

Metabolomic Data Analysis with MetaboAnalyst 5.0

Name: guest18019451723783111663

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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.^{1, 2}

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)*);

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

²Nam 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 Co

	Query	Match	HMDB	PubChem	KEGG	S
1	HMDB0000123	Glycine	HMDB0000123	750	C00037	C
2	HMDB0014691	Acetohydroxamic Acid	HMDB0014691	1990	C06808	C
3	HMDB0031239	Ethyl nitrite	HMDB0031239	8026		C
4	HMDB0161401	NA	NA	NA	NA	N
5	HMDB0001858	p-Cresol	HMDB0001858	2879	C01468	C
6	HMDB0033895	Anisole	HMDB0033895	7519	C01403	C
7	HMDB0003119	Benzyl alcohol	HMDB0003119	244	C03485	C
8	HMDB0002055	o-Cresol	HMDB0002055	335	C01542	C
9	HMDB0002048	m-Cresol	HMDB0002048	342	C01467	C
10	HMDB0003431	L-Histidinol	HMDB0003431	165271	C00860	C
11	HMDB0124942	NA	NA	NA	NA	N
12	HMDB0167829	NA	NA	NA	NA	N
13	HMDB0062810	NA	NA	NA	NA	N
14	HMDB0125535	NA	NA	NA	NA	N
15	HMDB0183895	NA	NA	NA	NA	N
16	HMDB0126385	NA	NA	NA	NA	N
17	HMDB0031459	3-Methoxybenzaldehyde	HMDB0031459	11569		C
18	HMDB0002340	2-Methylbenzoic acid	HMDB0002340	0	C07215	C
19	HMDB0041485	NA	NA	NA	NA	N
20	HMDB0033968	Methyl benzoate	HMDB0033968	7150		C
21	HMDB0032400	3-(5-Methyl-2-furyl)prop-2-enal	HMDB0032400	11434978		C
22	HMDB0032603	2-Hydroxy-4-methylbenzaldehyde	HMDB0032603	61200		C
23	HMDB0029686	4-Methoxybenzaldehyde	HMDB0029686	31244	C10761	C
24	HMDB0040733	Phenyl acetate	HMDB0040733	31229	C15583	C
25	HMDB0032568	2'-Hydroxyacetophenone	HMDB0032568	9398	C07189	C
26	HMDB0167830	NA	NA	NA	NA	N
27	HMDB0038176	NA	NA	NA	NA	N
28	HMDB0040638	NA	NA	NA	NA	N
29	HMDB0029635	4-Methylbenzoic acid	HMDB0029635	7470	C01454	C
30	HMDB0033128	4-(2-Furanyl)-3-buten-2-one	HMDB0033128	1549522		C
31	HMDB0003767	4-Hydroxyphenylacetaldehyde	HMDB0003767	440113	C03765	C
32	HMDB0033766	2-Methoxybenzaldehyde	HMDB0033766	8658		C
33	HMDB0000209	Phenylacetic acid	HMDB0000209	999	C07086	C
34	HMDB0126617	NA	NA	NA	NA	N
35	HMDB0169080	NA	NA	NA	NA	N
36	HMDB0059966	NA	NA	NA	NA	N
37	HMDB0131479	NA	NA	NA	NA	N
38	HMDB0135785	NA	NA	NA	NA	N
39	HMDB0146894	NA	NA	NA	NA	N
40	HMDB0146874	NA	NA	NA	NA	N
41	HMDB0131231	NA	NA	NA	NA	N
42	HMDB0131232	NA	NA	NA	NA	N
43	HMDB0125534	NA	NA	NA	NA	N
44	HMDB0037724	NA	NA	NA	NA	N
45	HMDB0005784	Hydroxytyrosol	HMDB0005784	82755		C
46	HMDB0030570	Sylvopinol	HMDB0030570	592986		C
47	HMDB0032012	4-Hydroxy-3-methoxybenzenemethanol	HMDB0032012	62348	C06317	C
48	HMDB0037728	NA	NA	NA	NA	N
49	HMDB0034158	2,6-Dimethoxyphenol	HMDB0034158	7041	C10787	C
50	HMDB0163703	NA	NA	NA	NA	N
51	HMDB0165581	NA	NA	NA	NA	N
52	HMDB0165584	NA	NA	NA	NA	N
53	HMDB0165583	NA	NA	NA	NA	N
54	HMDB0165582	NA	NA	NA	NA	N
55	HMDB0031501	3-Hexenoic acid	HMDB0031501	5355152		C
56	HMDB0163702	NA	NA	NA	NA	N
57	HMDB0163353	NA	NA	NA	NA	N
58	HMDB0163352	NA	NA	NA	NA	N
59	HMDB0031559	4-Methyl-2,3-pentanedione	HMDB0031559	24115		C

60	HMDB0031491	2,3-Hexanedione	HMDB0031491	19707			
61	HMDB0031560	2-Methyl-2-pentenoic acid	HMDB0031560	6436344			
62	HMDB0163350	NA	NA	NA	NA		
63	HMDB0163351	NA	NA	NA	NA		
64	HMDB0163354	NA	NA	NA	NA		
65	HMDB0169664	NA	NA	NA	NA		
66	HMDB0169695	NA	NA	NA	NA		
67	HMDB0033568	5-Oxohexanal	HMDB0033568	10953466			
68	HMDB0040328	NA	NA	NA	NA		
69	HMDB0031492	3,4-Hexanedione	HMDB0031492	62539			
70	HMDB0031561	4-Methyl-2-pentenoic acid	HMDB0031561	12216200			
71	HMDB0010719	trans-Hex-2-enoic acid	HMDB0010719	5282707			
72	HMDB0003843	Gamma-Caprolactone	HMDB0003843	12756			
73	HMDB0000453	Delta-Hexanolactone	HMDB0000453	13204			
74	HMDB0029487	Allyl propionate	HMDB0029487	61319			
75	HMDB0179342	NA	NA	NA	NA		
76	HMDB0179343	NA	NA	NA	NA		
77	HMDB0179341	NA	NA	NA	NA		
78	HMDB0179344	NA	NA	NA	NA		
79	HMDB0179345	NA	NA	NA	NA		
80	HMDB0179346	NA	NA	NA	NA		
81	HMDB0179351	NA	NA	NA	NA		
82	HMDB0031562	2-Methyl-3-pentenoic acid	HMDB0031562	71587183			
83	HMDB0031158	2-Methyl-4-pentenoic acid	HMDB0031158	549519			
84	HMDB0039581	NA	NA	NA	NA		
85	HMDB0032490	Prenyl formate	HMDB0032490	110373			
86	HMDB0060476	epsilon-Caprolactone	HMDB0060476	10401	C01880		
87	HMDB0240384	NA	NA	NA	NA		
88	HMDB0061929	NA	NA	NA	NA		
89	HMDB0061965	NA	NA	NA	NA		
90	HMDB0062135	NA	NA	NA	NA		
91	HMDB0162021	NA	NA	NA	NA		
92	HMDB0040972	NA	NA	NA	NA		
93	HMDB0038628	NA	NA	NA	NA		
94	HMDB0004073	5-Hydroxyindoleacetaldehyde	HMDB0004073	74688	C05634		
95	HMDB0000197	Indoleacetic acid	HMDB0000197	802	C00954		
96	HMDB0166095	NA	NA	NA	NA		
97	HMDB0060758	NA	NA	NA	NA		
98	HMDB0240317	NA	NA	NA	NA		
99	HMDB0162022	NA	NA	NA	NA		
100	HMDB0162020	NA	NA	NA	NA		
101	HMDB0162023	NA	NA	NA	NA		
102	HMDB0013292	p-Methylhippuric acid	HMDB0013292	97479			
103	HMDB0000821	Phenylacetyl glycine	HMDB0000821	68144	C05598		
104	HMDB0000859	Methyl hippurate	HMDB0000859	14566			
105	HMDB0011723	2-Methylhippuric acid	HMDB0011723	91637	C01586		
106	HMDB0060366	3-Carbamoyl-2-phenylpropionaldehyde	HMDB0060366	0	C16587		
107	HMDB0060389	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	HMDB0060389	0	C16595		
108	HMDB0034250	Betamipron	HMDB0034250	71651			
109	HMDB0032388	Methyl n-acetylanthranilate	HMDB0032388	17623	C06332		
110	HMDB0013245	m-Methylhippuric acid	HMDB0013245	99223			
111	HMDB0012309	Vanillylamine	HMDB0012309	70966	C16666		
112	HMDB0004825	p-Octopamine	HMDB0004825	440266	C04227		
113	HMDB0156498	NA	NA	NA	NA		
114	HMDB0000073	Dopamine	HMDB0000073	681	C03758		
115	HMDB0060277	NA	NA	NA	NA		
116	HMDB0037786	NA	NA	NA	NA		
117	HMDB0172919	NA	NA	NA	NA		
118	HMDB0129369	NA	NA	NA	NA		
119	HMDB0135530	NA	NA	NA	NA		
120	HMDB0135531	NA	NA	NA	NA		
121	HMDB0135533	NA	NA	NA	NA		
122	HMDB0128615	NA	NA	NA	NA		
123	HMDB0135532	NA	NA	NA	NA		
124	HMDB0033813	3-(3,4-Methylenedioxyphe nyl)propenal	HMDB0033813	5355018			
125	HMDB0032883	1,4,5-Naphthalenetriol	HMDB0032883	3083585			
126	HMDB0032990	7-Hydroxy-6-methyl-2H-1-benzopyran-2-one	HMDB0032990	5412913			
127	HMDB0163660	NA	NA	NA	NA		
128	HMDB0029758	Herniarin	HMDB0029758	10748	C09268		
129	HMDB0059622	NA	NA	NA	NA		
130	HMDB0031054	10-Hydroxy-2,8-decadiene-4,6-dienoic acid	HMDB0031054	131751124			
131	HMDB0060747	NA	NA	NA	NA		
132	HMDB0001434	3-Methoxytyrosine	HMDB0001434	1670			
133	HMDB0011754	Methyl dopa	HMDB0011754	38853	C07194		
134	HMDB0040003	NA	NA	NA	NA		
135	HMDB0172928	NA	NA	NA	NA		
136	HMDB0172925	NA	NA	NA	NA		
137	HMDB0151309	NA	NA	NA	NA		
138	HMDB0037153	NA	NA	NA	NA		
139	HMDB0151285	NA	NA	NA	NA		
140	HMDB0151284	NA	NA	NA	NA		
141	HMDB0062564	NA	NA	NA	NA		
142	HMDB0163545	NA	NA	NA	NA		
143	HMDB0031437	(-)-Bornesitol	HMDB0031437		C03659		
144	HMDB0029965	Methyl beta-D-glucopyranoside	HMDB0029965	94214			
145	HMDB0031449	Sequoiitol	HMDB0031449	439990	C03365		
146	HMDB0029915	D-4-O-Methyl-myo-inositol	HMDB0029915		C06353		

