

Metabolomic Data Analysis with MetaboAnalyst 5.0

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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.^{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*

	Query	Match	HMDB
1	HMDB0167366	NA	NA
2	HMDB0094692	NA	NA
3	HMDB0041945	NA	NA
4	HMDB0167367	NA	NA
5	HMDB0167365	NA	NA
6	HMDB0240305	NA	NA
7	HMDB0031654	3-Aminobutanoic acid	HMDB0031654
8	HMDB0094693	NA	NA
9	HMDB0002166	(S)-b-aminoisobutyric acid	HMDB0002166
10	HMDB0000452	L-Alpha-aminobutyric acid	HMDB0000452
11	HMDB0002299	(R)-b-aminoisobutyric acid	HMDB0002299
12	HMDB0001906	2-Aminoisobutyric acid	HMDB0001906
13	HMDB0003911	3-Aminoisobutanoic acid	HMDB0003911
14	HMDB0000112	Gamma-Aminobutyric acid	HMDB0000112
15	HMDB0038394	NA	NA
16	HMDB0031329	Butyl nitrite	HMDB0031329
17	HMDB0000092	Dimethylglycine	HMDB0000092
18	HMDB0000650	D-Alpha-aminobutyric acid	HMDB0000650
19	HMDB0061050	NA	NA
20	HMDB0167139	NA	NA
21	HMDB0167138	NA	NA
22	HMDB0000549	Gamma-Butyrolactone	HMDB0000549
23	HMDB0002523	Oxolan-3-one	HMDB0002523
24	HMDB0003407	Diacetyl	HMDB0003407
25	HMDB0031209	Ethenyl acetate	HMDB0031209
26	HMDB0034439	Isocrotonic acid	HMDB0034439
27	HMDB0033977	Methyl acrylate	HMDB0033977
28	HMDB0174868	NA	NA
29	HMDB0010720	But-2-enoic acid	HMDB0010720
30	HMDB0240288	NA	NA
31	HMDB0161316	NA	NA
32	HMDB0002994	Erythritol	HMDB0002994
33	HMDB0004136	D-Threitol	HMDB0004136
34	HMDB0094689	NA	NA
35	HMDB0165469	NA	NA
36	HMDB0165470	NA	NA
37	HMDB0062640	NA	NA
38	HMDB0126088	NA	NA
39	HMDB0000710	4-Hydroxybutyric acid	HMDB0000710
40	HMDB0000442	(S)-3-Hydroxybutyric acid	HMDB0000442
41	HMDB0000357	3-Hydroxybutyric acid	HMDB0000357
42	HMDB0000336	(R)-3-Hydroxyisobutyric acid	HMDB0000336
43	HMDB0000011	(R)-3-Hydroxybutyric acid	HMDB0000011
44	HMDB0000023	(S)-3-Hydroxyisobutyric acid	HMDB0000023
45	HMDB0000729	Alpha-Hydroxyisobutyric acid	HMDB0000729
46	HMDB0031212	Ethoxyacetic acid	HMDB0031212
47	HMDB0059748	NA	NA
48	HMDB0000008	2-Hydroxybutyric acid	HMDB0000008
49	HMDB0015507	Gamma Hydroxybutyric Acid	HMDB0015507
50	HMDB0061950	NA	NA
51	HMDB0000532	Acetyl glycine	HMDB0000532
52	HMDB0006454	L-2-Amino-3-oxobutanoic acid	HMDB0006454
53	HMDB0012249	L-Aspartate-semialdehyde	HMDB0012249
54	HMDB0161181	NA	NA
55	HMDB0187639	NA	NA
56	HMDB0032523	Succinic anhydride	HMDB0032523
57	HMDB0029389	(+)-threo-2-Amino-3,4-dihydroxybutanoic acid	HMDB0029389
58	HMDB0000034	Adenine	HMDB0000034
59	HMDB0003431	L-Histidinol	HMDB0003431

60	HMDB0128943	NA	NA
61	HMDB0132477	NA	NA
62	HMDB0129097	NA	NA
63	HMDB0168839	NA	NA
64	HMDB0128916	NA	NA
65	HMDB0012233	Glutarate semialdehyde	HMDB0012233
66	HMDB0029172	3-keto-2-Methylbutyrate	HMDB0029172
67	HMDB0001865	2-Oxovaleric acid	HMDB0001865
68	HMDB0000310	Methylacetoacetic acid	HMDB0000310
69	HMDB0031643	Ethyl pyruvate	HMDB0031643
70	HMDB0000019	Alpha-ketoisovaleric acid	HMDB0000019
71	HMDB0003771	2-Methylacetoacetic acid	HMDB0003771
72	HMDB0000720	Levulinic acid	HMDB0000720
73	HMDB0034466	Acetoxyacetone	HMDB0034466
74	HMDB0128917	NA	NA
75	HMDB0129096	NA	NA
76	HMDB0129098	NA	NA
77	HMDB0168838	NA	NA
78	HMDB0177210	NA	NA
79	HMDB0169666	NA	NA
80	HMDB0177209	NA	NA
81	HMDB0171727	NA	NA
82	HMDB0032356	N-Lactoyl ethanolamine	HMDB0032356
83	HMDB0039499	NA	NA
84	HMDB0031658	L-2-Amino-5-hydroxypentanoic acid	HMDB0031658
85	HMDB0039790	NA	NA
86	HMDB0038974	NA	NA
87	HMDB0039789	NA	NA
88	HMDB0000786	Oxypurinol	HMDB0000786
89	HMDB0000292	Xanthine	HMDB0000292
90	HMDB0001182	6,8-Dihydroxypurine	HMDB0001182
91	HMDB0000744	Malic acid	HMDB0000744
92	HMDB0031518	D-Malic acid	HMDB0031518
93	HMDB0000156	L-Malic acid	HMDB0000156
94	HMDB0032872	Velcorin	HMDB0032872
95	HMDB0061971	NA	NA
96	HMDB0000132	Guanine	HMDB0000132
97	HMDB0000403	2-Hydroxyadenine	HMDB0000403
98	HMDB0000542	8-Hydroxyadenine	HMDB0000542
99	HMDB0240251	NA	NA
100	HMDB0061880	NA	NA
101	HMDB0059659	Trans-3-hydroxy-L-proline	HMDB0059659
102	HMDB0002113	3-Hydroxy-L-proline	HMDB0002113
103	HMDB0000783	Propionylglycine	HMDB0000783
104	HMDB0000766	N-Acetyl-L-alanine	HMDB0000766
105	HMDB0000725	4-Hydroxyproline	HMDB0000725
106	HMDB0036576	NA	NA
107	HMDB0001149	5-Aminolevulinic acid	HMDB0001149
108	HMDB0002104	L-Glutamic gamma-semialdehyde	HMDB0002104
109	HMDB0006055	4-Hydroxy-L-proline	HMDB0006055
110	HMDB0060460	cis-4-Hydroxy-D-proline	HMDB0060460
111	HMDB0006272	5-Amino-2-oxopentanoic acid	HMDB0006272
112	HMDB0177404	NA	NA
113	HMDB0014389	Mesalazine	HMDB0014389
114	HMDB0164041	NA	NA
115	HMDB0059749	NA	NA
116	HMDB0001972	3-Aminosalicylic acid	HMDB0001972
117	HMDB0014378	Aminosalicylic Acid	HMDB0014378
118	HMDB0001476	3-Hydroxyanthranilic acid	HMDB0001476
119	HMDB0059811	NA	NA
120	HMDB0012289	Tetrahydrodipicolinate	HMDB0012289
121	HMDB0014447	Tranexamic Acid	HMDB0014447
122	HMDB0033433	(S)-Homostachydrine	HMDB0033433
123	HMDB0039651	NA	NA
124	HMDB0039680	NA	NA
125	HMDB0036176	NA	NA
126	HMDB0037625	NA	NA
127	HMDB0040526	NA	NA
128	HMDB0037196	NA	NA
129	HMDB0037167	NA	NA
130	HMDB0039652	NA	NA
131	HMDB0060682	NA	NA
132	HMDB0032311	2,4-Hexadienyl acetate	HMDB0032311
133	HMDB0039673	NA	NA
134	HMDB0040463	NA	NA
135	HMDB0039681	NA	NA
136	HMDB0033054	Ethyl isopropyl disulfide	HMDB0033054
137	HMDB0033053	Ethyl propyl disulfide	HMDB0033053
138	HMDB0031160	1-Pentanesulfenothioic acid	HMDB0031160
139	HMDB0000157	Hypoxanthine	HMDB0000157
140	HMDB0014581	Allopurinol	HMDB0014581
141	HMDB0000943	Threonic acid	HMDB0000943
142	HMDB0062620	NA	NA
143	HMDB0000613	Erythronic acid	HMDB0000613
144	HMDB0137818	NA	NA
145	HMDB0183470	NA	NA
146	HMDB0060348	Maleylacetic acid	HMDB0060348

147	HMDB0031210	Zymonic acid	HMDB0031210
148	HMDB0037759	NA	NA
149	HMDB0014273	NA	NA
150	HMDB0000044	Ascorbic acid	HMDB0000044
151	HMDB0031193	1,2,3-Propanetricarboxylic acid	HMDB0031193
152	HMDB0006355	D-Glucurono-6,3-lactone	HMDB0006355
153	HMDB0160667	NA	NA
154	HMDB0160666	NA	NA
155	HMDB0160406	NA	NA
156	HMDB0160407	NA	NA
157	HMDB0000694	L-2-Hydroxyglutaric acid	HMDB0000694
158	HMDB0000428	3-Hydroxyglutaric acid	HMDB0000428
159	HMDB0000426	Citramalic acid	HMDB0000426
160	HMDB0000606	D-2-Hydroxyglutaric acid	HMDB0000606
161	HMDB0059655	2-Hydroxyglutarate	HMDB0059655
162	HMDB0001900	Ribonolactone	HMDB0001900
163	HMDB0161319	NA	NA
164	HMDB0011676	D-Xylono-1,5-lactone	HMDB0011676
165	HMDB0061190	NA	NA
166	HMDB0062739	NA	NA
167	HMDB0160668	NA	NA
168	HMDB0041392	NA	NA
169	HMDB0033912	2-Propenyl propyl disulfide	HMDB0033912
170	HMDB0038890	NA	NA
171	HMDB0001566	3-Methylguanine	HMDB0001566
172	HMDB0000897	7-Methylguanine	HMDB0000897
173	HMDB0006040	N2-Methylguanine	HMDB0006040
174	HMDB0003282	1-Methylguanine	HMDB0003282
175	HMDB0011657	2,6-Diamino-4-hydroxy-5-N-methylformamidopyrimidine	HMDB0011657
176	HMDB0000232	Quinolinic acid	HMDB0000232
177	HMDB0033161	2,6-Pyridinedicarboxylic acid	HMDB0033161
178	HMDB0185628	NA	NA
179	HMDB0001330	2-Amino-3-carboxymuconic acid semialdehyde	HMDB0001330
180	HMDB0062578	NA	NA
181	HMDB0060260	NA	NA
182	HMDB0001552	2-Keto-glutaramic acid	HMDB0001552
183	HMDB0013988	N-Deschlorobenzoyl indomethacin	HMDB0013988
184	HMDB0038339	NA	NA
185	HMDB0033436	Nigellimine N-oxide	HMDB0033436
186	HMDB0038338	NA	NA
187	HMDB0139875	NA	NA
188	HMDB0033763	Ethyl N-methylanthranilate	HMDB0033763
189	HMDB0041931	NA	NA
190	HMDB0029223	alpha-Methylphenylalanine	HMDB0029223
191	HMDB0029224	N-methylphenylalanine	HMDB0029224
192	HMDB0042012	NA	NA
193	HMDB0030372	Maltosazine	HMDB0030372
194	HMDB0040021	NA	NA
195	HMDB0001189	2(N)-Methyl-norsalsolinol	HMDB0001189
196	HMDB0005199	(R)-Salsolinol	HMDB0005199
197	HMDB0031811	3,5-Dimethylphenyl methylcarbamate	HMDB0031811
198	HMDB0039655	NA	NA
199	HMDB0029034	Serylasparagine	HMDB0029034
200	HMDB0028740	Asparaginy-Serine	HMDB0028740
201	HMDB0032401	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	HMDB0032401
202	HMDB0001539	Asymmetric dimethylarginine	HMDB0001539
203	HMDB0003334	Symmetric dimethylarginine	HMDB0003334
204	HMDB0164284	NA	NA
205	HMDB0164282	NA	NA
206	HMDB0164283	NA	NA
207	HMDB0164280	NA	NA
208	HMDB0164279	NA	NA
209	HMDB0164281	NA	NA
210	HMDB0000933	Traumatic acid	HMDB0000933
211	HMDB0030994	5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	HMDB0030994
212	HMDB0037816	NA	NA
213	HMDB0037135	NA	NA
214	HMDB0032871	Sedanonic acid	HMDB0032871
215	HMDB0032797	Jasmonic acid	HMDB0032797
216	HMDB0037104	NA	NA
217	HMDB0041573	NA	NA
218	HMDB0037735	NA	NA
219	HMDB0033102	Dihydro-3-(2-octenyl)-2,5-furandione	HMDB0033102
220	HMDB0037642	NA	NA
221	HMDB0039669	NA	NA
222	HMDB0033640	7-Methyl-3-methylene-1,6,7-octanetriol	HMDB0033640
223	HMDB0038186	NA	NA
224	HMDB0010725	(R)-3-Hydroxydecanoic acid	HMDB0010725
225	HMDB0040329	NA	NA
226	HMDB0034783	cis-p-Menthane-1,7,8-triol	HMDB0034783
227	HMDB0033574	(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	HMDB0033574
228	HMDB0033201	9-Hydroxydecanoic acid	HMDB0033201
229	HMDB0039668	NA	NA
230	HMDB0039470	NA	NA
231	HMDB0039893	NA	NA
232	HMDB0180105	NA	NA
233	HMDB0180106	NA	NA

