# Metabolomic Data Analysis with MetaboAnalyst 6.0

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#### 1 Background

MSEA 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. <sup>1</sup>. <sup>2</sup>

#### 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));

<sup>&</sup>lt;sup>1</sup>Subramanian Gene set enrichment analysis: A knowledge-based approach for interpreting genome-wide expression profiles., Proc Natl Acad Sci USA. 2005 102(43): 15545-50

<sup>&</sup>lt;sup>2</sup>Nam D, Kim SY. Gene-set approach for expression pattern analysis, Briefings in Bioinformatics. 2008 9(3): 189-197.

• 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 Over Representation Analysis (ORA) which requires a list of compound names as input.

#### 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 contain the result can be found the downloaded file  $name\_map.csv$ 

Table 1: Result from Com

-		3.5	HMDD	D. I. GI	TIBAA	GMII DG
	Query	Match	HMDB	PubChem	KEGG	SMILES
1	O-Butanoylcarnitine	Butyrylcarnitine	HMDB0002013	213144	C02862	CCCC(=0)O[C@H](CC([O-])
2	Glutary l-carnitine	Glutarylcarnitine	HMDB0013130	53481699		C[N+](C)(C)C[C@@H](CC(O)
3	Arginine-Glutamine	Arginylglutamine	HMDB0028707	7019985	004404	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@H])
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[CC)
9	Glucose	D-Glucose	HMDB0000122	5793	C00031	OC[C@H]1O[C@@H](O)[C@H]
10	L-Octanoylcarnitine	Octanoylcarnitine	HMDB0000791	11953814	C02838	CCCCCCC(=O)O[C@H](CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
11	Creatinine	Creatinine	HMDB0000562	588	C00791	CN1CC(=O)NC1=N
12	Lysine-Glutamine	Lysylglutamine	HMDB0028949	196305	G00440	NCCCC[C@H](N)C(=O)N[CO]
13	Malate	Malic acid	HMDB0000156	222656	C00149	O[C@@H](CC(O)=O)C(O)=O
14	Guanidinoacetate	Guanidoacetic acid	HMDB0000128	763	C00581	NC(=N)NCC(O)=O
15	AMP	Adenosine monophosphate	HMDB0000045	6083	C00020	NC1=C2N=CN([C@@H]3O[C]
16	Uric acid	Uric acid	HMDB0000289	1175	C00366	O=C1NC2=C(N1)C(=O)NC(
17	Serine	Serine	HMDB0000187	5951	C00065	N[C@@H](CO)C(O)=O
18	Arginine-Valine	Arginylvaline	HMDB0028722	6992654	a	CC(C)[C@H](NC(=O)[C@@H]
19	Hypotaurine	Hypotaurine	HMDB0000965	107812	C00519	NCCS(O) = O
20	Asparagine	L-Asparagine	HMDB0000168	6267	C00152	N[C@@H](CC(N)=O)C(O)=0
21	Guanine	Guanine	HMDB0000132	764	C00242	NC1=NC(=O)C2=C(N1)N=0
22	Phenethylamine	Phenylethylamine	HMDB0012275	1001	C05332	NCCC1=CC=CC=C1
23	Cyclic AMP	Cyclic AMP	HMDB0000058	6076	C00575	[H][C@@]12COP(O)(=O)O[C
24	Thiamine	Thiamine	HMDB0000235	1130	C00378	CC1=C(CCO)SC=[N+]1CC1