147	HMDB0029916	4-O-Methyl-myo-inositol	HMDB0029916	164619	C06353	C
148	HMDB0033816	Mytilitol	HMDB0033816			C
149	HMDB0034219	D-Pinitol	HMDB0034219	0	C03844	C
150	HMDB0034222	L-Pinitol	HMDB0034222	164619	C03844	C
151	HMDB0034221	L-Quebrachitol	HMDB0034221	0	C08257	C
152	HMDB0033750	D-Glycero-D-galacto-heptitol	HMDB0033750	441436	C08255	C
153	HMDB0037295	NA	NA	NA	NA	N
154	HMDB0014962	Enprofylline	HMDB0014962	1676		C
155	HMDB0001847	Caffeine	HMDB0001847	2519	C07481	C
156	HMDB0039467	NA	NA	NA	NA	N
157	HMDB0031699	S-(3-Methyl-2-butenyl) 2-methylpropanethioate	HMDB0031699	71438214		C
158	HMDB0033843	Polyvidone	HMDB0033843	131751496		P
159	HMDB0028843	Glycyl-Histidine	HMDB0028843	7023107		N
160	HMDB0028885	Histidiny-Glycine	HMDB0028885	351662		C
161	HMDB0014814	Benzyl Benzoate	HMDB0014814	2345	C12537	C
162	HMDB0032039	Benzoin	HMDB0032039	8400	C01408	C
163	HMDB0059660	NA	NA	NA	NA	N
164	HMDB0000114	Glycerylphosphorylethanolamine	HMDB0000114	22833510	C01233	C
165	HMDB0033349	Casimiroin	HMDB0033349	124075	C10654	C
166	HMDB0013859	2-Dechloroethylifosfamide	HMDB0013859	0	C16555	N
167	HMDB0013858	3-Dechloroethylifosfamide	HMDB0013858	114861	C16550	C
168	HMDB0060881	NA	NA	NA	NA	N
169	HMDB0028776	Cysteinyl-Hydroxyproline	HMDB0028776	131750737		O
170	HMDB0028860	Hydroxypropyl-Cysteine	HMDB0028860	131750765		N
171	HMDB0032660	(2Z,4'Z)-2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene	HMDB0032660	14540699		C
172	HMDB0004821	Bisnorbiotin	HMDB0004821	86492	C20384	C
173	HMDB0060618	NA	NA	NA	NA	N
174	HMDB0059798	NA	NA	NA	NA	N
175	HMDB0059799	NA	NA	NA	NA	N
176	HMDB0059800	NA	NA	NA	NA	N
177	HMDB0059797	NA	NA	NA	NA	N
178	HMDB0059801	NA	NA	NA	NA	N
179	HMDB0181581	NA	NA	NA	NA	N
180	HMDB0028797	Glutaminyglycine	HMDB0028797	6992691		C
181	HMDB0028682	Alanyl-Asparagine	HMDB0028682	259612		C
182	HMDB0028724	Asparaginy-Alanine	HMDB0028724	9942455		C
183	HMDB0028855	Glycyl-Gamma-glutamate	HMDB0028855	87557032		N
184	HMDB0028839	Glycyl-Glutamine	HMDB0028839	597739		N
185	HMDB0033191	2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	HMDB0033191	100958560		C
186	HMDB0150426	NA	NA	NA	NA	N
187	HMDB0034046	1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene	HMDB0034046	617233		C
188	HMDB0037492	NA	NA	NA	NA	N
189	HMDB0040424	NA	NA	NA	NA	N
190	HMDB0061823	NA	NA	NA	NA	N
191	HMDB0061942	NA	NA	NA	NA	N
192	HMDB0032589	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	HMDB0032589	13308867		C
193	HMDB0132937	NA	NA	NA	NA	N
194	HMDB0132935	NA	NA	NA	NA	N
195	HMDB0132936	NA	NA	NA	NA	N
196	HMDB0132939	NA	NA	NA	NA	N
197	HMDB0132948	NA	NA	NA	NA	N
198	HMDB0151796	NA	NA	NA	NA	N
199	HMDB0151797	NA	NA	NA	NA	N
200	HMDB0151800	NA	NA	NA	NA	N
201	HMDB0151798	NA	NA	NA	NA	N
202	HMDB0151799	NA	NA	NA	NA	N
203	HMDB0151801	NA	NA	NA	NA	N
204	HMDB0132933	NA	NA	NA	NA	N
205	HMDB0151802	NA	NA	NA	NA	N
206	HMDB0001319	Pyridoxine 5'-phosphate	HMDB0001319	1055	C00627	C
207	HMDB0000210	Pantothenic acid	HMDB0000210	6613	C00864	C
208	HMDB0062717	NA	NA	NA	NA	N
209	HMDB0040349	NA	NA	NA	NA	N
210	HMDB0012204	Cis-zeatin	HMDB0012204	449093	C00371	C
211	HMDB0152315	NA	NA	NA	NA	N
212	HMDB0142172	NA	NA	NA	NA	N
213	HMDB0142174	NA	NA	NA	NA	N
214	HMDB0146404	NA	NA	NA	NA	N
215	HMDB0146402	NA	NA	NA	NA	N
216	HMDB0149145	NA	NA	NA	NA	N
217	HMDB0146405	NA	NA	NA	NA	N
218	HMDB0146406	NA	NA	NA	NA	N
219	HMDB0146407	NA	NA	NA	NA	N
220	HMDB0149144	NA	NA	NA	NA	N
221	HMDB0149143	NA	NA	NA	NA	N
222	HMDB0142171	NA	NA	NA	NA	N
223	HMDB0142170	NA	NA	NA	NA	N
224	HMDB0128183	NA	NA	NA	NA	N
225	HMDB0128665	NA	NA	NA	NA	N
226	HMDB0128667	NA	NA	NA	NA	N
227	HMDB0128668	NA	NA	NA	NA	N
228	HMDB0128674	NA	NA	NA	NA	N
229	HMDB0128673	NA	NA	NA	NA	N
230	HMDB0137280	NA	NA	NA	NA	N
231	HMDB0137283	NA	NA	NA	NA	N
232	HMDB0137284	NA	NA	NA	NA	N
233	HMDB0137291	NA	NA	NA	NA	N