234	HMDB0180104	NA	NA
235	HMDB0179930	NA	NA
236	HMDB0179931	NA	NA
237	HMDB0179932	NA	NA
238	HMDB0179929	NA	NA
239	HMDB0180588	NA	NA
240	HMDB0180587	NA	NA
241	HMDB0180586	NA	NA
242	HMDB0041600	NA	NA
243	HMDB0179928	NA	NA
244	HMDB0002203	3-Hydroxycapric acid	HMDB0002203
245	HMDB0094656	2-Hydroxydecanoate	HMDB0094656
246	HMDB0180585	NA	NA
247	HMDB0180589	NA	NA
248	HMDB0094651	PyroGlu-Val	HMDB0094651
249	HMDB0029018	Prolyl-Hydroxyproline	HMDB0029018
250	HMDB0028871	Hydroxyprolyl-Proline	HMDB0028871
251	HMDB0006695	Prolylhydroxyproline	HMDB0006695
252	HMDB0040573	NA	NA
253	HMDB0060747	NA	NA
254	HMDB0011754	Methyldopa	HMDB0011754
255	HMDB0001434	3-Methoxytyrosine	HMDB0001434
256	HMDB0011172	gamma-Glutamylvaline	HMDB0011172
257	HMDB0029162	NA	NA
258	HMDB0028756	Aspartyl-Isoleucine	HMDB0028756
259	HMDB0028903	Isoleucyl-Aspartate	HMDB0028903
260	HMDB0028925	Leucyl-Aspartate	HMDB0028925
261	HMDB0028832	Glutamylvaline	HMDB0028832
262	HMDB0059717	NA	NA
263	HMDB0029126	Valyl-Glutamate	HMDB0029126
264	HMDB0028757	Aspartyl-Leucine	HMDB0028757
265	HMDB0011166	L-beta-aspartyl-L-leucine	HMDB0011166
266	HMDB0151781	NA	NA
267	HMDB0151783	NA	NA
268	HMDB0151788	NA	NA
269	HMDB0151787	NA	NA
270	HMDB0151784	NA	NA
271	HMDB0035016	2-Phenylethyl pentanoate	HMDB0035016
272	HMDB0132932	NA	NA
273	HMDB0132940	NA	NA
274	HMDB0151780	NA	NA
275	HMDB0001925	Ibuprofen	HMDB0001925
276	HMDB0034472	3-Phenylpropyl 2-methylpropanoate	HMDB0034472
277	HMDB0034470	2-Phenylpropyl isobutyrate	HMDB0034470
278	HMDB0038605	NA	NA
279	HMDB0040431	NA	NA
280	HMDB0036391	NA	NA
281	HMDB0036025	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	HMDB0036025
282	HMDB0037194	NA	NA
283	HMDB0034469	2-Phenylpropyl butyrate	HMDB0034469
284	HMDB0037623	NA	NA
285	HMDB0036240	NA	NA
286	HMDB0035017	2-Phenylethyl 3-methylbutanoate	HMDB0035017
287	HMDB0037720	NA	NA
288	HMDB0035008	3-Methylbutyl phenylacetate	HMDB0035008
289	HMDB0036386	NA	NA
290	HMDB0033196	(E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one	HMDB0033196
291	HMDB0037604	NA	NA
292	HMDB0029669	Eremopetasinorone A	HMDB0029669
293	HMDB0035181	xi-8,9-Dehydrotheaspirone	HMDB0035181
294	HMDB0039101	NA	NA
295	HMDB0034556	3-Acetoxy-3-methyl-1-phenylbutane	HMDB0034556
296	HMDB0032176	Benzyl hexanoate	HMDB0032176
297	HMDB0163212	NA	NA
298	HMDB0151805	NA	NA
299	HMDB0151793	NA	NA
300	HMDB0151794	NA	NA
301	HMDB0151789	NA	NA
302	HMDB0151790	NA	NA
303	HMDB0151791	NA	NA
304	HMDB0151785	NA	NA
305	HMDB0151786	NA	NA
306	HMDB0151792	NA	NA
307	HMDB0014604	Nabumetone	HMDB0014604
308	HMDB0176774	NA	NA
309	HMDB0176773	NA	NA
310	HMDB0176775	NA	NA
311	HMDB0061836	NA	NA
312	HMDB0032133	Bisphenol A	HMDB0032133
313	HMDB0033878	(S)-Curzeone	HMDB0033878
314	HMDB0135597	NA	NA
315	HMDB0170855	NA	NA
316	HMDB0179330	NA	NA
317	HMDB0179331	NA	NA
318	HMDB0038202	NA	NA
319	HMDB0036767	NA	NA
320	HMDB0036455	NA	NA

321	HMDB0035902	Enokipodin B	HMDB0035902
322	HMDB0040903	NA	NA
323	HMDB0038188	NA	NA
324	HMDB0031916	5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran	HMDB0031916
325	HMDB0037558	NA	NA
326	HMDB0036473	NA	NA
327	HMDB0037801	NA	NA
328	HMDB0030911	2-Oxo-5,11(13)-eudesmadien-12,8-olide	HMDB0030911
329	HMDB0031900	Methyl (2E,4Z,6E,8E,10E)-4,8-dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoate	HMDB0031900
330	HMDB0036488	NA	NA
331	HMDB0038547	NA	NA
332	HMDB0041920	NA	NA
333	HMDB0179332	NA	NA
334	HMDB0001319	Pyridoxine 5'-phosphate	HMDB0001319
335	HMDB0001904	3-Nitrotyrosine	HMDB0001904
336	HMDB0015122	Cytarabine	HMDB0015122
337	HMDB0155273	NA	NA
338	HMDB0060478	gamma-Glutamyl-beta-cyanoalanine	HMDB0060478
339	HMDB0000089	Cytidine	HMDB0000089
340	HMDB0028751	Aspartyl-Glutamine	HMDB0028751
341	HMDB0028767	Aspartyl-Gamma-glutamate	HMDB0028767
342	HMDB0028814	Glutamylasparagine	HMDB0028814
343	HMDB0029144	gamma-Glutamylasparagine	HMDB0029144
344	HMDB0028793	Glutaminylaspartic acid	HMDB0028793
345	HMDB0028730	Asparaginy-Glutamate	HMDB0028730
346	HMDB0139892	NA	NA
347	HMDB0033701	Hydrocotarnine	HMDB0033701
348	HMDB0031770	Carbofuran	HMDB0031770
349	HMDB0014798	Metaxalone	HMDB0014798
350	HMDB0161832	NA	NA
351	HMDB0161833	NA	NA
352	HMDB0161834	NA	NA
353	HMDB0149051	NA	NA
354	HMDB0149050	NA	NA
355	HMDB0149006	NA	NA
356	HMDB0148541	NA	NA
357	HMDB0148540	NA	NA
358	HMDB0148786	NA	NA
359	HMDB0148785	NA	NA
360	HMDB0148998	NA	NA
361	HMDB0149048	NA	NA
362	HMDB0147226	NA	NA
363	HMDB0148542	NA	NA
364	HMDB0128505	NA	NA
365	HMDB0148539	NA	NA
366	HMDB0145646	NA	NA
367	HMDB0145647	NA	NA
368	HMDB0145645	NA	NA
369	HMDB0135172	NA	NA
370	HMDB0149007	NA	NA
371	HMDB0128506	NA	NA
372	HMDB0128503	NA	NA
373	HMDB0128504	NA	NA
374	HMDB0040876	NA	NA
375	HMDB0030946	(2E,11Z)-Wyerone acid	HMDB0030946
376	HMDB0041016	NA	NA
377	HMDB0030595	Suberenone	HMDB0030595
378	HMDB0033735	Graveolone	HMDB0033735
379	HMDB0039430	NA	NA
380	HMDB0004215	3,3',4'5-Tetrahydroxystilbene	HMDB0004215
381	HMDB0170845	NA	NA
382	HMDB0164057	NA	NA
383	HMDB0135900	NA	NA
384	HMDB0135902	NA	NA
385	HMDB0135904	NA	NA
386	HMDB0164055	NA	NA
387	HMDB0164056	NA	NA
388	HMDB0164058	NA	NA
389	HMDB0170846	NA	NA
390	HMDB0170974	NA	NA
391	HMDB0170976	NA	NA
392	HMDB0170979	NA	NA
393	HMDB0170978	NA	NA
394	HMDB0131284	NA	NA
395	HMDB0131285	NA	NA
396	HMDB0127824	NA	NA
397	HMDB0131281	NA	NA
398	HMDB0131283	NA	NA
399	HMDB0170977	NA	NA
400	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	HMDB0031668
401	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	HMDB0034056
402	HMDB0037681	NA	NA
403	HMDB0029470	Isodillapiole	HMDB0029470
404	HMDB0041379	NA	NA
405	HMDB0135906	NA	NA
406	HMDB0038563	NA	NA
407	HMDB0037130	NA	NA

