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: Res

	Query	Match	HMDB	PubChem	KEGG	SMILES
1	1-methylguanidine	Methylguanidine	HMDB0001522	10111	C02294	CNC(N)=N
2	1-methylxanthine	1-Methylxanthine	HMDB0010738	80220	C16358	CN1C(=O)NC2
3	1,2,3-butanetriol	NA	NA	NA	NA	NA
4	11beta-hydroxyandrosterone sulfate	NA	NA	NA	NA	NA
5	11beta-hydroxyetiocholanolone glucuronide	NA	NA	NA	NA	NA
6	2-acetamidophenol sulfate	NA	NA	NA	NA	NA
7	2-aminophenol sulfate	Pyrocatechol sulfate	HMDB0059724	3083879		OC1=C(OS(O)
8	2-ethylphenylsulfate	NA	NA	NA	NA	NA
9	2-piperidinone	2-Piperidinone	HMDB0011749	12665		O=C1CCCCN1

10	2,6-dihydroxybenzoic acid	2,6-Dihydroxybenzoic acid	HMDB0013676	9338	C21298	OC(=O)C1=C
11	21-hydroxypregnenolone disulfate	NA	NA	NA	NA	NA
12	3-ethylcatechol sulfate	NA	NA	NA	NA	NA
13	3-hydroxyhippurate	3-Hydroxyhippuric acid	HMDB0006116	450268		OC(=O)CNC(=
14	3-hydroxyisonicotinic acid	NA	NA	NA	NA	NA
15	3-hydroxyphenylacetate	3-Hydroxyphenylacetic acid	HMDB0000440	12122	C05593	OC(=O)CC1=C
16	3-hydroxyphenylacetoylglutamine	NA	NA	NA	NA	NA
17	3-hydroxypyridine glucuronide	NA	NA	NA	NA	NA
18	3-methoxycatechol sulfate	NA	NA	NA	NA	NA
19	3-methyl catechol sulfate	NA	NA	NA	NA	NA
20	3-sulfo-L-alanine	3-Sulfinoalanine	HMDB0000996	1549098	C00606	N[C@@H](CS(O
21	4-acetylcatechol sulfate	NA	NA	NA	NA	NA
22	4-allylphenol sulfate	NA	NA	NA	NA	NA
23	4-ethyl-2-methoxyphenol sulfate	NA	NA	NA	NA	NA
24	4-ethylcatechol sulfate	NA	NA	NA	NA	NA
25	4-ethylphenol glucuronide	NA	NA	NA	NA	NA
26	4-ethylphenyl sulfate	4-Ethylphenylsulfate	HMDB0062551	20822574		CCC1=CC=C(
27	4-hydroxycinnamate	4-Hydroxycinnamic acid	HMDB0002035	637542	C00811	OC(=O)\C=C
28	4-hydroxyglutamate	4-Hydroxy-L-glutamic acid	HMDB0002273	440854	C05947	N[C@@H](C[C
29	4'-hydroxypropiophenone sulfate	NA	NA	NA	NA	NA
30	acetylhydroquinone sulfate	NA	NA	NA	NA	NA
31	alpha-ketoglutarate	Oxoglutaric acid	HMDB0000208	51	C00026	OC(=O)CCC(=
32	androsterone glucuronide	Androsterone glucuronide	HMDB0002829	114833	C11135	[H][C@@]12CC
33	anserine	Anserine	HMDB0000194	112072	C01262	CN1C=NC=C1
34	beta-hydroxyisovalerylglycine	NA	NA	NA	NA	NA
35	catechol glucuronide	NA	NA	NA	NA	NA