234	HMDB0137290	NA	NA	NA	NA
235	HMDB0141325	NA	NA	NA	NA
236	HMDB0142075	NA	NA	NA	NA
237	HMDB0142076	NA	NA	NA	NA
238	HMDB0142169	NA	NA	NA	NA
239	HMDB0179746	NA	NA	NA	NA
240	HMDB0142173	NA	NA	NA	NA
241	HMDB0041691	NA	NA	NA	NA
242	HMDB0030018	Elenolide	HMDB0030018	10013857	C09506
243	HMDB0140920	NA	NA	NA	NA
244	HMDB0032616	Sinapic acid	HMDB0032616	637775	C00482
245	HMDB0034069	cis-Sinapic acid	HMDB0034069	1549091	NA
246	HMDB0127488	NA	NA	NA	NA
247	HMDB0014567	Methocarbamol	HMDB0014567	4107	NA
248	HMDB0040032	NA	NA	NA	NA
249	HMDB0013134	Fumarycarnitine	HMDB0013134	53481630	NA
250	HMDB0032769	Osmaronin	HMDB0032769	14559842	NA
251	HMDB0147191	NA	NA	NA	NA
252	HMDB0131062	NA	NA	NA	NA
253	HMDB0131065	NA	NA	NA	NA
254	HMDB0036050	NA	NA	NA	NA
255	HMDB0033771	Cyperine	HMDB0033771	182142	C09923
256	HMDB0030690	(E)-Suberenol	HMDB0030690	5375166	NA
257	HMDB0039592	NA	NA	NA	NA
258	HMDB0030788	Citrusal	HMDB0030788	5319433	NA
259	HMDB0135759	NA	NA	NA	NA
260	HMDB0135760	NA	NA	NA	NA
261	HMDB0135761	NA	NA	NA	NA
262	HMDB0141827	NA	NA	NA	NA
263	HMDB0151855	NA	NA	NA	NA
264	HMDB0153660	NA	NA	NA	NA
265	HMDB0135757	NA	NA	NA	NA
266	HMDB0135758	NA	NA	NA	NA
267	HMDB0129916	NA	NA	NA	NA
268	HMDB0129917	NA	NA	NA	NA
269	HMDB0129919	NA	NA	NA	NA
270	HMDB0129920	NA	NA	NA	NA
271	HMDB0129922	NA	NA	NA	NA
272	HMDB0131064	NA	NA	NA	NA
273	HMDB0131066	NA	NA	NA	NA
274	HMDB0131067	NA	NA	NA	NA
275	HMDB0132269	NA	NA	NA	NA
276	HMDB0129918	NA	NA	NA	NA
277	HMDB0030854	(S)-Auraptenol	HMDB0030854	13343540	NA
278	HMDB0030110	Celerin	HMDB0030110	156431	NA
279	HMDB0030948	Dihydrowyerone	HMDB0030948	131751105	NA
280	HMDB0039142	NA	NA	NA	NA
281	HMDB0041192	NA	NA	NA	NA
282	HMDB0034133	3-(1,1-Dimethylallyl)scopoletin	HMDB0034133	5377569	NA
283	HMDB0030853	(R)-Meranzin	HMDB0030853	3819217	NA
284	HMDB0033015	5,6-Dihydroyangonin	HMDB0033015	11623055	NA
285	HMDB0035254	7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone	HMDB0035254	86205980	NA
286	HMDB0033016	7,8-Dihydroyangonin	HMDB0033016	9992755	NA
287	HMDB0030578	Apigravin	HMDB0030578	85982833	NA
288	HMDB0032953	7-Methoxy-5-prenyloxy coumarin	HMDB0032953	15108314	NA
289	HMDB0061290	NA	NA	NA	NA
290	HMDB0061303	NA	NA	NA	NA
291	HMDB0039146	NA	NA	NA	NA
292	HMDB0037679	NA	NA	NA	NA
293	HMDB0035019	Phenethyl salicylate	HMDB0035019	62332	NA
294	HMDB0029302	1-Phenyl-6,7-dihydroxy-isochroman	HMDB0029302	131750844	NA
295	HMDB0036347	NA	NA	NA	NA
296	HMDB0002209	Equol	HMDB0002209	91469	C14131
297	HMDB0130495	NA	NA	NA	NA
298	HMDB0014713	Fenoprofen	HMDB0014713	3342	C06997
299	HMDB0135409	NA	NA	NA	NA
300	HMDB0135406	NA	NA	NA	NA
301	HMDB0135408	NA	NA	NA	NA
302	HMDB0135407	NA	NA	NA	NA
303	HMDB0135593	NA	NA	NA	NA
304	HMDB0135594	NA	NA	NA	NA
305	HMDB0135405	NA	NA	NA	NA
306	HMDB0130496	NA	NA	NA	NA
307	HMDB0135355	NA	NA	NA	NA
308	HMDB0135397	NA	NA	NA	NA
309	HMDB0135595	NA	NA	NA	NA
310	HMDB0151857	NA	NA	NA	NA
311	HMDB0130497	NA	NA	NA	NA
312	HMDB0168444	NA	NA	NA	NA
313	HMDB0135601	NA	NA	NA	NA
314	HMDB0168447	NA	NA	NA	NA
315	HMDB0148520	NA	NA	NA	NA
316	HMDB0168443	NA	NA	NA	NA
317	HMDB0182848	NA	NA	NA	NA
318	HMDB0168445	NA	NA	NA	NA
319	HMDB0168442	NA	NA	NA	NA
320	HMDB0135596	NA	NA	NA	NA

321	HMDB0168446	NA	NA	NA	NA
322	HMDB0029953	D-erythro-D-galacto-octitol	HMDB0029953	219890	NA
323	HMDB0161832	NA	NA	NA	NA
324	HMDB0161833	NA	NA	NA	NA
325	HMDB0161834	NA	NA	NA	NA
326	HMDB0149051	NA	NA	NA	NA
327	HMDB0149050	NA	NA	NA	NA
328	HMDB0149006	NA	NA	NA	NA
329	HMDB0148541	NA	NA	NA	NA
330	HMDB0148540	NA	NA	NA	NA
331	HMDB0148786	NA	NA	NA	NA
332	HMDB0148785	NA	NA	NA	NA
333	HMDB0148998	NA	NA	NA	NA
334	HMDB0149048	NA	NA	NA	NA
335	HMDB0147226	NA	NA	NA	NA
336	HMDB0148542	NA	NA	NA	NA
337	HMDB0128505	NA	NA	NA	NA
338	HMDB0148539	NA	NA	NA	NA
339	HMDB0145646	NA	NA	NA	NA
340	HMDB0145647	NA	NA	NA	NA
341	HMDB0145645	NA	NA	NA	NA
342	HMDB0135172	NA	NA	NA	NA
343	HMDB0149007	NA	NA	NA	NA
344	HMDB0128506	NA	NA	NA	NA
345	HMDB0128503	NA	NA	NA	NA
346	HMDB0128504	NA	NA	NA	NA
347	HMDB0040876	NA	NA	NA	NA
348	HMDB0030946	(2E,11Z)-Wyerone acid	HMDB0030946	131751103	NA
349	HMDB0041016	NA	NA	NA	NA
350	HMDB0030595	Suberenone	HMDB0030595	53218539	NA
351	HMDB0033735	Graveolone	HMDB0033735	177751	NA
352	HMDB0039430	NA	NA	NA	NA
353	HMDB0004215	3,3',4'5-Tetrahydroxystilbene	HMDB0004215	667639	C05901
354	HMDB0170845	NA	NA	NA	NA
355	HMDB0164057	NA	NA	NA	NA
356	HMDB0135900	NA	NA	NA	NA
357	HMDB0135902	NA	NA	NA	NA
358	HMDB0135904	NA	NA	NA	NA
359	HMDB0164055	NA	NA	NA	NA
360	HMDB0164056	NA	NA	NA	NA
361	HMDB0164058	NA	NA	NA	NA
362	HMDB0170846	NA	NA	NA	NA
363	HMDB0170974	NA	NA	NA	NA
364	HMDB0170976	NA	NA	NA	NA
365	HMDB0170979	NA	NA	NA	NA
366	HMDB0170978	NA	NA	NA	NA
367	HMDB0131284	NA	NA	NA	NA
368	HMDB0131285	NA	NA	NA	NA
369	HMDB0127824	NA	NA	NA	NA
370	HMDB0131281	NA	NA	NA	NA
371	HMDB0131283	NA	NA	NA	NA
372	HMDB0170977	NA	NA	NA	NA
373	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	HMDB0031668	76551322	NA
374	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	HMDB0034056	5321853	NA
375	HMDB0037681	NA	NA	NA	NA
376	HMDB0029470	Isodillapiole	HMDB0029470	11435991	NA
377	HMDB0041379	NA	NA	NA	NA
378	HMDB0135906	NA	NA	NA	NA
379	HMDB0038563	NA	NA	NA	NA
380	HMDB0037130	NA	NA	NA	NA
381	HMDB0094660	Diethyl phthalic acid	HMDB0094660	6781	C14175
382	HMDB0033776	Apiole	HMDB0033776	10659	C10429
383	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	HMDB0029226	3028410	NA
384	HMDB0135689	NA	NA	NA	NA
385	HMDB0013247	Monobutylphthalate	HMDB0013247	8575	NA
386	HMDB0030725	Dillapiol	HMDB0030725	10231	C10449
387	HMDB0002056	Monoisobutyl phthalic acid	HMDB0002056	92272	NA
388	HMDB0147179	NA	NA	NA	NA
389	HMDB0140340	NA	NA	NA	NA
390	HMDB0173973	NA	NA	NA	NA
391	HMDB0173971	NA	NA	NA	NA
392	HMDB0173972	NA	NA	NA	NA
393	HMDB0173975	NA	NA	NA	NA
394	HMDB0173976	NA	NA	NA	NA
395	HMDB0177472	NA	NA	NA	NA
396	HMDB0177470	NA	NA	NA	NA
397	HMDB0173974	NA	NA	NA	NA
398	HMDB0128944	NA	NA	NA	NA
399	HMDB0131630	NA	NA	NA	NA
400	HMDB0128958	NA	NA	NA	NA
401	HMDB0039027	NA	NA	NA	NA
402	HMDB0128963	NA	NA	NA	NA
403	HMDB0138052	NA	NA	NA	NA
404	HMDB0128962	NA	NA	NA	NA
405	HMDB0030882	(S)-Rutaretin	HMDB0030882	11108126	NA
406	HMDB0128960	NA	NA	NA	NA
407	HMDB0128961	NA	NA	NA	NA

