA	NA	NA
43	etiocholanolone glucuronide	Etiocholanolone glucuronide	HMDB0004484	443078	C11136	[H][C
44	formiminoglutamate	Formiminoglutamic acid	HMDB0000854	439233	C00439	OC(=
45	gamma-CEHC sulfate	NA	NA	NA	NA	NA
46	gamma-glutamylhistidine	gamma-Glutamylhistidine	HMDB0029151	7017195		N[C@
47	GlcNAc sulfate conjugate of C21H34O2 steroid	NA	NA	NA	NA	NA
48	glucose	D-Glucose	HMDB0000122	5793	C00031	OC[C
49	glucose 6-phosphate	Glucose 6-phosphate	HMDB0001401	5958	C00092	OC1C
50	glucuronide of C12H20O3	NA	NA	NA	NA	NA
51	glucuronide of C8H18O2	NA	NA	NA	NA	NA
52	glycerate	Glyceric acid	HMDB0000139	439194	C00258	OC[C
53	glycochenodeoxycholate	Chenodeoxycholic acid glycine conjugate	HMDB0000637	12544	C05466	[H][C
54	glycochenodeoxycholate 3-sulfate	Glycochenodeoxycholate-3-sulfate	HMDB0002497	21125002		[H][C
55	glycoursodeoxycholic acid sulfate	NA	NA	NA	NA	NA
56	glycylleucine	Glycylleucine	HMDB0000759	92843	C02155	CC(C
57	guaiacol sulfate	O-methoxycatechol-O-sulphate	HMDB0060013	22473		COC
58	guanosine-3	NA	NA	NA	NA	NA
59	hippurate	Hippuric acid	HMDB0000714	464	C01586	OC(=
60	homoarginine	Homo-L-arginine	HMDB0000670	9085	C01924	N[C@
61	hydroxyproline	4-Hydroxyproline	HMDB0000725	5810	C01157	O[C@
62	lanthionine	Lanthionine	HMDB0240656	98504		N[C@
63	methyl-4-hydroxybenzoate sulfate	Methyl-4-hydroxybenzoate sulfate	HMDB0168668	122164837		COC
64	N-acetyl-cadaverine	N-Acetylcadaverine	HMDB0002284	189087		CC(=
65	N-acetylglutamate	N-Acetyl-L-glutamic acid	HMDB0001138	70914	C00624	CC(=
66	N-acetylhistamine	N-Acetylhistamine	HMDB0013253	69602	C05135	CC(=
67	N-acetylisoleucine	N-Acetylisoleucine	HMDB0061684	7036275		CC[C
68	N-acetylvaline	N-Acetylvaline	HMDB0011757	66789		CC(C
69	N-methylpipecolate	NA	NA	NA	NA	NA
70	N-succinyl-isoleucine	NA	NA	NA	NA	NA
71	N-succinyl-phenylalanine	NA	NA	NA	NA	NA
72	N2-acetyl	N-alpha-Acetyl-L-lysine	HMDB0000446	92907	C12989	CC(=
73	nicotinamide N-oxide	Nicotinamide N-oxide	HMDB0002730	72661		NC(=
74	p-cresol glucuronide	p-Cresol glucuronide	HMDB0011686	154035		CC1=
75	phenethylamine	Phenylethylamine	HMDB0012275	1001	C05332	NCC
