

Metabolomic Data Analysis with MetaboAnalyst 5.0

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1 Background

The Pathway Analysis module combines results from powerful pathway enrichment analysis with pathway topology analysis to help researchers identify the most relevant pathways involved in the conditions under study.

There are many commercial pathway analysis software tools such as Pathway Studio, MetaCore, or Ingenuity Pathway Analysis (IPA), etc. Compared to these commercial tools, the pathway analysis module was specifically developed for metabolomics studies. It uses high-quality KEGG metabolic pathways as the backend knowledgebase. This module integrates many well-established (i.e. univariate analysis, over-representation analysis) methods, as well as novel algorithms and concepts (i.e. Global Test, GlobalAncova, network topology analysis) into pathway analysis. Another feature is a Google-Map style interactive visualization system to deliver the analysis results in an intuitive manner.

2 Data Input

The Pathway Analysis module accepts either a list of compound labels (common names, HMDB IDs or KEGG IDs) with one compound per row, or a compound concentration table with samples in rows and compounds in columns. The second column must be phenotype labels (binary, multi-group, or continuous). The table is uploaded as comma separated values (.csv).

3 Compound Name Matching

The first step is to standardize the compound labels used in user uploaded data. This is a necessary step since these compounds will be subsequently compared with compounds contained in the pathway library. There are three outcomes from the step - exact match, approximate match (for common names only), and no match. Users should click the textbfView button from the approximate matched results to manually select the correct one. Compounds without match will be excluded from the subsequently pathway analysis.

Table 1 shows the conversion results. Note: *1* indicates exact match, *2* indicates approximate match, and *0* indicates no match. A text file contain the result can be found the downloaded file *name_map.csv*

	Query	Match	HMDB
1	HMDB0000973	Hydrogen phosphate	HMDB0000973
2	HMDB0001429	Phosphate	HMDB0001429
3	HMDB0002105	Dihydrogen phosphate	HMDB0002105
4	HMDB0002142	Phosphoric acid	HMDB0002142
5	HMDB0031404	Cyclohexylamine	HMDB0031404
6	HMDB0032416	2-Methylpiperidine	HMDB0032416
7	HMDB0031544	3-Methylcyclopentene	HMDB0031544
8	HMDB0062716	NA	NA
9	HMDB0033971	2-Diethylaminoethanol	HMDB0033971

