

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	HMDB0060253	1-Methylpyrrolinium	HMDB0060253
2	HMDB0172632	NA	NA
3	HMDB0062600	NA	NA
4	HMDB0012815	5-Aminopentanal	HMDB0012815
5	HMDB0033529	(+)-2,3-Dihydro-3-methyl-1H-pyrrole	HMDB0033529
6	HMDB0040173	NA	NA
7	HMDB0061878	NA	NA
8	HMDB0001252	Betaine aldehyde	HMDB0001252
9	HMDB0000973	Hydrogen phosphate	HMDB0000973
10	HMDB0001429	Phosphate	HMDB0001429
11	HMDB0002105	Dihydrogen phosphate	HMDB0002105
12	HMDB0002142	Phosphoric acid	HMDB0002142
13	HMDB0062781	NA	NA
14	HMDB0059784	NA	NA
15	HMDB0161317	NA	NA
16	HMDB0160653	NA	NA
17	HMDB0160654	NA	NA
18	HMDB0000208	Oxoglutaric acid	HMDB0000208
19	HMDB0013701	3-Oxoglutaric acid	HMDB0013701
20	HMDB0164700	NA	NA
21	HMDB0161318	NA	NA
22	HMDB0041390	NA	NA
23	HMDB0041393	NA	NA
24	HMDB0033966	Di-2-propenyl disulfide, 9CI	HMDB0033966
25	HMDB0000139	Glyceric acid	HMDB0000139
26	HMDB0031818	D-2,3-Dihydroxypropanoic acid	HMDB0031818
27	HMDB0006372	L-Glyceric acid	HMDB0006372
28	HMDB0166738	NA	NA
29	HMDB0164724	NA	NA
30	HMDB0165094	NA	NA
31	HMDB0165096	NA	NA
32	HMDB0165095	NA	NA
33	HMDB0165097	NA	NA
34	HMDB0166737	NA	NA
35	HMDB0031484	2-Heptenoic acid	HMDB0031484
36	HMDB0038962	NA	NA
37	HMDB0031500	Methyl 2E-hexenoate	HMDB0031500
38	HMDB0166739	NA	NA
39	HMDB0029314	Isopentenyl acetate	HMDB0029314
40	HMDB0031477	3,4-Heptanedione	HMDB0031477
41	HMDB0031476	2,3-Heptanedione	HMDB0031476
42	HMDB0031504	Methyl (Z)-3-hexenoate	HMDB0031504
43	HMDB0031603	Ethyl 4-pentenoate	HMDB0031603
44	HMDB0040214	NA	NA
45	HMDB0031342	Cyclohexanecarboxylic acid	HMDB0031342
46	HMDB0038271	NA	NA
47	HMDB0031174	4-Methyl-5-hexanolide	HMDB0031174
48	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	HMDB0031681
49	HMDB0033793	4-Heptenoic acid	HMDB0033793
50	HMDB0031593	5-Methyl-2,3-hexanedione	HMDB0031593
51	HMDB0039819	NA	NA
52	HMDB0166736	NA	NA
53	HMDB0173760	NA	NA
54	HMDB0173761	NA	NA
55	HMDB0173762	NA	NA
56	HMDB0173763	NA	NA
57	HMDB0180322	NA	NA
58	HMDB0180323	NA	NA
59	HMDB0029165	1,3-Diacetylpropane	HMDB0029165

60	HMDB0031351	Cyclohexyl formate	HMDB0031351
61	HMDB0032460	4-Pentenyl acetate	HMDB0032460
62	HMDB0032391	3-Methyl-3-butenyl acetate	HMDB0032391
63	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	HMDB0030330
64	HMDB0059876	NA	NA
65	HMDB0040591	NA	NA
66	HMDB0145113	NA	NA
67	HMDB0145114	NA	NA
68	HMDB0145115	NA	NA
69	HMDB0145125	NA	NA
70	HMDB0145116	NA	NA
71	HMDB0094649	2-Amino-heptanoic acid	HMDB0094649
72	HMDB0001161	4-Trimethylammonibutanoic acid	HMDB0001161
73	HMDB0006831	3-Dehydroxycarnitine	HMDB0006831
74	HMDB0013811	1-Nitroheptane	HMDB0013811
75	HMDB0000895	Acetylcholine	HMDB0000895
76	HMDB0062183	NA	NA
77	HMDB0002393	N-Methyl-D-aspartic acid	HMDB0002393
78	HMDB0003011	O-Acetylserine	HMDB0003011
79	HMDB0003339	D-Glutamic acid	HMDB0003339
80	HMDB0006556	L-4-Hydroxyglutamate semialdehyde	HMDB0006556
81	HMDB0060475	DL-Glutamate	HMDB0060475
82	HMDB0033550	3-(Carboxymethylamino)propanoic acid	HMDB0033550
83	HMDB0002931	N-Acetylserine	HMDB0002931
84	HMDB0000148	L-Glutamic acid	HMDB0000148
85	HMDB0156263	NA	NA
86	HMDB0000634	Citraconic acid	HMDB0000634
87	HMDB0060365	2,5-Dioxopentanoate	HMDB0060365
88	HMDB0000620	Glutaconic acid	HMDB0000620
89	HMDB0061185	NA	NA
90	HMDB0033809	Methyl hydrogen fumarate	HMDB0033809
91	HMDB0013233	Gamma-delta-Dioxovaleric acid	HMDB0013233
92	HMDB0059743	NA	NA
93	HMDB0000749	Mesaconic acid	HMDB0000749
94	HMDB0002092	Itaconic acid	HMDB0002092
95	HMDB0000897	7-Methylguanine	HMDB0000897
96	HMDB0001566	3-Methylguanine	HMDB0001566
97	HMDB0003282	1-Methylguanine	HMDB0003282
98	HMDB0006040	N2-Methylguanine	HMDB0006040
99	HMDB0165786	NA	NA
100	HMDB0166497	NA	NA
101	HMDB0166498	NA	NA
102	HMDB0166499	NA	NA
103	HMDB0166500	NA	NA
104	HMDB0164728	NA	NA
105	HMDB0163403	NA	NA
106	HMDB0164729	NA	NA
107	HMDB0166501	NA	NA
108	HMDB0031176	Tetrahydrofurfuryl acetate	HMDB0031176
109	HMDB0040433	NA	NA
110	HMDB0036594	NA	NA
111	HMDB0037114	NA	NA
112	HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	HMDB0001988
113	HMDB0166747	NA	NA
114	HMDB0166744	NA	NA
115	HMDB0166746	NA	NA
116	HMDB0061990	NA	NA
117	HMDB0166745	NA	NA
118	HMDB0172013	NA	NA
119	HMDB0180327	NA	NA
120	HMDB0180326	NA	NA
121	HMDB0180835	NA	NA
122	HMDB0000062	L-Carnitine	HMDB0000062
123	HMDB0062496	Malonyl-Carnitin	HMDB0062496
124	HMDB0145126	NA	NA
125	HMDB0155786	NA	NA
126	HMDB0062634	NA	NA
127	HMDB0010207	L-Rhamnulose	HMDB0010207
128	HMDB0124735	NA	NA
129	HMDB0240304	NA	NA
130	HMDB0062489	NA	NA
131	HMDB0059625	NA	NA
132	HMDB0029196	D-Fucose	HMDB0029196
133	HMDB0000174	L-Fucose	HMDB0000174
134	HMDB0059624	NA	NA
135	HMDB0033821	2-O-Methyl-D-xylose	HMDB0033821
136	HMDB0000849	Rhamnose	HMDB0000849
137	HMDB0003081	Beta-D-Fucose	HMDB0003081
138	HMDB0012327	2-Deoxygalactopyranose	HMDB0012327
139	HMDB0002712	1,5-Anhydrosorbitol	HMDB0002712
140	HMDB0062477	NA	NA
141	HMDB0062498	NA	NA
142	HMDB0062499	NA	NA
143	HMDB0005876	3-Deoxyfructose	HMDB0005876
144	HMDB0060267	L-Fuculose	HMDB0060267
145	HMDB0033050	Butyl isopropyl disulfide	HMDB0033050
146	HMDB0033051	Butyl propyl disulfide	HMDB0033051

147	HMDB0039783	NA	NA
148	HMDB0132202	NA	NA
149	HMDB0041026	NA	NA
150	HMDB0041031	NA	NA
151	HMDB0035593	Rishitin	HMDB0035593
152	HMDB0037605	NA	NA
153	HMDB0036790	NA	NA
154	HMDB0036791	NA	NA
155	HMDB0037820	NA	NA
156	HMDB0040178	NA	NA
157	HMDB0160293	NA	NA
158	HMDB0160295	NA	NA
159	HMDB0160291	NA	NA
160	HMDB0160290	NA	NA
161	HMDB0160289	NA	NA
162	HMDB0160292	NA	NA
163	HMDB0160296	NA	NA
164	HMDB0160294	NA	NA
165	HMDB0160298	NA	NA
166	HMDB0160297	NA	NA
167	HMDB0032369	L-Menthyl acetoacetate	HMDB0032369
168	HMDB0033619	Hexyl hexanoate	HMDB0033619
169	HMDB0059868	NA	NA
170	HMDB0032440	Nonanal propyleneglycol acetal	HMDB0032440
171	HMDB0061988	NA	NA
172	HMDB0035410	(R)-Dihydrocitronellol acetate	HMDB0035410
173	HMDB0000638	Dodecanoic acid	HMDB0000638
174	HMDB0040166	NA	NA
175	HMDB0030998	Ethyl decanoate	HMDB0030998
176	HMDB0034137	Octyl 2-methylpropanoate	HMDB0034137
177	HMDB0036225	NA	NA
178	HMDB0034136	Octyl butanoate	HMDB0034136
179	HMDB0034128	Isopropyl nonanoate	HMDB0034128
180	HMDB0032310	2-Heptyl butyrate	HMDB0032310
181	HMDB0168119	NA	NA
182	HMDB0168120	NA	NA
183	HMDB0168121	NA	NA
184	HMDB0015050	Phenformin	HMDB0015050
185	HMDB0004231	Pantothenol	HMDB0004231
186	HMDB0038259	NA	NA
187	HMDB0032342	Isobornyl isobutyrate	HMDB0032342
188	HMDB0032053	alpha-Terpineol butanoate	HMDB0032053
189	HMDB0030427	Linalyl butyrate	HMDB0030427
190	HMDB0038260	NA	NA
191	HMDB0038246	NA	NA
192	HMDB0036424	NA	NA
193	HMDB0037814	NA	NA
194	HMDB0032524	Terpinyl isobutyrate	HMDB0032524
195	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	HMDB0031015
196	HMDB0030426	Linalyl isobutyrate	HMDB0030426
197	HMDB0000560	5,8-Tetradecadienoic acid	HMDB0000560
198	HMDB0039129	NA	NA
199	HMDB0159801	NA	NA
200	HMDB0159802	NA	NA
201	HMDB0176319	NA	NA
202	HMDB0176320	NA	NA
203	HMDB0159803	NA	NA
204	HMDB0159799	NA	NA
205	HMDB0159800	NA	NA
206	HMDB0030982	6-Ketomyristic acid	HMDB0030982
207	HMDB0010730	3-Oxotetradecanoic acid	HMDB0010730
208	HMDB0032370	L-Menthyl (R,S)-3-hydroxybutyrate	HMDB0032370
209	HMDB0159614	NA	NA
210	HMDB0159613	NA	NA
211	HMDB0159611	NA	NA
212	HMDB0159610	NA	NA
213	HMDB0159612	NA	NA
214	HMDB0159609	NA	NA
215	HMDB0168123	NA	NA
216	HMDB0032153	Acetaldehyde diisoamyl acetal	HMDB0032153
217	HMDB0037310	NA	NA
218	HMDB0168122	NA	NA
219	HMDB0062248	NA	NA
220	HMDB0094671	NA	NA
221	HMDB0062243	NA	NA
222	HMDB0000499	5-Tetradecenoic acid	HMDB0000499
223	HMDB0037189	NA	NA
224	HMDB0037188	NA	NA
225	HMDB0031073	12-Methyl-13-tridecanolide	HMDB0031073
226	HMDB0034561	Houttuynin	HMDB0034561
227	HMDB0038056	NA	NA
228	HMDB0030921	(R)-14-Methyloxacyclotetradecan-2-one	HMDB0030921
229	HMDB0031029	Ethyl (E)-2-dodecenoate	HMDB0031029
230	HMDB0037633	NA	NA
231	HMDB0010732	trans-Tetra-dec-2-enoic acid	HMDB0010732
232	HMDB0005051	Tsuzuic acid	HMDB0005051
233	HMDB0002000	Myristoleic acid	HMDB0002000