408	HMDB0094660	Diethyl phthalic acid	HMDB0094660
409	HMDB0033776	Apiole	HMDB0033776
410	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	HMDB0029226
411	HMDB0135689	NA	NA
412	HMDB0013247	Monobutylphthalate	HMDB0013247
413	HMDB0030725	Dillapiol	HMDB0030725
414	HMDB0002056	Monoisobutyl phthalic acid	HMDB0002056
415	HMDB0147179	NA	NA
416	HMDB0140340	NA	NA
417	HMDB0173973	NA	NA
418	HMDB0173971	NA	NA
419	HMDB0173972	NA	NA
420	HMDB0173975	NA	NA
421	HMDB0173976	NA	NA
422	HMDB0177472	NA	NA
423	HMDB0177470	NA	NA
424	HMDB0173974	NA	NA
425	HMDB0128944	NA	NA
426	HMDB0131630	NA	NA
427	HMDB0128958	NA	NA
428	HMDB0039027	NA	NA
429	HMDB0128963	NA	NA
430	HMDB0138052	NA	NA
431	HMDB0128962	NA	NA
432	HMDB0030882	(S)-Rutaretin	HMDB0030882
433	HMDB0128960	NA	NA
434	HMDB0128961	NA	NA
435	HMDB0032838	Dorsteniol	HMDB0032838
436	HMDB0131653	NA	NA
437	HMDB0147178	NA	NA
438	HMDB0131691	NA	NA
439	HMDB0131700	NA	NA
440	HMDB0167944	NA	NA
441	HMDB0163475	NA	NA
442	HMDB0171044	NA	NA
443	HMDB0167134	NA	NA
444	HMDB0028752	Aspartyl-Glutamate	HMDB0028752
445	HMDB0029145	NA	NA
446	HMDB0030419	gamma-Glutamylaspartic acid	HMDB0030419
447	HMDB0062501	NA	NA
448	HMDB0028815	Glutamylaspartic acid	HMDB0028815
449	HMDB0030413	NA	NA
450	HMDB0011164	L-beta-aspartyl-L-glutamic acid	HMDB0011164
451	HMDB0000767	Pseudouridine	HMDB0000767
452	HMDB0000296	Uridine	HMDB0000296
453	HMDB0156330	NA	NA
454	HMDB0126635	NA	NA
455	HMDB0130466	NA	NA
456	HMDB0130477	NA	NA
457	HMDB0006794	5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate	HMDB0006794
458	HMDB0157260	NA	NA
459	HMDB0157259	NA	NA
460	HMDB0125157	NA	NA
461	HMDB0166885	NA	NA
462	HMDB0155302	NA	NA
463	HMDB0180914	NA	NA
464	HMDB0177249	NA	NA
465	HMDB0163614	NA	NA
466	HMDB0032924	3-Furanmethanol glucoside	HMDB0032924
467	HMDB0130798	NA	NA
468	HMDB0130839	NA	NA
469	HMDB0126546	NA	NA
470	HMDB0167013	NA	NA
471	HMDB0175219	NA	NA
472	HMDB0167016	NA	NA
473	HMDB0002091	Isovalerylglucuronide	HMDB0002091
474	HMDB0167014	NA	NA
475	HMDB0175223	NA	NA
476	HMDB0143217	NA	NA
477	HMDB0175224	NA	NA
478	HMDB0175227	NA	NA
479	HMDB0175220	NA	NA
480	HMDB0033065	(x)-1,2-Propanediol 1-O-b-D-glucopyranoside	HMDB0033065
481	HMDB0060917	NA	NA
482	HMDB0144816	NA	NA
483	HMDB0184077	NA	NA
484	HMDB0029155	NA	NA
485	HMDB0034367	gamma-Glutamylmethionine	HMDB0034367
486	HMDB0028972	Methionyl-Glutamate	HMDB0028972
487	HMDB0028825	Glutamylmethionine	HMDB0028825
488	HMDB0060663	NA	NA
489	HMDB0161782	NA	NA
490	HMDB0161783	NA	NA
491	HMDB0161780	NA	NA
492	HMDB0161778	NA	NA
493	HMDB0161779	NA	NA
494	HMDB0177722	NA	NA

495	HMDB0040790	NA	NA
496	HMDB0033351	Methoxybrassinin	HMDB0033351
497	HMDB0155171	NA	NA
498	HMDB0002062	Norepinephrine sulfate	HMDB0002062
499	HMDB0156032	NA	NA
500	HMDB0155175	NA	NA
501	HMDB0155133	NA	NA
502	HMDB0156031	NA	NA
503	HMDB0155132	NA	NA
504	HMDB0240695	NA	NA
505	HMDB0168085	NA	NA
506	HMDB0167573	NA	NA
507	HMDB0153240	NA	NA
508	HMDB0148680	NA	NA
509	HMDB0130908	NA	NA
510	HMDB0150257	NA	NA
511	HMDB0150666	NA	NA
512	HMDB0150667	NA	NA
513	HMDB0151413	NA	NA
514	HMDB0151710	NA	NA
515	HMDB0151717	NA	NA
516	HMDB0151989	NA	NA
517	HMDB0152004	NA	NA
518	HMDB0152130	NA	NA
519	HMDB0153396	NA	NA
520	HMDB0147592	NA	NA
521	HMDB0128588	NA	NA
522	HMDB0130320	NA	NA
523	HMDB0130374	NA	NA
524	HMDB0130909	NA	NA
525	HMDB0130905	NA	NA
526	HMDB0130928	NA	NA
527	HMDB0130926	NA	NA
528	HMDB0132873	NA	NA
529	HMDB0140458	NA	NA
530	HMDB0140466	NA	NA
531	HMDB0140465	NA	NA
532	HMDB0140471	NA	NA
533	HMDB0140478	NA	NA
534	HMDB0141217	NA	NA
535	HMDB0128584	NA	NA
536	HMDB0146278	NA	NA
537	HMDB0132455	NA	NA
538	HMDB0130379	NA	NA
539	HMDB0036629	NA	NA
540	HMDB0029522	5,7-Dihydroxy-3-methoxyflavone	HMDB0029522
541	HMDB0133330	NA	NA
542	HMDB0132457	NA	NA
543	HMDB0031428	Farnisin	HMDB0031428
544	HMDB0039166	NA	NA
545	HMDB0039578	NA	NA
546	HMDB0005781	Glycitein	HMDB0005781
547	HMDB0002338	Biochanin A	HMDB0002338
548	HMDB0034127	Prunetin	HMDB0034127
549	HMDB0180733	NA	NA
550	HMDB0147591	NA	NA
551	HMDB0041758	NA	NA
552	HMDB0041776	NA	NA
553	HMDB0031720	Xenognosin B	HMDB0031720
554	HMDB0030768	2-(6-Hydroxy-2-methoxy-3,4-methylenedioxyphenyl)benzofuran	HMDB0030768
555	HMDB0141945	NA	NA
556	HMDB0132850	NA	NA
557	HMDB0147530	NA	NA
558	HMDB0150245	NA	NA
559	HMDB0132886	NA	NA
560	HMDB0130929	NA	NA
561	HMDB0134889	NA	NA
562	HMDB0137557	NA	NA
563	HMDB0125118	NA	NA
564	HMDB0145984	NA	NA
565	HMDB0175189	NA	NA
566	HMDB0175187	NA	NA
567	HMDB0175188	NA	NA
568	HMDB0162484	NA	NA
569	HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	HMDB0033197
570	HMDB0036047	NA	NA
571	HMDB0059661	NA	NA
572	HMDB0015088	Rizatriptan	HMDB0015088
573	HMDB0014873	Naftifine	HMDB0014873
574	HMDB0014578	Cyproheptadine	HMDB0014578
575	HMDB0240660	NA	NA
576	HMDB0166396	NA	NA
577	HMDB0155323	NA	NA
578	HMDB0125616	NA	NA
579	HMDB0157443	NA	NA
580	HMDB0125615	NA	NA
581	HMDB0155324	NA	NA

582	HMDB0155326	NA	NA
583	HMDB0155327	NA	NA
584	HMDB0157445	NA	NA
585	HMDB0157442	NA	NA
586	HMDB0166395	NA	NA
587	HMDB0156225	NA	NA
588	HMDB0156223	NA	NA
589	HMDB0156224	NA	NA
590	HMDB0156222	NA	NA
591	HMDB0155825	NA	NA
592	HMDB0166394	NA	NA
593	HMDB0125614	NA	NA
594	HMDB0125613	NA	NA
595	HMDB0157444	NA	NA
596	HMDB0155325	NA	NA
597	HMDB0164008	NA	NA
598	HMDB0062577	NA	NA
599	HMDB0003950	7-Methylinosine	HMDB0003950
600	HMDB0002721	1-Methylinosine	HMDB0002721
601	HMDB0033060	Piperolactam A	HMDB0033060
602	HMDB0034319	Furofoline	HMDB0034319
603	HMDB0038882	NA	NA
604	HMDB0038880	NA	NA
605	HMDB0029918	Arabinofuranobiose	HMDB0029918
606	HMDB0029894	Xylobiose	HMDB0029894
607	HMDB0038855	NA	NA
608	HMDB0029619	Arabinopyranobiose	HMDB0029619
609	HMDB0038881	NA	NA
610	HMDB0179982	NA	NA
611	HMDB0179983	NA	NA
612	HMDB0179984	NA	NA
613	HMDB0028745	Asparaginylnl-Gamma-glutamate	HMDB0028745
614	HMDB0028792	Glutaminylnlasparagine	HMDB0028792
615	HMDB0028729	Asparaginylnl-Glutamine	HMDB0028729
616	HMDB0126535	NA	NA
617	HMDB0126543	NA	NA
618	HMDB0126529	NA	NA
619	HMDB0126544	NA	NA
620	HMDB0126525	NA	NA
621	HMDB0126540	NA	NA
622	HMDB0126536	NA	NA
623	HMDB0126532	NA	NA
624	HMDB0126531	NA	NA
625	HMDB0126528	NA	NA
626	HMDB0126526	NA	NA
627	HMDB0140895	NA	NA
628	HMDB0140584	NA	NA
629	HMDB0140434	NA	NA
630	HMDB0240404	NA	NA
631	HMDB0132291	NA	NA
632	HMDB0140896	NA	NA
633	HMDB0140901	NA	NA
634	HMDB0140900	NA	NA
635	HMDB0172131	NA	NA
636	HMDB0171705	NA	NA
637	HMDB0168714	NA	NA
638	HMDB0168707	NA	NA
639	HMDB0159585	NA	NA
640	HMDB0157245	NA	NA
641	HMDB0152783	NA	NA
642	HMDB0145741	NA	NA
643	HMDB0145740	NA	NA
644	HMDB0172133	NA	NA
645	HMDB0134099	NA	NA
646	HMDB0159586	NA	NA
647	HMDB0132292	NA	NA
648	HMDB0041648	NA	NA
649	HMDB0041721	NA	NA
650	HMDB0059967	NA	NA
651	HMDB0061117	NA	NA
652	HMDB0011719	Homovanillic acid sulfate	HMDB0011719
653	HMDB0002899	Ellagic acid	HMDB0002899
654	HMDB0015039	Ethacrynic acid	HMDB0015039
655	HMDB0060626	NA	NA
656	HMDB0015401	Nelarabine	HMDB0015401
657	HMDB0005862	2-Methylguanosine	HMDB0005862
658	HMDB0006038	3'-O-Methylguanosine	HMDB0006038
659	HMDB0001563	1-Methylguanosine	HMDB0001563
660	HMDB0001107	7-Methylguanosine	HMDB0001107
661	HMDB0029076	Tryptophyl-Alanine	HMDB0029076
662	HMDB0028698	Alanyl-Tryptophan	HMDB0028698
663	HMDB0142223	NA	NA
664	HMDB0013209	Alanyltryptophan	HMDB0013209
665	HMDB0165476	NA	NA
666	HMDB0165475	NA	NA
667	HMDB0165471	NA	NA
668	HMDB0165472	NA	NA