10	HMDB0000630	Cytosine	HMDB0000630
11	HMDB0031335	2-Chloro-1-propanol	HMDB0031335
12	HMDB0062781	NA	NA
13	HMDB0059784	NA	NA
14	HMDB0161317	NA	NA
15	HMDB0160653	NA	NA
16	HMDB0160654	NA	NA
17	HMDB0000208	Oxoglutaric acid	HMDB0000208
18	HMDB0013701	3-Oxoglutaric acid	HMDB0013701
19	HMDB0164700	NA	NA
20	HMDB0161318	NA	NA
21	HMDB0041390	NA	NA
22	HMDB0041393	NA	NA
23	HMDB0033966	Di-2-propenyl disulfide, 9CI	HMDB0033966
24	HMDB0000139	Glyceric acid	HMDB0000139
25	HMDB0031818	D-2,3-Dihydroxypropanoic acid	HMDB0031818
26	HMDB0006372	L-Glyceric acid	HMDB0006372
27	HMDB0166738	NA	NA
28	HMDB0164724	NA	NA
29	HMDB0165094	NA	NA
30	HMDB0165096	NA	NA
31	HMDB0165095	NA	NA
32	HMDB0165097	NA	NA
33	HMDB0166737	NA	NA
34	HMDB0031484	2-Heptenoic acid	HMDB0031484
35	HMDB0038962	NA	NA
36	HMDB0031500	Methyl 2E-hexenoate	HMDB0031500
37	HMDB0166739	NA	NA
38	HMDB0029314	Isopentenyl acetate	HMDB0029314
39	HMDB0031477	3,4-Heptanedione	HMDB0031477
40	HMDB0031476	2,3-Heptanedione	HMDB0031476
41	HMDB0031504	Methyl (Z)-3-hexenoate	HMDB0031504
42	HMDB0031603	Ethyl 4-pentenoate	HMDB0031603
43	HMDB0040214	NA	NA
44	HMDB0031342	Cyclohexanecarboxylic acid	HMDB0031342
45	HMDB0038271	NA	NA
46	HMDB0031174	4-Methyl-5-hexanolide	HMDB0031174
47	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	HMDB0031681
48	HMDB0033793	4-Heptenoic acid	HMDB0033793
49	HMDB0031593	5-Methyl-2,3-hexanedione	HMDB0031593
50	HMDB0039819	NA	NA
51	HMDB0166736	NA	NA
52	HMDB0173760	NA	NA
53	HMDB0173761	NA	NA
54	HMDB0173762	NA	NA
55	HMDB0173763	NA	NA
56	HMDB0180322	NA	NA
57	HMDB0180323	NA	NA