76	phenol glucuronide	Phenol glucuronide	HMDB0060014	87235		O[C@
77	phenyllactate	D-Phenyllactic acid	HMDB0000563	444718	C05607	[H][C
78	phenylpropionylglycine	Phenylpropionylglycine	HMDB0000860	152323		OC(=
79	phosphocholine	Phosphorylcholine	HMDB0001565	1014	C00588	C[N+
80	phosphoethanolamine	O-Phosphoethanolamine	HMDB0000224	1015	C00346	NCC
81	prolylglycine	Prolylglycine	HMDB0011178	6426709		OC(=
82	S-carboxymethyl-L-cysteine	S-Carboxymethyl-L-cysteine	HMDB0029415	1080		NC(C
83	sarcosine	Sarcosine	HMDB0000271	1088	C00213	CNC
84	tartarate	Tartaric acid	HMDB0000956	444305	C00898	O[C@
85	taurine	Taurine	HMDB0000251	1123	C00245	NCC
86	tetrahydrocortisone	Tetrahydrocortisone	HMDB0000903	12444617	C05470	[H][C
87	tryptamine	Tryptamine	HMDB0000303	1150	C00398	NCC
88	tyramine	Tyramine	HMDB0000306	5610	C00483	NCC
89	umbelliferone sulfate	4-Methylumbelliferone sulfate	HMDB0240465		C11585	CC1=

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

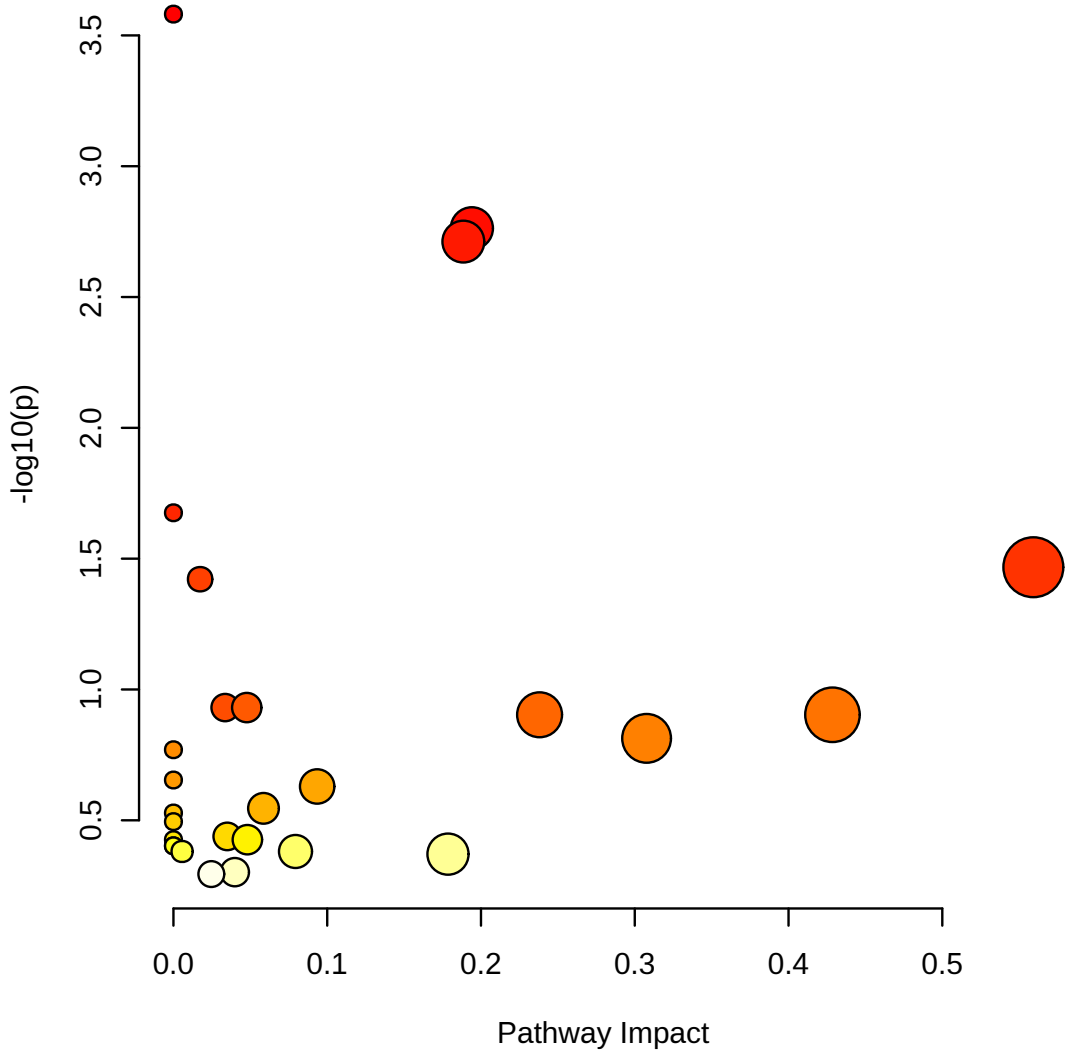

Figure 1: Summary of Pathway Analysis

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
Neomycin, kanamycin and gentamicin biosynthesis	2	0.03	2	2.62E-04	3.58E+00	2.10E-02	2.10E-02	0.00
Glycine, serine and threonine metabolism	33	0.54	4	1.73E-03	2.76E+00	1.36E-01	5.18E-02	0.19
Histidine metabolism	16	0.26	3	1.94E-03	2.71E+00	1.51E-01	5.18E-02	0.19
Arginine biosynthesis	14	0.23	2	2.11E-02	1.68E+00	1.00E+00	4.22E-01	0.00
Starch and sucrose metabolism	18	0.30	2	3.41E-02	1.47E+00	1.00E+00	5.05E-01	0.56
Primary bile acid biosynthesis	46	0.76	3	3.79E-02	1.42E+00	1.00E+00	5.05E-01	0.02
Glycerophospholipid metabolism	36	0.59	2	1.17E-01	9.31E-01	1.00E+00	1.00E+00	0.03
Arginine and proline metabolism	36	0.59	2	1.17E-01	9.31E-01	1.00E+00	1.00E+00	0.05
Phenylalanine metabolism	8	0.13	1	1.25E-01	9.03E-01	1.00E+00	1.00E+00	0.24
Taurine and hypotaurine metabolism	8	0.13	1	1.25E-01	9.03E-01	1.00E+00	1.00E+00	0.43
Caffeine metabolism	10	0.17	1	1.54E-01	8.13E-01	1.00E+00	1.00E+00	0.31
Steroid hormone biosynthesis	87	1.44	3	1.70E-01	7.70E-01	1.00E+00	1.00E+00	0.00
Butanoate metabolism	15	0.25	1	2.22E-01	6.54E-01	1.00E+00	1.00E+00	0.00