25	Histidine	Histidine	HMDB0000177	6274	C00135	N[C@@H](CC1=CN=CN1)C(
$\frac{26}{27}$	Hypoxanthine	Hypoxanthine	HMDB0000157 HMDB0059655	790 43	C00262 $C02630$	OC1=NC=NC2=C1NC=N2
28	2-Hydroxyglutarate Glutamine	2-Hydroxyglutarate Glutamine	HMDB0009635	45 5961	C02030 C00064	OC(CCC(O)=O)C(O)=O N[C@@H](CCC(N)=O)C(O)=O
$\frac{26}{29}$	Nicotinamide riboside	Nicotinamide riboside	HMDB0000855	439924	C00004 C03150	NC(=O)C1=C[N+](=CC=C1
30	N-acetyl-L-ornithine	N2-Acetylornithine	HMDB0000833	439232	C03130 C00437	CC(=0)C1=C[N+](=CC=C1) CC(=0)N[C@@H](CCCN)C(0)
31	NADH	NADH	HMDB0003337	439153	C00437	NC(=O)C1=CN(C=CC1)[C@
32	Cellobiose	Cellobiose	HMDB00001487	10712	C00004 C00185	OC[C@H]10[C@@H](O[C@H]
33	Norvaline	Norvaline	HMDB0000000	439575	C01799	CCC[C@@H](N)C(O)=O
34	Indole	Indole	HMDB000737	798	C00463	N1C=CC2=C1C=CC=C2
35	Orotate	Orotic acid	HMDB0000226	967	C00295	OC(=O)C1=CC(=O)NC(=O
36	Phosphocholine	Phosphorylcholine	HMDB0001565	1014	C00588	C[N+](C)(C)CCOP(O)(O)=0
37	Nicotinate	Nicotinic acid	HMDB0001488	938	C00253	OC(=O)C1=CN=CC=C1
38	Fructose	D-Fructose	HMDB0000660	439709	C00095	OC[C@H]10[C@](O)(CO)[C@
39	5-Methylthioadenosine	5'-Methylthioadenosine	HMDB0001173	439176	C00170	CSĊ[C@Ĥ]1Ò[C@Ĥ](ÌC@Ĥ](C
40	UMP	Uridine 5'-monophosphate	HMDB0000288	6030	C00105	O[C@H]1[C@@H](O)[C@@H](
41	Uridine	Uridine	HMDB0000296	6029	C00299	ос[с@н]10[с@н]([с@н](о́)
42	Ornithine	Ornithine	HMDB0000214	6262	C00077	NCCC[C@H](N)C(O)=O
43	Glucuronic acid	D-Glucuronic acid	HMDB0000127	444791	C00191	O[C@H]1O[C@@H]([C@@H](
44	Cytosine	Cytosine	HMDB0000630	597	C00380	NC1=CC=NC(=O)N1
45	L-Palmitoy lcarnitine	L-Palmitoylcarnitine	${\rm HMDB0240774}$	16902		[H][C@](CC([O-])=O)(C[N+])
$^{46}$	ADP-D-Glucose	ADP-glucose	HMDB0006557	16500	C00498	NC1=C2N=CN([C@@H]3O[C
$^{47}$	Carnitine	L-Carnitine	${\rm HMDB0000062}$	10917	C00487	C[N+](C)(C)C[C@H](O)CC(C
48	Montiporic Acid C	NA	NA	NA	NA	NA
$^{49}$	Montiporic Acid D	NA	NA	NA	NA	NA
50	Nicotinamide ribotide	Nicotinamide ribotide	${ m HMDB0000229}$	14181	C00455	NC(=O)C1=C[N+](=CC=C1
51	Montiporic Acid A	NA	NA	NA	NΑ	NA
52	Montiporic Acid B	NA	NA	NA	NΑ	NA
53	Tryptophan	L-Tryptophan	HMDB0000929	6305	C00078	N[C@@H](CC1=CNC2=C1C)
54	a-ketoglutarate	Oxoglutaric acid	HMDB0000208	51	C00026	OC(=O)CCC(=O)C(O)=O
55	Dihydroxyacetone phosphate	Dihydroxyacetone phosphate	HMDB0001473	668	C00111	OCC(=O)COP(O)(O)=O
56	N-octanoylglycine	Capry loylgly cine	HMDB0000832	84290	G00	CCCCCCC(=0)NCC(0)=0
57	Porphobilinogen	Porphobilinogen	HMDB0000245	1021	C00931	NCC1=C(CC(O)=O)C(CCC(O)=O)
58	GMP	Guanosine monophosphate	HMDB0001397	6804	C00144	NC1=NC2=C(N=CN2[C@@F