58	HMDB0029165	1,3-Diacetylpropane	HMDB0029165
59	HMDB0031351	Cyclohexyl formate	HMDB0031351
60	HMDB0032460	4-Pentenyl acetate	HMDB0032460
61	HMDB0032391	3-Methyl-3-butenyl acetate	HMDB0032391
62	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	HMDB0030330
63	HMDB0059876	NA	NA
64	HMDB0040591	NA	NA
65	HMDB0145113	NA	NA
66	HMDB0145114	NA	NA
67	HMDB0145115	NA	NA
68	HMDB0145125	NA	NA
69	HMDB0145116	NA	NA
70	HMDB0094649	2-Amino-heptanoic acid	HMDB0094649
71	HMDB0001161	4-Trimethylammoniobutanoic acid	HMDB0001161
72	HMDB0006831	3-Dehydroxycarnitine	HMDB0006831
73	HMDB0013811	1-Nitroheptane	HMDB0013811
74	HMDB0000895	Acetylcholine	HMDB0000895
75	HMDB0062183	NA	NA
76	HMDB0002393	N-Methyl-D-aspartic acid	HMDB0002393
77	HMDB0003011	O-Acetylserine	HMDB0003011
78	HMDB0003339	D-Glutamic acid	HMDB0003339
79	HMDB0006556	L-4-Hydroxyglutamate semialdehyde	HMDB0006556
80	HMDB0060475	DL-Glutamate	HMDB0060475
81	HMDB0033550	3-(Carboxymethylamino)propanoic acid	HMDB0033550
82	HMDB0002931	N-Acetylserine	HMDB0002931
83	HMDB0000148	L-Glutamic acid	HMDB0000148
84	HMDB0156263	NA	NA
85	HMDB0000634	Citraconic acid	HMDB0000634
86	HMDB0060365	2,5-Dioxopentanoate	HMDB0060365
87	HMDB0000620	Glutaconic acid	HMDB0000620
88	HMDB0061185	NA	NA
89	HMDB0033809	Methyl hydrogen fumarate	HMDB0033809
90	HMDB0013233	Gamma-delta-Dioxovaleric acid	HMDB0013233
91	HMDB0059743	NA	NA
92	HMDB0000749	Mesaconic acid	HMDB0000749
93	HMDB0002092	Itaconic acid	HMDB0002092
94	HMDB0000897	7-Methylguanine	HMDB0000897
95	HMDB0001566	3-Methylguanine	HMDB0001566
96	HMDB0003282	1-Methylguanine	HMDB0003282