669	HMDB0126113	NA	NA
670	HMDB0130135	NA	NA
671	HMDB0130132	NA	NA
672	HMDB0130129	NA	NA
673	HMDB0145822	NA	NA
674	HMDB0130130	NA	NA
675	HMDB0164665	NA	NA
676	HMDB0130133	NA	NA
677	HMDB0130019	NA	NA
678	HMDB0126116	NA	NA
679	HMDB0126115	NA	NA
680	HMDB0130136	NA	NA
681	HMDB0126114	NA	NA
682	HMDB0178290	NA	NA
683	HMDB0178289	NA	NA
684	HMDB0181208	NA	NA
685	HMDB0167459	NA	NA
686	HMDB0167457	NA	NA
687	HMDB0167445	NA	NA
688	HMDB0167443	NA	NA
689	HMDB0167442	NA	NA
690	HMDB0167444	NA	NA
691	HMDB0167441	NA	NA
692	HMDB0167440	NA	NA
693	HMDB0167439	NA	NA
694	HMDB0003573	Scopolamine	HMDB0003573
695	HMDB0061074	NA	NA
696	HMDB0061075	NA	NA
697	HMDB0060544	NA	NA
698	HMDB0060543	NA	NA
699	HMDB0061076	NA	NA
700	HMDB0015405	Fenoterol	HMDB0015405
701	HMDB0015043	Cocaine	HMDB0015043
702	HMDB0131583	NA	NA
703	HMDB0132858	NA	NA
704	HMDB0140840	NA	NA
705	HMDB0146937	NA	NA
706	HMDB0151950	NA	NA
707	HMDB0153673	NA	NA
708	HMDB0034024	Isosativan	HMDB0034024
709	HMDB0133974	NA	NA
710	HMDB0131551	NA	NA
711	HMDB0130572	NA	NA
712	HMDB0041671	NA	NA
713	HMDB0041680	NA	NA
714	HMDB0041169	NA	NA
715	HMDB0030521	Sativan	HMDB0030521
716	HMDB0041168	NA	NA
717	HMDB0030152	4'-Hydroxy-5,7-dimethoxyflavan	HMDB0030152
718	HMDB0130384	NA	NA
719	HMDB0132908	NA	NA
720	HMDB0126611	NA	NA
721	HMDB0061205	NA	NA
722	HMDB0039423	NA	NA
723	HMDB0028813	Glutamylarginine	HMDB0028813
724	HMDB0028708	Arginyl-Glutamate	HMDB0028708
725	HMDB0029143	gamma-Glutamylarginine	HMDB0029143
726	HMDB0135641	NA	NA
727	HMDB0179385	NA	NA
728	HMDB0179388	NA	NA
729	HMDB0179383	NA	NA
730	HMDB0179382	NA	NA
731	HMDB0163720	NA	NA
732	HMDB0173550	NA	NA
733	HMDB0135574	NA	NA
734	HMDB0135576	NA	NA
735	HMDB0135572	NA	NA
736	HMDB0135564	NA	NA
737	HMDB0135568	NA	NA
738	HMDB0134573	NA	NA
739	HMDB0134571	NA	NA
740	HMDB0135570	NA	NA
741	HMDB0158752	NA	NA
742	HMDB0158753	NA	NA
743	HMDB0155927	NA	NA
744	HMDB0155928	NA	NA
745	HMDB0161130	NA	NA
746	HMDB0041096	NA	NA
747	HMDB0158750	NA	NA
748	HMDB0158751	NA	NA
749	HMDB0159487	NA	NA
750	HMDB0159488	NA	NA
751	HMDB0159490	NA	NA
752	HMDB0159830	NA	NA
753	HMDB0161128	NA	NA
754	HMDB0161127	NA	NA
755	HMDB0161129	NA	NA

756	HMDB0161132	NA	NA
757	HMDB0161133	NA	NA
758	HMDB0166865	NA	NA
759	HMDB0159483	NA	NA
760	HMDB0159484	NA	NA
761	HMDB0159482	NA	NA
762	HMDB0158755	NA	NA
763	HMDB0158759	NA	NA
764	HMDB0158758	NA	NA
765	HMDB0159491	NA	NA
766	HMDB0158756	NA	NA
767	HMDB0158876	NA	NA
768	HMDB0158877	NA	NA
769	HMDB0159485	NA	NA
770	HMDB0061135	NA	NA
771	HMDB0015176	Melphalan	HMDB0015176
772	HMDB0127928	NA	NA
773	HMDB0037110	NA	NA
774	HMDB0145098	NA	NA
775	HMDB0175072	NA	NA
776	HMDB0041450	NA	NA
777	HMDB0038322	NA	NA
778	HMDB0032909	2-(4-Methoxyphenyl)naphthalic anhydride	HMDB0032909
779	HMDB0175074	NA	NA
780	HMDB0175080	NA	NA
781	HMDB0175081	NA	NA
782	HMDB0175083	NA	NA
783	HMDB0175073	NA	NA
784	HMDB0175082	NA	NA
785	HMDB0163581	NA	NA
786	HMDB0163582	NA	NA
787	HMDB0163584	NA	NA
788	HMDB0000495	Androstanediol	HMDB0000495
789	HMDB0159493	NA	NA
790	HMDB0158029	NA	NA
791	HMDB0000554	Dihydroandrosterone	HMDB0000554
792	HMDB0000551	Etiocholanediol	HMDB0000551
793	HMDB0000458	5a-Androstane-3a,17a-diol	HMDB0000458
794	HMDB0000383	3a,17a-Dihydroxy-5b-androstane	HMDB0000383
795	HMDB0000493	5a-Androstane-3b,17b-diol	HMDB0000493
796	HMDB0000369	3b,17b-Dihydroxyetiocholanone	HMDB0000369
797	HMDB0000412	3b,17a-Dihydroxy-5a-androstane	HMDB0000412
798	HMDB0060437	Androstan-3alpha,17beta-diol	HMDB0060437
799	HMDB0167160	NA	NA
800	HMDB0167157	NA	NA
801	HMDB0156083	NA	NA
802	HMDB0167154	NA	NA
803	HMDB0167155	NA	NA
804	HMDB0167156	NA	NA
805	HMDB0062521	NA	NA
806	HMDB0167161	NA	NA
807	HMDB0167158	NA	NA
808	HMDB0173640	NA	NA
809	HMDB0186461	NA	NA
810	HMDB0167171	NA	NA
811	HMDB0167170	NA	NA
812	HMDB0186443	NA	NA
813	HMDB0167159	NA	NA
814	HMDB0167165	NA	NA
815	HMDB0167163	NA	NA
816	HMDB0167162	NA	NA
817	HMDB0167164	NA	NA
818	HMDB0167169	NA	NA
819	HMDB0167168	NA	NA
820	HMDB0167167	NA	NA
821	HMDB0167166	NA	NA
822	HMDB0014613	Dronabinol	HMDB0014613
823	HMDB0038533	NA	NA
824	HMDB0013121	7-Dehydropregnenolone	HMDB0013121
825	HMDB0031924	4-Nerolidylcatechol	HMDB0031924
826	HMDB0041865	NA	NA
827	HMDB0001830	Progesterone	HMDB0001830
828	HMDB0156085	NA	NA
829	HMDB0137415	NA	NA
830	HMDB0137402	NA	NA
831	HMDB0156084	NA	NA
832	HMDB0156089	NA	NA
833	HMDB0186441	NA	NA
834	HMDB0186440	NA	NA
835	HMDB0186438	NA	NA
836	HMDB0186439	NA	NA
837	HMDB0186444	NA	NA
838	HMDB0186457	NA	NA
839	HMDB0186462	NA	NA
840	HMDB0186435	NA	NA
841	HMDB0186437	NA	NA
842	HMDB0156091	NA	NA

843	HMDB0156092	NA	NA
844	HMDB0156093	NA	NA
845	HMDB0156090	NA	NA
846	HMDB0156094	NA	NA
847	HMDB0156095	NA	NA
848	HMDB0156840	NA	NA
849	HMDB0158166	NA	NA
850	HMDB0173643	NA	NA
851	HMDB0173642	NA	NA
852	HMDB0173641	NA	NA
853	HMDB0173645	NA	NA
854	HMDB0173644	NA	NA
855	HMDB0173646	NA	NA
856	HMDB0173647	NA	NA
857	HMDB0173648	NA	NA
858	HMDB0186436	NA	NA
859	HMDB0062609	NA	NA
860	HMDB0060424	7alpha-Hydroxypregnenolone	HMDB0060424
861	HMDB0060407	5alpha-Dihydrodeoxycorticosterone	HMDB0060407
862	HMDB0031462	[10]-Shogaol	HMDB0031462
863	HMDB0033918	(15alpha,20R)-15,20-Dihydroxypregn-4-en-3-one	HMDB0033918
864	HMDB0011653	17-alpha,20-alpha-Dihydroxypregn-4-en-3-one	HMDB0011653
865	HMDB0004026	21-Hydroxypregnenolone	HMDB0004026
866	HMDB0003851	3a,7a-Dihydroxy-5b-cholestanate	HMDB0003851
867	HMDB0000363	17a-Hydroxypregnenolone	HMDB0000363
868	HMDB0000315	16-a-Hydroxypregnenolone	HMDB0000315
869	HMDB0173549	NA	NA
870	HMDB0125510	NA	NA
871	HMDB0125509	NA	NA
872	HMDB0060017	NA	NA
873	HMDB0125511	NA	NA
874	HMDB0125508	NA	NA
875	HMDB0125512	NA	NA
876	HMDB0187598	NA	NA
877	HMDB0015513	Fludiazepam	HMDB0015513
878	HMDB0162772	NA	NA
879	HMDB0162714	NA	NA
880	HMDB0162760	NA	NA
881	HMDB0162710	NA	NA
882	HMDB0162708	NA	NA
883	HMDB0162758	NA	NA
884	HMDB0033374	Benzyl glycinate 4-methylbenzenesulfonate salt	HMDB0033374
885	HMDB0161228	NA	NA
886	HMDB0161229	NA	NA
887	HMDB0159742	NA	NA
888	HMDB0185385	NA	NA
889	HMDB0181751	NA	NA
890	HMDB0181741	NA	NA
891	HMDB0039733	NA	NA
892	HMDB0004662	S-(Hydroxymethyl)glutathione	HMDB0004662
893	HMDB0014848	Ibandronate	HMDB0014848
894	HMDB0033608	2-Heptadecylfuran	HMDB0033608
895	HMDB0034373	N-(14-Methylhexadecanoyl)pyrrolidine	HMDB0034373
896	HMDB0240592	NA	NA
897	HMDB0033108	Semilepidinoside B	HMDB0033108
898	HMDB0240296	NA	NA
899	HMDB0166033	NA	NA
900	HMDB0012492	1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylate	HMDB0012492
901	HMDB0029992	Tetrahydropentoxylone	HMDB0029992
902	HMDB0166038	NA	NA
903	HMDB0166035	NA	NA
904	HMDB0166036	NA	NA
905	HMDB0014720	Voriconazole	HMDB0014720
906	HMDB0014258	R-138727	HMDB0014258
907	HMDB0131015	NA	NA
908	HMDB0131014	NA	NA
909	HMDB0131011	NA	NA
910	HMDB0131013	NA	NA
911	HMDB0136701	NA	NA
912	HMDB0140161	NA	NA
913	HMDB0171360	NA	NA
914	HMDB0171359	NA	NA
915	HMDB0171362	NA	NA
916	HMDB0171358	NA	NA
917	HMDB0171355	NA	NA
918	HMDB0171354	NA	NA
919	HMDB0032955	5-(6-Hydroxy-3,7-dimethyl-2,7-octadienyloxy)-7-methoxycoumarin	HMDB0032955
920	HMDB0038690	NA	NA
921	HMDB0171361	NA	NA
922	HMDB0034179	Malabaricano	HMDB0034179
923	HMDB0031889	(1(10)E,4E,6a,8b)-8-Angeloyloxy-14-oxo-1(10),4,11(13)-germacatrien-12,6-olide	HMDB0031889
924	HMDB0031753	2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol	HMDB0031753
925	HMDB0038219	NA	NA
926	HMDB0040388	NA	NA
927	HMDB0040421	NA	NA
928	HMDB0036691	NA	NA
929	HMDB0039610	NA	NA