36	catechol sulfate	Pyrocatechol sulfate	HMDB0059724	3083879		OC1=C(OS(O)
37	cinnamoylglycine	Cinnamoylglycine	HMDB0011621	709625		OC(=O)CNC(=
38	cis-urocanate	NA	NA	NA	NA	NA
39	citraconate/glutaconate	NA	NA	NA	NA	NA
40	daidzein 7-O-glucuronide	Daidzein 7-O-glucuronide	HMDB0041718	11316354		O[C@@H]1[C@
41	dehydroandrosterone glucuronide	NA	NA	NA	NA	NA
42	dimethylglycine	Dimethylglycine	HMDB0000092	673	C01026	CN(C)CC(O)=
43	epiandrosterone glucuronide	NA	NA	NA	NA	NA
44	epiandrosterone sulfate	Epiandrosterone sulfate	HMDB0062657	9929317		[H][C@@]12CC
45	ethyl alpha-glucopyranoside	NA	NA	NA	NA	NA
46	etiocholanolone glucuronide	Etiocholanolone glucuronide	HMDB0004484	443078	C11136	[H][C@@]12CC
47	galactonate	Galactonic acid	HMDB0000565	128869	C00880	OC[C@@H](O)
48	gamma-aminobutyrate	gamma-Aminobutyric acid	HMDB0000112	119	C00334	NCCCC(O)=O
49	GlcNAc sulfate conjugate of C21H34O2 steroid	NA	NA	NA	NA	NA
50	glucose 6-phosphate	Glucose 6-phosphate	HMDB0001401	5958	C00092	OC1O[C@H](C
51	glucuronide of C10H14O2 (2)	NA	NA	NA	NA	NA
52	glucuronide of C12H20O3 (1)	NA	NA	NA	NA	NA
53	glucuronide of C8H18O2 (1)	NA	NA	NA	NA	NA
54	glucuronide of C8H18O2 (2)	NA	NA	NA	NA	NA
55	glycerate	Glyceric acid	HMDB0000139	439194	C00258	OC[C@@H](O)
56	glycylleucine	Glycylleucine	HMDB0000759	92843	C02155	CC(C)C[C@H](
57	guaiacol sulfate	O-methoxycatechol-O-sulphate	HMDB0060013	22473		COC1=CC=CC
58	guanosine	Guanosine	HMDB0000133	6802	C00387	NC1=NC2=C(
59	hippurate	Hippuric acid	HMDB0000714	464	C01586	OC(=O)CNC(=
60	homoarginine	Homo-L-arginine	HMDB0000670	9085	C01924	N[C@@H](CCC
61	hydroquinone sulfate	NA	NA	NA	NA	NA
62	lyxonate	L-Lyxonic acid	HMDB0060255	644110	C05412	OC[C@H](O)[C
63	methylurea	N-Methylurea	METPA1296		C16363	
64	N-acetylalanine	N-Acetyl-L-alanine	HMDB0000766	88064		C[C@H](NC(C)
65	N-acetylhistamine	N-Acetylhistamine	HMDB0013253	69602	C05135	CC(=O)NCCC
66	N-methylpipecolate	NA	NA	NA	NA	NA
67	N,N-dimethyl-5-aminovalerate	NA	NA	NA	NA	NA
68	N2-acetyl,N6-methyllysine	NA	NA	NA	NA	NA
69	N2-acetyl,N6,N6-dimethyllysine	NA	NA	NA	NA	NA
70	nicotinamide riboside	Nicotinamide riboside	HMDB0000855	439924	C03150	NC(=O)C1=C[
71	o-cresol sulfate	p-Cresol sulfate	HMDB0011635	4615423		CC1=CC=C(O