Glycerolipid metabolism	16	0.26	1	2.35E-01	6.29E-01	1.00E+00	1.00E+00	0.09
Citrate cycle (TCA cycle)	20	0.33	1	2.85E-01	5.46E-01	1.00E+00	1.00E+00	0.06
beta-Alanine metabolism	21	0.35	1	2.97E-01	5.28E-01	1.00E+00	1.00E+00	0.00
Pentose phosphate pathway	23	0.38	1	3.20E-01	4.95E-01	1.00E+00	1.00E+00	0.00
Galactose metabolism	27	0.45	1	3.64E-01	4.38E-01	1.00E+00	1.00E+00	0.03
Lipoic acid metabolism	28	0.46	1	3.75E-01	4.26E-01	1.00E+00	1.00E+00	0.00
Alanine, aspartate and glutamate metabolism	28	0.46	1	3.75E-01	4.26E-01	1.00E+00	1.00E+00	0.05
Lysine degradation	30	0.50	1	3.96E-01	4.02E-01	1.00E+00	1.00E+00	0.00
Inositol phosphate metabolism	30	0.50	1	3.96E-01	4.02E-01	1.00E+00	1.00E+00	0.00
Sphingolipid metabolism	32	0.53	1	4.16E-01	3.81E-01	1.00E+00	1.00E+00	0.01
Glyoxylate and dicarboxylate metabolism	32	0.53	1	4.16E-01	3.81E-01	1.00E+00	1.00E+00	0.08
Cysteine and methionine metabolism	33	0.54	1	4.26E-01	3.71E-01	1.00E+00	1.00E+00	0.18
Tryptophan metabolism	41	0.68	1	4.99E-01	3.02E-01	1.00E+00	1.00E+00	0.04
Tyrosine metabolism	42	0.69	1	5.08E-01	2.94E-01	1.00E+00	1.00E+00	0.02

6 Appendix: R Command History

```
 [1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
 [2] "cmpd.vec<-c(\"1-carboxyethylhistidine\",\"1-carboxyethylisoleucine\",\"1-carboxyethylleucine\"
 [3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
 [4] "mSet<-CrossReferencing(mSet, \"name\");"
 [5] "mSet<-CreateMappingResultTable(mSet)"
 [6] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylhistidine\");"
 [7] "mSet<-GetCandidateList(mSet);"
 [8] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylisoleucine\");"
 [9] "mSet<-GetCandidateList(mSet);"
[10] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylleucine\");"
[11] "mSet<-GetCandidateList(mSet);"
[12] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethyltyrosine\");"
[13] "mSet<-GetCandidateList(mSet);"
[14] "mSet<-PerformDetailMatch(mSet, \"1-carboxyethylvaline\");"
[15] "mSet<-GetCandidateList(mSet);"
[16] "mSet<-PerformDetailMatch(mSet, \"1-ribosyl-imidazoleacetate\");"