59	Citrate	Citric acid	${ m HMDB0000094}$	311	C00158	OC(=O)CC(O)(CC(O)=O)C
60	ADP	ADP	HMDB0001341	6022	C00008	NC1=NC=NC2=C1N=CN2
61	Thymidine	Thymidine	${ m HMDB0000273}$	5789	C00214	CC1=CN([C@H]2C[C@H](O)
62	1-Methylimidazole acetic acid	Methylimidazoleacetic acid	${ m HMDB0002820}$	75810	C05828	CN1C=NC(CC(O)=O)=C1
63	ADP-ribose	Adenosine diphosphate ribose	${ m HMDB0001178}$	192	C00301	NC1=C2N=CN(C3OC(COP(
64	Carbamoyl phosphate	Carbamoyl phosphate	$_{ m HMDB0001096}$	278	C00169	NC(=O)OP(O)(O)=O
65	Cresol	p-Cresol	${ m HMDB0001858}$	2879	C01468	CC1=CC=C(O)C=C1
66	Itaconic acid	Itaconic acid	${ m HMDB0002092}$	811	C00490	OC(=O)CC(=C)C(O)=O
67	Phenylalanine	Phenylalanine	${ m HMDB0000159}$	6140	C00079	N[C@@H](CC1=CC=CC=C1
68	Isoleucine	Isoleucine	${ m HMDB0000172}$	6306	C00407	CC[C@H](C)[C@H](N)C(O)=
69	4-Aminobutyrate	gamma-Aminobutyric acid	HMDB0000112	119	C00334	NCCCC(O) = O
70	Pterin	Pterin	${ m HMDB0000802}$	73000	C00715	NC1=NC2=NC=CN=C2C(=
71	Hippuric acid	Hippuric acid	${ m HMDB0000714}$	464	C01586	OC(=O)CNC(=O)C1=CC=O
72	GTP	Guanosine triphosphate	${ m HMDB0001273}$	6830	C00044	NC1=NC2=C(N=CN2[C@@I
73	ATP	Adenosine triphosphate	${ m HMDB0000538}$	5957	C00002	NC1=NC=NC2=C1N=CN2[
74	Glutamate	Glutamic acid	${ m HMDB0000148}$	33032	C00025	N[C@@H](CCC(O)=O)C(O)
75	Glucose-6-phosphate	Glucose 6-phosphate	${ m HMDB0001401}$	5958	C00092	OC1O[C@H](COP(O)(O)=O
76	Methionine	Methionine	${ m HMDB0000696}$	6137	C00073	CSCC[C@H](N)C(O)=O
77	Coenzyme A	Coenzyme A	${ m HMDB0001423}$	87642	C00010	CC(C)(COP(O)(=O)OP(O)(
78	Succinate	Succinic acid	${ m HMDB0000254}$	1110	C00042	OC(=O)CCC(O)=O
79	Lumichrome	NA	NA	NA	NA	NA

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.

## 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 99 entries);
- Disease associated metabolite sets (reported in blood) (currently contains 344 entries);
- Disease associated metabolite sets (reported in urine) (currently contains 384 entries)
- Disease associated metabolite sets (reported in CSF) (currently contains 166 entries)
- Metabolite sets associated with SNPs (currently contains 4598 entries)
- Predicted metabolite sets based on computational enzyme knockout model (currently contains 912 entries)
- Metabolite sets based on locations (currently contains 73 entries)
- Drug pathway associated metabolite sets (currently contains 461 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

Over Representation Analysis (ORA) is performed when a list of compound names is provided. The list of compound list can be obtained through conventional feature selection methods, or from a clustering algorithm, or from the compounds with abnormal concentrations detected in SSP, to investigate if some biologically meaningful patterns can be identified.

ORA was implemented using the *hypergeometric test* to evaluate whether a particular metabolite set is represented more than expected by chance within the given compound list. One-tailed p values are provided after adjusting for multiple testing. **Figure 2** below summarizes the result.