72	orcinol sulfate	NA	NA	NA	NA	NA
73	pentose acid	Valeric acid	HMDB0000892	7991	C00803	CCCCC(O)=O
74	phenylpropionylglycine	Phenylpropionylglycine	HMDB0000860	152323		OC(=O)CNC(=
75	phosphoethanolamine	O-Phosphoethanolamine	HMDB0000224	1015	C00346	NCCOP(O)(O)
76	pregnanediol-3-glucuronide	Pregnanediol 3-O-glucuronide	HMDB0010318	123796	C03033	[H][C@@]1(CC[
77	prolylglycine	Prolylglycine	HMDB0011178	6426709		OC(=O)CNC(=
78	quinate	Quinic acid	HMDB0003072	6508	C00296	O[C@@H]1C[C
79	syringol sulfate	NA	NA	NA	NA	NA
80	tartarate	Tartaric acid	HMDB0000956	444305	C00898	O[C@H]([C@@H
81	threonate	Threonic acid	HMDB0000943	5460407	C01620	OC[C@H](O)[C
82	tricarballylate	1,2,3-Propanetricarboxylic acid	HMDB0031193	14925	C19806	OC(=O)CC(CC
83	trigonelline	Trigonelline	HMDB0000875	5570	C01004	C[N+]1=CC=C
84	uracil	Uracil	HMDB0000300	1174	C00106	O=C1NC=CC(

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

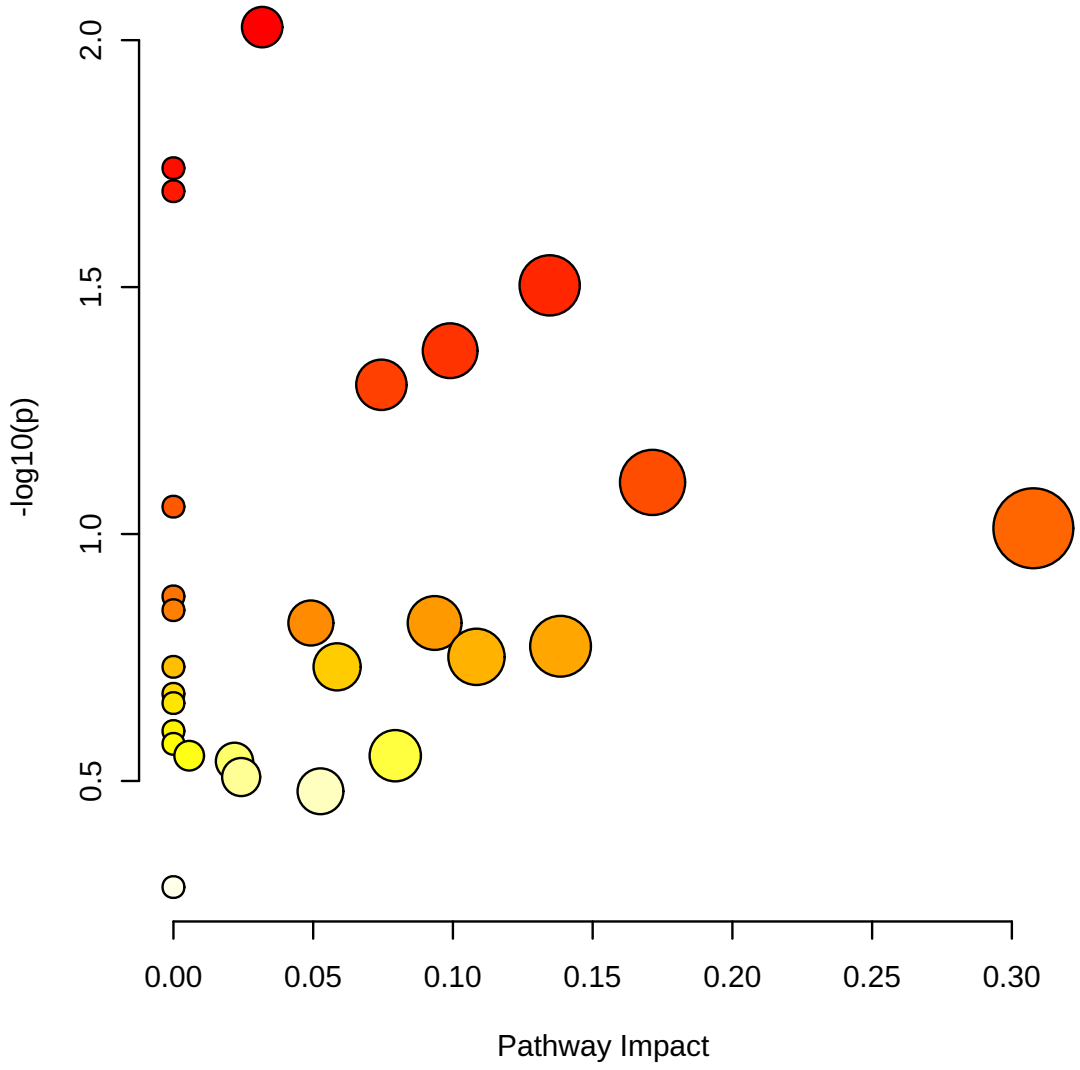

Figure 1: Summary of Pathway Analysis

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
Butanoate metabolism	15	0.15	2	9.41E-03	2.03E+00	7.53E-01	5.39E-01	0.03
beta-Alanine metabolism	21	0.21	2	1.82E-02	1.74E+00	1.00E+00	5.39E-01	0.00
Neomycin, kanamycin and gentamicin biosynthesis	2	0.02	1	2.02E-02	1.69E+00	1.00E+00	5.39E-01	0.00
Alanine, aspartate and glutamate metabolism	28	0.28	2	3.14E-02	1.50E+00	1.00E+00	6.27E-01	0.13
Glycine, serine and threonine metabolism	33	0.34	2	4.25E-02	1.37E+00	1.00E+00	6.65E-01	0.10
Arginine and proline metabolism	36	0.37	2	4.99E-02	1.30E+00	1.00E+00	6.65E-01	0.07
Taurine and hypotaurine metabolism	8	0.08	1	7.86E-02	1.10E+00	1.00E+00	8.65E-01	0.17
Ascorbate and aldarate metabolism	9	0.09	1	8.80E-02	1.06E+00	1.00E+00	8.65E-01	0.00
Caffeine metabolism	10	0.10	1	9.73E-02	1.01E+00	1.00E+00	8.65E-01	0.31
Arginine biosynthesis	14	0.14	1	1.34E-01	8.74E-01	1.00E+00	8.74E-01	0.00
Nicotinate and nicotinamide metabolism	15	0.15	1	1.43E-01	8.46E-01	1.00E+00	8.74E-01	0.00
Histidine metabolism	16	0.16	1	1.51E-01	8.20E-01	1.00E+00	8.74E-01	0.05
Glycerolipid metabolism	16	0.16	1	1.51E-01	8.20E-01	1.00E+00	8.74E-01	0.09
Starch and sucrose metabolism	18	0.18	1	1.69E-01	7.73E-01	1.00E+00	8.74E-01	0.14