234	HMDB0000521	5Z-Tetradecenoic acid	HMDB0000521
235	HMDB0037227	NA	NA
236	HMDB0037228	NA	NA
237	HMDB0037369	NA	NA
238	HMDB0061991	NA	NA
239	HMDB0032152	Acetaldehyde di-cis-3-hexenyl acetal	HMDB0032152
240	HMDB0032321	2-Hexenyl octanoate	HMDB0032321
241	HMDB0040228	NA	NA
242	HMDB0171056	NA	NA
243	HMDB0176323	NA	NA
244	HMDB0176321	NA	NA
245	HMDB0176322	NA	NA
246	HMDB0176324	NA	NA
247	HMDB0061656	3-hydroxytetradecanoic acid	HMDB0061656
248	HMDB0010731	(R)-3-Hydroxy-tetradecanoic acid	HMDB0010731
249	HMDB0002261	2-Hydroxy-myristic acid	HMDB0002261
250	HMDB0094672	NA	NA
251	HMDB0059850	NA	NA
252	HMDB0171057	NA	NA
253	HMDB0032417	3-(L-Menthoxyl)-2-methylpropane-1,2-diol	HMDB0032417
254	HMDB0028925	Leucyl-Aspartate	HMDB0028925
255	HMDB0011166	L-beta-aspartyl-L-leucine	HMDB0011166
256	HMDB0028757	Aspartyl-Leucine	HMDB0028757
257	HMDB0028756	Aspartyl-Isoleucine	HMDB0028756
258	HMDB0028903	Isoleucyl-Aspartate	HMDB0028903
259	HMDB0029126	Valyl-Glutamate	HMDB0029126
260	HMDB0011172	gamma-Glutamylvaline	HMDB0011172
261	HMDB0029162	NA	NA
262	HMDB0028832	Glutamylvaline	HMDB0028832
263	HMDB0059717	NA	NA
264	HMDB0151784	NA	NA
265	HMDB0151780	NA	NA
266	HMDB0151794	NA	NA
267	HMDB0151781	NA	NA
268	HMDB0151783	NA	NA
269	HMDB0151789	NA	NA
270	HMDB0151790	NA	NA
271	HMDB0151792	NA	NA
272	HMDB0151788	NA	NA
273	HMDB0151787	NA	NA
274	HMDB0151786	NA	NA
275	HMDB0151785	NA	NA
276	HMDB0132940	NA	NA
277	HMDB0001925	Ibuprofen	HMDB0001925
278	HMDB0035016	2-Phenylethyl pentanoate	HMDB0035016
279	HMDB0036386	NA	NA
280	HMDB0035008	3-Methylbutyl phenylacetate	HMDB0035008
281	HMDB0034472	3-Phenylpropyl 2-methylpropanoate	HMDB0034472
282	HMDB0034470	2-Phenylpropyl isobutyrate	HMDB0034470
283	HMDB0038605	NA	NA
284	HMDB0040431	NA	NA
285	HMDB0036391	NA	NA
286	HMDB0036025	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	HMDB0036025
287	HMDB0037194	NA	NA
288	HMDB0034469	2-Phenylpropyl butyrate	HMDB0034469
289	HMDB0034556	3-Acetoxy-3-methyl-1-phenylbutane	HMDB0034556
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	HMDB0037623	NA	NA
296	HMDB0036240	NA	NA
297	HMDB0132932	NA	NA
298	HMDB0163212	NA	NA
299	HMDB0151805	NA	NA
300	HMDB0151793	NA	NA
301	HMDB0151791	NA	NA
302	HMDB0037720	NA	NA
303	HMDB0032176	Benzyl hexanoate	HMDB0032176
304	HMDB0035017	2-Phenylethyl 3-methylbutanoate	HMDB0035017
305	HMDB0028871	Hydroxyprolyl-Proline	HMDB0028871
306	HMDB0006695	Prolylhydroxyproline	HMDB0006695
307	HMDB0094651	PyroGlu-Val	HMDB0094651
308	HMDB0040573	NA	NA
309	HMDB0029018	Prolyl-Hydroxyproline	HMDB0029018
310	HMDB0060747	NA	NA
311	HMDB0001434	3-Methoxytyrosine	HMDB0001434
312	HMDB0011754	Methyldopa	HMDB0011754
313	HMDB0061836	NA	NA
314	HMDB0033878	(S)-Curzeone	HMDB0033878
315	HMDB0032133	Bisphenol A	HMDB0032133
316	HMDB0014604	Nabumetone	HMDB0014604
317	HMDB0176774	NA	NA
318	HMDB0176775	NA	NA
319	HMDB0135597	NA	NA
320	HMDB0176773	NA	NA

321	HMDB0036455	NA	NA
322	HMDB0036767	NA	NA
323	HMDB0038202	NA	NA
324	HMDB0041920	NA	NA
325	HMDB0031900	Methyl (2E,4Z,6E,8E,10E)-4,8-dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoate	HMDB0031900
326	HMDB0035902	Enokipodin B	HMDB0035902
327	HMDB0040903	NA	NA
328	HMDB0179330	NA	NA
329	HMDB0170855	NA	NA
330	HMDB0038547	NA	NA
331	HMDB0036488	NA	NA
332	HMDB0030911	2-Oxo-5,11(13)-eudesmadien-12,8-olide	HMDB0030911
333	HMDB0037801	NA	NA
334	HMDB0036473	NA	NA
335	HMDB0037558	NA	NA
336	HMDB0031916	5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran	HMDB0031916
337	HMDB0038188	NA	NA
338	HMDB0179331	NA	NA
339	HMDB0179332	NA	NA
340	HMDB0033349	Casimiroin	HMDB0033349
341	HMDB0183398	NA	NA
342	HMDB0183400	NA	NA
343	HMDB0240342	NA	NA
344	HMDB0061316	NA	NA
345	HMDB0183397	NA	NA
346	HMDB0029051	Seryltyrosine	HMDB0029051
347	HMDB0029114	Tyrosyl-Serine	HMDB0029114
348	HMDB0171478	NA	NA
349	HMDB0171479	NA	NA
350	HMDB0171476	NA	NA
351	HMDB0171477	NA	NA
352	HMDB0041422	NA	NA
353	HMDB0033791	(E)-3-Hexadecenoic acid	HMDB0033791
354	HMDB0038958	NA	NA
355	HMDB0031711	15-Hexadecanolide	HMDB0031711
356	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	HMDB0031145
357	HMDB0035877	(Z)-13-Hexadecenoic acid	HMDB0035877
358	HMDB0031053	(E)-6-Hexadecenoic acid	HMDB0031053
359	HMDB0032638	(Z)-5-Hexadecenoic acid	HMDB0032638
360	HMDB0012328	Palmitelaidic acid	HMDB0012328
361	HMDB0002186	Hypogeic acid	HMDB0002186
362	HMDB0003229	Palmitoleic acid	HMDB0003229
363	HMDB0010735	Trans-Hexa-dec-2-enoic acid	HMDB0010735
364	HMDB0037647	NA	NA
365	HMDB0061979	NA	NA
366	HMDB0062548	NA	NA
367	HMDB0184174	NA	NA
368	HMDB0184176	NA	NA
369	HMDB0112192	NA	NA
370	HMDB0184180	NA	NA
371	HMDB0184177	NA	NA
372	HMDB0184328	NA	NA
373	HMDB0184175	NA	NA
374	HMDB0031057	(R)-2-Hydroxyhexadecanoic acid	HMDB0031057
375	HMDB0061658	NA	NA
376	HMDB0184178	NA	NA
377	HMDB0112190	NA	NA
378	HMDB0112191	NA	NA
379	HMDB0010734	(R)-3-Hydroxy-hexadecanoic acid	HMDB0010734
380	HMDB0006294	16-Hydroxy hexadecanoic acid	HMDB0006294
381	HMDB0155887	NA	NA
382	HMDB0112186	NA	NA
383	HMDB0112189	NA	NA
384	HMDB0112185	NA	NA
385	HMDB0112187	NA	NA
386	HMDB0112184	NA	NA
387	HMDB0155886	NA	NA
388	HMDB0112188	NA	NA
389	HMDB0175409	NA	NA
390	HMDB0175412	NA	NA
391	HMDB0175413	NA	NA
392	HMDB0175414	NA	NA
393	HMDB0175415	NA	NA
394	HMDB0175408	NA	NA
395	HMDB0175410	NA	NA
396	HMDB0175411	NA	NA
397	HMDB0160594	NA	NA
398	HMDB0173892	NA	NA
399	HMDB0175402	NA	NA
400	HMDB0175403	NA	NA
401	HMDB0175404	NA	NA
402	HMDB0175405	NA	NA
403	HMDB0175406	NA	NA
404	HMDB0175407	NA	NA
405	HMDB0030964	Linolenelaidic acid	HMDB0030964
406	HMDB0001388	Alpha-Linolenic acid	HMDB0001388
407	HMDB0003073	Gamma-Linolenic acid	HMDB0003073

408	HMDB0030962	Calendic acid	HMDB0030962
409	HMDB0030963	Punicic acid	HMDB0030963
410	HMDB0160589	NA	NA
411	HMDB0160588	NA	NA
412	HMDB0112194	NA	NA
413	HMDB0062652	NA	NA
414	HMDB0173890	NA	NA
415	HMDB0160590	NA	NA
416	HMDB0160592	NA	NA
417	HMDB0160591	NA	NA
418	HMDB0160593	NA	NA
419	HMDB0160595	NA	NA
420	HMDB0173886	NA	NA
421	HMDB0173885	NA	NA
422	HMDB0173887	NA	NA
423	HMDB0173889	NA	NA
424	HMDB0173891	NA	NA
425	HMDB0173888	NA	NA
426	HMDB0173893	NA	NA
427	HMDB0004667	13S-hydroxyoctadecadienoic acid	HMDB0004667
428	HMDB0061708	NA	NA
429	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	HMDB0029796
430	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid	HMDB0029998
431	HMDB0029978	Avenoleic acid	HMDB0029978
432	HMDB0010223	9-HODE	HMDB0010223
433	HMDB0004701	9,10-Epoxyoctadecenoic acid	HMDB0004701
434	HMDB0004702	12,13-EpOME	HMDB0004702
435	HMDB0004670	Alpha-dimorphecolic acid	HMDB0004670
436	HMDB0000220	Palmitic acid	HMDB0000220
437	HMDB0060083	NA	NA
438	HMDB0061373	NA	NA
439	HMDB0032324	Hexyl decanoate	HMDB0032324
440	HMDB0032249	Dodecyl butyrate	HMDB0032249
441	HMDB0033166	Octyl octanoate	HMDB0033166
442	HMDB0032065	Butyl dodecanoate	HMDB0032065
443	HMDB0036210	NA	NA
444	HMDB0034153	Ethyl tetradecanoate	HMDB0034153
445	HMDB0031068	Isopalmitic acid	HMDB0031068
446	HMDB0002396	Trimethyltridecanoic acid	HMDB0002396
447	HMDB0062238	NA	NA
448	HMDB0061864	Dihomolinoleic acid	HMDB0061864
449	HMDB0005048	10E,12Z-Octadecadienoic acid	HMDB0005048
450	HMDB0062784	NA	NA
451	HMDB0030430	Linalyl caprylate	HMDB0030430
452	HMDB0029800	Mangiferic acid	HMDB0029800
453	HMDB0031097	5-Octadecynoic acid	HMDB0031097
454	HMDB0031051	Ethyl 2E,4Z-hexadecadienoate	HMDB0031051
455	HMDB0006270	Linoelaidic acid	HMDB0006270
456	HMDB0005047	9E,11E-Octadecadienoic acid	HMDB0005047
457	HMDB0003797	Bovinic acid	HMDB0003797
458	HMDB0000673	Linoleic acid	HMDB0000673
459	HMDB0173874	NA	NA
460	HMDB0155791	NA	NA
461	HMDB0160378	NA	NA
462	HMDB0160379	NA	NA
463	HMDB0160380	NA	NA
464	HMDB0160377	NA	NA
465	HMDB0155790	NA	NA
466	HMDB0155794	NA	NA
467	HMDB0155793	NA	NA
468	HMDB0155792	NA	NA
469	HMDB0187012	NA	NA
470	HMDB0187010	NA	NA
471	HMDB0160381	NA	NA
472	HMDB0187015	NA	NA
473	HMDB0187014	NA	NA
474	HMDB0187013	NA	NA
475	HMDB0187011	NA	NA
476	HMDB0030979	9-Oxoctadecanoic acid	HMDB0030979
477	HMDB0034074	5-Oxoctadecanoic acid	HMDB0034074
478	HMDB0030980	10-Oxoctadecanoic acid	HMDB0030980
479	HMDB0031127	5-Hexyltetrahydro-2-furanoctanoic acid	HMDB0031127
480	HMDB0034297	Ricinoleic acid	HMDB0034297
481	HMDB0030981	11-Oxoctadecanoic acid	HMDB0030981
482	HMDB0010736	3-Oxoctadecanoic acid	HMDB0010736
483	HMDB0002080	Petroselinic acid	HMDB0002080
484	HMDB0003231	Vaccenic acid	HMDB0003231
485	HMDB0062703	NA	NA
486	HMDB0062242	NA	NA
487	HMDB0041480	NA	NA
488	HMDB0062218	NA	NA
489	HMDB0062093	NA	NA
490	HMDB0059871	NA	NA
491	HMDB0000573	Elaidic acid	HMDB0000573
492	HMDB0240219	cis-Vaccenic acid	HMDB0240219
493	HMDB0000207	Oleic acid	HMDB0000207
494	HMDB0112180	NA	NA