#### **Enrichment Overview (top 25)**

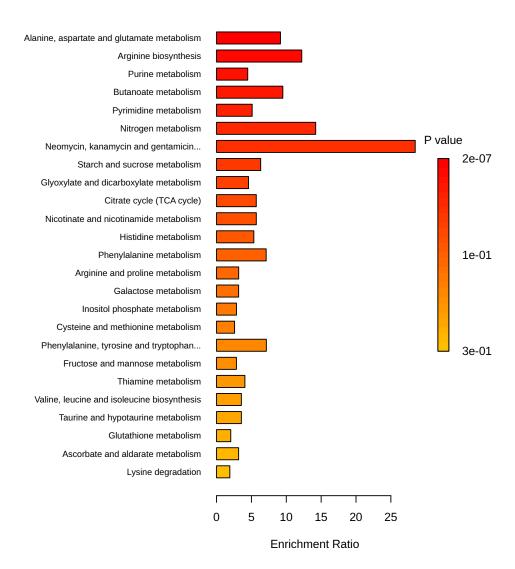


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Alanine, aspartate and glutamate metabolism	28	0.98	9	1.69E-07	1.35E-05	1.35E-05
Arginine biosynthesis	14	0.49	6	3.41E-06	2.70E-04	1.37E-04
Purine metabolism	70	2.46	11	1.57E-05	1.22E-03	4.18E-04
Butanoate metabolism	15	0.53	5	1.01E-04	7.81E-03	2.03E-03
Pyrimidine metabolism	39	1.37	7	2.84E-04	2.16E-02	4.55E-03
Nitrogen metabolism	6	0.21	3	7.59E-04	5.69E-02	1.01E-02
Neomycin, kanamycin and gentamicin		0.07	2	1.21E-03	8.95E-02	1.38E-02
biosynthesis	_		_			
Starch and sucrose metabolism	18	0.63	4	2.88E-03	2.10E-01	2.88E-02
Glyoxylate and dicarboxylate metabolism	31	1.09	5	3.74E-03	2.69E-01	3.32E-02
Citrate cycle (TCA cycle)	20	0.70	4	4.32E-03	3.07E-01	3.46E-02
Nicotinate and nicotinamide metabolism	15	0.53	3	1.38E-02	9.65E-01	1.00E-01
Histidine metabolism	16	0.56	3	1.65E-02	1.00E+00	1.10E-01
Phenylalanine metabolism	8	0.28	2	2.95E-02	1.00E+00	1.82E-01
Arginine and proline metabolism	36	1.26	4	3.47E-02	1.00E + 00	1.98E-01
Galactose metabolism	27	0.95	3	6.59E-02	1.00E+00	3.52E-01
Inositol phosphate metabolism	30	1.05	3	8.51E-02	1.00E+00	4.25E-01
Cysteine and methionine metabolism	33	1.16	3	1.06E-01	1.00E+00	5.00E-01
Phenylalanine, tyrosine and tryptophan biosynthesis	4	0.14	1	1.33E-01	1.00E+00	5.92E-01
Fructose and mannose metabolism	20	0.70	2	1.54E-01	1.00E+00	6.47E-01
Thiamine metabolism	7	0.70	1	2.22E-01	1.00E+00 1.00E+00	8.86E-01
Valine, leucine and isoleucine biosynthe-	8	0.28	1	2.49E-01	1.00E+00 1.00E+00	8.95E-01
sis	0	0.26	1	2.4915-01	1.001	0.9515-01
Taurine and hypotaurine metabolism	8	0.28	1	2.49E-01	1.00E+00	8.95E-01
Glutathione metabolism	28	0.98	2	2.57E-01	1.00E+00	8.95E-01
Ascorbate and aldarate metabolism	9	0.32	1	2.76E-01	1.00E+00	9.09E-01
Lysine degradation	30	1.05	2	2.84E-01	1.00E+00	9.09E-01
Porphyrin metabolism	31	1.09	2	2.97E-01	1.00E+00	9.14E-01
Glycine, serine and threonine metabolism	33	1.16	2	3.24E-01	1.00E+00	9.59E-01
Glycerophospholipid metabolism	36	1.26	2	3.63E-01	1.00E+00	1.00E+00
D-Amino acid metabolism	15	0.53	1	4.16E-01	1.00E+00	1.00E+00
Glycerolipid metabolism	16	0.56	1	4.37E-01	1.00E+00	1.00E+00
Pentose and glucuronate interconversions	19	0.67	1	4.95E-01	1.00E+00	1.00E+00
Pantothenate and CoA biosynthesis	20	0.70	1	5.13E-01	1.00E+00	1.00E+00
beta- Alanine metabolism	21	0.74	1	5.30E-01	1.00E+00	1.00E+00
Propanoate metabolism	21	0.74	1	5.30E-01	1.00E+00	1.00E+00
Pyruvate metabolism	23	0.81	1	5.63E-01	1.00E+00	1.00E+00
Glycolysis / Gluconeogenesis	26	0.91	1	6.08E-01	1.00E+00	1.00E+00
Folate biosynthesis	26	0.91	1	6.08E-01	1.00E+00	1.00E+00
Lipoic acid metabolism	28	0.98	1	6.35E-01	1.00E+00	1.00E+00
Sphingolipid metabolism	32	1.12	1	6.85E-01	1.00E+00	1.00E+00
Fatty acid degradation	39	1.37	1	7.56E-01	1.00E+00	1.00E+00
Valine, leucine and isoleucine degrada-	39	1.37	1	7.56E-01	1.00E+00	1.00E+00
tion	""	1.5.	*		1.552,55	1.552,0
Tryptophan metabolism	41	1.44	1	7.73E-01	1.00E+00	1.00E+00
Amino sugar and nucleotide sugar	42	1.47	1	7.81E-01	1.00E+00	1.00E+00
metabolism			-			