408	HMDB0032838	Dorsteniol	HMDB0032838	71438319		
409	HMDB0131653	NA	NA	NA	NA	NA
410	HMDB0147178	NA	NA	NA	NA	NA
411	HMDB0131691	NA	NA	NA	NA	NA
412	HMDB0131700	NA	NA	NA	NA	NA
413	HMDB0167944	NA	NA	NA	NA	NA
414	HMDB0163475	NA	NA	NA	NA	NA
415	HMDB0171044	NA	NA	NA	NA	NA
416	HMDB0167134	NA	NA	NA	NA	NA
417	HMDB0028752	Aspartyl-Glutamate	HMDB0028752	4130574		
418	HMDB0029145	NA	NA	NA	NA	NA
419	HMDB0030419	gamma-Glutamylaspartic acid	HMDB0030419	5122061		
420	HMDB0062501	NA	NA	NA	NA	NA
421	HMDB0028815	Glutamylaspartic acid	HMDB0028815	99716		
422	HMDB0030413	NA	NA	NA	NA	NA
423	HMDB0011164	L-beta-aspartyl-L-glutamic acid	HMDB0011164	25207301		
424	HMDB0000767	Pseudouridine	HMDB0000767	15047	C02067	C02067
425	HMDB0000296	Uridine	HMDB0000296	6029	C00299	C00299
426	HMDB0156330	NA	NA	NA	NA	NA
427	HMDB0126635	NA	NA	NA	NA	NA
428	HMDB0130466	NA	NA	NA	NA	NA
429	HMDB0130477	NA	NA	NA	NA	NA
430	HMDB0006794	5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate	HMDB0006794	0	C05655	C05655
431	HMDB0157260	NA	NA	NA	NA	NA
432	HMDB0157259	NA	NA	NA	NA	NA
433	HMDB0125157	NA	NA	NA	NA	NA
434	HMDB0166885	NA	NA	NA	NA	NA
435	HMDB0155302	NA	NA	NA	NA	NA
436	HMDB0180914	NA	NA	NA	NA	NA
437	HMDB0177249	NA	NA	NA	NA	NA
438	HMDB0163614	NA	NA	NA	NA	NA
439	HMDB0038582	NA	NA	NA	NA	NA
440	HMDB0154970	NA	NA	NA	NA	NA
441	HMDB0156936	NA	NA	NA	NA	NA
442	HMDB0158197	NA	NA	NA	NA	NA
443	HMDB0158606	NA	NA	NA	NA	NA
444	HMDB0012782	4-Methoxy-17beta-estradiol	HMDB0012782	68578	C05302	C05302
445	HMDB0155194	NA	NA	NA	NA	NA
446	HMDB0155195	NA	NA	NA	NA	NA
447	HMDB0137388	NA	NA	NA	NA	NA
448	HMDB0137399	NA	NA	NA	NA	NA
449	HMDB0154971	NA	NA	NA	NA	NA
450	HMDB0154972	NA	NA	NA	NA	NA
451	HMDB0154973	NA	NA	NA	NA	NA
452	HMDB0154976	NA	NA	NA	NA	NA
453	HMDB0154995	NA	NA	NA	NA	NA
454	HMDB0155190	NA	NA	NA	NA	NA
455	HMDB0155192	NA	NA	NA	NA	NA
456	HMDB0155191	NA	NA	NA	NA	NA
457	HMDB0155189	NA	NA	NA	NA	NA
458	HMDB0155193	NA	NA	NA	NA	NA
459	HMDB0006773	11b-Hydroxyandrost-4-ene-3,17-dione	HMDB0006773	94141	C07432	C07432
460	HMDB0039568	NA	NA	NA	NA	NA
461	HMDB0034167	Falcarindiol 3-acetate	HMDB0034167	131751532		
462	HMDB0040927	NA	NA	NA	NA	NA
463	HMDB0033125	[8]-Dehydroshogaol	HMDB0033125	131751378		
464	HMDB0006771	7a-Hydroxyandrost-4-ene-3,17-dione	HMDB0006771	65542	C05296	C05296
465	HMDB0006774	16a-Hydroxyandrost-4-ene-3,17-dione	HMDB0006774	440574	C05140	C05140
466	HMDB0003959	19-Oxotestosterone	HMDB0003959	7048589	C05295	C05295
467	HMDB0003955	19-Hydroxyandrost-4-ene-3,17-dione	HMDB0003955	252379	C05290	C05290
468	HMDB0000405	2-Methoxyestradiol	HMDB0000405	66414	C05302	C05302
469	HMDB0000380	2-Hydroxyestradiol-3-methyl ether	HMDB0000380	13267935		
470	HMDB0034028	2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone	HMDB0034028	14236605		
471	HMDB0154977	NA	NA	NA	NA	NA
472	HMDB0041204	NA	NA	NA	NA	NA
473	HMDB0031038	(2Z,8S,9Z)-2,9-Heptadecadiene-8-hydroxy-4,6-diyne-1-yl acetate	HMDB0031038	131751121		
474	HMDB0036696	NA	NA	NA	NA	NA
475	HMDB0060359	2,3-Epoxymenaquinone	HMDB0060359	71448979	C20265	C20265
476	HMDB0184900	NA	NA	NA	NA	NA
477	HMDB0184898	NA	NA	NA	NA	NA
478	HMDB0184895	NA	NA	NA	NA	NA
479	HMDB0184897	NA	NA	NA	NA	NA
480	HMDB0184899	NA	NA	NA	NA	NA
481	HMDB0184896	NA	NA	NA	NA	NA
482	HMDB0184903	NA	NA	NA	NA	NA
483	HMDB0184902	NA	NA	NA	NA	NA
484	HMDB0184904	NA	NA	NA	NA	NA
485	HMDB0184908	NA	NA	NA	NA	NA
486	HMDB0184905	NA	NA	NA	NA	NA
487	HMDB0184901	NA	NA	NA	NA	NA
488	HMDB0005038	Citalopram	HMDB0005038	2771	C07572	C07572
489	HMDB0005028	Escitalopram	HMDB0005028	6101829		
490	HMDB0186295	NA	NA	NA	NA	NA
491	HMDB0186306	NA	NA	NA	NA	NA
492	HMDB0186305	NA	NA	NA	NA	NA
493	HMDB0186302	NA	NA	NA	NA	NA
494	HMDB0186303	NA	NA	NA	NA	NA