930	HMDB0125864	NA	NA
931	HMDB0172929	NA	NA
932	HMDB0148194	NA	NA
933	HMDB0040834	NA	NA
934	HMDB0040809	NA	NA
935	HMDB0041100	NA	NA
936	HMDB0041417	NA	NA
937	HMDB0035427	Glicoisoflavanone	HMDB0035427
938	HMDB0014559	Ampicillin	HMDB0014559
939	HMDB0015428	Cefradine	HMDB0015428
940	HMDB0062731	Dodecamethylpentasiloxane	HMDB0062731
941	HMDB0012983	Kinetensin 1-3	HMDB0012983
942	HMDB0011568	MG(18:2(9Z,12Z)/0:0/0:0)	HMDB0011568
943	HMDB0011538	MG(0:0/18:2(9Z,12Z)/0:0)	HMDB0011538
944	HMDB0012868	9'-Carboxy-gamma-chromanol	HMDB0012868
945	HMDB0167759	NA	NA
946	HMDB0039278	NA	NA
947	HMDB0011550	MG(0:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	HMDB0011550
948	HMDB0011580	MG(20:5(5Z,8Z,11Z,14Z,17Z)/0:0/0:0)	HMDB0011580
949	HMDB0013651	2-(14,15-Epoxyeicosatrienoyl) Glycerol	HMDB0013651
950	HMDB0012530	11-Hydroxyeicosatetraenoate glyceryl ester	HMDB0012530
951	HMDB0030281	Calycanthidine	HMDB0030281
952	HMDB0013038	Prostaglandin E2 ethanolamide	HMDB0013038
953	HMDB0013629	PGD2 ethanolamide	HMDB0013629
954	HMDB0183162	NA	NA
955	HMDB0004038	Resolvin D5	HMDB0004038
956	HMDB0030454	Macrophorin A	HMDB0030454
957	HMDB0031848	Butylated hydroxyanisole	HMDB0031848
958	HMDB0061063	NA	NA
959	HMDB0185005	NA	NA
960	HMDB0003689	Neuroprotectin D1	HMDB0003689
961	HMDB0062285	NA	NA
962	HMDB0062277	NA	NA
963	HMDB0167634	NA	NA
964	HMDB0167632	NA	NA
965	HMDB0167633	NA	NA
966	HMDB0167631	NA	NA
967	HMDB0167629	NA	NA
968	HMDB0167630	NA	NA
969	HMDB0165170	NA	NA
970	HMDB0167636	NA	NA
971	HMDB0167635	NA	NA
972	HMDB0167638	NA	NA
973	HMDB0185004	NA	NA
974	HMDB0185001	NA	NA
975	HMDB0185003	NA	NA
976	HMDB0185002	NA	NA
977	HMDB0184999	NA	NA
978	HMDB0167640	NA	NA
979	HMDB0167639	NA	NA
980	HMDB0167637	NA	NA
981	HMDB0061065	NA	NA
982	HMDB0061064	NA	NA
983	HMDB0011131	MG(18:0/0:0/0:0)	HMDB0011131
984	HMDB0031075	Glycerol 1-octadecanoate	HMDB0031075
985	HMDB0072842	NA	NA
986	HMDB0011535	MG(0:0/18:0/0:0)	HMDB0011535
987	HMDB0072877	NA	NA
988	HMDB0032735	Isopersin	HMDB0032735
989	HMDB0039403	NA	NA
990	HMDB0011577	MG(20:3(8Z,11Z,14Z)/0:0/0:0)	HMDB0011577
991	HMDB0011576	MG(20:3(5Z,8Z,11Z)/0:0/0:0)	HMDB0011576
992	HMDB0011575	MG(20:3(11Z,14Z,17Z)/0:0/0:0)	HMDB0011575
993	HMDB0011547	MG(0:0/20:3(8Z,11Z,14Z)/0:0)	HMDB0011547
994	HMDB0011545	MG(0:0/20:3(11Z,14Z,17Z)/0:0)	HMDB0011545
995	HMDB0011546	MG(0:0/20:3(5Z,8Z,11Z)/0:0)	HMDB0011546
996	HMDB0041103	NA	NA
997	HMDB0140016	NA	NA
998	HMDB0140097	NA	NA
999	HMDB0039021	NA	NA
1000	HMDB0039020	NA	NA
1001	HMDB0039019	NA	NA
1002	HMDB0005066	Tetradecanoylcarnitine	HMDB0005066
1003	HMDB0013335	3-Hydroxyhexadecadienoylcarnitine	HMDB0013335
1004	HMDB0240762	NA	NA
1005	HMDB0060833	NA	NA
1006	HMDB0185381	NA	NA
1007	HMDB0002873	Deacetyldiltiazem	HMDB0002873
1008	HMDB0124912	NA	NA
1009	HMDB0124915	NA	NA
1010	HMDB0124828	NA	NA
1011	HMDB0124911	NA	NA
1012	HMDB0124914	NA	NA
1013	HMDB0124913	NA	NA
1014	HMDB0125800	NA	NA
1015	HMDB0131078	NA	NA
1016	HMDB0131080	NA	NA

1017	HMDB0131077	NA	NA
1018	HMDB0130292	NA	NA
1019	HMDB0130291	NA	NA
1020	HMDB0130288	NA	NA
1021	HMDB0130290	NA	NA
1022	HMDB0130289	NA	NA
1023	HMDB0130100	NA	NA
1024	HMDB0130099	NA	NA
1025	HMDB0124817	NA	NA
1026	HMDB0124816	NA	NA
1027	HMDB0124815	NA	NA
1028	HMDB0124810	NA	NA
1029	HMDB0124811	NA	NA
1030	HMDB0124813	NA	NA
1031	HMDB0124812	NA	NA
1032	HMDB0133480	NA	NA
1033	HMDB0149865	NA	NA
1034	HMDB0149860	NA	NA
1035	HMDB0149855	NA	NA
1036	HMDB0149846	NA	NA
1037	HMDB0149841	NA	NA
1038	HMDB0149835	NA	NA
1039	HMDB0149834	NA	NA
1040	HMDB0146994	NA	NA
1041	HMDB0146992	NA	NA
1042	HMDB0146993	NA	NA
1043	HMDB0146989	NA	NA
1044	HMDB0133520	NA	NA
1045	HMDB0133514	NA	NA
1046	HMDB0133513	NA	NA
1047	HMDB0133493	NA	NA
1048	HMDB0133492	NA	NA
1049	HMDB0133481	NA	NA
1050	HMDB0146939	NA	NA
1051	HMDB0131836	NA	NA
1052	HMDB0131837	NA	NA
1053	HMDB0131838	NA	NA
1054	HMDB0133527	NA	NA
1055	HMDB0133537	NA	NA
1056	HMDB0137511	NA	NA
1057	HMDB0146987	NA	NA
1058	HMDB0146988	NA	NA
1059	HMDB0146986	NA	NA
1060	HMDB0146947	NA	NA
1061	HMDB0146945	NA	NA
1062	HMDB0146944	NA	NA
1063	HMDB0146941	NA	NA
1064	HMDB0146940	NA	NA
1065	HMDB0146938	NA	NA
1066	HMDB0138813	NA	NA
1067	HMDB0131079	NA	NA
1068	HMDB0039066	NA	NA
1069	HMDB0041416	NA	NA
1070	HMDB0030826	2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-methylenedioxyphenyl)-1-propanol	HMDB0030826
1071	HMDB0035182	Licoriphenone	HMDB0035182
1072	HMDB0032733	(8R,8'R,9S)-9-Hydroxy-3,4-dimethoxy-3',4'-methylenoxy-9,9'-epoxylignan	HMDB0032733
1073	HMDB0005789	Tetrahydrocurcumin	HMDB0005789
1074	HMDB0030087	(-)-Arctigenin	HMDB0030087
1075	HMDB0032734	9-Hydroxy-3',4'-dimethoxy-3,4-methylenedioxy-9,9'-epoxylignan	HMDB0032734
1076	HMDB0164958	NA	NA
1077	HMDB0029510	Garcinone B	HMDB0029510
1078	HMDB0034436	Rotenone	HMDB0034436
1079	HMDB0036984	NA	NA
1080	HMDB0148796	NA	NA
1081	HMDB0146129	NA	NA
1082	HMDB0173953	NA	NA
1083	HMDB0184813	NA	NA
1084	HMDB0184985	NA	NA
1085	HMDB0184812	NA	NA
1086	HMDB0184811	NA	NA
1087	HMDB0184810	NA	NA
1088	HMDB0173968	NA	NA
1089	HMDB0173965	NA	NA
1090	HMDB0173956	NA	NA
1091	HMDB0039867	NA	NA
1092	HMDB0035584	1-Phenyl-1,3-nonadecanediol	HMDB0035584
1093	HMDB0038506	NA	NA
1094	HMDB0174608	NA	NA
1095	HMDB0173235	NA	NA
1096	HMDB0171546	NA	NA
1097	HMDB0036848	NA	NA
1098	HMDB0039022	NA	NA
1099	HMDB0036849	NA	NA
1100	HMDB0040749	NA	NA
1101	HMDB0040765	NA	NA
1102	HMDB0015567	Calcipotriol	HMDB0015567
1103	HMDB0015434	Forasartan	HMDB0015434

1104	HMDB0014940	Alfentanil	HMDB0014940
1105	HMDB0182768	NA	NA
1106	HMDB0182223	NA	NA
1107	HMDB0187634	NA	NA
1108	HMDB0182254	NA	NA
1109	HMDB0172273	NA	NA
1110	HMDB0172275	NA	NA
1111	HMDB0172274	NA	NA
1112	HMDB0174261	NA	NA
1113	HMDB0174260	NA	NA
1114	HMDB0174265	NA	NA
1115	HMDB0174262	NA	NA
1116	HMDB0174263	NA	NA
1117	HMDB0174264	NA	NA
1118	HMDB0174266	NA	NA
1119	HMDB0155085	NA	NA
1120	HMDB0155087	NA	NA
1121	HMDB0154867	NA	NA
1122	HMDB0154866	NA	NA
1123	HMDB0155080	NA	NA
1124	HMDB0155083	NA	NA
1125	HMDB0155082	NA	NA
1126	HMDB0155081	NA	NA
1127	HMDB0155084	NA	NA
1128	HMDB0155086	NA	NA
1129	HMDB0174267	NA	NA
1130	HMDB0174268	NA	NA
1131	HMDB0184842	NA	NA
1132	HMDB0184845	NA	NA
1133	HMDB0184846	NA	NA
1134	HMDB0184848	NA	NA
1135	HMDB0184847	NA	NA
1136	HMDB0184849	NA	NA
1137	HMDB0184851	NA	NA
1138	HMDB0184850	NA	NA
1139	HMDB0185576	NA	NA
1140	HMDB0185577	NA	NA
1141	HMDB0184843	NA	NA
1142	HMDB0184841	NA	NA
1143	HMDB0184144	NA	NA
1144	HMDB0184143	NA	NA
1145	HMDB0184146	NA	NA
1146	HMDB0184145	NA	NA
1147	HMDB0184147	NA	NA
1148	HMDB0184148	NA	NA
1149	HMDB0184150	NA	NA
1150	HMDB0184149	NA	NA
1151	HMDB0184168	NA	NA
1152	HMDB0184844	NA	NA
1153	HMDB0185578	NA	NA
1154	HMDB0003550	Calcidiol	HMDB0003550
1155	HMDB0060132	NA	NA
1156	HMDB0060131	NA	NA
1157	HMDB0015504	Alfacalcidol	HMDB0015504
1158	HMDB0000501	7-Ketocholesterol	HMDB0000501
1159	HMDB0001993	7a-Hydroxy-cholestene-3-one	HMDB0001993
1160	HMDB0006722	25-Hydroxytachysterol3	HMDB0006722
1161	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	HMDB0006721
1162	HMDB0035585	1-Phenyl-1,3-heneicosanedione	HMDB0035585
1163	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	HMDB0034328
1164	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	HMDB0036012
1165	HMDB0039871	NA	NA
1166	HMDB0159655	NA	NA
1167	HMDB0159658	NA	NA
1168	HMDB0159656	NA	NA
1169	HMDB0159657	NA	NA
1170	HMDB0159654	NA	NA
1171	HMDB0159653	NA	NA
1172	HMDB0159651	NA	NA
1173	HMDB0159652	NA	NA
1174	HMDB0062675	NA	NA
1175	HMDB0062664	NA	NA
1176	HMDB0062419	NA	NA
1177	HMDB0062420	NA	NA
1178	HMDB0062607	NA	NA
1179	HMDB0172263	NA	NA
1180	HMDB0172264	NA	NA
1181	HMDB0185568	NA	NA
1182	HMDB0185570	NA	NA
1183	HMDB0185567	NA	NA
1184	HMDB0185569	NA	NA
1185	HMDB0185572	NA	NA
1186	HMDB0185575	NA	NA
1187	HMDB0185571	NA	NA
1188	HMDB0185574	NA	NA
1189	HMDB0185566	NA	NA
1190	HMDB0172272	NA	NA