### 7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"msetora\", FALSE)"
 [2] "cmpd.vec<-c(\"0-Butanoylcarnitine\",\"Glutaryl-carnitine\",\"Arginine-Glutamine\",\"Deoxycarn
 [3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
 [4] "mSet<-CrossReferencing(mSet, \"name\");"</pre>
 [5] "mSet<-CreateMappingResultTable(mSet)"
 [6] "mSet<-PerformDetailMatch(mSet, \"Glutaryl-carnitine\");"</pre>
 [7] "mSet<-GetCandidateList(mSet);"</pre>
 [8] "mSet<-SetCandidate(mSet, \"Glutaryl-carnitine\", \"Glutarylcarnitine\");"
 [9] "mSet<-PerformDetailMatch(mSet, \"Arginine-Glutamine\");"
[10] "mSet<-GetCandidateList(mSet);"</pre>
[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\");"</pre>
[16] "mSet<-GetCandidateList(mSet);"</pre>
[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, \"1-Methylimidazole acetic acid\");"
[22] "mSet<-GetCandidateList(mSet);"</pre>
[23] "mSet<-SetCandidate(mSet, \"1-Methylimidazole acetic acid\", \"Methylimidazoleacetic acid\");"
[24] "mSet<-PerformDetailMatch(mSet, \"Cresol\");"
[25] "mSet<-GetCandidateList(mSet);"</pre>
[26] "mSet<-SetCandidate(mSet, \"Cresol\", \"p-Cresol\");"</pre>
[27] "mSet<-PerformDetailMatch(mSet, \"Lumichrome\");"
[28] "mSet<-GetCandidateList(mSet);"</pre>
[29] "mSet<-SetMetabolomeFilter(mSet, F);"</pre>
[30] "mSet<-SetCurrentMsetLib(mSet, \"kegg_pathway\", 2);"
[31] "mSet<-CalculateHyperScore(mSet)"
[32] "mSet<-PlotORA(mSet, \"ora_0_\", \"net\", \"png\", 72, width=NA)"
[33] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_0_\", \"png\", 72, width=NA)"
[34] "mSet<-CalculateHyperScore(mSet)"
[35] "mSet<-PlotORA(mSet, \"ora_1_\", \"net\", \"png\", 72, width=NA)"
[36] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_1_\", \"png\", 72, width=NA)"
[37] "mSet<-CalculateHyperScore(mSet)"
[38] "mSet<-PlotORA(mSet, \"ora_2_\", \"net\", \"png\", 72, width=NA)"
[39] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_2_\", \"png\", 72, width=NA)"
[40] "mSet<-CalculateHyperScore(mSet)"
[41] "mSet<-PlotORA(mSet, \"ora_3_\", \"net\", \"png\", 72, width=NA)"
[42] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_3_\", \"png\", 72, width=NA)"
[43] "mSet<-CalculateHyperScore(mSet)"
[44] "mSet<-PlotORA(mSet, \"ora_4_\", \"net\", \"png\", 72, width=NA)"
[45] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_4_\", \"png\", 72, width=NA)"
[46] "mSet<-CalculateHyperScore(mSet)"
[47] "mSet<-PlotORA(mSet, \"ora_5_\", \"net\", \"png\", 72, width=NA)"
[48] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_5_\", \"png\", 72, width=NA)"
[49] "mSet<-CalculateHyperScore(mSet)"
[50] "mSet<-PlotORA(mSet, \"ora_6_\", \"net\", \"png\", 72, width=NA)"
[51] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_6_\", \"png\", 72, width=NA)"
[52] "mSet<-CalculateHyperScore(mSet)"</pre>
[53] "mSet<-PlotORA(mSet, \"ora_7_\", \"net\", \"png\", 72, width=NA)"
[54] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_7_\", \"png\", 72, width=NA)"
[55] "mSet<-CalculateHyperScore(mSet)"
[56] "mSet<-PlotORA(mSet, \"ora_8_\", \"net\", \"png\", 72, width=NA)"
```