97	HMDB0006040	N2-Methylguanine	HMDB0006040
98	HMDB0165786	NA	NA
99	HMDB0166497	NA	NA
100	HMDB0166498	NA	NA
101	HMDB0166499	NA	NA
102	HMDB0166500	NA	NA
103	HMDB0164728	NA	NA
104	HMDB0163403	NA	NA
105	HMDB0164729	NA	NA
106	HMDB0166501	NA	NA
107	HMDB0031176	Tetrahydrofurfuryl acetate	HMDB0031176
108	HMDB0040433	NA	NA
109	HMDB0036594	NA	NA
110	HMDB0037114	NA	NA
111	HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	HMDB0001988
112	HMDB0166747	NA	NA
113	HMDB0166744	NA	NA
114	HMDB0166746	NA	NA
115	HMDB0061990	NA	NA
116	HMDB0166745	NA	NA
117	HMDB0172013	NA	NA
118	HMDB0180327	NA	NA
119	HMDB0180326	NA	NA
120	HMDB0180835	NA	NA
121	HMDB0000062	L-Carnitine	HMDB0000062
122	HMDB0062496	Malonyl-Carnitin	HMDB0062496
123	HMDB0145126	NA	NA
124	HMDB0155786	NA	NA
125	HMDB0062634	NA	NA
126	HMDB0010207	L-Rhamnulose	HMDB0010207
127	HMDB0124735	NA	NA
128	HMDB0240304	NA	NA
129	HMDB0062489	NA	NA
130	HMDB0059625	NA	NA
131	HMDB0029196	D-Fucose	HMDB0029196
132	HMDB0000174	L-Fucose	HMDB0000174
133	HMDB0059624	NA	NA
134	HMDB0033821	2-O-Methyl-D-xylose	HMDB0033821
135	HMDB0000849	Rhamnose	HMDB0000849
136	HMDB0003081	Beta-D-Fucose	HMDB0003081
137	HMDB0012327	2-Deoxygalactopyranose	HMDB0012327
138	HMDB0002712	1,5-Anhydrosorbitol	HMDB0002712
139	HMDB0062477	NA	NA
140	HMDB0062498	NA	NA
141	HMDB0062499	NA	NA
142	HMDB0005876	3-Deoxyfructose	HMDB0005876
143	HMDB0060267	L-Fuculose	HMDB0060267
144	HMDB0033050	Butyl isopropyl disulfide	HMDB0033050
145	HMDB0033051	Butyl propyl disulfide	HMDB0033051
146	HMDB0039783	NA	NA
147	HMDB0132202	NA	NA
148	HMDB0041026	NA	NA
149	HMDB0041031	NA	NA
150	HMDB0149524	NA	NA
151	HMDB0041862	NA	NA
152	HMDB0062803	NA	NA
153	HMDB0000094	Citric acid	HMDB0000094
154	HMDB0000193	Isocitric acid	HMDB0000193
155	HMDB0001874	D-threo-Isocitric acid	HMDB0001874
156	HMDB0005971	Diketogulonic acid	HMDB0005971
157	HMDB0006511	2,3-Diketo-L-gulonate	HMDB0006511
158	HMDB0033717	(1R,2R)-Isocitric acid	HMDB0033717
159	HMDB0035145	Chrycolide	HMDB0035145
160	HMDB0180803	NA	NA
161	HMDB0168872	NA	NA
162	HMDB0033845	(Z)-5-[(5-Methyl-2-thienyl)methylene]-2(5H)-furanone	HMDB0033845
163	HMDB0035593	Rishitin	HMDB0035593
164	HMDB0037605	NA	NA
165	HMDB0036790	NA	NA
166	HMDB0036791	NA	NA
167	HMDB0037820	NA	NA
168	HMDB0040178	NA	NA
169	HMDB0160293	NA	NA
170	HMDB0160295	NA	NA
171	HMDB0160291	NA	NA
172	HMDB0160290	NA	NA
173	HMDB0160289	NA	NA
174	HMDB0160292	NA	NA
175	HMDB0160296	NA	NA
176	HMDB0160294	NA	NA
177	HMDB0160298	NA	NA
178	HMDB0160297	NA	NA
179	HMDB0032369	L-Menthyl acetoacetate	HMDB0032369
180	HMDB0033619	Hexyl hexanoate	HMDB0033619
181	HMDB0059868	NA	NA
182	HMDB0032440	Nonanal propyleneglycol acetal	HMDB0032440
183	HMDB0061988	NA	NA