495	HMDB0112182	NA	NA
496	HMDB0112193	NA	NA
497	HMDB0240324	NA	NA
498	HMDB0240330	NA	NA
499	HMDB0062549	2-Hydroxystearic acid	HMDB0062549
500	HMDB0112181	NA	NA
501	HMDB0010737	(R)-3-Hydroxy-Octadecanoic acid	HMDB0010737
502	HMDB0037396	xi-10-Hydroxyoctadecanoic acid	HMDB0037396
503	HMDB0061662	NA	NA
504	HMDB0061661	NA	NA
505	HMDB0061706	NA	NA
506	HMDB0171068	NA	NA
507	HMDB0171069	NA	NA
508	HMDB0112183	NA	NA
509	HMDB0002171	Glycylprolylhydroxyproline	HMDB0002171
510	HMDB0039423	NA	NA
511	HMDB0032305	N-(Heptan-4-yl)benzo[d][1,3]dioxole-5-carboxamide	HMDB0032305
512	HMDB0178285	NA	NA
513	HMDB0015692	Isothipendyl	HMDB0015692
514	HMDB0015061	Phenoxybenzamine	HMDB0015061
515	HMDB0240223	NA	NA
516	HMDB0163450	NA	NA
517	HMDB0147448	NA	NA
518	HMDB0032056	Eugenyl benzoate	HMDB0032056
519	HMDB0014472	Hydromorphone	HMDB0014472
520	HMDB0040987	NA	NA
521	HMDB0032961	Secodemethylclausenamide	HMDB0032961
522	HMDB0030256	Erysopine	HMDB0030256
523	HMDB0060657	Norcodeine	HMDB0060657
524	HMDB0061070	NA	NA
525	HMDB0029377	Piperine	HMDB0029377
526	HMDB0139474	NA	NA
527	HMDB0014440	Morphine	HMDB0014440
528	HMDB0167447	NA	NA
529	HMDB0167440	NA	NA
530	HMDB0167439	NA	NA
531	HMDB0167441	NA	NA
532	HMDB0167457	NA	NA
533	HMDB0167445	NA	NA
534	HMDB0167443	NA	NA
535	HMDB0167442	NA	NA
536	HMDB0167459	NA	NA
537	HMDB0167444	NA	NA
538	HMDB0061075	NA	NA
539	HMDB0061074	NA	NA
540	HMDB0061076	NA	NA
541	HMDB0060544	NA	NA
542	HMDB0060543	NA	NA
543	HMDB0003573	Scopolamine	HMDB0003573
544	HMDB0015043	Cocaine	HMDB0015043
545	HMDB0015405	Fenoterol	HMDB0015405
546	HMDB0171728	NA	NA
547	HMDB0000230	N-Acetylneuraminic acid	HMDB0000230
548	HMDB0000773	N-Acetyl-a-neuraminic acid	HMDB0000773
549	HMDB0161436	NA	NA
550	HMDB0167290	NA	NA
551	HMDB0167291	NA	NA
552	HMDB0167294	NA	NA
553	HMDB0167293	NA	NA
554	HMDB0167296	NA	NA
555	HMDB0167297	NA	NA
556	HMDB0179979	NA	NA
557	HMDB0179980	NA	NA
558	HMDB0153318	NA	NA
559	HMDB0172140	NA	NA
560	HMDB0028880	Histidinyl-Asparagine	HMDB0028880
561	HMDB0028733	Asparaginylnl-Histidine	HMDB0028733
562	HMDB0061039	NA	NA
563	HMDB0031766	Alachlor	HMDB0031766
564	HMDB0038584	NA	NA
565	HMDB0170783	NA	NA
566	HMDB0170784	NA	NA
567	HMDB0170785	NA	NA
568	HMDB0170788	NA	NA
569	HMDB0170786	NA	NA
570	HMDB0170787	NA	NA
571	HMDB0033359	Cryptodrine	HMDB0033359
572	HMDB0039096	NA	NA
573	HMDB0173636	NA	NA
574	HMDB0041314	NA	NA
575	HMDB0130350	NA	NA
576	HMDB0130347	NA	NA
577	HMDB0175079	NA	NA
578	HMDB0178312	NA	NA
579	HMDB0141160	NA	NA
580	HMDB0141105	NA	NA
581	HMDB0141099	NA	NA

582	HMDB0141080	NA	NA
583	HMDB0141122	NA	NA
584	HMDB0141079	NA	NA
585	HMDB0141126	NA	NA
586	HMDB0141149	NA	NA
587	HMDB0141119	NA	NA
588	HMDB0040889	NA	NA
589	HMDB0129039	NA	NA
590	HMDB0138953	NA	NA
591	HMDB0141045	NA	NA
592	HMDB0138954	NA	NA
593	HMDB0138952	NA	NA
594	HMDB0138951	NA	NA
595	HMDB0138956	NA	NA
596	HMDB0140994	NA	NA
597	HMDB0138959	NA	NA
598	HMDB0138955	NA	NA
599	HMDB0138957	NA	NA
600	HMDB0138958	NA	NA
601	HMDB0141056	NA	NA
602	HMDB0141150	NA	NA
603	HMDB0141152	NA	NA
604	HMDB0141153	NA	NA
605	HMDB0141164	NA	NA
606	HMDB0146848	NA	NA
607	HMDB0146849	NA	NA
608	HMDB0141181	NA	NA
609	HMDB0141151	NA	NA
610	HMDB0141180	NA	NA
611	HMDB0141162	NA	NA
612	HMDB0141161	NA	NA
613	HMDB0141169	NA	NA
614	HMDB0141163	NA	NA
615	HMDB0141145	NA	NA
616	HMDB0141146	NA	NA
617	HMDB0141057	NA	NA
618	HMDB0141101	NA	NA
619	HMDB0141102	NA	NA
620	HMDB0141100	NA	NA
621	HMDB0141103	NA	NA
622	HMDB0141106	NA	NA
623	HMDB0141107	NA	NA
624	HMDB0141120	NA	NA
625	HMDB0141121	NA	NA
626	HMDB0141130	NA	NA
627	HMDB0141129	NA	NA
628	HMDB0141128	NA	NA
629	HMDB0141127	NA	NA
630	HMDB0141139	NA	NA
631	HMDB0141140	NA	NA
632	HMDB0141170	NA	NA
633	HMDB0036635	NA	NA
634	HMDB0041298	NA	NA
635	HMDB0033310	Moracin C	HMDB0033310
636	HMDB0031744	Artocarbene	HMDB0031744
637	HMDB0141044	NA	NA
638	HMDB0138682	NA	NA
639	HMDB0011741	gamma-Glutamyltyrosine	HMDB0011741
640	HMDB0029161	NA	NA
641	HMDB0029104	Tyrosyl-Glutamate	HMDB0029104
642	HMDB0028831	Glutamyltyrosine	HMDB0028831
643	HMDB0062553	NA	NA
644	HMDB0041309	NA	NA
645	HMDB0000839	Pentaporphyrin I	HMDB0000839
646	HMDB0029428	Hypoglycin B	HMDB0029428
647	HMDB0061318	NA	NA
648	HMDB0015102	Desloratadine	HMDB0015102
649	HMDB0013034	Palmitoylglycine	HMDB0013034
650	HMDB0072849	NA	NA
651	HMDB0072862	NA	NA
652	HMDB0072865	NA	NA
653	HMDB0072878	NA	NA
654	HMDB0011532	MG(0:0/15:0/0:0)	HMDB0011532
655	HMDB0011563	MG(15:0/0:0/0:0)	HMDB0011563
656	HMDB0031008	(+)-15,16-Dihydroxyoctadecanoic acid	HMDB0031008
657	HMDB0059633	NA	NA
658	HMDB0038580	NA	NA
659	HMDB0033631	Lactapiperanol D	HMDB0033631
660	HMDB0180021	NA	NA
661	HMDB0180098	NA	NA
662	HMDB0180100	NA	NA
663	HMDB0180099	NA	NA
664	HMDB0180102	NA	NA
665	HMDB0034780	Capsiate	HMDB0034780
666	HMDB0180103	NA	NA
667	HMDB0184951	NA	NA
668	HMDB0184949	NA	NA

669	HMDB0184953	NA	NA
670	HMDB0012799	5'-Carboxy-gamma-chromanol	HMDB0012799
671	HMDB0184954	NA	NA
672	HMDB0184950	NA	NA
673	HMDB0061677	NA	NA
674	HMDB0000552	3-Methylglutaryl carnitine	HMDB0000552
675	HMDB0039044	NA	NA
676	HMDB0131544	NA	NA
677	HMDB0153683	NA	NA
678	HMDB0134716	NA	NA
679	HMDB0131577	NA	NA
680	HMDB0140842	NA	NA
681	HMDB0039858	NA	NA
682	HMDB0150310	NA	NA
683	HMDB0150311	NA	NA
684	HMDB0030019	4'-Methoxymucidin	HMDB0030019
685	HMDB0125543	NA	NA
686	HMDB0125544	NA	NA
687	HMDB0125545	NA	NA
688	HMDB0125547	NA	NA
689	HMDB0125546	NA	NA
690	HMDB0125548	NA	NA
691	HMDB0129031	NA	NA
692	HMDB0129032	NA	NA
693	HMDB0141104	NA	NA
694	HMDB0141131	NA	NA
695	HMDB0141141	NA	NA
696	HMDB0141165	NA	NA
697	HMDB0141171	NA	NA
698	HMDB0129034	NA	NA
699	HMDB0149106	NA	NA
700	HMDB0140204	NA	NA
701	HMDB0140116	NA	NA
702	HMDB0129033	NA	NA
703	HMDB0129035	NA	NA
704	HMDB0129037	NA	NA
705	HMDB0129036	NA	NA
706	HMDB0129038	NA	NA
707	HMDB0140114	NA	NA
708	HMDB0140118	NA	NA
709	HMDB0140117	NA	NA
710	HMDB0140115	NA	NA
711	HMDB0146850	NA	NA
712	HMDB0040670	NA	NA
713	HMDB0176556	NA	NA
714	HMDB0037839	NA	NA
715	HMDB0029089	Tryptophyl-Methionine	HMDB0029089
716	HMDB0028984	Methionyl-Tryptophan	HMDB0028984
717	HMDB0000489	Aspartylglycosamine	HMDB0000489
718	HMDB0136315	NA	NA
719	HMDB0136311	NA	NA
720	HMDB0136314	NA	NA
721	HMDB0136313	NA	NA
722	HMDB0136316	NA	NA
723	HMDB0005037	Sumatriptan	HMDB0005037
724	HMDB0153675	NA	NA
725	HMDB0153676	NA	NA
726	HMDB0151629	NA	NA
727	HMDB0151909	NA	NA
728	HMDB0153670	NA	NA
729	HMDB0153672	NA	NA
730	HMDB0153671	NA	NA
731	HMDB0153674	NA	NA
732	HMDB0146373	NA	NA
733	HMDB0140280	NA	NA
734	HMDB0136509	NA	NA
735	HMDB0130773	NA	NA
736	HMDB0130772	NA	NA
737	HMDB0130769	NA	NA
738	HMDB0130768	NA	NA
739	HMDB0130580	NA	NA
740	HMDB0138454	NA	NA
741	HMDB0130574	NA	NA
742	HMDB0130573	NA	NA
743	HMDB0130576	NA	NA
744	HMDB0130899	NA	NA
745	HMDB0132853	NA	NA
746	HMDB0134815	NA	NA
747	HMDB0133983	NA	NA
748	HMDB0133985	NA	NA
749	HMDB0133980	NA	NA
750	HMDB0133300	NA	NA
751	HMDB0133299	NA	NA
752	HMDB0132915	NA	NA
753	HMDB0132911	NA	NA
754	HMDB0132909	NA	NA
755	HMDB0130569	NA	NA