[17] "mSet<-GetCandidateList(mSet);"
[18] "mSet<-SetCandidate(mSet, \"1-ribosyl-imidazoleacetate\", \"Imidazoleacetic acid riboside\");"
[19] "mSet<-PerformDetailMatch(mSet, \"11beta-hydroxyandrosterone sulfate\");"
[20] "mSet<-GetCandidateList(mSet);"
[21] "mSet<-PerformDetailMatch(mSet, \"11beta-hydroxyetiocholanolone glucuronide\");"
[22] "mSet<-GetCandidateList(mSet);"
[23] "mSet<-PerformDetailMatch(mSet, \"2-keto-3-deoxy-gluconate\");"
[24] "mSet<-GetCandidateList(mSet);"
[25] "mSet<-SetCandidate(mSet, \"2-keto-3-deoxy-gluconate\", \"2-Keto-3-deoxy-D-gluconic acid\");"
[26] "mSet<-PerformDetailMatch(mSet, \"2-methoxyhydroquinone glucuronide\");"
[27] "mSet<-GetCandidateList(mSet);"
[28] "mSet<-PerformDetailMatch(mSet, \"3-carboxy-4-methyl-5-pentyl-2-furanpropionate\");"
[29] "mSet<-GetCandidateList(mSet);"
[30] "mSet<-PerformDetailMatch(mSet, \"3-methoxytyramine sulfate\");"
[31] "mSet<-GetCandidateList(mSet);"
[32] "mSet<-PerformDetailMatch(mSet, \"3-S-cysteinyl-2-methylpropanoate\");"
[33] "mSet<-GetCandidateList(mSet);"
[34] "mSet<-PerformDetailMatch(mSet, \"3-sulfo-L-alanine\");"
[35] "mSet<-GetCandidateList(mSet);"
[36] "mSet<-PerformDetailMatch(mSet, \"4-ethylphenol glucuronide\");"
[37] "mSet<-GetCandidateList(mSet);"
[38] "mSet<-PerformDetailMatch(mSet, \"6-bromotryptophan\");"
[39] "mSet<-GetCandidateList(mSet);"
[40] "mSet<-PerformDetailMatch(mSet, \"adenosine 3\");"
[41] "mSet<-GetCandidateList(mSet);"
[42] "mSet<-SetCandidate(mSet, \"adenosine 3\", \"Cyclic AMP\");"
[43] "mSet<-PerformDetailMatch(mSet, \"beta-hydroxyisovalerylglycine\");"
[44] "mSet<-GetCandidateList(mSet);"
[45] "mSet<-PerformDetailMatch(mSet, \"catechol glucuronide\");"
[46] "mSet<-GetCandidateList(mSet);"
[47] "mSet<-PerformDetailMatch(mSet, \"cortolone glucuronide\");"
[48] "mSet<-GetCandidateList(mSet);"
[49] "mSet<-PerformDetailMatch(mSet, \"dehydroandrosterone glucuronide\");"
[50] "mSet<-GetCandidateList(mSet);"
[51] "mSet<-PerformDetailMatch(mSet, \"epiandrosterone glucuronide\");"
[52] "mSet<-GetCandidateList(mSet);"
[53] "mSet<-PerformDetailMatch(mSet, \"ethyl alpha-glucopyranoside\");"