495	HMDB0186304	NA	NA	NA	NA
496	HMDB0186299	NA	NA	NA	NA
497	HMDB0186301	NA	NA	NA	NA
498	HMDB0186297	NA	NA	NA	NA
499	HMDB0186300	NA	NA	NA	NA
500	HMDB0186296	NA	NA	NA	NA
501	HMDB0029525	7-(4-Hydroxy-3-methoxyphenyl)-5-methoxy-1-phenyl-3-heptanone	HMDB0029525	5319454	NA
502	HMDB0131863	NA	NA	NA	NA
503	HMDB0060117	NA	NA	NA	NA
504	HMDB0002007	Tetracosahexaenoic acid	HMDB0002007	11792612	NA
505	HMDB0013025	6,9,12,15,18,21-Tetracosahexaenoic acid	HMDB0013025	53481586	NA
506	HMDB00036330	NA	NA	NA	NA
507	HMDB0240359	NA	NA	NA	NA
508	HMDB0184493	NA	NA	NA	NA
509	HMDB0184482	NA	NA	NA	NA
510	HMDB0184312	NA	NA	NA	NA
511	HMDB0161169	NA	NA	NA	NA
512	HMDB0158249	NA	NA	NA	NA
513	HMDB0038522	NA	NA	NA	NA
514	HMDB0041453	NA	NA	NA	NA
515	HMDB0000308	3b-Hydroxy-5-cholenoic acid	HMDB0000308	92997	NA
516	HMDB0031099	(all-Z)-7,10,13-Docosatrienoic acid	HMDB0031099	131751134	NA
517	HMDB0002823	Docosatrienoic acid	HMDB0002823	5312557	NA
518	HMDB0167412	NA	NA	NA	NA
519	HMDB0167408	NA	NA	NA	NA
520	HMDB0184483	NA	NA	NA	NA
521	HMDB0013326	trans-2-Dodecenoylcarnitine	HMDB0013326	53481671	NA
522	HMDB0061714	Docosadienoate (22:2n6)	HMDB0061714	5282807	C16533
523	HMDB0062219	NA	NA	NA	NA
524	HMDB0005076	13,14-Dihydro PGF-1a	HMDB0005076	5311239	NA
525	HMDB0158242	NA	NA	NA	NA
526	HMDB0158243	NA	NA	NA	NA
527	HMDB0158241	NA	NA	NA	NA
528	HMDB0158247	NA	NA	NA	NA
529	HMDB0158244	NA	NA	NA	NA
530	HMDB0158245	NA	NA	NA	NA
531	HMDB0158248	NA	NA	NA	NA
532	HMDB0184305	NA	NA	NA	NA
533	HMDB0158246	NA	NA	NA	NA
534	HMDB0184490	NA	NA	NA	NA
535	HMDB0184492	NA	NA	NA	NA
536	HMDB0184489	NA	NA	NA	NA
537	HMDB0184488	NA	NA	NA	NA
538	HMDB0184491	NA	NA	NA	NA
539	HMDB0184487	NA	NA	NA	NA
540	HMDB0184485	NA	NA	NA	NA
541	HMDB0184486	NA	NA	NA	NA
542	HMDB0184484	NA	NA	NA	NA
543	HMDB0184311	NA	NA	NA	NA
544	HMDB0184308	NA	NA	NA	NA
545	HMDB0184309	NA	NA	NA	NA
546	HMDB0184310	NA	NA	NA	NA
547	HMDB0184306	NA	NA	NA	NA
548	HMDB0184307	NA	NA	NA	NA
549	HMDB0000946	Ursodeoxycholic acid	HMDB0000946	31401	C07880
550	HMDB0002451	7b,12a-Dihydroxycholanoic acid	HMDB0002451	5283839	NA
551	HMDB0000811	Murocholic acid	HMDB0000811	5283821	C15515
552	HMDB0000733	Hyodeoxycholic acid	HMDB0000733	9963687	C15517
553	HMDB0000686	Isoursodeoxycholic acid	HMDB0000686	127601	C17662
554	HMDB0000664	Isohyodeoxycholic acid	HMDB0000664	5283822	NA
555	HMDB0000626	Deoxycholic acid	HMDB0000626	222528	C04483
556	HMDB0000514	Allochenodeoxycholic acid	HMDB0000514	96024007	C17664
557	HMDB0000518	Chenodeoxycholic acid	HMDB0000518	10133	C02528
558	HMDB0000478	Allodeoxycholic acid	HMDB0000478	96024028	C17687
559	HMDB0000438	3b,12a-Dihydroxy-5b-cholanoic acid	HMDB0000438	160530	NA
560	HMDB0000411	3a,12b-Dihydroxy-5b-cholanoic acid	HMDB0000411	5283831	C17646
561	HMDB0000384	3a,7a-Dihydroxycholanoic acid	HMDB0000384	21252245	NA
562	HMDB0000361	3b,7a-Dihydroxy-5b-cholanoic acid	HMDB0000361	164673	C17660
563	HMDB0000348	3b,12a-Dihydroxy-5a-cholanoic acid	HMDB0000348	5283835	NA
564	HMDB0002488	7a,12b-dihydroxy-5b-Cholan-24-oic acid	HMDB0002488	5283838	NA
565	HMDB0002536	Isodeoxycholic acid	HMDB0002536	164672	C17661
566	HMDB0002585	3b,12b-Dihydroxy-5b-cholanoic acid	HMDB0002585	5283832	NA
567	HMDB0094648	Leu-Leu-Leu	HMDB0094648	259327	NA
568	HMDB0161492	NA	NA	NA	NA
569	HMDB0161493	NA	NA	NA	NA
570	HMDB0161490	NA	NA	NA	NA
571	HMDB0029360	Isorheagenine	HMDB0029360	609840	NA
572	HMDB0029401	Ochratoxin B	HMDB0029401	609663	NA
573	HMDB0015068	Mesoridazine	HMDB0015068	4078	C07143
574	HMDB0030785	Mammeigin	HMDB0030785	5319255	NA
575	HMDB0015248	Trimethaphan	HMDB0015248	23576	C07174
576	HMDB0180131	NA	NA	NA	NA
577	HMDB0180133	NA	NA	NA	NA
578	HMDB0180134	NA	NA	NA	NA
579	HMDB0180137	NA	NA	NA	NA
580	HMDB0180138	NA	NA	NA	NA
581	HMDB0180139	NA	NA	NA	NA

582	HMDB0180595	NA	NA	NA	NA
583	HMDB0180596	NA	NA	NA	NA
584	HMDB0180594	NA	NA	NA	NA
585	HMDB0180593	NA	NA	NA	NA
586	HMDB0180599	NA	NA	NA	NA
587	HMDB0180598	NA	NA	NA	NA
588	HMDB0180601	NA	NA	NA	NA
589	HMDB0180602	NA	NA	NA	NA
590	HMDB0180604	NA	NA	NA	NA
591	HMDB0180605	NA	NA	NA	NA
592	HMDB0179947	NA	NA	NA	NA
593	HMDB0180130	NA	NA	NA	NA
594	HMDB0180128	NA	NA	NA	NA
595	HMDB0180129	NA	NA	NA	NA
596	HMDB0179950	NA	NA	NA	NA
597	HMDB0179946	NA	NA	NA	NA
598	HMDB0179945	NA	NA	NA	NA
599	HMDB0179942	NA	NA	NA	NA
600	HMDB0179943	NA	NA	NA	NA
601	HMDB0179941	NA	NA	NA	NA
602	HMDB0164899	NA	NA	NA	NA
603	HMDB0164897	NA	NA	NA	NA
604	HMDB0164898	NA	NA	NA	NA
605	HMDB0163827	NA	NA	NA	NA
606	HMDB0163828	NA	NA	NA	NA
607	HMDB0179951	NA	NA	NA	NA
608	HMDB0179955	NA	NA	NA	NA
609	HMDB0163826	NA	NA	NA	NA
610	HMDB0179962	NA	NA	NA	NA
611	HMDB0179960	NA	NA	NA	NA
612	HMDB0179961	NA	NA	NA	NA
613	HMDB0179957	NA	NA	NA	NA
614	HMDB0179956	NA	NA	NA	NA
615	HMDB0180124	NA	NA	NA	NA
616	HMDB0180118	NA	NA	NA	NA
617	HMDB0180115	NA	NA	NA	NA
618	HMDB0180117	NA	NA	NA	NA
619	HMDB0180112	NA	NA	NA	NA
620	HMDB0180114	NA	NA	NA	NA
621	HMDB0012240	Isopentenyladenine-9-N-glucoside	HMDB0012240	53481394	C
622	HMDB0014828	Flurazepam	HMDB0014828	3393	C
623	HMDB0126243	NA	NA	NA	NA
624	HMDB0133257	NA	NA	NA	NA
625	HMDB0133256	NA	NA	NA	NA
626	HMDB0133260	NA	NA	NA	NA
627	HMDB0133258	NA	NA	NA	NA
628	HMDB0133261	NA	NA	NA	NA
629	HMDB0133254	NA	NA	NA	NA
630	HMDB0133265	NA	NA	NA	NA
631	HMDB0133262	NA	NA	NA	NA
632	HMDB0133264	NA	NA	NA	NA
633	HMDB0132557	NA	NA	NA	NA
634	HMDB0135675	NA	NA	NA	NA
635	HMDB0133252	NA	NA	NA	NA
636	HMDB0126244	NA	NA	NA	NA
637	HMDB0126245	NA	NA	NA	NA
638	HMDB0126247	NA	NA	NA	NA
639	HMDB0126372	NA	NA	NA	NA
640	HMDB0132287	NA	NA	NA	NA
641	HMDB0132286	NA	NA	NA	NA
642	HMDB0132293	NA	NA	NA	NA
643	HMDB0132294	NA	NA	NA	NA
644	HMDB0126241	NA	NA	NA	NA
645	HMDB0132556	NA	NA	NA	NA
646	HMDB0133251	NA	NA	NA	NA
647	HMDB0135697	NA	NA	NA	NA
648	HMDB0151258	NA	NA	NA	NA
649	HMDB0163653	NA	NA	NA	NA
650	HMDB0163655	NA	NA	NA	NA
651	HMDB0163657	NA	NA	NA	NA
652	HMDB0163654	NA	NA	NA	NA
653	HMDB0163658	NA	NA	NA	NA
654	HMDB0164136	NA	NA	NA	NA
655	HMDB0164140	NA	NA	NA	NA
656	HMDB0164138	NA	NA	NA	NA
657	HMDB0166270	NA	NA	NA	NA
658	HMDB0166272	NA	NA	NA	NA
659	HMDB0182840	NA	NA	NA	NA
660	HMDB0163651	NA	NA	NA	NA
661	HMDB0163650	NA	NA	NA	NA
662	HMDB0151257	NA	NA	NA	NA
663	HMDB0151255	NA	NA	NA	NA
664	HMDB0151261	NA	NA	NA	NA
665	HMDB0151262	NA	NA	NA	NA
666	HMDB0151267	NA	NA	NA	NA
667	HMDB0151269	NA	NA	NA	NA
668	HMDB0152804	NA	NA	NA	NA