756	HMDB0130570	NA	NA
757	HMDB0130578	NA	NA
758	HMDB0146408	NA	NA
759	HMDB0146435	NA	NA
760	HMDB0147284	NA	NA
761	HMDB0147288	NA	NA
762	HMDB0150246	NA	NA
763	HMDB0150244	NA	NA
764	HMDB0151165	NA	NA
765	HMDB0146372	NA	NA
766	HMDB0130397	NA	NA
767	HMDB0130393	NA	NA
768	HMDB0130373	NA	NA
769	HMDB0130370	NA	NA
770	HMDB0130369	NA	NA
771	HMDB0128539	NA	NA
772	HMDB0126073	NA	NA
773	HMDB0140838	NA	NA
774	HMDB0140839	NA	NA
775	HMDB0151166	NA	NA
776	HMDB0130571	NA	NA
777	HMDB0030875	2',4'-Dihydroxy-4',6'-dimethoxychalcone	HMDB0030875
778	HMDB0033861	3-Hydroxy-2,9-dimethoxypterocarpan	HMDB0033861
779	HMDB0034116	Homopisatin	HMDB0034116
780	HMDB0033142	Melilotocarpan A	HMDB0033142
781	HMDB0041321	NA	NA
782	HMDB0038812	NA	NA
783	HMDB0033292	8-Hydroxy-3,9-dimethoxypterocarpan	HMDB0033292
784	HMDB0031421	Heliannone B	HMDB0031421
785	HMDB0038110	NA	NA
786	HMDB0034008	Methylnissolin	HMDB0034008
787	HMDB0031705	Heliannone A	HMDB0031705
788	HMDB0041322	NA	NA
789	HMDB0034001	3-Hydroxy-4,9-dimethoxypterocarpan	HMDB0034001
790	HMDB0130378	NA	NA
791	HMDB0140279	NA	NA
792	HMDB0130568	NA	NA
793	HMDB0140278	NA	NA
794	HMDB0030341	Piplartine	HMDB0030341
795	HMDB0137020	NA	NA
796	HMDB0137023	NA	NA
797	HMDB0137024	NA	NA
798	HMDB0137022	NA	NA
799	HMDB0137025	NA	NA
800	HMDB0137027	NA	NA
801	HMDB0137026	NA	NA
802	HMDB0137021	NA	NA
803	HMDB0136330	NA	NA
804	HMDB0136329	NA	NA
805	HMDB0136327	NA	NA
806	HMDB0136328	NA	NA
807	HMDB0136326	NA	NA
808	HMDB0136325	NA	NA
809	HMDB0061634	NA	NA
810	HMDB0241696	NA	NA
811	HMDB0241698	NA	NA
812	HMDB0241742	NA	NA
813	HMDB0062287	NA	NA
814	HMDB0062294	NA	NA
815	HMDB0062302	NA	NA
816	HMDB0062431	NA	NA
817	HMDB0062433	NA	NA
818	HMDB0112071	NA	NA
819	HMDB0112068	NA	NA
820	HMDB0004673	11,12-Epoxyeicosatrienoic acid	HMDB0004673
821	HMDB0038694	NA	NA
822	HMDB0038520	NA	NA
823	HMDB0038689	NA	NA
824	HMDB0038688	NA	NA
825	HMDB0036705	NA	NA
826	HMDB0036810	NA	NA
827	HMDB0036262	NA	NA
828	HMDB0011136	19(S)-HETE	HMDB0011136
829	HMDB0012598	17-HETE	HMDB0012598
830	HMDB0012567	13-HETE	HMDB0012567
831	HMDB0012508	10-HETE	HMDB0012508
832	HMDB0011134	5-HETE	HMDB0011134
833	HMDB0010409	11,12-EpETrE	HMDB0010409
834	HMDB0060101	NA	NA
835	HMDB0006111	12-HETE	HMDB0006111
836	HMDB0061118	NA	NA
837	HMDB0061119	NA	NA
838	HMDB0002190	5,6-Epoxy-8,11,14-eicosatrienoic acid	HMDB0002190
839	HMDB0002232	8,9-Epoxyeicosatrienoic acid	HMDB0002232
840	HMDB0010222	9-HETE	HMDB0010222
841	HMDB0006245	18-Hydroxyarachidonic acid	HMDB0006245
842	HMDB0005998	20-Hydroxyeicosatetraenoic acid	HMDB0005998

843	HMDB0004682	11(R)-HETE	HMDB0004682
844	HMDB0004679	8-HETE	HMDB0004679
845	HMDB0004680	16(R)-HETE	HMDB0004680
846	HMDB0004264	14,15-Epoxy-5,8,11-eicosatrienoic acid	HMDB0004264
847	HMDB0003876	15(S)-HETE	HMDB0003876
848	HMDB0002283	14R,15S-EpETrE	HMDB0002283
849	HMDB0184684	NA	NA
850	HMDB0035379	Sterebin E	HMDB0035379
851	HMDB0002995	12-Keto-tetrahydro-leukotriene B4	HMDB0002995
852	HMDB0002343	5,6-DHET	HMDB0002343
853	HMDB0002314	11,12-DiHETrE	HMDB0002314
854	HMDB0002311	8,9-DiHETrE	HMDB0002311
855	HMDB0012504	10,11-dihydro-leukotriene B4	HMDB0012504
856	HMDB0060106	NA	NA
857	HMDB0012838	6,7-dihydro-12-epi-LTB4	HMDB0012838
858	HMDB0002265	14,15-DiHETrE	HMDB0002265
859	HMDB0013220	Beta-Citryl-L-glutamic acid	HMDB0013220
860	HMDB0155333	NA	NA
861	HMDB0187538	NA	NA
862	HMDB0002044	8-Hydroxyguanosine	HMDB0002044
863	HMDB0141391	NA	NA
864	HMDB0141389	NA	NA
865	HMDB0135622	NA	NA
866	HMDB0135448	NA	NA
867	HMDB0001570	Thymidine 3',5'-cyclic monophosphate	HMDB0001570
868	HMDB0154811	NA	NA
869	HMDB0154812	NA	NA
870	HMDB0178281	NA	NA
871	HMDB0154815	NA	NA
872	HMDB0154816	NA	NA
873	HMDB0014618	Chlordiazepoxide	HMDB0014618
874	HMDB0173604	NA	NA
875	HMDB0173603	NA	NA
876	HMDB0173602	NA	NA
877	HMDB0173601	NA	NA
878	HMDB0173600	NA	NA
879	HMDB0173596	NA	NA
880	HMDB0173594	NA	NA
881	HMDB0173595	NA	NA
882	HMDB0173598	NA	NA
883	HMDB0173597	NA	NA
884	HMDB0015536	Imipenem	HMDB0015536
885	HMDB0060628	NA	NA
886	HMDB0013624	Alpha-Linolenoyl ethanolamide	HMDB0013624
887	HMDB0179589	NA	NA
888	HMDB0179592	NA	NA
889	HMDB0179590	NA	NA
890	HMDB0179591	NA	NA
891	HMDB0185649	NA	NA
892	HMDB0179587	NA	NA
893	HMDB0179586	NA	NA
894	HMDB0179588	NA	NA
895	HMDB0014996	Drostanolone	HMDB0014996
896	HMDB0036829	NA	NA
897	HMDB0039702	NA	NA
898	HMDB0036702	NA	NA
899	HMDB0001043	Arachidonic acid	HMDB0001043
900	HMDB0060102	Arachidonate	HMDB0060102
901	HMDB0002177	Cis-8,11,14,17-Eicosatetraenoic acid	HMDB0002177
902	HMDB0006036	Mesterolone	HMDB0006036
903	HMDB0036830	NA	NA
904	HMDB0037824	NA	NA
905	HMDB0036721	NA	NA
906	HMDB0036754	NA	NA
907	HMDB0039687	NA	NA
908	HMDB0013631	Oleoyl glycine	HMDB0013631
909	HMDB0062571	NA	NA
910	HMDB0062807	NA	NA
911	HMDB0040423	NA	NA
912	HMDB0001480	3-Dehydrosphinganine	HMDB0001480
913	HMDB0002100	Palmitoylethanolamide	HMDB0002100
914	HMDB0000252	Sphingosine	HMDB0000252
915	HMDB0171015	NA	NA
916	HMDB0171016	NA	NA
917	HMDB0171017	NA	NA
918	HMDB0146077	NA	NA
919	HMDB0060088	NA	NA
920	HMDB0169559	NA	NA
921	HMDB0137378	NA	NA
922	HMDB0015031	Testolactone	HMDB0015031
923	HMDB0038684	NA	NA
924	HMDB0000010	2-Methoxyestrone	HMDB0000010
925	HMDB0006768	19-Oxoandrost-4-ene-3,17-dione	HMDB0006768
926	HMDB0006772	Adrenosterone	HMDB0006772
927	HMDB0011195	2-Hydroxy-3-methoxyestrone	HMDB0011195
928	HMDB0039569	NA	NA
929	HMDB0015097	Zaleplon	HMDB0015097

930	HMDB0133470	NA	NA
931	HMDB0125851	NA	NA
932	HMDB0124921	NA	NA
933	HMDB0124820	NA	NA
934	HMDB0030799	5-Deoxymyricanone	HMDB0030799
935	HMDB0036401	NA	NA
936	HMDB0036399	NA	NA
937	HMDB0034010	4',7-Dihydroxy-2'-methoxy-3'-prenylisoflavan	HMDB0034010
938	HMDB0032737	2,2-Bis[4-(2,3-epoxypropoxy)phenyl]propane	HMDB0032737
939	HMDB0031929	Zanthodioline	HMDB0031929
940	HMDB0015607	Lucanthone	HMDB0015607
941	HMDB0014915	Propiomazine	HMDB0014915
942	HMDB0015204	Mequitazine	HMDB0015204
943	HMDB0185647	NA	NA
944	HMDB0185650	NA	NA
945	HMDB0185648	NA	NA
946	HMDB0185644	NA	NA
947	HMDB0185646	NA	NA
948	HMDB0185645	NA	NA
949	HMDB0185643	NA	NA
950	HMDB0185642	NA	NA
951	HMDB0185639	NA	NA
952	HMDB0185641	NA	NA
953	HMDB0185640	NA	NA
954	HMDB0185638	NA	NA
955	HMDB0185636	NA	NA
956	HMDB0185637	NA	NA
957	HMDB0112104	NA	NA
958	HMDB0112091	NA	NA
959	HMDB0062747	NA	NA
960	HMDB0062290	NA	NA
961	HMDB0061647	NA	NA
962	HMDB0061645	NA	NA
963	HMDB0060052	NA	NA
964	HMDB0036802	NA	NA
965	HMDB0005045	15(S)-Hydroxyeicosatrienoic acid	HMDB0005045
966	HMDB0000269	Sphinganine	HMDB0000269
967	HMDB0174156	NA	NA
968	HMDB0174155	NA	NA
969	HMDB0174154	NA	NA
970	HMDB0174153	NA	NA
971	HMDB0174151	NA	NA
972	HMDB0174149	NA	NA
973	HMDB0174152	NA	NA
974	HMDB0174150	NA	NA
975	HMDB0174106	NA	NA
976	HMDB0174105	NA	NA
977	HMDB0174104	NA	NA
978	HMDB0174101	NA	NA
979	HMDB0174100	NA	NA
980	HMDB0174102	NA	NA
981	HMDB0174103	NA	NA
982	HMDB0174097	NA	NA
983	HMDB0174157	NA	NA
984	HMDB0174160	NA	NA
985	HMDB0174161	NA	NA
986	HMDB0174158	NA	NA
987	HMDB0174159	NA	NA
988	HMDB0174098	NA	NA
989	HMDB0174099	NA	NA
990	HMDB0174096	NA	NA
991	HMDB0174095	NA	NA
992	HMDB0174093	NA	NA
993	HMDB0174094	NA	NA
994	HMDB0060039	NA	NA
995	HMDB0036835	NA	NA
996	HMDB0031058	Sciadonic acid	HMDB0031058
997	HMDB0010378	5,8,11-Eicosatrienoic acid	HMDB0010378
998	HMDB0002925	8,11,14-Eicosatrienoic acid	HMDB0002925
999	HMDB0012252	Linoleoyl ethanolamide	HMDB0012252
1000	HMDB0013308	Stearoylglycine	HMDB0013308
1001	HMDB0062338	NA	NA
1002	HMDB0041906	NA	NA
1003	HMDB0147295	NA	NA
1004	HMDB0141110	NA	NA
1005	HMDB0141111	NA	NA
1006	HMDB0141134	NA	NA
1007	HMDB0141135	NA	NA
1008	HMDB0141142	NA	NA
1009	HMDB0141168	NA	NA
1010	HMDB0141174	NA	NA
1011	HMDB0141173	NA	NA
1012	HMDB0147032	NA	NA
1013	HMDB0147293	NA	NA
1014	HMDB0147294	NA	NA
1015	HMDB0147297	NA	NA
1016	HMDB0147298	NA	NA