```
[57] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_8_\", \"png\", 72, width=NA)"
[58] "mSet<-CalculateHyperScore(mSet)"
[59] "mSet<-PlotORA(mSet, \"ora_9_\", \"net\", \"png\", 72, width=NA)"
[60] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_9_\", \"png\", 72, width=NA)"
[61] "mSet<-CalculateHyperScore(mSet)"
[62] "mSet<-PlotORA(mSet, \"ora_10_\", \"net\", \"png\", 72, width=NA)"
[63] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_10_\", \"png\", 72, width=NA)"
[64] "mSet<-CalculateHyperScore(mSet)"
[65] "mSet<-PlotORA(mSet, \"ora_11_\", \"net\", \"png\", 72, width=NA)"
[66] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_11_\", \"png\", 72, width=NA)"
[67] "mSet<-CalculateHyperScore(mSet)"
[68] "mSet<-PlotORA(mSet, \"ora_12_\", \"net\", \"png\", 72, width=NA)"
[69] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_12_\", \"png\", 72, width=NA)"
[70] "mSet<-CalculateHyperScore(mSet)"
[71] "mSet<-PlotORA(mSet, \"ora_13_\", \"net\", \"png\", 72, width=NA)"
[72] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_13_\", \"png\", 72, width=NA)"
[73] "mSet<-CalculateHyperScore(mSet)"
[74] "mSet<-PlotORA(mSet, \"ora_14_\", \"net\", \"png\", 72, width=NA)"
[75] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_14_\", \"png\", 72, width=NA)"
[76] "mSet<-CalculateHyperScore(mSet)"
[77] "mSet<-PlotORA(mSet, \"ora_15_\", \"net\", \"png\", 72, width=NA)"
[78] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_15_\", \"png\", 72, width=NA)"
[79] "mSet<-CalculateHyperScore(mSet)"
[80] "mSet<-PlotORA(mSet, \"ora_16_\\", \"net\", \"png\", 72, width=NA)"
[81] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_16_\", \"png\", 72, width=NA)"
[82] "mSet<-CalculateHyperScore(mSet)"
[83] "mSet<-PlotORA(mSet, \"ora_17_\", \"net\", \"png\", 72, width=NA)"
[84] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_17_\", \"png\", 72, width=NA)"
[85] "mSet<-CalculateHyperScore(mSet)"
[86] "mSet<-PlotORA(mSet, \"ora_18_\", \"net\", \"png\", 72, width=NA)"
[87] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_18_\", \"png\", 72, width=NA)"
[88] "mSet<-CalculateHyperScore(mSet)"
[89] "mSet<-PlotORA(mSet, \"ora_19_\", \"net\", \"png\", 72, width=NA)"
[90] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_19_\", \"png\", 72, width=NA)"
[91] "mSet<-CalculateHyperScore(mSet)"
[92] "mSet<-PlotORA(mSet, \"ora_20_\", \"net\", \"png\", 72, width=NA)"
[93] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_20_\", \"png\", 72, width=NA)"
[94] "mSet<-CalculateHyperScore(mSet)"
[95] "mSet<-Plot0RA(mSet, \"ora_21_\", \"net\", \"png\", 72, width=NA)"
[96] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_21_\", \"png\", 72, width=NA)"
[97] "mSet<-CalculateHyperScore(mSet)"
[98] "mSet<-PlotORA(mSet, \"ora_22_\", \"net\", \"png\", 72, width=NA)"
[99] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_22_\", \"png\", 72, width=NA)"
[100] "mSet<-SaveTransformedData(mSet)"
```

[101] "mSet<-PreparePDFReport(mSet, \"guest17754256662783239768\")\n"

The report was generated on Tue Jun 18  $18:44:19\ 2024$  with R version  $4.3.2\ (2023-10-31)$ , OS system: Linux.