669	HMDB0152821	NA	NA	NA	NA
670	HMDB0163644	NA	NA	NA	NA
671	HMDB0163645	NA	NA	NA	NA
672	HMDB0163647	NA	NA	NA	NA
673	HMDB0163646	NA	NA	NA	NA
674	HMDB0163652	NA	NA	NA	NA
675	HMDB0059980	NA	NA	NA	NA
676	HMDB0040865	NA	NA	NA	NA
677	HMDB0041115	NA	NA	NA	NA
678	HMDB0030380	Brevianamide B	HMDB0030380	99771	C
679	HMDB0153959	NA	NA	NA	NA
680	HMDB0176911	NA	NA	NA	NA
681	HMDB0165595	NA	NA	NA	NA
682	HMDB0061060	NA	NA	NA	NA
683	HMDB0061059	NA	NA	NA	NA
684	HMDB0031754	Nequinatate	HMDB0031754	26383	C
685	HMDB0165504	NA	NA	NA	NA
686	HMDB0014902	Mometasone	HMDB0014902	441335	C07816
687	HMDB0149450	NA	NA	NA	NA
688	HMDB0165831	NA	NA	NA	NA
689	HMDB0138170	NA	NA	NA	NA
690	HMDB0138169	NA	NA	NA	NA
691	HMDB0138189	NA	NA	NA	NA
692	HMDB0138192	NA	NA	NA	NA
693	HMDB0138175	NA	NA	NA	NA
694	HMDB0138176	NA	NA	NA	NA
695	HMDB0138179	NA	NA	NA	NA
696	HMDB0138182	NA	NA	NA	NA
697	HMDB0138183	NA	NA	NA	NA
698	HMDB0138186	NA	NA	NA	NA
699	HMDB0138188	NA	NA	NA	NA
700	HMDB0138191	NA	NA	NA	NA
701	HMDB0138195	NA	NA	NA	NA
702	HMDB0138172	NA	NA	NA	NA
703	HMDB0138173	NA	NA	NA	NA
704	HMDB0171434	NA	NA	NA	NA
705	HMDB0171377	NA	NA	NA	NA
706	HMDB0171432	NA	NA	NA	NA
707	HMDB0171436	NA	NA	NA	NA
708	HMDB0180057	NA	NA	NA	NA
709	HMDB0180127	NA	NA	NA	NA
710	HMDB0183179	NA	NA	NA	NA
711	HMDB0183180	NA	NA	NA	NA
712	HMDB0167778	NA	NA	NA	NA
713	HMDB0172090	NA	NA	NA	NA
714	HMDB0144261	NA	NA	NA	NA
715	HMDB0136130	NA	NA	NA	NA
716	HMDB0136128	NA	NA	NA	NA
717	HMDB0130041	NA	NA	NA	NA
718	HMDB0130042	NA	NA	NA	NA
719	HMDB0130038	NA	NA	NA	NA
720	HMDB0130035	NA	NA	NA	NA
721	HMDB0130037	NA	NA	NA	NA
722	HMDB0136134	NA	NA	NA	NA
723	HMDB0141975	NA	NA	NA	NA
724	HMDB0154071	NA	NA	NA	NA
725	HMDB0154072	NA	NA	NA	NA
726	HMDB0148956	NA	NA	NA	NA
727	HMDB0145713	NA	NA	NA	NA
728	HMDB0144028	NA	NA	NA	NA
729	HMDB0141974	NA	NA	NA	NA
730	HMDB0138050	NA	NA	NA	NA
731	HMDB0138003	NA	NA	NA	NA
732	HMDB0137957	NA	NA	NA	NA
733	HMDB0136144	NA	NA	NA	NA
734	HMDB0136137	NA	NA	NA	NA
735	HMDB0145714	NA	NA	NA	NA
736	HMDB0136139	NA	NA	NA	NA
737	HMDB0038066	NA	NA	NA	NA
738	HMDB0180987	NA	NA	NA	NA
739	HMDB0164391	NA	NA	NA	NA
740	HMDB0164389	NA	NA	NA	NA
741	HMDB0164395	NA	NA	NA	NA
742	HMDB0036334	NA	NA	NA	NA
743	HMDB0029900	Lucuminoside	HMDB0029900	656493	C08335
744	HMDB0014780	Pemetrexed	HMDB0014780	60843	C
745	HMDB0037260	NA	NA	NA	NA
746	HMDB0158333	NA	NA	NA	NA
747	HMDB0150478	NA	NA	NA	NA
748	HMDB0150475	NA	NA	NA	NA
749	HMDB0162509	NA	NA	NA	NA
750	HMDB0150477	NA	NA	NA	NA
751	HMDB0038347	NA	NA	NA	NA
752	HMDB0150474	NA	NA	NA	NA
753	HMDB0150463	NA	NA	NA	NA
754	HMDB0150458	NA	NA	NA	NA
755	HMDB0150468	NA	NA	NA	NA

756	HMDB0150470	NA	NA	NA	NA
757	HMDB0150457	NA	NA	NA	NA
758	HMDB0150453	NA	NA	NA	NA
759	HMDB0150469	NA	NA	NA	NA
760	HMDB0150452	NA	NA	NA	NA
761	HMDB0149868	NA	NA	NA	NA
762	HMDB0150462	NA	NA	NA	NA
763	HMDB0140070	NA	NA	NA	NA
764	HMDB0153459	NA	NA	NA	NA
765	HMDB0153444	NA	NA	NA	NA
766	HMDB0153474	NA	NA	NA	NA
767	HMDB0153627	NA	NA	NA	NA
768	HMDB0153466	NA	NA	NA	NA
769	HMDB0139521	NA	NA	NA	NA
770	HMDB0139520	NA	NA	NA	NA
771	HMDB0139517	NA	NA	NA	NA
772	HMDB0139504	NA	NA	NA	NA
773	HMDB0139507	NA	NA	NA	NA
774	HMDB0139514	NA	NA	NA	NA
775	HMDB0149502	NA	NA	NA	NA
776	HMDB0153458	NA	NA	NA	NA
777	HMDB0153451	NA	NA	NA	NA
778	HMDB0153443	NA	NA	NA	NA
779	HMDB0139516	NA	NA	NA	NA
780	HMDB0139508	NA	NA	NA	NA
781	HMDB0139513	NA	NA	NA	NA
782	HMDB0164958	NA	NA	NA	NA
783	HMDB0035876	Mesuagin	HMDB0035876	5319380	NA
784	HMDB0180147	NA	NA	NA	NA
785	HMDB0013842	O-Deethylated candesartan	HMDB0013842	10047287	NA
786	HMDB0144444	NA	NA	NA	NA
787	HMDB0144965	NA	NA	NA	NA
788	HMDB0144871	NA	NA	NA	NA
789	HMDB0142647	NA	NA	NA	NA
790	HMDB0144859	NA	NA	NA	NA
791	HMDB0144408	NA	NA	NA	NA
792	HMDB0144379	NA	NA	NA	NA
793	HMDB0142761	NA	NA	NA	NA
794	HMDB0142694	NA	NA	NA	NA
795	HMDB0144418	NA	NA	NA	NA
796	HMDB0144964	NA	NA	NA	NA
797	HMDB0142682	NA	NA	NA	NA
798	HMDB0144733	NA	NA	NA	NA
799	HMDB0030041	Lupulone	HMDB0030041	51397980	C10706
800	HMDB0030140	Adlupulone	HMDB0030140		NA
801	HMDB0012516	11'-Carboxy-alpha-tocotrienol	HMDB0012516	53481452	NA
802	HMDB0173226	NA	NA	NA	NA
803	HMDB0173228	NA	NA	NA	NA
804	HMDB0173227	NA	NA	NA	NA
805	HMDB0173225	NA	NA	NA	NA
806	HMDB0173223	NA	NA	NA	NA
807	HMDB0173224	NA	NA	NA	NA
808	HMDB0014792	Latanoprost	HMDB0014792	5311221	NA
809	HMDB0187221	NA	NA	NA	NA
810	HMDB0187222	NA	NA	NA	NA
811	HMDB0015041	Bimatoprost	HMDB0015041	5311027	NA
812	HMDB0015073	Salmeterol	HMDB0015073	5152	C07241
813	HMDB0187634	NA	NA	NA	NA
814	HMDB0182254	NA	NA	NA	NA
815	HMDB0039018	NA	NA	NA	NA
816	HMDB0014660	Trandolapril	HMDB0014660	5484727	NA
817	HMDB0033479	Sinapoylspermine	HMDB0033479	131751433	NA
818	HMDB0140060	NA	NA	NA	NA
819	HMDB0171482	NA	NA	NA	NA
820	HMDB0171480	NA	NA	NA	NA
821	HMDB0166472	NA	NA	NA	NA
822	HMDB0160977	NA	NA	NA	NA
823	HMDB0171485	NA	NA	NA	NA
824	HMDB0171483	NA	NA	NA	NA
825	HMDB0184333	NA	NA	NA	NA
826	HMDB0184203	NA	NA	NA	NA
827	HMDB0184202	NA	NA	NA	NA
828	HMDB0184199	NA	NA	NA	NA
829	HMDB0155893	NA	NA	NA	NA
830	HMDB0155894	NA	NA	NA	NA
831	HMDB0155897	NA	NA	NA	NA
832	HMDB0155896	NA	NA	NA	NA
833	HMDB0155899	NA	NA	NA	NA
834	HMDB0155900	NA	NA	NA	NA
835	HMDB0184187	NA	NA	NA	NA
836	HMDB0184189	NA	NA	NA	NA
837	HMDB0184192	NA	NA	NA	NA
838	HMDB0184190	NA	NA	NA	NA
839	HMDB0184193	NA	NA	NA	NA
840	HMDB0184200	NA	NA	NA	NA
841	HMDB0184197	NA	NA	NA	NA
842	HMDB0184196	NA	NA	NA	NA