1017	HMDB0147299	NA	NA
1018	HMDB0147300	NA	NA
1019	HMDB0141074	NA	NA
1020	HMDB0141073	NA	NA
1021	HMDB0128989	NA	NA
1022	HMDB0128988	NA	NA
1023	HMDB0128986	NA	NA
1024	HMDB0128987	NA	NA
1025	HMDB0128991	NA	NA
1026	HMDB0128990	NA	NA
1027	HMDB0128992	NA	NA
1028	HMDB0141065	NA	NA
1029	HMDB0141066	NA	NA
1030	HMDB0147302	NA	NA
1031	HMDB0141087	NA	NA
1032	HMDB0146924	NA	NA
1033	HMDB0033535	Honyudisin	HMDB0033535
1034	HMDB0030600	4-(3-Methyl-1-butenyl)-3,3',4',5-tetrahydroxystilbene	HMDB0030600
1035	HMDB0037586	NA	NA
1036	HMDB0035478	2',3,4',5-Tetrahydroxy-4-prenylstilbene	HMDB0035478
1037	HMDB0173719	NA	NA
1038	HMDB0038724	NA	NA
1039	HMDB0003601	(S)-Reticuline	HMDB0003601
1040	HMDB0177097	NA	NA
1041	HMDB0173722	NA	NA
1042	HMDB0173723	NA	NA
1043	HMDB0173724	NA	NA
1044	HMDB0173726	NA	NA
1045	HMDB0177092	NA	NA
1046	HMDB0173721	NA	NA
1047	HMDB0173720	NA	NA
1048	HMDB0149429	NA	NA
1049	HMDB0177099	NA	NA
1050	HMDB0177098	NA	NA
1051	HMDB0177111	NA	NA
1052	HMDB0177112	NA	NA
1053	HMDB0154672	NA	NA
1054	HMDB0154674	NA	NA
1055	HMDB0154675	NA	NA
1056	HMDB0154673	NA	NA
1057	HMDB0154671	NA	NA
1058	HMDB0154670	NA	NA
1059	HMDB0029566	Isopulegone caffeate	HMDB0029566
1060	HMDB0154668	NA	NA
1061	HMDB0134704	NA	NA
1062	HMDB0147915	NA	NA
1063	HMDB0154665	NA	NA
1064	HMDB0154669	NA	NA
1065	HMDB0154666	NA	NA
1066	HMDB0154667	NA	NA
1067	HMDB0148183	NA	NA
1068	HMDB0153649	NA	NA
1069	HMDB0125854	NA	NA
1070	HMDB0141256	NA	NA
1071	HMDB0124819	NA	NA
1072	HMDB0125836	NA	NA
1073	HMDB0125842	NA	NA
1074	HMDB0133467	NA	NA
1075	HMDB0041386	NA	NA
1076	HMDB0034412	2'-O-Methylphaseollinisoflavan	HMDB0034412
1077	HMDB0039439	NA	NA
1078	HMDB0033672	4'-O-Methylglabridin	HMDB0033672
1079	HMDB0029514	Licochalcone A	HMDB0029514
1080	HMDB0033782	Bergamottin	HMDB0033782
1081	HMDB0039309	NA	NA
1082	HMDB0030846	Archangelin	HMDB0030846
1083	HMDB0039438	NA	NA
1084	HMDB0033671	2'-O-Methylglabridin	HMDB0033671
1085	HMDB0032665	Licoagrocarpin	HMDB0032665
1086	HMDB0031633	Orientanol B	HMDB0031633
1087	HMDB0001272	Nicotine glucuronide	HMDB0001272
1088	HMDB0032808	Niazirinin	HMDB0032808
1089	HMDB0131864	NA	NA
1090	HMDB0124924	NA	NA
1091	HMDB0131867	NA	NA
1092	HMDB0133539	NA	NA
1093	HMDB0124927	NA	NA
1094	HMDB0125807	NA	NA
1095	HMDB0131075	NA	NA
1096	HMDB0133516	NA	NA
1097	HMDB0133495	NA	NA
1098	HMDB0133485	NA	NA
1099	HMDB0133468	NA	NA
1100	HMDB0131866	NA	NA
1101	HMDB0131865	NA	NA
1102	HMDB0124928	NA	NA
1103	HMDB0124929	NA	NA

1104	HMDB0124838	NA	NA
1105	HMDB0124800	NA	NA
1106	HMDB0124826	NA	NA
1107	HMDB0124829	NA	NA
1108	HMDB0124835	NA	NA
1109	HMDB0124837	NA	NA
1110	HMDB0124922	NA	NA
1111	HMDB0130876	NA	NA
1112	HMDB0138809	NA	NA
1113	HMDB0150217	NA	NA
1114	HMDB0150219	NA	NA
1115	HMDB0124822	NA	NA
1116	HMDB0150216	NA	NA
1117	HMDB0150218	NA	NA
1118	HMDB0150215	NA	NA
1119	HMDB0147761	NA	NA
1120	HMDB0147762	NA	NA
1121	HMDB0147765	NA	NA
1122	HMDB0147767	NA	NA
1123	HMDB0147766	NA	NA
1124	HMDB0147764	NA	NA
1125	HMDB0147768	NA	NA
1126	HMDB0147769	NA	NA
1127	HMDB0149836	NA	NA
1128	HMDB0150181	NA	NA
1129	HMDB0150186	NA	NA
1130	HMDB0150185	NA	NA
1131	HMDB0150182	NA	NA
1132	HMDB0150184	NA	NA
1133	HMDB0150187	NA	NA
1134	HMDB0150214	NA	NA
1135	HMDB0035440	alpha,beta-Dihydroxanthohumol	HMDB0035440
1136	HMDB0030666	Chalepin acetate	HMDB0030666
1137	HMDB0035403	Gingerenone A	HMDB0035403
1138	HMDB0030798	Myricanone	HMDB0030798
1139	HMDB0033880	Mammea B/AC cyclo D	HMDB0033880
1140	HMDB0033879	Mammea B/AD cyclo D	HMDB0033879
1141	HMDB0030333	Fragransol C	HMDB0030333
1142	HMDB0041401	NA	NA
1143	HMDB0138808	NA	NA
1144	HMDB0184970	NA	NA
1145	HMDB0184809	NA	NA
1146	HMDB0165813	NA	NA
1147	HMDB0173729	NA	NA
1148	HMDB0036987	NA	NA
1149	HMDB0033354	Cassythicine	HMDB0033354
1150	HMDB0032143	Palaudine	HMDB0032143
1151	HMDB0030245	Nornantenine	HMDB0030245
1152	HMDB0038145	NA	NA
1153	HMDB0033360	Isodomesticine	HMDB0033360
1154	HMDB0168557	NA	NA
1155	HMDB0168558	NA	NA
1156	HMDB0032717	Lepidine C	HMDB0032717
1157	HMDB0033437	Lepidine	HMDB0033437
1158	HMDB0041826	NA	NA
1159	HMDB0179308	NA	NA
1160	HMDB0179323	NA	NA
1161	HMDB0179326	NA	NA
1162	HMDB0179329	NA	NA
1163	HMDB0179320	NA	NA
1164	HMDB0015288	Trimetrexate	HMDB0015288
1165	HMDB0014808	Pirenzepine	HMDB0014808
1166	HMDB0172326	NA	NA
1167	HMDB0172325	NA	NA
1168	HMDB0012996	Lipoyllysine	HMDB0012996
1169	HMDB0114763	NA	NA
1170	HMDB0062319	NA	NA
1171	HMDB0176802	NA	NA
1172	HMDB0176822	NA	NA
1173	HMDB0031877	Acetylsalvipisone	HMDB0031877
1174	HMDB0161644	NA	NA
1175	HMDB0161632	NA	NA
1176	HMDB0161627	NA	NA
1177	HMDB0161628	NA	NA
1178	HMDB0161629	NA	NA
1179	HMDB0161622	NA	NA
1180	HMDB0161624	NA	NA
1181	HMDB0161626	NA	NA
1182	HMDB0161623	NA	NA
1183	HMDB0161625	NA	NA
1184	HMDB0015227	Fluvastatin	HMDB0015227
1185	HMDB0185383	NA	NA
1186	HMDB0158037	NA	NA
1187	HMDB0015439	Tasosartan	HMDB0015439
1188	HMDB0153809	NA	NA
1189	HMDB0033906	2'-Hydroxy-3',4',5',7,8-pentamethoxyflavan	HMDB0033906
1190	HMDB0039032	NA	NA

1191	HMDB0032731	(1E,4Z,6a,8b,10a)-8-Angeloyloxy-10,15-dihydroxy-3-oxo-1,4,11(13)-germacatrien-12,6-olide	HMDB0032731
1192	HMDB0035108	Diosbulbin A	HMDB0035108
1193	HMDB0036780	NA	NA
1194	HMDB0032105	1,2-Anhydridoniveusin	HMDB0032105
1195	HMDB0030081	Carissanol	HMDB0030081
1196	HMDB0039575	NA	NA
1197	HMDB0178288	NA	NA
1198	HMDB0038581	NA	NA
1199	HMDB0014671	Erlotinib	HMDB0014671
1200	HMDB0038643	NA	NA
1201	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol	HMDB0011644
1202	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al	HMDB0006894
1203	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one	HMDB0006887
1204	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one	HMDB0006886
1205	HMDB0006764	17a,20a-Dihydroxycholesterol	HMDB0006764
1206	HMDB0006763	20a,22b-Dihydroxycholesterol	HMDB0006763
1207	HMDB0006281	7-a,27-Dihydroxycholesterol	HMDB0006281
1208	HMDB0060136	7alpha,24S-Dihydroxycholesterol	HMDB0060136
1209	HMDB0006280	7-a,25-Dihydroxycholesterol	HMDB0006280
1210	HMDB0159657	NA	NA
1211	HMDB0172272	NA	NA
1212	HMDB0172271	NA	NA
1213	HMDB0172269	NA	NA
1214	HMDB0172270	NA	NA
1215	HMDB0172267	NA	NA
1216	HMDB0172265	NA	NA
1217	HMDB0172268	NA	NA
1218	HMDB0172266	NA	NA
1219	HMDB0185566	NA	NA
1220	HMDB0185568	NA	NA
1221	HMDB0185575	NA	NA
1222	HMDB0185573	NA	NA
1223	HMDB0185574	NA	NA
1224	HMDB0185571	NA	NA
1225	HMDB0185572	NA	NA
1226	HMDB0185569	NA	NA
1227	HMDB0185567	NA	NA
1228	HMDB0185570	NA	NA
1229	HMDB0172262	NA	NA
1230	HMDB0172264	NA	NA
1231	HMDB0062675	NA	NA
1232	HMDB0062664	NA	NA
1233	HMDB0062607	NA	NA
1234	HMDB0062420	NA	NA
1235	HMDB0062419	NA	NA
1236	HMDB0159652	NA	NA
1237	HMDB0159656	NA	NA
1238	HMDB0172263	NA	NA
1239	HMDB0159658	NA	NA
1240	HMDB0159655	NA	NA
1241	HMDB0159654	NA	NA
1242	HMDB0159653	NA	NA
1243	HMDB0159651	NA	NA
1244	HMDB0184845	NA	NA
1245	HMDB0184846	NA	NA
1246	HMDB0155084	NA	NA
1247	HMDB0184842	NA	NA
1248	HMDB0184843	NA	NA
1249	HMDB0184841	NA	NA
1250	HMDB0184844	NA	NA
1251	HMDB0184848	NA	NA
1252	HMDB0184847	NA	NA
1253	HMDB0184849	NA	NA
1254	HMDB0184851	NA	NA
1255	HMDB0184850	NA	NA
1256	HMDB0185576	NA	NA
1257	HMDB0185577	NA	NA
1258	HMDB0185578	NA	NA
1259	HMDB0184168	NA	NA
1260	HMDB0003550	Calcidiol	HMDB0003550
1261	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	HMDB0036012
1262	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	HMDB0034328
1263	HMDB0035585	1-Phenyl-1,3-heneicosanedione	HMDB0035585
1264	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	HMDB0006721
1265	HMDB0006722	25-Hydroxytachysterol3	HMDB0006722
1266	HMDB0001993	7a-Hydroxy-cholestene-3-one	HMDB0001993
1267	HMDB0000501	7-Ketocholesterol	HMDB0000501
1268	HMDB0015504	Alfacalcidol	HMDB0015504
1269	HMDB0039871	NA	NA
1270	HMDB0060132	NA	NA
1271	HMDB0060131	NA	NA
1272	HMDB0184149	NA	NA
1273	HMDB0174260	NA	NA
1274	HMDB0174261	NA	NA
1275	HMDB0172274	NA	NA
1276	HMDB0172275	NA	NA
1277	HMDB0172273	NA	NA