1191	HMDB0172262	NA	NA
1192	HMDB0172266	NA	NA
1193	HMDB0172268	NA	NA
1194	HMDB0172265	NA	NA
1195	HMDB0172267	NA	NA
1196	HMDB0172270	NA	NA
1197	HMDB0172269	NA	NA
1198	HMDB0172271	NA	NA
1199	HMDB0185573	NA	NA
1200	HMDB0006280	7-a,25-Dihydroxycholesterol	HMDB0006280
1201	HMDB0060136	7alpha,24S-Dihydroxycholesterol	HMDB0060136
1202	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol	HMDB0011644
1203	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al	HMDB0006894
1204	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one	HMDB0006887
1205	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one	HMDB0006886
1206	HMDB0006764	17a,20a-Dihydroxycholesterol	HMDB0006764
1207	HMDB0006763	20a,22b-Dihydroxycholesterol	HMDB0006763
1208	HMDB0006281	7-a,27-Dihydroxycholesterol	HMDB0006281
1209	HMDB0035951	Erucylacetone	HMDB0035951
1210	HMDB0037260	NA	NA
1211	HMDB0158333	NA	NA
1212	HMDB0150478	NA	NA
1213	HMDB0150475	NA	NA
1214	HMDB0162509	NA	NA
1215	HMDB0150477	NA	NA
1216	HMDB0038347	NA	NA
1217	HMDB0150474	NA	NA
1218	HMDB0150463	NA	NA
1219	HMDB0150458	NA	NA
1220	HMDB0150468	NA	NA
1221	HMDB0150470	NA	NA
1222	HMDB0150457	NA	NA
1223	HMDB0150453	NA	NA
1224	HMDB0150469	NA	NA
1225	HMDB0150452	NA	NA
1226	HMDB0149868	NA	NA
1227	HMDB0150462	NA	NA
1228	HMDB0140070	NA	NA
1229	HMDB0153459	NA	NA
1230	HMDB0153444	NA	NA
1231	HMDB0153474	NA	NA
1232	HMDB0153627	NA	NA
1233	HMDB0153466	NA	NA
1234	HMDB0139521	NA	NA
1235	HMDB0139520	NA	NA
1236	HMDB0139517	NA	NA
1237	HMDB0139504	NA	NA
1238	HMDB0139507	NA	NA
1239	HMDB0139514	NA	NA
1240	HMDB0149502	NA	NA
1241	HMDB0153458	NA	NA
1242	HMDB0153451	NA	NA
1243	HMDB0153443	NA	NA
1244	HMDB0139516	NA	NA
1245	HMDB0139508	NA	NA
1246	HMDB0139513	NA	NA
1247	HMDB0035876	Mesuagin	HMDB0035876
1248	HMDB0180147	NA	NA
1249	HMDB0013842	O-Deethylated candesartan	HMDB0013842
1250	HMDB0144444	NA	NA
1251	HMDB0144965	NA	NA
1252	HMDB0144871	NA	NA
1253	HMDB0142647	NA	NA
1254	HMDB0144859	NA	NA
1255	HMDB0144408	NA	NA
1256	HMDB0144379	NA	NA
1257	HMDB0142761	NA	NA
1258	HMDB0142694	NA	NA
1259	HMDB0144418	NA	NA
1260	HMDB0144964	NA	NA
1261	HMDB0142682	NA	NA
1262	HMDB0144733	NA	NA
1263	HMDB0011503	LysoPE(16:0/0:0)	HMDB0011503
1264	HMDB0011473	LysoPE(0:0/16:0)	HMDB0011473
1265	HMDB0160383	NA	NA
1266	HMDB0007851	LysoPA(0:0/18:1(9Z))	HMDB0007851
1267	HMDB0007855	LysoPA(18:1(9Z)/0:0)	HMDB0007855
1268	HMDB0187017	NA	NA
1269	HMDB0155795	NA	NA
1270	HMDB0160382	NA	NA
1271	HMDB0011133	DHAP(18:0)	HMDB0011133
1272	HMDB0187016	NA	NA
1273	HMDB0161139	NA	NA
1274	HMDB0041085	NA	NA
1275	HMDB0032798	(R)-1-O-[b-D-Apiofuranosyl-(1->2)-b-D-glucopyranoside]-1,3-octanediol	HMDB0032798
1276	HMDB0159681	NA	NA
1277	HMDB0159673	NA	NA

1278	HMDB0157616	NA	NA
1279	HMDB0159671	NA	NA
1280	HMDB0159668	NA	NA
1281	HMDB0159669	NA	NA
1282	HMDB0157629	NA	NA
1283	HMDB0157630	NA	NA
1284	HMDB0157615	NA	NA
1285	HMDB0062712	NA	NA
1286	HMDB0062686	NA	NA
1287	HMDB0062400	NA	NA
1288	HMDB0062399	NA	NA
1289	HMDB0159672	NA	NA
1290	HMDB0159676	NA	NA
1291	HMDB0159675	NA	NA
1292	HMDB0062794	NA	NA
1293	HMDB0159670	NA	NA
1294	HMDB0159683	NA	NA
1295	HMDB0159684	NA	NA
1296	HMDB0159682	NA	NA
1297	HMDB0159680	NA	NA
1298	HMDB0159679	NA	NA
1299	HMDB0159678	NA	NA
1300	HMDB0159677	NA	NA
1301	HMDB0159674	NA	NA
1302	HMDB0012454	3beta,7alpha-Dihydroxy-5-cholestenoate	HMDB0012454
1303	HMDB0062211	NA	NA
1304	HMDB0060134	NA	NA
1305	HMDB0006228	24-Hydroxycalcitriol	HMDB0006228
1306	HMDB0030702	Neochlorogenin	HMDB0030702
1307	HMDB0033769	Rockogenin	HMDB0033769
1308	HMDB0173231	NA	NA
1309	HMDB0036850	NA	NA
1310	HMDB0006710	Ubiquinone-4	HMDB0006710
1311	HMDB0012556	13'-Carboxy-alpha-tocotrienol	HMDB0012556
1312	HMDB0035112	(3beta,17alpha,23R)-17,23-Epoxy-3,29-dihydroxy-27-norlanost-8-ene-15,24-dione	HMDB0035112
1313	HMDB0035843	(23S,24S)-17,23-Epoxy-24,29-dihydroxy-27-norlanost-8-ene-3,15-dione	HMDB0035843
1314	HMDB0035624	(17alpha,23S)-Epoxy-28,29-dihydroxy-27-norlanost-8-ene-3,24-dione	HMDB0035624
1315	HMDB0175485	NA	NA
1316	HMDB0175491	NA	NA
1317	HMDB0175488	NA	NA
1318	HMDB0175481	NA	NA
1319	HMDB0175475	NA	NA
1320	HMDB0175477	NA	NA
1321	HMDB0175479	NA	NA
1322	HMDB0175474	NA	NA
1323	HMDB0240598	NA	NA
1324	HMDB0160534	NA	NA
1325	HMDB0160531	NA	NA
1326	HMDB0160532	NA	NA
1327	HMDB0160533	NA	NA
1328	HMDB0160538	NA	NA
1329	HMDB0160535	NA	NA
1330	HMDB0160536	NA	NA
1331	HMDB0160537	NA	NA
1332	HMDB0039079	NA	NA
1333	HMDB0039024	NA	NA
1334	HMDB0160175	NA	NA
1335	HMDB0160176	NA	NA
1336	HMDB0160173	NA	NA
1337	HMDB0160172	NA	NA
1338	HMDB0160170	NA	NA
1339	HMDB0160169	NA	NA
1340	HMDB0160171	NA	NA
1341	HMDB0157668	NA	NA
1342	HMDB0157667	NA	NA
1343	HMDB0157669	NA	NA
1344	HMDB0157665	NA	NA
1345	HMDB0157666	NA	NA
1346	HMDB0160174	NA	NA
1347	HMDB0160180	NA	NA
1348	HMDB0160177	NA	NA
1349	HMDB0160512	NA	NA
1350	HMDB0160514	NA	NA
1351	HMDB0160511	NA	NA
1352	HMDB0160513	NA	NA
1353	HMDB0160510	NA	NA
1354	HMDB0160508	NA	NA
1355	HMDB0160507	NA	NA
1356	HMDB0160509	NA	NA
1357	HMDB0160182	NA	NA
1358	HMDB0160181	NA	NA
1359	HMDB0160178	NA	NA
1360	HMDB0160179	NA	NA
1361	HMDB0157663	NA	NA
1362	HMDB0157664	NA	NA
1363	HMDB0157661	NA	NA
1364	HMDB0062534	NA	NA

1365	HMDB0157659	NA	NA
1366	HMDB0157660	NA	NA
1367	HMDB0157662	NA	NA
1368	HMDB0157655	NA	NA
1369	HMDB0157658	NA	NA
1370	HMDB0157657	NA	NA
1371	HMDB0157656	NA	NA
1372	HMDB0039015	NA	NA
1373	HMDB0184086	NA	NA
1374	HMDB0002385	Celastrol	HMDB0002385
1375	HMDB0015057	Buprenorphine	HMDB0015057
1376	HMDB0062331	NA	NA
1377	HMDB0010379	LysoPC(14:0)	HMDB0010379
1378	HMDB0061691	NA	NA
1379	HMDB0161447	NA	NA
1380	HMDB0179451	NA	NA
1381	HMDB0062337	NA	NA
1382	HMDB0010381	LysoPC(15:0)	HMDB0010381
1383	HMDB0011130	LysoPE(18:0/0:0)	HMDB0011130
1384	HMDB0011129	LysoPE(0:0/18:0)	HMDB0011129
1385	HMDB0062305	NA	NA
1386	HMDB0172584	NA	NA
1387	HMDB0172583	NA	NA
1388	HMDB0154880	NA	NA
1389	HMDB0184865	NA	NA
1390	HMDB0172431	NA	NA
1391	HMDB0175550	NA	NA
1392	HMDB0172429	NA	NA
1393	HMDB0175542	NA	NA
1394	HMDB0175548	NA	NA
1395	HMDB0175549	NA	NA
1396	HMDB0160542	NA	NA
1397	HMDB0160540	NA	NA
1398	HMDB0160539	NA	NA
1399	HMDB0160541	NA	NA
1400	HMDB0160543	NA	NA
1401	HMDB0160544	NA	NA
1402	HMDB0160545	NA	NA
1403	HMDB0034216	Adouetine X	HMDB0034216
1404	HMDB0030199	Frangulanine	HMDB0030199
1405	HMDB0032879	all-trans-Carophyll yellow	HMDB0032879
1406	HMDB0010380	LysoPC(14:1(9Z))	HMDB0010380
1407	HMDB0170639	NA	NA
1408	HMDB0170632	NA	NA
1409	HMDB0170638	NA	NA
1410	HMDB0170641	NA	NA
1411	HMDB0170637	NA	NA
1412	HMDB0170661	NA	NA
1413	HMDB0170640	NA	NA
1414	HMDB0170634	NA	NA
1415	HMDB0170636	NA	NA
1416	HMDB0170633	NA	NA
1417	HMDB0170635	NA	NA
1418	HMDB0170642	NA	NA
1419	HMDB0011481	LysoPE(0:0/20:0)	HMDB0011481
1420	HMDB0012108	LysoPC(17:0)	HMDB0012108
1421	HMDB0011511	LysoPE(20:0/0:0)	HMDB0011511
1422	HMDB0114750	NA	NA
1423	HMDB0062304	NA	NA
1424	HMDB0030291	Daphniphylline	HMDB0030291
1425	HMDB0183973	NA	NA
1426	HMDB0174607	NA	NA
1427	HMDB0174422	NA	NA
1428	HMDB0171595	NA	NA
1429	HMDB0167550	NA	NA
1430	HMDB0167544	NA	NA
1431	HMDB0167357	NA	NA
1432	HMDB0166718	NA	NA
1433	HMDB0166240	NA	NA
1434	HMDB0162256	NA	NA
1435	HMDB0011149	LysoPC(O-18:0)	HMDB0011149
1436	HMDB0062689	NA	NA
1437	HMDB0176475	NA	NA
1438	HMDB0183620	NA	NA
1439	HMDB0183626	NA	NA
1440	HMDB0183623	NA	NA
1441	HMDB0062314	NA	NA
1442	HMDB0114749	NA	NA
1443	HMDB0114769	NA	NA
1444	HMDB0011490	LysoPE(0:0/22:0)	HMDB0011490
1445	HMDB0011520	LysoPE(22:0/0:0)	HMDB0011520
1446	HMDB0114757	NA	NA
1447	HMDB0165392	NA	NA
1448	HMDB0171540	NA	NA
1449	HMDB0015129	Neomycin	HMDB0015129
1450	HMDB0002160	Harderoporpyrinogen	HMDB0002160
1451	HMDB0039454	NA	NA