184	HMDB0035410	(R)-Dihydrocitronellol acetate	HMDB0035410
185	HMDB0000638	Dodecanoic acid	HMDB0000638
186	HMDB0040166	NA	NA
187	HMDB0030998	Ethyl decanoate	HMDB0030998
188	HMDB0034137	Octyl 2-methylpropanoate	HMDB0034137
189	HMDB0036225	NA	NA
190	HMDB0034136	Octyl butanoate	HMDB0034136
191	HMDB0034128	Isopropyl nonanoate	HMDB0034128
192	HMDB0032310	2-Heptyl butyrate	HMDB0032310
193	HMDB0168119	NA	NA
194	HMDB0168120	NA	NA
195	HMDB0168121	NA	NA
196	HMDB0015050	Phenformin	HMDB0015050
197	HMDB0004231	Pantothenol	HMDB0004231
198	HMDB0038259	NA	NA
199	HMDB0032342	Isobornyl isobutyrate	HMDB0032342
200	HMDB0032053	alpha-Terpineol butanoate	HMDB0032053
201	HMDB0030427	Linalyl butyrate	HMDB0030427
202	HMDB0038260	NA	NA
203	HMDB0038246	NA	NA
204	HMDB0036424	NA	NA
205	HMDB0037814	NA	NA
206	HMDB0032524	Terpinyl isobutyrate	HMDB0032524
207	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	HMDB0031015
208	HMDB0030426	Linalyl isobutyrate	HMDB0030426
209	HMDB0000560	5,8-Tetradecadienoic acid	HMDB0000560
210	HMDB0039129	NA	NA
211	HMDB0159801	NA	NA
212	HMDB0159802	NA	NA
213	HMDB0176319	NA	NA
214	HMDB0176320	NA	NA
215	HMDB0159803	NA	NA
216	HMDB0159799	NA	NA
217	HMDB0159800	NA	NA
218	HMDB0030982	6-Ketomyristic acid	HMDB0030982
219	HMDB0010730	3-Oxotetradecanoic acid	HMDB0010730
220	HMDB0032370	L-Menthyl (R,S)-3-hydroxybutyrate	HMDB0032370
221	HMDB0159614	NA	NA
222	HMDB0159613	NA	NA
223	HMDB0159611	NA	NA
224	HMDB0159610	NA	NA
225	HMDB0159612	NA	NA
226	HMDB0159609	NA	NA
227	HMDB0168123	NA	NA
228	HMDB0032153	Acetaldehyde diisoamyl acetal	HMDB0032153
229	HMDB0037310	NA	NA
230	HMDB0168122	NA	NA
231	HMDB0061683	NA	NA
232	HMDB0031813	N-Carbamoyl-2-amino-2-(4-hydroxyphenyl)acetic acid	HMDB0031813
233	HMDB0000014	Deoxycytidine	HMDB0000014
234	HMDB0028732	Asparaginyln-Hydroxyproline	HMDB0028732
235	HMDB0028858	Hydroxypropyl-Asparagine	HMDB0028858
236	HMDB0040046	NA	NA
237	HMDB0161863	NA	NA
238	HMDB0161860	NA	NA
239	HMDB0041444	NA	NA
240	HMDB0033452	Koenoline	HMDB0033452
241	HMDB0161862	NA	NA
242	HMDB0161861	NA	NA
243	HMDB0161859	NA	NA
244	HMDB0161858	NA	NA
245	HMDB0161857	NA	NA
246	HMDB0028925	Leucyl-Aspartate	HMDB0028925
247	HMDB0011166	L-beta-aspartyl-L-leucine	HMDB0011166
248	HMDB0028757	Aspartyl-Leucine	HMDB0028757
249	HMDB0028756	Aspartyl-Isoleucine	HMDB0028756
250	HMDB0028903	Isoleucyl-Aspartate	HMDB0028903
251	HMDB0029126	Valyl-Glutamate	HMDB0029126
252	HMDB0011172	gamma-Glutamylvaline	HMDB0011172
253	HMDB0029162	NA	NA
254	HMDB0028832	Glutamylvaline	HMDB0028832
255	HMDB0059717	NA	NA
256	HMDB0151784	NA	NA
257	HMDB0151780	NA	NA
258	HMDB0151794	NA	NA
259	HMDB0151781	NA	NA
260	HMDB0151783	NA	NA
261	HMDB0151789	NA	NA
262	HMDB0151790	NA	NA
263	HMDB0151792	NA	NA
264	HMDB0151788	NA	NA
265	HMDB0151787	NA	NA
266	HMDB0151786	NA	NA
267	HMDB0151785	NA	NA
268	HMDB0132940	NA	NA
269	HMDB0001925	Ibuprofen	HMDB0001925
270	HMDB0035016	2-Phenylethyl pentanoate	HMDB0035016