843	HMDB0160543	NA	NA	NA	NA
844	HMDB0160539	NA	NA	NA	NA
845	HMDB0160541	NA	NA	NA	NA
846	HMDB0160540	NA	NA	NA	NA
847	HMDB0160542	NA	NA	NA	NA
848	HMDB0160544	NA	NA	NA	NA
849	HMDB0160545	NA	NA	NA	NA
850	HMDB0160516	NA	NA	NA	NA
851	HMDB0160517	NA	NA	NA	NA
852	HMDB0160518	NA	NA	NA	NA
853	HMDB0160515	NA	NA	NA	NA
854	HMDB0160519	NA	NA	NA	NA
855	HMDB0160522	NA	NA	NA	NA
856	HMDB0160521	NA	NA	NA	NA
857	HMDB0160520	NA	NA	NA	NA
858	HMDB0160523	NA	NA	NA	NA
859	HMDB0160526	NA	NA	NA	NA
860	HMDB0160524	NA	NA	NA	NA
861	HMDB0160525	NA	NA	NA	NA
862	HMDB0160528	NA	NA	NA	NA
863	HMDB0160529	NA	NA	NA	NA
864	HMDB0160527	NA	NA	NA	NA
865	HMDB0160530	NA	NA	NA	NA
866	HMDB0172528	NA	NA	NA	NA
867	HMDB0170464	NA	NA	NA	NA
868	HMDB0059931	NA	NA	NA	NA
869	HMDB0040118	NA	NA	NA	NA
870	HMDB0037794	NA	NA	NA	NA
871	HMDB0038743	NA	NA	NA	NA
872	HMDB0143644	NA	NA	NA	NA
873	HMDB0173692	NA	NA	NA	NA
874	HMDB0173693	NA	NA	NA	NA
875	HMDB0041431	NA	NA	NA	NA
876	HMDB0113034	NA	NA	NA	NA
877	HMDB0113594	NA	NA	NA	NA
878	HMDB0113893	NA	NA	NA	NA
879	HMDB0113951	NA	NA	NA	NA
880	HMDB0116711	NA	NA	NA	NA
881	HMDB0114495	NA	NA	NA	NA
882	HMDB0114355	NA	NA	NA	NA
883	HMDB0113972	NA	NA	NA	NA
884	HMDB0113993	NA	NA	NA	NA
885	HMDB0114019	NA	NA	NA	NA
886	HMDB0114018	NA	NA	NA	NA
887	HMDB0114045	NA	NA	NA	NA
888	HMDB0114046	NA	NA	NA	NA
889	HMDB0114073	NA	NA	NA	NA
890	HMDB0114100	NA	NA	NA	NA
891	HMDB0114101	NA	NA	NA	NA
892	HMDB0114129	NA	NA	NA	NA
893	HMDB0114130	NA	NA	NA	NA
894	HMDB0114157	NA	NA	NA	NA
895	HMDB0114272	NA	NA	NA	NA
896	HMDB0114300	NA	NA	NA	NA
897	HMDB0114327	NA	NA	NA	NA
898	HMDB0113971	NA	NA	NA	NA
899	HMDB0007950	PC(15:0/20:4(8Z,11Z,14Z,17Z))	HMDB0007950	53478649	C00157
900	HMDB0009259	PE(20:1(11Z)/18:3(6Z,9Z,12Z))	HMDB0009259	52924556	C00350
901	HMDB0009291	PE(20:2(11Z,14Z)/18:2(9Z,12Z))	HMDB0009291	52924585	C00350
902	HMDB0009322	PE(20:3(5Z,8Z,11Z)/18:1(11Z))	HMDB0009322	53479748	C00350
903	HMDB0009323	PE(20:3(5Z,8Z,11Z)/18:1(9Z))	HMDB0009323	53479749	C00350
904	HMDB0009356	PE(20:3(8Z,11Z,14Z)/18:1(9Z))	HMDB0009356	52924615	C00350
905	HMDB0009355	PE(20:3(8Z,11Z,14Z)/18:1(11Z))	HMDB0009355	53479775	C00350
906	HMDB0009387	PE(20:4(5Z,8Z,11Z,14Z)/18:0)	HMDB0009387	52924644	C00350
907	HMDB0009420	PE(20:4(8Z,11Z,14Z,17Z)/18:0)	HMDB0009420	53479804	C00350
908	HMDB0009583	PE(22:4(7Z,10Z,13Z,16Z)/16:0)	HMDB0009583	52924809	C00350
909	HMDB0009260	PE(20:1(11Z)/18:3(9Z,12Z,15Z))	HMDB0009260	52924557	C00350
910	HMDB0009228	PE(20:0/18:4(6Z,9Z,12Z,15Z))	HMDB0009228	9546815	C00350
911	HMDB0007949	PC(15:0/20:4(5Z,8Z,11Z,14Z))	HMDB0007949	52922330	C00157
912	HMDB0008428	PC(20:4(5Z,8Z,11Z,14Z)/15:0)	HMDB0008428	52923279	C00157
913	HMDB0008461	PC(20:4(8Z,11Z,14Z,17Z)/15:0)	HMDB0008461	53479061	C00157
914	HMDB0008943	PE(16:0/22:4(7Z,10Z,13Z,16Z))	HMDB0008943	9546817	C00350
915	HMDB0008969	PE(16:1(9Z)/20:3(8Z,11Z,14Z))	HMDB0008969	53479598	C00350
916	HMDB0009004	PE(18:0/20:4(8Z,11Z,14Z,17Z))	HMDB0009004	53479610	C00350
917	HMDB0009003	PE(18:0/20:4(5Z,8Z,11Z,14Z))	HMDB0009003	5289133	C00350
918	HMDB0009034	PE(18:1(11Z)/20:3(5Z,8Z,11Z))	HMDB0009034	53479633	C00350
919	HMDB0009035	PE(18:1(11Z)/20:3(8Z,11Z,14Z))	HMDB0009035	53479634	C00350
920	HMDB0009068	PE(18:1(9Z)/20:3(8Z,11Z,14Z))	HMDB0009068	52924349	C00350
921	HMDB0009067	PE(18:1(9Z)/20:3(5Z,8Z,11Z))	HMDB0009067	9546816	C00350
922	HMDB0009099	PE(18:2(9Z,12Z)/20:2(11Z,14Z))	HMDB0009099	52924372	C00350
923	HMDB0009131	PE(18:3(6Z,9Z,12Z)/20:1(11Z))	HMDB0009131	52924400	C00350
924	HMDB0009164	PE(18:3(9Z,12Z,15Z)/20:1(11Z))	HMDB0009164	52924428	C00350
925	HMDB0009196	PE(18:4(6Z,9Z,12Z,15Z)/20:0)	HMDB0009196	52924458	C00350
926	HMDB0115462	NA	NA	NA	NA
927	HMDB0115461	NA	NA	NA	NA
928	HMDB0115551	NA	NA	NA	NA
929	HMDB0115589	NA	NA	NA	NA

930	HMDB0115436	NA	NA	NA	NA
931	HMDB0115308	NA	NA	NA	NA
932	HMDB0116706	NA	NA	NA	NA
933	HMDB0115084	NA	NA	NA	NA
934	HMDB0114971	NA	NA	NA	NA
935	HMDB0114945	NA	NA	NA	NA
936	HMDB0114920	NA	NA	NA	NA
937	HMDB0115110	NA	NA	NA	NA
938	HMDB0114279	NA	NA	NA	NA
939	HMDB0114168	NA	NA	NA	NA
940	HMDB0114167	NA	NA	NA	NA
941	HMDB0114141	NA	NA	NA	NA
942	HMDB0114140	NA	NA	NA	NA
943	HMDB0113982	NA	NA	NA	NA
944	HMDB0114084	NA	NA	NA	NA
945	HMDB0114112	NA	NA	NA	NA
946	HMDB0114307	NA	NA	NA	NA
947	HMDB0114333	NA	NA	NA	NA
948	HMDB0114334	NA	NA	NA	NA
949	HMDB0114580	NA	NA	NA	NA
950	HMDB0114389	NA	NA	NA	NA
951	HMDB0114361	NA	NA	NA	NA
952	HMDB0114362	NA	NA	NA	NA
953	HMDB0114111	NA	NA	NA	NA
954	HMDB0009045	PE(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0009045	53479643	C00350
955	HMDB0009431	PE(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z))	HMDB0009431	53479815	C00350
956	HMDB0009462	PE(20:5(5Z,8Z,11Z,14Z,17Z)/20:2(11Z,14Z))	HMDB0009462	52924683	C00350
957	HMDB0009589	PE(22:4(7Z,10Z,13Z,16Z)/18:3(6Z,9Z,12Z))	HMDB0009589	52924817	C00350
958	HMDB0009590	PE(22:4(7Z,10Z,13Z,16Z)/18:3(9Z,12Z,15Z))	HMDB0009590	52924818	C00350
959	HMDB0009621	PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z))	HMDB0009621	53479917	C00350
960	HMDB0009654	PE(22:5(7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z))	HMDB0009654	53479950	C00350
961	HMDB0009685	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z))	HMDB0009685	53479975	C00350
962	HMDB0009686	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z))	HMDB0009686	52924844	C00350
963	HMDB0009430	PE(20:4(8Z,11Z,14Z,17Z)/20:3(5Z,8Z,11Z))	HMDB0009430	53479814	C00350
964	HMDB0009397	PE(20:4(5Z,8Z,11Z,14Z)/20:3(5Z,8Z,11Z))	HMDB0009397	53479788	C00350
965	HMDB0009078	PE(18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0009078	52922113	C00350
966	HMDB0009110	PE(18:2(9Z,12Z)/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0009110	53479666	C00350
967	HMDB0009109	PE(18:2(9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0009109	53479665	C00350
968	HMDB0009141	PE(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	HMDB0009141	52924409	C00350
969	HMDB0009174	PE(18:3(9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z))	HMDB0009174	52924437	C00350
970	HMDB0009302	PE(20:2(11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z))	HMDB0009302	52924596	C00350
971	HMDB0009334	PE(20:3(5Z,8Z,11Z)/20:4(8Z,11Z,14Z,17Z))	HMDB0009334	53479760	C00350
972	HMDB0009333	PE(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0009333	53479759	C00350
973	HMDB0009366	PE(20:3(8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0009366	52924626	C00350
974	HMDB0009367	PE(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z))	HMDB0009367	53479777	C00350
975	HMDB0009398	PE(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z))	HMDB0009398	52924655	C00350
976	HMDB0112301	NA	NA	NA	NA
977	HMDB0112736	NA	NA	NA	NA
978	HMDB0112708	NA	NA	NA	NA
979	HMDB0112543	NA	NA	NA	NA
980	HMDB0112388	NA	NA	NA	NA
981	HMDB0112515	NA	NA	NA	NA
982	HMDB0112289	NA	NA	NA	NA
983	HMDB0112279	NA	NA	NA	NA
984	HMDB0012389	PS(18:1(9Z)/18:0)	HMDB0012389	9547094	C02737
985	HMDB0010163	PS(18:0/18:1(9Z))	HMDB0010163	59720717	C02737
986	HMDB0112287	NA	NA	NA	NA
987	HMDB0112286	NA	NA	NA	NA
988	HMDB0115170	NA	NA	NA	NA
989	HMDB0115471	NA	NA	NA	NA
990	HMDB0115367	NA	NA	NA	NA
991	HMDB0115197	NA	NA	NA	NA
992	HMDB0115222	NA	NA	NA	NA
993	HMDB0115265	NA	NA	NA	NA
994	HMDB0115264	NA	NA	NA	NA
995	HMDB0115341	NA	NA	NA	NA
996	HMDB0115392	NA	NA	NA	NA
997	HMDB0115445	NA	NA	NA	NA
998	HMDB0115470	NA	NA	NA	NA
999	HMDB0115290	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.