Pentose and glucuronate interconversions	19	0.19	1	1.77E-01	7.51E-01	1.00E+00	8.74E-01	0.11
Pantothenate and CoA biosynthesis	20	0.20	1	1.86E-01	7.31E-01	1.00E+00	8.74E-01	0.00
Citrate cycle (TCA cycle)	20	0.20	1	1.86E-01	7.31E-01	1.00E+00	8.74E-01	0.06
Pentose phosphate pathway	23	0.23	1	2.11E-01	6.76E-01	1.00E+00	9.26E-01	0.00
Steroid hormone biosynthesis	87	0.88	2	2.20E-01	6.58E-01	1.00E+00	9.26E-01	0.00
Lipoic acid metabolism	28	0.28	1	2.51E-01	6.01E-01	1.00E+00	9.62E-01	0.00
Inositol phosphate metabolism	30	0.30	1	2.66E-01	5.75E-01	1.00E+00	9.62E-01	0.00
Sphingolipid metabolism	32	0.33	1	2.81E-01	5.51E-01	1.00E+00	9.62E-01	0.01
Glyoxylate and dicarboxylate metabolism	32	0.33	1	2.81E-01	5.51E-01	1.00E+00	9.62E-01	0.08
Cysteine and methionine metabolism	33	0.34	1	2.89E-01	5.40E-01	1.00E+00	9.62E-01	0.02
Glycerophospholipid metabolism	36	0.37	1	3.10E-01	5.08E-01	1.00E+00	9.94E-01	0.02
Pyrimidine metabolism	39	0.40	1	3.32E-01	4.79E-01	1.00E+00	1.00E+00	0.05
Purine metabolism	70	0.71	1	5.19E-01	2.85E-01	1.00E+00	1.00E+00	0.00

6 Appendix: R Command History

```
 [1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
 [2] "cmpd.vec<-c(\"1-methylguanidine\",\"1-methylxanthine\",\"1,2,3-butanetriol\",\"11beta-hydroxya
 [3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
 [4] "mSet<-CrossReferencing(mSet, \"name\");"
 [5] "mSet<-CreateMappingResultTable(mSet)"
 [6] "mSet<-PerformDetailMatch(mSet, \"1,2,3-butanetriol\");"
 [7] "mSet<-GetCandidateList(mSet);"
 [8] "mSet<-PerformDetailMatch(mSet, \"11beta-hydroxyandrosterone sulfate\");"
 [9] "mSet<-GetCandidateList(mSet);"
[10] "mSet<-PerformDetailMatch(mSet, \"2-acetamidophenol sulfate\");"
[11] "mSet<-GetCandidateList(mSet);"
[12] "mSet<-PerformDetailMatch(mSet, \"2-ethylphenylsulfate\");"
[13] "mSet<-GetCandidateList(mSet);"
[14] "mSet<-PerformDetailMatch(mSet, \"21-hydroxypregnenolone disulfate\");"
[15] "mSet<-GetCandidateList(mSet);"
[16] "mSet<-PerformDetailMatch(mSet, \"3-ethylcatechol sulfate\");"
[17] "mSet<-GetCandidateList(mSet);"
[18] "mSet<-PerformDetailMatch(mSet, \"21-hydroxypregnenolone disulfate\");"
[19] "mSet<-GetCandidateList(mSet);"