271	HMDB0036386	NA	NA
272	HMDB0035008	3-Methylbutyl phenylacetate	HMDB0035008
273	HMDB0034472	3-Phenylpropyl 2-methylpropanoate	HMDB0034472
274	HMDB0034470	2-Phenylpropyl isobutyrate	HMDB0034470
275	HMDB0038605	NA	NA
276	HMDB0040431	NA	NA
277	HMDB0036391	NA	NA
278	HMDB0036025	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	HMDB0036025
279	HMDB0037194	NA	NA
280	HMDB0034469	2-Phenylpropyl butyrate	HMDB0034469
281	HMDB0034556	3-Acetoxy-3-methyl-1-phenylbutane	HMDB0034556
282	HMDB0033196	(E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one	HMDB0033196
283	HMDB0037604	NA	NA
284	HMDB0029669	Eremopetasinorone A	HMDB0029669
285	HMDB0035181	xi-8,9-Dehydrotheaspirone	HMDB0035181
286	HMDB0039101	NA	NA
287	HMDB0037623	NA	NA
288	HMDB0036240	NA	NA
289	HMDB0132932	NA	NA
290	HMDB0163212	NA	NA
291	HMDB0151805	NA	NA
292	HMDB0151793	NA	NA
293	HMDB0151791	NA	NA
294	HMDB0037720	NA	NA
295	HMDB0032176	Benzyl hexanoate	HMDB0032176
296	HMDB0035017	2-Phenylethyl 3-methylbutanoate	HMDB0035017
297	HMDB0028871	Hydroxyprolyl-Proline	HMDB0028871
298	HMDB0006695	Prolylhydroxyproline	HMDB0006695
299	HMDB0094651	PyroGlu-Val	HMDB0094651
300	HMDB0040573	NA	NA
301	HMDB0029018	Prolyl-Hydroxyproline	HMDB0029018
302	HMDB0060747	NA	NA
303	HMDB0001434	3-Methoxytyrosine	HMDB0001434
304	HMDB0011754	Methyldopa	HMDB0011754
305	HMDB0061836	NA	NA
306	HMDB0033878	(S)-Curzeone	HMDB0033878
307	HMDB0032133	Bisphenol A	HMDB0032133
308	HMDB0014604	Nabumetone	HMDB0014604
309	HMDB0176774	NA	NA
310	HMDB0176775	NA	NA
311	HMDB0135597	NA	NA
312	HMDB0176773	NA	NA
313	HMDB0036455	NA	NA
314	HMDB0036767	NA	NA
315	HMDB0038202	NA	NA
316	HMDB0041920	NA	NA
317	HMDB0031900	Methyl (2E,4Z,6E,8E,10E)-4,8-dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoate	HMDB0031900
318	HMDB0035902	Enokipodin B	HMDB0035902
319	HMDB0040903	NA	NA
320	HMDB0179330	NA	NA
321	HMDB0170855	NA	NA
322	HMDB0038547	NA	NA
323	HMDB0036488	NA	NA
324	HMDB0030911	2-Oxo-5,11(13)-eudesmadien-12,8-olide	HMDB0030911
325	HMDB0037801	NA	NA
326	HMDB0036473	NA	NA
327	HMDB0037558	NA	NA
328	HMDB0031916	5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran	HMDB0031916
329	HMDB0038188	NA	NA
330	HMDB0179331	NA	NA
331	HMDB0179332	NA	NA
332	HMDB0037153	NA	NA
333	HMDB0151309	NA	NA
334	HMDB0033750	D-Glycero-D-galacto-heptitol	HMDB0033750
335	HMDB0014814	Benzyl Benzoate	HMDB0014814
336	HMDB0032039	Benzoin	HMDB0032039
337	HMDB0028885	Histidinyl-Glycine	HMDB0028885
338	HMDB0028843	Glycyl-Histidine	HMDB0028843
339	HMDB0186509	NA	NA
340	HMDB0184957	NA	NA
341	HMDB0184936	NA	NA
342	HMDB0062677	NA	NA
343	HMDB0004590	19-Nor-5-androstenediol	HMDB0004590
344	HMDB0032464	Phenethyl decanoate	HMDB0032464
345	HMDB0002697	19-Norandrosterone	HMDB0002697
346	HMDB0032672	4,8,12,15-Octadecatetraenoic acid	HMDB0032672
347	HMDB0005886	19-Noretiocholanolone	HMDB0005886
348	HMDB0034382	(E,E)-11,13-Octadecadien-9-ynoic acid	HMDB0034382
349	HMDB0006547	Stearidonic acid	HMDB0006547
350	HMDB0186501	NA	NA
351	HMDB0186507	NA	NA
352	HMDB0186508	NA	NA
353	HMDB0062288	NA	NA
354	HMDB0186510	NA	NA
355	HMDB0186500	NA	NA
356	HMDB0186506	NA	NA
357	HMDB0186505	NA	NA