Metabolite Sets Enrichment Overview

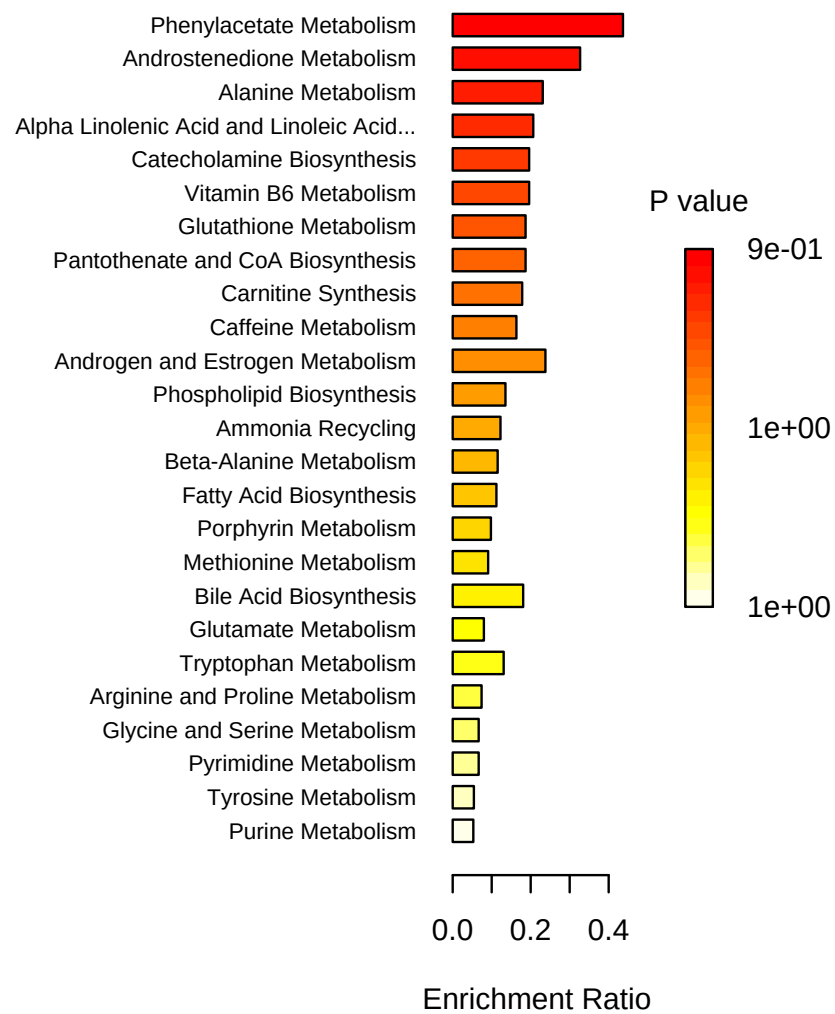


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Phenylacetate Metabolism	9	2.29	1	9.30E-01	1.00E+00	1.00E+00
Androstenedione Metabolism	24	6.12	2	9.93E-01	1.00E+00	1.00E+00
Alanine Metabolism	17	4.33	1	9.94E-01	1.00E+00	1.00E+00
Alpha Linolenic Acid and Linoleic Acid Metabolism	19	4.84	1	9.96E-01	1.00E+00	1.00E+00
Catecholamine Biosynthesis	20	5.10	1	9.97E-01	1.00E+00	1.00E+00
Vitamin B6 Metabolism	20	5.10	1	9.97E-01	1.00E+00	1.00E+00
Glutathione Metabolism	21	5.35	1	9.98E-01	1.00E+00	1.00E+00
Pantothenate and CoA Biosynthesis	21	5.35	1	9.98E-01	1.00E+00	1.00E+00
Carnitine Synthesis	22	5.61	1	9.99E-01	1.00E+00	1.00E+00
Caffeine Metabolism	24	6.12	1	9.99E-01	1.00E+00	1.00E+00
Androgen and Estrogen Metabolism	33	8.41	2	9.99E-01	1.00E+00	1.00E+00
Phospholipid Biosynthesis	29	7.39	1	1.00E+00	1.00E+00	1.00E+00
Ammonia Recycling	32	8.16	1	1.00E+00	1.00E+00	1.00E+00
Beta-Alanine Metabolism	34	8.67	1	1.00E+00	1.00E+00	1.00E+00
Fatty Acid Biosynthesis	35	8.92	1	1.00E+00	1.00E+00	1.00E+00
Porphyrin Metabolism	40	10.20	1	1.00E+00	1.00E+00	1.00E+00
Methionine Metabolism	43	11.00	1	1.00E+00	1.00E+00	1.00E+00
Bile Acid Biosynthesis	65	16.60	3	1.00E+00	1.00E+00	1.00E+00
Glutamate Metabolism	49	12.50	1	1.00E+00	1.00E+00	1.00E+00
Tryptophan Metabolism	60	15.30	2	1.00E+00	1.00E+00	1.00E+00
Arginine and Proline Metabolism	53	13.50	1	1.00E+00	1.00E+00	1.00E+00
Glycine and Serine Metabolism	59	15.00	1	1.00E+00	1.00E+00	1.00E+00
Pyrimidine Metabolism	59	15.00	1	1.00E+00	1.00E+00	1.00E+00
Tyrosine Metabolism	72	18.40	1	1.00E+00	1.00E+00	1.00E+00
Purine Metabolism	74	18.90	1	1.00E+00	1.00E+00	1.00E+00

7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "cmpd.vec<-c(\"HMDB0000123\", \"HMDB0014691\", \"HMDB0031239\", \"HMDB0161401\", \"HMDB0001858\", \"I
[3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
[4] "mSet<-CrossReferencing(mSet, \"hmdb\");"
[5] "mSet<-CreateMappingResultTable(mSet)"
[6] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[7] "mSet<-SetMetabolomeFilter(mSet, F);"
[8] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[9] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA)"
[10] "mSet<-SaveTransformedData(mSet)"
[11] "UpdateDataObjects(\"conc\", \"msetora\", FALSE)"
[12] "mSet<-SetMetabolomeFilter(mSet, F);"
[13] "mSet<-SetCurrentMsetLib(mSet, \"smpdb_pathway\", 2);"
[14] "mSet<-CalculateHyperScore(mSet)"
[15] "mSet<-PlotORA(mSet, \"ora_0_\", \"net\", \"png\", 72, width=NA)"
[16] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_0_\", \"png\", 72, width=NA)"
[17] "mSet<-CalculateHyperScore(mSet)"
[18] "mSet<-PlotORA(mSet, \"ora_1_\", \"net\", \"png\", 72, width=NA)"
[19] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_1_\", \"png\", 72, width=NA)"
[20] "mSet<-SaveTransformedData(mSet)"
[21] "mSet<-PreparePDFReport(mSet, \"guest18019451723783111663\")\n"
```

The report was generated on Mon May 24 15:16:33 2021 with R version 4.0.2 (2020-06-22).