[20] "mSet<-PerformDetailMatch(mSet, \"3-ethylcatechol sulfate\");"
[21] "mSet<-GetCandidateList(mSet);"
[22] "mSet<-PerformDetailMatch(mSet, \"3-hydroxyisonicotinic acid\");"
[23] "mSet<-GetCandidateList(mSet);"
[24] "mSet<-PerformDetailMatch(mSet, \"3-hydroxyphenylacetoylglutamine\");"
[25] "mSet<-GetCandidateList(mSet);"
[26] "mSet<-PerformDetailMatch(mSet, \"3-hydroxypyridine glucuronide\");"
[27] "mSet<-GetCandidateList(mSet);"
[28] "mSet<-PerformDetailMatch(mSet, \"3-methoxycatechol sulfate\");"
[29] "mSet<-GetCandidateList(mSet);"
[30] "mSet<-PerformDetailMatch(mSet, \"3-methyl catechol sulfate\");"
[31] "mSet<-GetCandidateList(mSet);"
[32] "mSet<-PerformDetailMatch(mSet, \"3-sulfo-L-alanine\");"
[33] "mSet<-GetCandidateList(mSet);"
[34] "mSet<-SetCandidate(mSet, \"3-sulfo-L-alanine\", \"3-Sulfinoalanine\");"
[35] "mSet<-PerformDetailMatch(mSet, \"4-acetylcatechol sulfate\");"
[36] "mSet<-GetCandidateList(mSet);"
[37] "mSet<-PerformDetailMatch(mSet, \"4-allylphenol sulfate\");"
[38] "mSet<-GetCandidateList(mSet);"
[39] "mSet<-PerformDetailMatch(mSet, \"4-ethyl-2-methoxyphenol sulfate\");"
[40] "mSet<-GetCandidateList(mSet);"
[41] "mSet<-PerformDetailMatch(mSet, \"4-ethylcatechol sulfate\");"
[42] "mSet<-GetCandidateList(mSet);"
[43] "mSet<-PerformDetailMatch(mSet, \"4-ethylphenol glucuronide\");"
[44] "mSet<-GetCandidateList(mSet);"
[45] "mSet<-PerformDetailMatch(mSet, \"4-ethylphenyl sulfate\");"
[46] "mSet<-GetCandidateList(mSet);"
[47] "mSet<-SetCandidate(mSet, \"4-ethylphenyl sulfate\", \"4-Ethylphenylsulfate\");"
[48] "mSet<-PerformDetailMatch(mSet, \"4'-hydroxypropiophenone sulfate\");"
[49] "mSet<-GetCandidateList(mSet);"
[50] "mSet<-PerformDetailMatch(mSet, \"acetylhydroquinone sulfate\");"
[51] "mSet<-GetCandidateList(mSet);"
[52] "mSet<-PerformDetailMatch(mSet, \"beta-hydroxyisovalerylglycine\");"
[53] "mSet<-GetCandidateList(mSet);"
[54] "mSet<-PerformDetailMatch(mSet, \"catechol glucuronide\");"
[55] "mSet<-GetCandidateList(mSet);"
[56] "mSet<-PerformDetailMatch(mSet, \"cis-urocanate\");"
```

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[57] "mSet<-GetCandidateList(mSet);"
[58] "mSet<-PerformDetailMatch(mSet, \"citraconate/glutaconate\");"