[54] "mSet<-GetCandidateList(mSet);"
[55] "mSet<-PerformDetailMatch(mSet, \"gamma-CEHC sulfate\");"
[56] "mSet<-GetCandidateList(mSet);"
```

```
[57] "mSet<-PerformDetailMatch(mSet, \"glycochenodeoxycholate 3-sulfate\");"
[58] "mSet<-GetCandidateList(mSet);"
[59] "mSet<-SetCandidate(mSet, \"glycochenodeoxycholate 3-sulfate\", \"Glycochenodeoxycholate-3-sulf
[60] "mSet<-PerformDetailMatch(mSet, \"glycoursodeoxycholic acid sulfate\");"
[61] "mSet<-GetCandidateList(mSet);"
[62] "mSet<-PerformDetailMatch(mSet, \"guaiacol sulfate\");"
[63] "mSet<-GetCandidateList(mSet);"
[64] "mSet<-SetCandidate(mSet, \"guaiacol sulfate\", \"O-methoxycatechol-O-sulphate\");"
[65] "mSet<-PerformDetailMatch(mSet, \"guanosine-3\");"
[66] "mSet<-GetCandidateList(mSet);"
[67] "mSet<-PerformDetailMatch(mSet, \"N-acetyl-cadaverine\");"
[68] "mSet<-GetCandidateList(mSet);"
[69] "mSet<-SetCandidate(mSet, \"N-acetyl-cadaverine\", \"N-Acetylcadaverine\");"
[70] "mSet<-PerformDetailMatch(mSet, \"N-methylpipecolate\");"
[71] "mSet<-GetCandidateList(mSet);"
[72] "mSet<-PerformDetailMatch(mSet, \"N-succinyl-isoleucine\");"
[73] "mSet<-GetCandidateList(mSet);"
[74] "mSet<-PerformDetailMatch(mSet, \"N-succinyl-phenylalanine\");"
[75] "mSet<-GetCandidateList(mSet);"
[76] "mSet<-PerformDetailMatch(mSet, \"N2-acetyl\");"
[77] "mSet<-GetCandidateList(mSet);"
[78] "mSet<-SetCandidate(mSet, \"N2-acetyl\", \"N-alpha-Acetyl-L-lysine\");"
[79] "mSet<-PerformDetailMatch(mSet, \"umbelliferone sulfate\");"
[80] "mSet<-GetCandidateList(mSet);"
[81] "mSet<-SetCandidate(mSet, \"umbelliferone sulfate\", \"4-Methylumbelliferone sulfate\");"
[82] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[83] "mSet<-SetMetabolomeFilter(mSet, F);"
[84] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[85] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA, NA, NA )"
[86] "mSet<-SaveTransformedData(mSet)"
[87] "mSet<-PreparePDFReport(mSet, \"guest11776700090262172234\")\n"
```

The report was generated on Mon Oct 7 14:31:24 2024 with R version 4.3.2 (2023-10-31), OS system: Linux.