1278	HMDB0155085	NA	NA
1279	HMDB0155087	NA	NA
1280	HMDB0155086	NA	NA
1281	HMDB0155081	NA	NA
1282	HMDB0155082	NA	NA
1283	HMDB0174265	NA	NA
1284	HMDB0174262	NA	NA
1285	HMDB0174263	NA	NA
1286	HMDB0184150	NA	NA
1287	HMDB0184148	NA	NA
1288	HMDB0184147	NA	NA
1289	HMDB0184145	NA	NA
1290	HMDB0184146	NA	NA
1291	HMDB0184144	NA	NA
1292	HMDB0174268	NA	NA
1293	HMDB0174267	NA	NA
1294	HMDB0174266	NA	NA
1295	HMDB0174264	NA	NA
1296	HMDB0155083	NA	NA
1297	HMDB0155080	NA	NA
1298	HMDB0184143	NA	NA
1299	HMDB0154867	NA	NA
1300	HMDB0154866	NA	NA
1301	HMDB0035951	Erucylacetone	HMDB0035951
1302	HMDB0164879	NA	NA
1303	HMDB0006351	Vaccenyl carnitine	HMDB0006351
1304	HMDB0013337	2-Hydroxyhexadecanoylcarnitine	HMDB0013337
1305	HMDB0013338	11Z-Octadecenylcarnitine	HMDB0013338
1306	HMDB0005065	Oleoylcarnitine	HMDB0005065
1307	HMDB0094687	NA	NA
1308	HMDB0006464	Elaidic carnitine	HMDB0006464
1309	HMDB0062772	NA	NA
1310	HMDB0013154	12-Hydroxy-12-octadecanoylcarnitine	HMDB0013154
1311	HMDB0002126	27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	HMDB0002126
1312	HMDB0036883	NA	NA
1313	HMDB0159770	NA	NA
1314	HMDB0159769	NA	NA
1315	HMDB0159767	NA	NA
1316	HMDB0159766	NA	NA
1317	HMDB0159765	NA	NA
1318	HMDB0159768	NA	NA
1319	HMDB0062421	NA	NA
1320	HMDB0062416	NA	NA
1321	HMDB0159772	NA	NA
1322	HMDB0159774	NA	NA
1323	HMDB0159773	NA	NA
1324	HMDB0159897	NA	NA
1325	HMDB0159894	NA	NA
1326	HMDB0159896	NA	NA
1327	HMDB0159893	NA	NA
1328	HMDB0159889	NA	NA
1329	HMDB0159890	NA	NA
1330	HMDB0159892	NA	NA
1331	HMDB0159891	NA	NA
1332	HMDB0000558	5a-Cholestane-3a,7a,12a,23,25-pentol	HMDB0000558
1333	HMDB0002208	Cholestane-3,7,12,24,25-pentol	HMDB0002208
1334	HMDB0000483	5b-Cholestane-3a,7a,12a,23S,25-pentol	HMDB0000483
1335	HMDB0000556	5b-Cholestane-3a,7a,12a,24,25-pentol	HMDB0000556
1336	HMDB0000513	5b-Cholestane-3a,7a,12a,23R,25-pentol	HMDB0000513
1337	HMDB0002180	5b-Cholestane-3a,7a,12a,25,26-pentol	HMDB0002180
1338	HMDB0011187	TG(8:0/8:0/8:0)	HMDB0011187
1339	HMDB0059930	NA	NA
1340	HMDB0167285	NA	NA
1341	HMDB0179976	NA	NA
1342	HMDB0179977	NA	NA
1343	HMDB0179975	NA	NA
1344	HMDB0167287	NA	NA
1345	HMDB0179974	NA	NA
1346	HMDB0167288	NA	NA
1347	HMDB0167286	NA	NA
1348	HMDB0036131	NA	NA
1349	HMDB0168857	NA	NA
1350	HMDB0062445	NA	NA
1351	HMDB0145193	NA	NA
1352	HMDB0161711	NA	NA
1353	HMDB0145200	NA	NA
1354	HMDB0161709	NA	NA
1355	HMDB0161720	NA	NA
1356	HMDB0145201	NA	NA
1357	HMDB0145177	NA	NA
1358	HMDB0145180	NA	NA
1359	HMDB0145185	NA	NA
1360	HMDB0145187	NA	NA
1361	HMDB0145189	NA	NA
1362	HMDB0145196	NA	NA
1363	HMDB0145197	NA	NA
1364	HMDB0145190	NA	NA

1365	HMDB0145192	NA	NA
1366	HMDB0145181	NA	NA
1367	HMDB0165633	NA	NA
1368	HMDB0163398	NA	NA
1369	HMDB0169690	NA	NA
1370	HMDB0169689	NA	NA
1371	HMDB0163397	NA	NA
1372	HMDB0163729	NA	NA
1373	HMDB0163728	NA	NA
1374	HMDB0240233	NA	NA
1375	HMDB0133638	NA	NA
1376	HMDB0133618	NA	NA
1377	HMDB0176615	NA	NA
1378	HMDB0176621	NA	NA
1379	HMDB0176619	NA	NA
1380	HMDB0176620	NA	NA
1381	HMDB0176618	NA	NA
1382	HMDB0176617	NA	NA
1383	HMDB0176614	NA	NA
1384	HMDB0176613	NA	NA
1385	HMDB0176612	NA	NA
1386	HMDB0176616	NA	NA
1387	HMDB0037783	NA	NA
1388	HMDB0034532	Camelliagenin C	HMDB0034532
1389	HMDB0034525	Barringtonenol C	HMDB0034525
1390	HMDB0035853	Fasciculol C	HMDB0035853
1391	HMDB0035150	2'-Apo-beta-carotenal	HMDB0035150
1392	HMDB0158633	NA	NA
1393	HMDB0158234	NA	NA
1394	HMDB0158235	NA	NA
1395	HMDB0158642	NA	NA
1396	HMDB0158238	NA	NA
1397	HMDB0158621	NA	NA
1398	HMDB0158636	NA	NA
1399	HMDB0158629	NA	NA
1400	HMDB0158625	NA	NA
1401	HMDB0158226	NA	NA
1402	HMDB0158231	NA	NA
1403	HMDB0158228	NA	NA
1404	HMDB0157580	NA	NA
1405	HMDB0158210	NA	NA
1406	HMDB0158213	NA	NA
1407	HMDB0158219	NA	NA
1408	HMDB0158216	NA	NA
1409	HMDB0158221	NA	NA
1410	HMDB0158223	NA	NA
1411	HMDB0158225	NA	NA
1412	HMDB0158639	NA	NA
1413	HMDB0158646	NA	NA
1414	HMDB0158643	NA	NA
1415	HMDB0169111	NA	NA
1416	HMDB0171254	NA	NA
1417	HMDB0171269	NA	NA
1418	HMDB0171253	NA	NA
1419	HMDB0171257	NA	NA
1420	HMDB0171258	NA	NA
1421	HMDB0171264	NA	NA
1422	HMDB0171268	NA	NA
1423	HMDB0171273	NA	NA
1424	HMDB0171272	NA	NA
1425	HMDB0169110	NA	NA
1426	HMDB0169105	NA	NA
1427	HMDB0169108	NA	NA
1428	HMDB0158650	NA	NA
1429	HMDB0158654	NA	NA
1430	HMDB0158656	NA	NA
1431	HMDB0158660	NA	NA
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1433	HMDB0169099	NA	NA
1434	HMDB0169097	NA	NA
1435	HMDB0169101	NA	NA
1436	HMDB0169103	NA	NA
1437	HMDB0169107	NA	NA
1438	HMDB0033412	Gibberellin A20 13-glucoside	HMDB0033412
1439	HMDB0037084	NA	NA
1440	HMDB0038610	NA	NA
1441	HMDB0171261	NA	NA
1442	HMDB0015181	Fluocinonide	HMDB0015181
1443	HMDB0140090	NA	NA
1444	HMDB0033177	Sapiol	HMDB0033177
1445	HMDB0038738	NA	NA
1446	HMDB0157582	NA	NA
1447	HMDB0179952	NA	NA
1448	HMDB0179953	NA	NA
1449	HMDB0174900	NA	NA
1450	HMDB0167227	NA	NA
1451	HMDB0167180	NA	NA

1452	HMDB0035700	Lucidenic acid J	HMDB0035700
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1454	HMDB0167174	NA	NA
1455	HMDB0167200	NA	NA
1456	HMDB0167223	NA	NA
1457	HMDB0167220	NA	NA
1458	HMDB0167217	NA	NA
1459	HMDB0167216	NA	NA
1460	HMDB0167195	NA	NA
1461	HMDB0167213	NA	NA
1462	HMDB0167206	NA	NA
1463	HMDB0167209	NA	NA
1464	HMDB0167203	NA	NA
1465	HMDB0167186	NA	NA
1466	HMDB0167183	NA	NA
1467	HMDB0167177	NA	NA
1468	HMDB0167189	NA	NA
1469	HMDB0167192	NA	NA
1470	HMDB0167196	NA	NA
1471	HMDB0167197	NA	NA
1472	HMDB0173045	NA	NA
1473	HMDB0033471	N1,N10-Diferuloylspermidine	HMDB0033471
1474	HMDB0158489	NA	NA
1475	HMDB0158490	NA	NA
1476	HMDB0158494	NA	NA
1477	HMDB0158485	NA	NA
1478	HMDB0158502	NA	NA
1479	HMDB0158497	NA	NA
1480	HMDB0158498	NA	NA
1481	HMDB0158486	NA	NA
1482	HMDB0158501	NA	NA
1483	HMDB0158493	NA	NA
1484	HMDB0030685	Cycloheterophyllin	HMDB0030685
1485	HMDB0034665	Artonin A	HMDB0034665
1486	HMDB0029471	Isocycloheterophyllin	HMDB0029471
1487	HMDB0035187	Artonin F	HMDB0035187
1488	HMDB0034667	Artonin B	HMDB0034667
1489	HMDB0187390	NA	NA
1490	HMDB0187391	NA	NA
1491	HMDB0187182	NA	NA
1492	HMDB0187392	NA	NA
1493	HMDB0035167	Cinnacsiol C1 19-glucoside	HMDB0035167
1494	HMDB0168850	NA	NA
1495	HMDB0183642	NA	NA
1496	HMDB0177911	NA	NA
1497	HMDB0168858	NA	NA
1498	HMDB0168859	NA	NA
1499	HMDB0177908	NA	NA
1500	HMDB0183653	NA	NA
1501	HMDB0183640	NA	NA
1502	HMDB0183646	NA	NA
1503	HMDB0183661	NA	NA
1504	HMDB0183660	NA	NA
1505	HMDB0183664	NA	NA
1506	HMDB0183663	NA	NA
1507	HMDB0183666	NA	NA
1508	HMDB0183667	NA	NA
1509	HMDB0183668	NA	NA
1510	HMDB0183671	NA	NA
1511	HMDB0183670	NA	NA
1512	HMDB0183659	NA	NA
1513	HMDB0183662	NA	NA
1514	HMDB0183655	NA	NA
1515	HMDB0183644	NA	NA
1516	HMDB0183645	NA	NA
1517	HMDB0183656	NA	NA
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1520	HMDB0183649	NA	NA
1521	HMDB0183651	NA	NA
1522	HMDB0183652	NA	NA
1523	HMDB0183657	NA	NA
1524	HMDB0183672	NA	NA
1525	HMDB0035603	Mascaroside	HMDB0035603
1526	HMDB0183641	NA	NA
1527	HMDB0037083	NA	NA
1528	HMDB0036903	NA	NA
1529	HMDB0040672	NA	NA
1530	HMDB0162428	NA	NA
1531	HMDB0162427	NA	NA
1532	HMDB0038028	NA	NA
1533	HMDB0145256	NA	NA
1534	HMDB0145259	NA	NA
1535	HMDB0145255	NA	NA
1536	HMDB0145268	NA	NA
1537	HMDB0145246	NA	NA
1538	HMDB0145249	NA	NA