[59] "mSet<-GetCandidateList(mSet);"
[60] "mSet<-PerformDetailMatch(mSet, \"cis-urocanate\");"
[61] "mSet<-GetCandidateList(mSet);"
[62] "mSet<-PerformDetailMatch(mSet, \"dehydroandrosterone glucuronide\");"
[63] "mSet<-GetCandidateList(mSet);"
[64] "mSet<-PerformDetailMatch(mSet, \"epiandrosterone glucuronide\");"
[65] "mSet<-GetCandidateList(mSet);"
[66] "mSet<-PerformDetailMatch(mSet, \"ethyl alpha-glucopyranoside\");"
[67] "mSet<-GetCandidateList(mSet);"
[68] "mSet<-PerformDetailMatch(mSet, \"guaiacol sulfate\");"
[69] "mSet<-GetCandidateList(mSet);"
[70] "mSet<-SetCandidate(mSet, \"guaiacol sulfate\", \"O-methoxycatechol-O-sulphate\");"
[71] "mSet<-PerformDetailMatch(mSet, \"hydroquinone sulfate\");"
[72] "mSet<-GetCandidateList(mSet);"
[73] "mSet<-PerformDetailMatch(mSet, \"N-methylpipecolate\");"
[74] "mSet<-GetCandidateList(mSet);"
[75] "mSet<-PerformDetailMatch(mSet, \"N,N-dimethyl-5-aminovalerate\");"
[76] "mSet<-GetCandidateList(mSet);"
[77] "mSet<-PerformDetailMatch(mSet, \"N2-acetyl,N6-methyllysine\");"
[78] "mSet<-GetCandidateList(mSet);"
[79] "mSet<-PerformDetailMatch(mSet, \"N2-acetyl,N6,N6-dimethyllysine\");"
[80] "mSet<-GetCandidateList(mSet);"
[81] "mSet<-PerformDetailMatch(mSet, \"o-cresol sulfate\");"
[82] "mSet<-GetCandidateList(mSet);"
[83] "mSet<-SetCandidate(mSet, \"o-cresol sulfate\", \"p-Cresol sulfate\");"
[84] "mSet<-PerformDetailMatch(mSet, \"orcinol sulfate\");"
[85] "mSet<-GetCandidateList(mSet);"
[86] "mSet<-PerformDetailMatch(mSet, \"pentose acid\");"
[87] "mSet<-GetCandidateList(mSet);"
[88] "mSet<-SetCandidate(mSet, \"pentose acid\", \"Valeric acid\");"
[89] "mSet<-PerformDetailMatch(mSet, \"syringol sulfate\");"
[90] "mSet<-GetCandidateList(mSet);"
[91] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[92] "mSet<-SetMetabolomeFilter(mSet, F);"
[93] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[94] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA, NA, NA )"
[95] "mSet<-SaveTransformedData(mSet)"
[96] "mSet<-PreparePDFReport(mSet, \"guest56257720172848102 43\")\n"
```

The report was generated on Mon Oct 7 15:06:17 2024 with R version 4.3.2 (2023-10-31), OS system: Linux.