1452	HMDB0173693	NA	NA
1453	HMDB0173692	NA	NA
1454	HMDB0173699	NA	NA
1455	HMDB0173698	NA	NA
1456	HMDB0142988	NA	NA
1457	HMDB0142998	NA	NA
1458	HMDB0142997	NA	NA
1459	HMDB0143001	NA	NA
1460	HMDB0142987	NA	NA
1461	HMDB0142978	NA	NA
1462	HMDB0142977	NA	NA
1463	HMDB0142917	NA	NA
1464	HMDB0142918	NA	NA
1465	HMDB0142919	NA	NA
1466	HMDB0142921	NA	NA
1467	HMDB0142920	NA	NA
1468	HMDB0142926	NA	NA
1469	HMDB0142929	NA	NA
1470	HMDB0142928	NA	NA
1471	HMDB0142927	NA	NA
1472	HMDB0143002	NA	NA
1473	HMDB0143007	NA	NA
1474	HMDB0143006	NA	NA
1475	HMDB0143108	NA	NA
1476	HMDB0143104	NA	NA
1477	HMDB0143098	NA	NA
1478	HMDB0143093	NA	NA
1479	HMDB0143086	NA	NA
1480	HMDB0143085	NA	NA
1481	HMDB0143076	NA	NA
1482	HMDB0143075	NA	NA
1483	HMDB0143066	NA	NA
1484	HMDB0143065	NA	NA
1485	HMDB0143061	NA	NA
1486	HMDB0143060	NA	NA
1487	HMDB0143022	NA	NA
1488	HMDB0143012	NA	NA
1489	HMDB0143011	NA	NA
1490	HMDB0143021	NA	NA
1491	HMDB0142916	NA	NA
1492	HMDB0142915	NA	NA
1493	HMDB0142901	NA	NA
1494	HMDB0142899	NA	NA
1495	HMDB0142902	NA	NA
1496	HMDB0142900	NA	NA
1497	HMDB0142905	NA	NA
1498	HMDB0142904	NA	NA
1499	HMDB0142903	NA	NA
1500	HMDB0142908	NA	NA
1501	HMDB0142911	NA	NA
1502	HMDB0142913	NA	NA
1503	HMDB0142914	NA	NA
1504	HMDB0142912	NA	NA
1505	HMDB0142930	NA	NA
1506	HMDB0165936	NA	NA
1507	HMDB0165918	NA	NA
1508	HMDB0173230	NA	NA
1509	HMDB0173229	NA	NA
1510	HMDB0165966	NA	NA
1511	HMDB0164809	NA	NA
1512	HMDB0034433	Riboflavine 2',3',4',5'-tetrabutanoate	HMDB0034433
1513	HMDB0157944	NA	NA
1514	HMDB0157945	NA	NA
1515	HMDB0157949	NA	NA
1516	HMDB0157950	NA	NA
1517	HMDB0157951	NA	NA
1518	HMDB0157955	NA	NA
1519	HMDB0157956	NA	NA
1520	HMDB0157943	NA	NA
1521	HMDB0157938	NA	NA
1522	HMDB0157939	NA	NA
1523	HMDB0157937	NA	NA
1524	HMDB0157933	NA	NA
1525	HMDB0157932	NA	NA
1526	HMDB0157931	NA	NA
1527	HMDB0157898	NA	NA
1528	HMDB0157896	NA	NA
1529	HMDB0157957	NA	NA
1530	HMDB0158932	NA	NA
1531	HMDB0158968	NA	NA
1532	HMDB0158964	NA	NA
1533	HMDB0158963	NA	NA
1534	HMDB0158958	NA	NA
1535	HMDB0158959	NA	NA
1536	HMDB0158953	NA	NA
1537	HMDB0158954	NA	NA
1538	HMDB0158949	NA	NA

1539	HMDB0158948	NA	NA
1540	HMDB0158944	NA	NA
1541	HMDB0158943	NA	NA
1542	HMDB0158937	NA	NA
1543	HMDB0158938	NA	NA
1544	HMDB0158939	NA	NA
1545	HMDB0158933	NA	NA
1546	HMDB0158969	NA	NA
1547	HMDB0157897	NA	NA
1548	HMDB0157050	NA	NA
1549	HMDB0157221	NA	NA
1550	HMDB0157842	NA	NA
1551	HMDB0157841	NA	NA
1552	HMDB0157843	NA	NA
1553	HMDB0157847	NA	NA
1554	HMDB0157846	NA	NA
1555	HMDB0157851	NA	NA
1556	HMDB0157848	NA	NA
1557	HMDB0157853	NA	NA
1558	HMDB0157215	NA	NA
1559	HMDB0157218	NA	NA
1560	HMDB0157212	NA	NA
1561	HMDB0157051	NA	NA
1562	HMDB0157054	NA	NA
1563	HMDB0157057	NA	NA
1564	HMDB0157060	NA	NA
1565	HMDB0157066	NA	NA
1566	HMDB0157063	NA	NA
1567	HMDB0157206	NA	NA
1568	HMDB0157205	NA	NA
1569	HMDB0157209	NA	NA
1570	HMDB0157852	NA	NA
1571	HMDB0157856	NA	NA
1572	HMDB0157857	NA	NA
1573	HMDB0157876	NA	NA
1574	HMDB0157881	NA	NA
1575	HMDB0157882	NA	NA
1576	HMDB0157883	NA	NA
1577	HMDB0157886	NA	NA
1578	HMDB0157887	NA	NA
1579	HMDB0157888	NA	NA
1580	HMDB0157891	NA	NA
1581	HMDB0157892	NA	NA
1582	HMDB0157893	NA	NA
1583	HMDB0157878	NA	NA
1584	HMDB0157877	NA	NA
1585	HMDB0157858	NA	NA
1586	HMDB0157861	NA	NA
1587	HMDB0157862	NA	NA
1588	HMDB0157863	NA	NA
1589	HMDB0157866	NA	NA
1590	HMDB0157867	NA	NA
1591	HMDB0157868	NA	NA
1592	HMDB0157871	NA	NA
1593	HMDB0157873	NA	NA
1594	HMDB0157872	NA	NA
1595	HMDB0165986	NA	NA
1596	HMDB0165987	NA	NA
1597	HMDB0166012	NA	NA
1598	HMDB0166013	NA	NA
1599	HMDB0166011	NA	NA
1600	HMDB0166007	NA	NA
1601	HMDB0170721	NA	NA
1602	HMDB0166009	NA	NA
1603	HMDB0166010	NA	NA
1604	HMDB0166004	NA	NA
1605	HMDB0166005	NA	NA
1606	HMDB0166003	NA	NA
1607	HMDB0166006	NA	NA
1608	HMDB0167988	NA	NA
1609	HMDB0167989	NA	NA
1610	HMDB0168064	NA	NA
1611	HMDB0170719	NA	NA
1612	HMDB0170718	NA	NA
1613	HMDB0168079	NA	NA
1614	HMDB0168080	NA	NA
1615	HMDB0168077	NA	NA
1616	HMDB0168076	NA	NA
1617	HMDB0168068	NA	NA
1618	HMDB0168067	NA	NA
1619	HMDB0168065	NA	NA
1620	HMDB0166001	NA	NA
1621	HMDB0166002	NA	NA
1622	HMDB0170734	NA	NA
1623	HMDB0165975	NA	NA
1624	HMDB0165973	NA	NA
1625	HMDB0165879	NA	NA

1626	HMDB0165880	NA	NA
1627	HMDB0170735	NA	NA
1628	HMDB0170737	NA	NA
1629	HMDB0166008	NA	NA
1630	HMDB0165977	NA	NA
1631	HMDB0165978	NA	NA
1632	HMDB0165999	NA	NA
1633	HMDB0165985	NA	NA
1634	HMDB0165984	NA	NA
1635	HMDB0165976	NA	NA
1636	HMDB0165983	NA	NA
1637	HMDB0165980	NA	NA
1638	HMDB0165981	NA	NA
1639	HMDB0165982	NA	NA
1640	HMDB0165979	NA	NA
1641	HMDB0177535	NA	NA
1642	HMDB0177543	NA	NA
1643	HMDB0177537	NA	NA
1644	HMDB0177545	NA	NA
1645	HMDB0177544	NA	NA
1646	HMDB0177546	NA	NA
1647	HMDB0177536	NA	NA
1648	HMDB0166014	NA	NA
1649	HMDB0165988	NA	NA
1650	HMDB0143644	NA	NA
1651	HMDB0041431	NA	NA
1652	HMDB0175661	NA	NA
1653	HMDB0175651	NA	NA
1654	HMDB0175656	NA	NA
1655	HMDB0175652	NA	NA
1656	HMDB0175662	NA	NA
1657	HMDB0175657	NA	NA
1658	HMDB0186380	NA	NA
1659	HMDB0186379	NA	NA
1660	HMDB0186374	NA	NA
1661	HMDB0186377	NA	NA
1662	HMDB0186373	NA	NA
1663	HMDB0186376	NA	NA
1664	HMDB0164570	NA	NA
1665	HMDB0030751	1,26-Hexacosanediol diferulate	HMDB0030751
1666	HMDB0038064	NA	NA
1667	HMDB0156198	NA	NA
1668	HMDB0156204	NA	NA
1669	HMDB0156203	NA	NA
1670	HMDB0156205	NA	NA
1671	HMDB0156202	NA	NA
1672	HMDB0156200	NA	NA
1673	HMDB0156199	NA	NA
1674	HMDB0156201	NA	NA
1675	HMDB0156197	NA	NA
1676	HMDB0008880	PE(14:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0008880
1677	HMDB0009680	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/14:1(9Z))	HMDB0009680
1678	HMDB0009194	PE(18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	HMDB0009194
1679	HMDB0009193	PE(18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	HMDB0009193
1680	HMDB0009129	PE(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	HMDB0009129
1681	HMDB0009162	PE(18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	HMDB0009162
1682	HMDB0012375	PS(18:0/14:1(9Z))	HMDB0012375
1683	HMDB0012345	PS(14:1(9Z)/18:0)	HMDB0012345
1684	HMDB0012355	PS(16:0/16:1(9Z))	HMDB0012355
1685	HMDB0012365	PS(16:1(9Z)/16:0)	HMDB0012365
1686	HMDB0012335	PS(14:0/18:1(9Z))	HMDB0012335
1687	HMDB0112269	NA	NA
1688	HMDB0112266	NA	NA
1689	HMDB0012385	PS(18:1(9Z)/14:0)	HMDB0012385
1690	HMDB0115537	NA	NA
1691	HMDB0114811	NA	NA
1692	HMDB0114845	NA	NA
1693	HMDB0114865	NA	NA
1694	HMDB0114907	NA	NA
1695	HMDB0114932	NA	NA
1696	HMDB0114958	NA	NA
1697	HMDB0115097	NA	NA
1698	HMDB0115098	NA	NA
1699	HMDB0115274	NA	NA
1700	HMDB0115299	NA	NA
1701	HMDB0115456	NA	NA
1702	HMDB0115514	NA	NA
1703	HMDB0115070	NA	NA
1704	HMDB0112956	NA	NA
1705	HMDB0112955	NA	NA
1706	HMDB0112957	NA	NA
1707	HMDB0113920	NA	NA
1708	HMDB0113309	NA	NA
1709	HMDB0114067	NA	NA
1710	HMDB0112984	NA	NA
1711	HMDB0113337	NA	NA
1712	HMDB0113167	NA	NA