1539	HMDB0145247	NA	NA
1540	HMDB0145253	NA	NA
1541	HMDB0145260	NA	NA
1542	HMDB0145261	NA	NA
1543	HMDB0145267	NA	NA
1544	HMDB0145263	NA	NA
1545	HMDB0145250	NA	NA
1546	HMDB0145262	NA	NA
1547	HMDB0145264	NA	NA
1548	HMDB0145265	NA	NA
1549	HMDB0145258	NA	NA
1550	HMDB0145252	NA	NA
1551	HMDB0145270	NA	NA
1552	HMDB0014433	Amcinonide	HMDB0014433
1553	HMDB0034339	Ixocarpalactone B	HMDB0034339
1554	HMDB0034059	4beta-Hydroxywithanolide E	HMDB0034059
1555	HMDB0034400	Withaperuvins F	HMDB0034400
1556	HMDB0034191	Withaperuvins B	HMDB0034191
1557	HMDB0031355	28-Hydroxywithanolide E	HMDB0031355
1558	HMDB0033943	Withaperuvins G	HMDB0033943
1559	HMDB0030362	Cavipetin B	HMDB0030362
1560	HMDB0170358	NA	NA
1561	HMDB0187402	NA	NA
1562	HMDB0185457	NA	NA
1563	HMDB0015393	Darunavir	HMDB0015393
1564	HMDB0168629	NA	NA
1565	HMDB0168628	NA	NA
1566	HMDB0161739	NA	NA
1567	HMDB0161740	NA	NA
1568	HMDB0072546	NA	NA
1569	HMDB0072531	NA	NA
1570	HMDB0072529	NA	NA
1571	HMDB0072338	NA	NA
1572	HMDB0072333	NA	NA
1573	HMDB0072245	NA	NA
1574	HMDB0072206	NA	NA
1575	HMDB0071968	NA	NA
1576	HMDB0071738	NA	NA
1577	HMDB0100886	NA	NA
1578	HMDB0100885	NA	NA
1579	HMDB0100884	NA	NA
1580	HMDB0096650	NA	NA
1581	HMDB0096651	NA	NA
1582	HMDB0096564	NA	NA
1583	HMDB0096562	NA	NA
1584	HMDB0096563	NA	NA
1585	HMDB0071685	NA	NA
1586	HMDB0071676	NA	NA
1587	HMDB0071663	NA	NA
1588	HMDB0096649	NA	NA
1589	HMDB0071443	NA	NA
1590	HMDB0071222	NA	NA
1591	HMDB0071165	NA	NA
1592	HMDB0143851	NA	NA
1593	HMDB0143714	NA	NA
1594	HMDB0143713	NA	NA
1595	HMDB0143708	NA	NA
1596	HMDB0143707	NA	NA
1597	HMDB0143710	NA	NA
1598	HMDB0143705	NA	NA
1599	HMDB0143706	NA	NA
1600	HMDB0143704	NA	NA
1601	HMDB0143701	NA	NA
1602	HMDB0143700	NA	NA
1603	HMDB0143716	NA	NA
1604	HMDB0143717	NA	NA
1605	HMDB0143850	NA	NA
1606	HMDB0143819	NA	NA
1607	HMDB0143820	NA	NA
1608	HMDB0143810	NA	NA
1609	HMDB0143809	NA	NA
1610	HMDB0143780	NA	NA
1611	HMDB0143759	NA	NA
1612	HMDB0143760	NA	NA
1613	HMDB0143720	NA	NA
1614	HMDB0143861	NA	NA
1615	HMDB0143718	NA	NA
1616	HMDB0143702	NA	NA
1617	HMDB0143697	NA	NA
1618	HMDB0143695	NA	NA
1619	HMDB0143779	NA	NA
1620	HMDB0143719	NA	NA
1621	HMDB0060144	NA	NA
1622	HMDB0143907	NA	NA
1623	HMDB0143902	NA	NA
1624	HMDB0143896	NA	NA
1625	HMDB0143888	NA	NA

1626	HMDB0143860	NA	NA
1627	HMDB0143870	NA	NA
1628	HMDB0143871	NA	NA
1629	HMDB0143880	NA	NA
1630	HMDB0143881	NA	NA
1631	HMDB0174790	NA	NA
1632	HMDB0174789	NA	NA
1633	HMDB0174791	NA	NA
1634	HMDB0174792	NA	NA
1635	HMDB0167228	NA	NA
1636	HMDB0167225	NA	NA
1637	HMDB0167224	NA	NA
1638	HMDB0167221	NA	NA
1639	HMDB0167229	NA	NA
1640	HMDB0034194	Jurubine	HMDB0034194
1641	HMDB0164367	NA	NA
1642	HMDB0164368	NA	NA
1643	HMDB0164358	NA	NA
1644	HMDB0164359	NA	NA
1645	HMDB0164350	NA	NA
1646	HMDB0164349	NA	NA
1647	HMDB0164341	NA	NA
1648	HMDB0164340	NA	NA
1649	HMDB0033477	NA	NA
1650	HMDB0166351	NA	NA
1651	HMDB0166343	NA	NA
1652	HMDB0166344	NA	NA
1653	HMDB0166348	NA	NA
1654	HMDB0184268	NA	NA
1655	HMDB0184266	NA	NA
1656	HMDB0183468	NA	NA
1657	HMDB0183465	NA	NA
1658	HMDB0166347	NA	NA
1659	HMDB0166355	NA	NA
1660	HMDB0166356	NA	NA
1661	HMDB0166352	NA	NA
1662	HMDB0183463	NA	NA
1663	HMDB0184827	NA	NA
1664	HMDB0062478	NA	NA
1665	HMDB0060155	NA	NA
1666	HMDB0013061	S-(PGA1)-glutathione	HMDB0013061
1667	HMDB0013060	S-(9-hydroxy-PGA2)-glutathione	HMDB0013060
1668	HMDB0013057	S-(9-deoxy-delta12-PGD2)-glutathione	HMDB0013057
1669	HMDB0013056	S-(11-OH-9-deoxy-delta9,12-PGD2)-glutathione	HMDB0013056
1670	HMDB0183885	NA	NA
1671	HMDB0183879	NA	NA
1672	HMDB0183878	NA	NA
1673	HMDB0183884	NA	NA
1674	HMDB0001198	Leukotriene C4	HMDB0001198
1675	HMDB0183882	NA	NA
1676	HMDB0005095	11-trans-Leukotriene C4	HMDB0005095
1677	HMDB0183888	NA	NA
1678	HMDB0183887	NA	NA
1679	HMDB0183881	NA	NA
1680	HMDB0178719	NA	NA
1681	HMDB0178728	NA	NA
1682	HMDB0178720	NA	NA
1683	HMDB0178718	NA	NA
1684	HMDB0178717	NA	NA
1685	HMDB0178729	NA	NA
1686	HMDB0178730	NA	NA
1687	HMDB0178727	NA	NA
1688	HMDB0160619	NA	NA
1689	HMDB0160620	NA	NA
1690	HMDB0160617	NA	NA
1691	HMDB0160616	NA	NA
1692	HMDB0173931	NA	NA
1693	HMDB0173932	NA	NA
1694	HMDB0014351	Reserpine	HMDB0014351
1695	HMDB0030172	Oxyacanthine	HMDB0030172
1696	HMDB0015330	Tubocurarine	HMDB0015330
1697	HMDB0185009	NA	NA
1698	HMDB0185010	NA	NA
1699	HMDB0014964	Natamycin	HMDB0014964
1700	HMDB0040917	NA	NA
1701	HMDB0015032	Benzylpenicilloyl Polylysine	HMDB0015032
1702	HMDB0184092	NA	NA
1703	HMDB0184087	NA	NA
1704	HMDB0015183	Ergoloid mesylate	HMDB0015183
1705	HMDB0168627	NA	NA
1706	HMDB0161735	NA	NA
1707	HMDB0161734	NA	NA
1708	HMDB0161733	NA	NA
1709	HMDB0168626	NA	NA
1710	HMDB0161736	NA	NA
1711	HMDB0184371	NA	NA
1712	HMDB0184657	NA	NA

1713	HMDB0184663	NA	NA
1714	HMDB0168002	NA	NA
1715	HMDB0168000	NA	NA
1716	HMDB0167999	NA	NA
1717	HMDB0168001	NA	NA
1718	HMDB0167998	NA	NA
1719	HMDB0167996	NA	NA
1720	HMDB0167997	NA	NA
1721	HMDB0168003	NA	NA
1722	HMDB0168005	NA	NA
1723	HMDB0168009	NA	NA
1724	HMDB0168007	NA	NA
1725	HMDB0168006	NA	NA
1726	HMDB0168008	NA	NA
1727	HMDB0167992	NA	NA
1728	HMDB0168004	NA	NA
1729	HMDB0167993	NA	NA
1730	HMDB0165890	NA	NA
1731	HMDB0165885	NA	NA
1732	HMDB0165884	NA	NA
1733	HMDB0165888	NA	NA
1734	HMDB0165889	NA	NA
1735	HMDB0165891	NA	NA
1736	HMDB0165899	NA	NA
1737	HMDB0165896	NA	NA
1738	HMDB0165898	NA	NA
1739	HMDB0165897	NA	NA
1740	HMDB0165895	NA	NA
1741	HMDB0165893	NA	NA
1742	HMDB0165892	NA	NA
1743	HMDB0165894	NA	NA
1744	HMDB0034699	Fumonisin A2	HMDB0034699
1745	HMDB0148903	NA	NA
1746	HMDB0148904	NA	NA
1747	HMDB0167769	NA	NA
1748	HMDB0167768	NA	NA
1749	HMDB0173103	NA	NA
1750	HMDB0169616	NA	NA
1751	HMDB0165411	NA	NA
1752	HMDB0173104	NA	NA
1753	HMDB0164420	NA	NA
1754	HMDB0164423	NA	NA
1755	HMDB0164424	NA	NA
1756	HMDB0164421	NA	NA
1757	HMDB0164422	NA	NA
1758	HMDB0164419	NA	NA
1759	HMDB0164418	NA	NA
1760	HMDB0015518	Metrizamide	HMDB0015518
1761	HMDB0127545	NA	NA
1762	HMDB0127546	NA	NA
1763	HMDB0036339	NA	NA
1764	HMDB0177744	NA	NA
1765	HMDB0177747	NA	NA
1766	HMDB0177749	NA	NA
1767	HMDB0177748	NA	NA
1768	HMDB0177746	NA	NA
1769	HMDB0177745	NA	NA
1770	HMDB0177743	NA	NA
1771	HMDB0178532	NA	NA
1772	HMDB0178529	NA	NA
1773	HMDB0178528	NA	NA
1774	HMDB0178530	NA	NA
1775	HMDB0178531	NA	NA
1776	HMDB0178527	NA	NA
1777	HMDB0114630	NA	NA
1778	HMDB0114658	NA	NA
1779	HMDB0004889	Ganglioside GA2 (d18:1/9Z-18:1)	HMDB0004889
1780	HMDB0001543	Diguanosine hexaphosphate	HMDB0001543
1781	HMDB0006563	Hexaglutamyl folate	HMDB0006563
1782	HMDB0060217	NA	NA
1783	HMDB0032781	Acetylujuboside B	HMDB0032781
1784	HMDB0056929	NA	NA
1785	HMDB0056930	NA	NA
1786	HMDB0056950	NA	NA
1787	HMDB0056954	NA	NA
1788	HMDB0056985	NA	NA
1789	HMDB0056995	NA	NA
1790	HMDB0057012	NA	NA
1791	HMDB0057013	NA	NA
1792	HMDB0056834	NA	NA
1793	HMDB0056782	NA	NA
1794	HMDB0056503	NA	NA
1795	HMDB0056504	NA	NA
1796	HMDB0056524	NA	NA
1797	HMDB0056528	NA	NA
1798	HMDB0057019	NA	NA
1799	HMDB0057029	NA	NA