358	HMDB0186504	NA	NA
359	HMDB0186502	NA	NA
360	HMDB0186497	NA	NA
361	HMDB0186499	NA	NA
362	HMDB0186498	NA	NA
363	HMDB0112093	NA	NA
364	HMDB0112099	NA	NA
365	HMDB0112102	NA	NA
366	HMDB0112103	NA	NA
367	HMDB0186503	NA	NA
368	HMDB0034586	(9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid	HMDB0034586
369	HMDB0031088	12,13-Epoxy-9,15-octadecadienoic acid	HMDB0031088
370	HMDB0029969	Squamosanal A	HMDB0029969
371	HMDB0031103	2-Hydroxylinolenic acid	HMDB0031103
372	HMDB0036832	NA	NA
373	HMDB0030950	15,16-Epoxy-9,12-octadecadienoic acid	HMDB0030950
374	HMDB0029786	10-Oxo-11-octadecen-13-olide	HMDB0029786
375	HMDB0011108	17-Hydroxylinolenic acid	HMDB0011108
376	HMDB0010224	9-HOTE	HMDB0010224
377	HMDB0010220	9(10)-EpODE	HMDB0010220
378	HMDB0010206	15(16)-EpODE	HMDB0010206
379	HMDB0010200	A-12(13)-EpODE	HMDB0010200
380	HMDB0010203	13-HOTE	HMDB0010203
381	HMDB0004669	9-OxoODE	HMDB0004669
382	HMDB0004668	13-OxoODE	HMDB0004668
383	HMDB0031934	(9S,10E,12Z,15Z)-9-Hydroxy-10,12,15-octadecatrienoic acid	HMDB0031934
384	HMDB0030995	(2'E,4'Z,8E)-Colneleic acid	HMDB0030995
385	HMDB0061644	NA	NA
386	HMDB0039603	NA	NA
387	HMDB0061979	NA	NA
388	HMDB0033791	(E)-3-Hexadecenoic acid	HMDB0033791
389	HMDB0038958	NA	NA
390	HMDB0031711	15-Hexadecanolide	HMDB0031711
391	HMDB0003229	Palmitoleic acid	HMDB0003229
392	HMDB0010735	Trans-Hexa-dec-2-enoic acid	HMDB0010735
393	HMDB0037647	NA	NA
394	HMDB0041422	NA	NA
395	HMDB0032638	(Z)-5-Hexadecenoic acid	HMDB0032638
396	HMDB0031053	(E)-6-Hexadecenoic acid	HMDB0031053
397	HMDB0035877	(Z)-13-Hexadecenoic acid	HMDB0035877
398	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	HMDB0031145
399	HMDB0002186	Hypogeic acid	HMDB0002186
400	HMDB0171478	NA	NA
401	HMDB0171479	NA	NA
402	HMDB0171477	NA	NA
403	HMDB0012328	Palmitelaidic acid	HMDB0012328
404	HMDB0171476	NA	NA
405	HMDB0000756	L-Hexanoylcarnitine	HMDB0000756
406	HMDB0000705	Hexanoylcarnitine	HMDB0000705
407	HMDB0014413	Ropinirole	HMDB0014413
408	HMDB0015070	Oxymetazoline	HMDB0015070
409	HMDB0061189	NA	NA
410	HMDB0062555	hydroxyisovaleroyl carnitine	HMDB0062555
411	HMDB0240421	NA	NA
412	HMDB0040904	NA	NA
413	HMDB0168550	NA	NA
414	HMDB0168551	NA	NA
415	HMDB0168552	NA	NA
416	HMDB0168553	NA	NA
417	HMDB0168554	NA	NA
418	HMDB0168549	NA	NA
419	HMDB0137260	NA	NA
420	HMDB0137271	NA	NA
421	HMDB0030974	8-Acetoxy-4-acoren-3-one	HMDB0030974
422	HMDB0031928	Panaxytriol	HMDB0031928
423	HMDB0030801	1-(4-Hydroxy-3-methoxyphenyl)-3-decanone	HMDB0030801
424	HMDB0039251	NA	NA
425	HMDB0134775	NA	NA
426	HMDB0038798	NA	NA
427	HMDB0035075	Tanacetol B	HMDB0035075
428	HMDB0060952	NA	NA
429	HMDB0014521	Palonosetron	HMDB0014521
430	HMDB0030283	Hydrocinchonine	HMDB0030283
431	HMDB0175409	NA	NA
432	HMDB0175412	NA	NA
433	HMDB0175413	NA	NA
434	HMDB0175414	NA	NA
435	HMDB0175415	NA	NA
436	HMDB0175408	NA	NA
437	HMDB0175410	NA	NA
438	HMDB0175411	NA	NA
439	HMDB0160594	NA	NA
440	HMDB0173892	NA	NA
441	HMDB0175402	NA	NA
442	HMDB0175403	NA	NA
443	HMDB0175404	NA	NA
444	HMDB0175405	NA	NA