1713	HMDB0113141	NA	NA
1714	HMDB0113114	NA	NA
1715	HMDB0113042	NA	NA
1716	HMDB0008901	PE(15:0/20:2(11Z,14Z))	HMDB0008901
1717	HMDB0009285	PE(20:2(11Z,14Z)/15:0)	HMDB0009285
1718	HMDB0008130	PC(18:2(9Z,12Z)/14:0)	HMDB0008130
1719	HMDB0007874	PC(14:0/18:2(9Z,12Z))	HMDB0007874
1720	HMDB0008098	PC(18:1(9Z)/14:1(9Z))	HMDB0008098
1721	HMDB0008002	PC(16:1(9Z)/16:1(9Z))	HMDB0008002
1722	HMDB0007906	PC(14:1(9Z)/18:1(9Z))	HMDB0007906
1723	HMDB0007905	PC(14:1(9Z)/18:1(11Z))	HMDB0007905
1724	HMDB0008065	PC(18:1(11Z)/14:1(9Z))	HMDB0008065
1725	HMDB0008460	PC(20:4(8Z,11Z,14Z,17Z)/14:1(9Z))	HMDB0008460
1726	HMDB0007885	PC(14:0/20:5(5Z,8Z,11Z,14Z,17Z))	HMDB0007885
1727	HMDB0007917	PC(14:1(9Z)/20:4(8Z,11Z,14Z,17Z))	HMDB0007917
1728	HMDB0007916	PC(14:1(9Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0007916
1729	HMDB0008233	PC(18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	HMDB0008233
1730	HMDB0008427	PC(20:4(5Z,8Z,11Z,14Z)/14:1(9Z))	HMDB0008427
1731	HMDB0008492	PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:0)	HMDB0008492
1732	HMDB0008911	PE(15:0/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0008911
1733	HMDB0008912	PE(15:0/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0008912
1734	HMDB0009615	PE(22:5(4Z,7Z,10Z,13Z,16Z)/15:0)	HMDB0009615
1735	HMDB0009648	PE(22:5(7Z,10Z,13Z,16Z,19Z)/15:0)	HMDB0009648
1736	HMDB0008009	PC(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	HMDB0008009
1737	HMDB0113482	NA	NA
1738	HMDB0113173	NA	NA
1739	HMDB0116726	NA	NA
1740	HMDB0113229	NA	NA
1741	HMDB0113256	NA	NA
1742	HMDB0113257	NA	NA
1743	HMDB0113426	NA	NA
1744	HMDB0113454	NA	NA
1745	HMDB0113174	NA	NA
1746	HMDB0113146	NA	NA
1747	HMDB0113119	NA	NA
1748	HMDB0112994	NA	NA
1749	HMDB0112995	NA	NA
1750	HMDB0113012	NA	NA
1751	HMDB0113051	NA	NA
1752	HMDB0113072	NA	NA
1753	HMDB0113073	NA	NA
1754	HMDB0113593	NA	NA
1755	HMDB0113620	NA	NA
1756	HMDB0114383	NA	NA
1757	HMDB0113646	NA	NA
1758	HMDB0113930	NA	NA
1759	HMDB0055799	NA	NA
1760	HMDB0010560	TG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0010560
1761	HMDB0004879	Trihexosylceramide (d18:1/16:0)	HMDB0004879
1762	HMDB0055889	NA	NA
1763	HMDB0055139	NA	NA
1764	HMDB0055937	NA	NA
1765	HMDB0010561	TG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0010561
1766	HMDB0054899	NA	NA
1767	HMDB0055091	NA	NA
1768	HMDB0055131	NA	NA
1769	HMDB0055138	NA	NA
1770	HMDB0010554	TG(22:5(7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0010554
1771	HMDB0055871	NA	NA
1772	HMDB0055133	NA	NA
1773	HMDB0055888	NA	NA
1774	HMDB0055935	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)

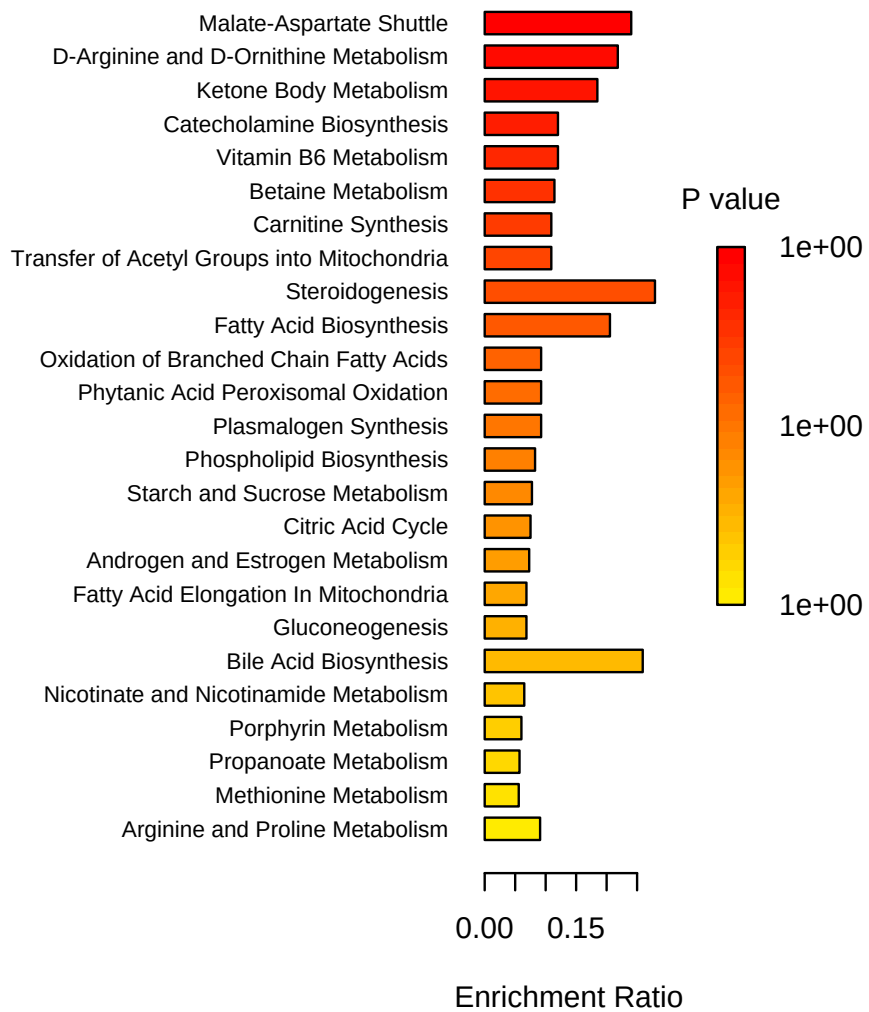


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Malate-Aspartate Shuttle	10	4.16	1	9.96E-01	1.00E+00	1.00E+00
D-Arginine and D-Ornithine Metabolism	11	4.58	1	9.97E-01	1.00E+00	1.00E+00
Ketone Body Metabolism	13	5.41	1	9.99E-01	1.00E+00	1.00E+00
Catecholamine Biosynthesis	20	8.32	1	1.00E+00	1.00E+00	1.00E+00
Vitamin B6 Metabolism	20	8.32	1	1.00E+00	1.00E+00	1.00E+00
Betaine Metabolism	21	8.74	1	1.00E+00	1.00E+00	1.00E+00
Carnitine Synthesis	22	9.15	1	1.00E+00	1.00E+00	1.00E+00
Transfer of Acetyl Groups into Mitochondria	22	9.15	1	1.00E+00	1.00E+00	1.00E+00
Steroidogenesis	43	17.90	5	1.00E+00	1.00E+00	1.00E+00
Fatty Acid Biosynthesis	35	14.60	3	1.00E+00	1.00E+00	1.00E+00
Oxidation of Branched Chain Fatty Acids	26	10.80	1	1.00E+00	1.00E+00	1.00E+00
Phytanic Acid Peroxisomal Oxidation	26	10.80	1	1.00E+00	1.00E+00	1.00E+00
Plasmalogen Synthesis	26	10.80	1	1.00E+00	1.00E+00	1.00E+00
Phospholipid Biosynthesis	29	12.10	1	1.00E+00	1.00E+00	1.00E+00
Starch and Sucrose Metabolism	31	12.90	1	1.00E+00	1.00E+00	1.00E+00
Citric Acid Cycle	32	13.30	1	1.00E+00	1.00E+00	1.00E+00
Androgen and Estrogen Metabolism	33	13.70	1	1.00E+00	1.00E+00	1.00E+00
Fatty Acid Elongation In Mitochondria	35	14.60	1	1.00E+00	1.00E+00	1.00E+00
Gluconeogenesis	35	14.60	1	1.00E+00	1.00E+00	1.00E+00
Bile Acid Biosynthesis	65	27.00	7	1.00E+00	1.00E+00	1.00E+00
Nicotinate and Nicotinamide Metabolism	37	15.40	1	1.00E+00	1.00E+00	1.00E+00
Porphyrin Metabolism	40	16.60	1	1.00E+00	1.00E+00	1.00E+00
Propanoate Metabolism	42	17.50	1	1.00E+00	1.00E+00	1.00E+00
Methionine Metabolism	43	17.90	1	1.00E+00	1.00E+00	1.00E+00
Arginine and Proline Metabolism	53	22.00	2	1.00E+00	1.00E+00	1.00E+00
Glycine and Serine Metabolism	59	24.50	3	1.00E+00	1.00E+00	1.00E+00
Pyrimidine Metabolism	59	24.50	3	1.00E+00	1.00E+00	1.00E+00
Valine, Leucine and Isoleucine Degradation	60	25.00	3	1.00E+00	1.00E+00	1.00E+00
Tryptophan Metabolism	60	25.00	3	1.00E+00	1.00E+00	1.00E+00
Pyruvate Metabolism	48	20.00	1	1.00E+00	1.00E+00	1.00E+00
Glutamate Metabolism	49	20.40	1	1.00E+00	1.00E+00	1.00E+00
Purine Metabolism	74	30.80	4	1.00E+00	1.00E+00	1.00E+00
Warburg Effect	58	24.10	1	1.00E+00	1.00E+00	1.00E+00
Tyrosine Metabolism	72	30.00	1	1.00E+00	1.00E+00	1.00E+00
Arachidonic Acid Metabolism	69	28.70	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(\"HMDB0167366\", \"HMDB0094692\", \"HMDB0041945\", \"HMDB0167367\", \"HMDB0167365\", \"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, \"guest4067896030607704141\")\n"
```

The report was generated on Mon May 24 15:11:37 2021 with R version 4.0.2 (2020-06-22).