1800	HMDB0057095	NA	NA
1801	HMDB0057127	NA	NA
1802	HMDB0057147	NA	NA
1803	HMDB0057179	NA	NA
1804	HMDB0057244	NA	NA
1805	HMDB0057248	NA	NA
1806	HMDB0057913	NA	NA
1807	HMDB0058366	NA	NA
1808	HMDB0010256	CL(20:1(11Z)/18:2(9Z,12Z)/18:1(9Z)/18:1(11Z))	HMDB0010256
1809	HMDB0010257	CL(20:1(11Z)/18:2(9Z,12Z)/18:1(9Z)/18:1(9Z))	HMDB0010257
1810	HMDB0010255	CL(20:1(11Z)/18:2(9Z,12Z)/18:1(11Z)/18:1(9Z))	HMDB0010255
1811	HMDB0010254	CL(20:1(11Z)/18:2(9Z,12Z)/18:1(11Z)/18:1(11Z))	HMDB0010254

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)

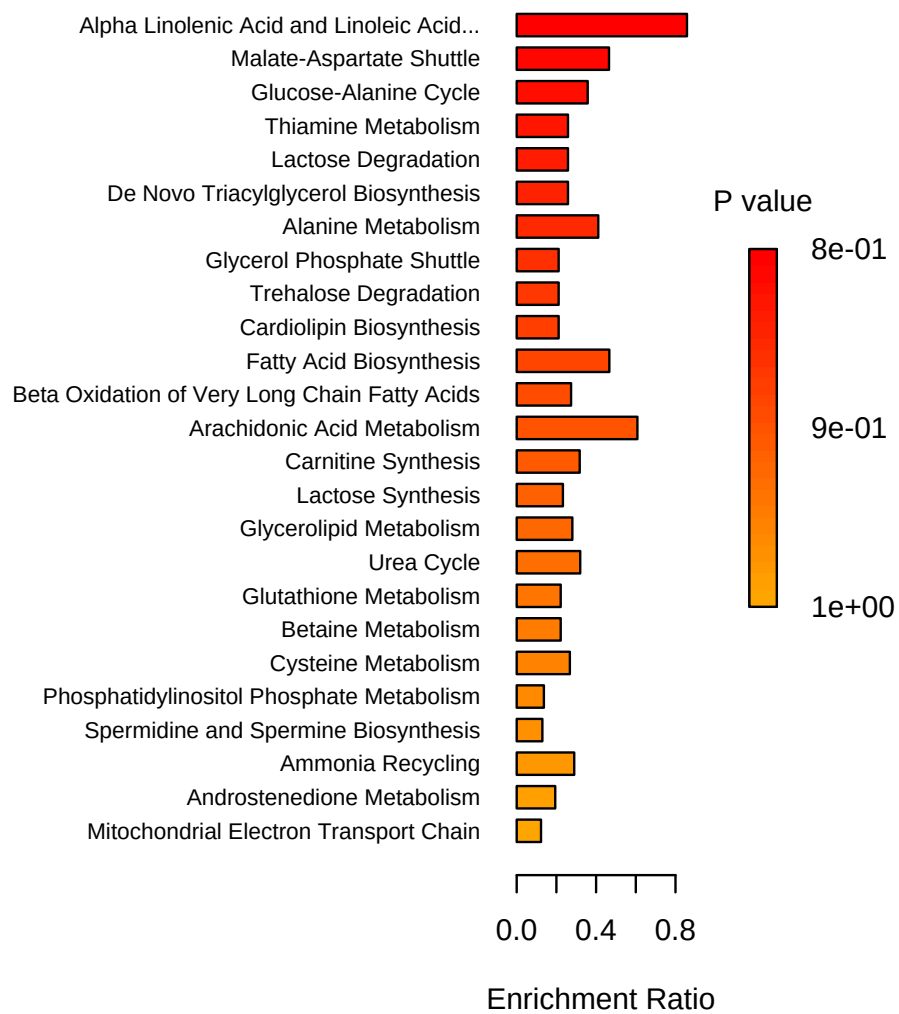


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Alpha Linolenic Acid and Linoleic Acid Metabolism	19	8.16	7	7.80E-01	1.00E+00	1.00E+00
Malate-Aspartate Shuttle	10	4.30	2	9.70E-01	1.00E+00	1.00E+00
Glucose-Alanine Cycle	13	5.59	2	9.93E-01	1.00E+00	1.00E+00
Thiamine Metabolism	9	3.87	1	9.94E-01	1.00E+00	1.00E+00
Lactose Degradation	9	3.87	1	9.94E-01	1.00E+00	1.00E+00
De Novo Triacylglycerol Biosynthesis	9	3.87	1	9.94E-01	1.00E+00	1.00E+00
Alanine Metabolism	17	7.30	3	9.94E-01	1.00E+00	1.00E+00
Glycerol Phosphate Shuttle	11	4.73	1	9.98E-01	1.00E+00	1.00E+00
Trehalose Degradation	11	4.73	1	9.98E-01	1.00E+00	1.00E+00
Cardiolipin Biosynthesis	11	4.73	1	9.98E-01	1.00E+00	1.00E+00
Fatty Acid Biosynthesis	35	15.00	7	9.99E-01	1.00E+00	1.00E+00
Beta Oxidation of Very Long Chain Fatty Acids	17	7.30	2	9.99E-01	1.00E+00	1.00E+00
Arachidonic Acid Metabolism	69	29.60	18	9.99E-01	1.00E+00	1.00E+00
Carnitine Synthesis	22	9.45	3	9.99E-01	1.00E+00	1.00E+00
Lactose Synthesis	20	8.59	2	1.00E+00	1.00E+00	1.00E+00
Glycerolipid Metabolism	25	10.70	3	1.00E+00	1.00E+00	1.00E+00
Urea Cycle	29	12.50	4	1.00E+00	1.00E+00	1.00E+00
Glutathione Metabolism	21	9.02	2	1.00E+00	1.00E+00	1.00E+00
Betaine Metabolism	21	9.02	2	1.00E+00	1.00E+00	1.00E+00
Cysteine Metabolism	26	11.20	3	1.00E+00	1.00E+00	1.00E+00
Phosphatidylinositol Metabolism	17	7.30	1	1.00E+00	1.00E+00	1.00E+00
Spermidine and Spermine Biosynthesis	18	7.73	1	1.00E+00	1.00E+00	1.00E+00
Ammonia Recycling	32	13.80	4	1.00E+00	1.00E+00	1.00E+00
Androstenedione Metabolism	24	10.30	2	1.00E+00	1.00E+00	1.00E+00
Mitochondrial Electron Transport Chain	19	8.16	1	1.00E+00	1.00E+00	1.00E+00
Glycolysis	25	10.70	2	1.00E+00	1.00E+00	1.00E+00
Vitamin B6 Metabolism	20	8.59	1	1.00E+00	1.00E+00	1.00E+00
Riboflavin Metabolism	20	8.59	1	1.00E+00	1.00E+00	1.00E+00
Oxidation of Branched Chain Fatty Acids	26	11.20	2	1.00E+00	1.00E+00	1.00E+00
Inositol Phosphate Metabolism	26	11.20	2	1.00E+00	1.00E+00	1.00E+00
Pantothenate and CoA Biosynthesis	21	9.02	1	1.00E+00	1.00E+00	1.00E+00
Fructose and Mannose Degradation	32	13.80	3	1.00E+00	1.00E+00	1.00E+00
Sulfate/Sulfite Metabolism	22	9.45	1	1.00E+00	1.00E+00	1.00E+00
Transfer of Acetyl Groups into Mitochondria	22	9.45	1	1.00E+00	1.00E+00	1.00E+00
Phenylalanine and Tyrosine Metabolism	28	12.00	2	1.00E+00	1.00E+00	1.00E+00
Amino Sugar Metabolism	33	14.20	3	1.00E+00	1.00E+00	1.00E+00
Folate Metabolism	29	12.50	2	1.00E+00	1.00E+00	1.00E+00
Estrone Metabolism	24	10.30	1	1.00E+00	1.00E+00	1.00E+00
Lysine Degradation	30	12.90	2	1.00E+00	1.00E+00	1.00E+00
Aspartate Metabolism	35	15.00	3	1.00E+00	1.00E+00	1.00E+00
Gluconeogenesis	35	15.00	3	1.00E+00	1.00E+00	1.00E+00
Sphingolipid Metabolism	40	17.20	4	1.00E+00	1.00E+00	1.00E+00
Phytanic Acid Peroxisomal Oxidation	26	11.20	1	1.00E+00	1.00E+00	1.00E+00
Plasmalogen Synthesis	26	11.20	1	1.00E+00	1.00E+00	1.00E+00
Citric Acid Cycle	32	13.80	2	1.00E+00	1.00E+00	1.00E+00
Nicotinate and Nicotinamide Metabolism	37	15.90	3	1.00E+00	1.00E+00	1.00E+00
Mitochondrial Beta-Oxidation of Short Chain Saturated Fatty Acids	27	11.60	1	1.00E+00	1.00E+00	1.00E+00
Mitochondrial Beta-Oxidation of Medium Chain Saturated Fatty Acids	27	11.60	1	1.00E+00	1.00E+00	1.00E+00
Inositol Metabolism	33	14.20	2	1.00E+00	1.00E+00	1.00E+00
Selenoamino Acid Metabolism	28	12.00	1	1.00E+00	1.00E+00	1.00E+00
Mitochondrial Beta-Oxidation of Long Chain Saturated Fatty Acids	28	12.00	1	1.00E+00	1.00E+00	1.00E+00
Beta-Alanine Metabolism	34	14.60	2	1.00E+00	1.00E+00	1.00E+00
Phospholipid Biosynthesis	29	12.50	1	1.00E+00	1.00E+00	1.00E+00
Pentose Phosphate Pathway	29	12.50	1	1.00E+00	1.00E+00	1.00E+00
Starch and Sucrose Metabolism	31	13.30	1	1.00E+00	1.00E+00	1.00E+00
Propanoate Metabolism	42	18.00	3	1.00E+00	1.00E+00	1.00E+00
Arginine and Proline Metabolism	53	22.80	5	1.00E+00	1.00E+00	1.00E+00
Androgen and Estrogen Metabolism	33	14.20	1	1.00E+00	1.00E+00	1.00E+00
Glutamate Metabolism	49	21.10	4	1.00E+00	1.00E+00	1.00E+00
Fatty Acid Elongation In Mitochondria	35	15.00	1	1.00E+00	1.00E+00	1.00E+00
Bile Acid Biosynthesis	65	27.90	7	1.00E+00	1.00E+00	1.00E+00
Histidine Metabolism	43	18.50	2	1.00E+00	1.00E+00	1.00E+00
Fatty acid Metabolism	43	18.50	2	1.00E+00	1.00E+00	1.00E+00
Steroidogenesis	43	18.50	2	1.00E+00	1.00E+00	1.00E+00
Galactose Metabolism	38	16.30	1	1.00E+00	1.00E+00	1.00E+00
Warburg Effect	58	24.90	4	1.00E+00	1.00E+00	1.00E+00
Steroid Biosynthesis	48	20.60	2	1.00E+00	1.00E+00	1.00E+00
Pyruvate Metabolism	48	20.60	2	1.00E+00	1.00E+00	1.00E+00
Glycine and Serine Metabolism	59	25.40	4	1.00E+00	1.00E+00	1.00E+00
Methionine Metabolism	43	18.50	1	1.00E+00	1.00E+00	1.00E+00
Valine, Leucine and Isoleucine Degradation	60	25.80	3	1.00E+00	1.00E+00	1.00E+00
Pyrimidine Metabolism	59	25.40	2	1.00E+00	1.00E+00	1.00E+00
Tryptophan Metabolism	60	25.80	2	1.00E+00	1.00E+00	1.00E+00
Purine Metabolism	74	31.80	3	1.00E+00	1.00E+00	1.00E+00
Tyrosine Metabolism	72	30.90	2	1.00E+00	1.00E+00	1.00E+00

7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "cmpd.vec<-c(\"HMDB0060253\", \"HMDB0172632\", \"HMDB0062600\", \"HMDB0012815\", \"HMDB0033529\", \"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, \"guest7111968406616392300\")\n"
```

The report was generated on Mon May 24 15:14:50 2021 with R version 4.0.2 (2020-06-22).