445	HMDB0175406	NA	NA
446	HMDB0175407	NA	NA
447	HMDB0030964	Linolenelaidic acid	HMDB0030964
448	HMDB0001388	Alpha-Linolenic acid	HMDB0001388
449	HMDB0003073	Gamma-Linolenic acid	HMDB0003073
450	HMDB0030962	Calendic acid	HMDB0030962
451	HMDB0030963	Punicic acid	HMDB0030963
452	HMDB0160589	NA	NA
453	HMDB0160588	NA	NA
454	HMDB0112194	NA	NA
455	HMDB0062652	NA	NA
456	HMDB0173890	NA	NA
457	HMDB0160590	NA	NA
458	HMDB0160592	NA	NA
459	HMDB0160591	NA	NA
460	HMDB0160593	NA	NA
461	HMDB0160595	NA	NA
462	HMDB0173886	NA	NA
463	HMDB0173885	NA	NA
464	HMDB0173887	NA	NA
465	HMDB0173889	NA	NA
466	HMDB0173891	NA	NA
467	HMDB0173888	NA	NA
468	HMDB0173893	NA	NA
469	HMDB0004667	13S-hydroxyoctadecadienoic acid	HMDB0004667
470	HMDB0061708	NA	NA
471	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	HMDB0029796
472	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid	HMDB0029998
473	HMDB0029978	Avenoleic acid	HMDB0029978
474	HMDB0010223	9-HODE	HMDB0010223
475	HMDB0004701	9,10-Epoxyoctadecenoic acid	HMDB0004701
476	HMDB0004702	12,13-EpOME	HMDB0004702
477	HMDB0004670	Alpha-dimorphecolic acid	HMDB0004670
478	HMDB0000220	Palmitic acid	HMDB0000220
479	HMDB0060083	NA	NA
480	HMDB0061373	NA	NA
481	HMDB0032324	Hexyl decanoate	HMDB0032324
482	HMDB0032249	Dodecyl butyrate	HMDB0032249
483	HMDB0033166	Octyl octanoate	HMDB0033166
484	HMDB0032065	Butyl dodecanoate	HMDB0032065
485	HMDB0036210	NA	NA
486	HMDB0034153	Ethyl tetradecanoate	HMDB0034153
487	HMDB0031068	Isopalmitic acid	HMDB0031068
488	HMDB0002396	Trimethyltridecanoic acid	HMDB0002396
489	HMDB0240660	NA	NA
490	HMDB0166396	NA	NA
491	HMDB0155323	NA	NA
492	HMDB0125616	NA	NA
493	HMDB0157443	NA	NA
494	HMDB0125615	NA	NA
495	HMDB0155324	NA	NA
496	HMDB0155326	NA	NA
497	HMDB0155327	NA	NA
498	HMDB0157445	NA	NA
499	HMDB0157442	NA	NA
500	HMDB0166395	NA	NA
501	HMDB0156225	NA	NA
502	HMDB0156223	NA	NA
503	HMDB0156224	NA	NA
504	HMDB0156222	NA	NA
505	HMDB0155825	NA	NA
506	HMDB0166394	NA	NA
507	HMDB0125614	NA	NA
508	HMDB0125613	NA	NA
509	HMDB0157444	NA	NA
510	HMDB0155325	NA	NA
511	HMDB0164008	NA	NA
512	HMDB0062577	NA	NA
513	HMDB0140895	NA	NA
514	HMDB0140584	NA	NA
515	HMDB0140434	NA	NA
516	HMDB0240404	NA	NA
517	HMDB0132291	NA	NA
518	HMDB0140896	NA	NA
519	HMDB0140901	NA	NA
520	HMDB0140900	NA	NA
521	HMDB0172131	NA	NA
522	HMDB0171705	NA	NA
523	HMDB0168714	NA	NA
524	HMDB0168707	NA	NA
525	HMDB0159585	NA	NA
526	HMDB0157245	NA	NA
527	HMDB0152783	NA	NA
528	HMDB0145741	NA	NA
529	HMDB0145740	NA	NA
530	HMDB0172133	NA	NA
531	HMDB0134099	NA	NA

532	HMDB0159586	NA	NA
533	HMDB0132292	NA	NA
534	HMDB0041648	NA	NA
535	HMDB0041721	NA	NA
536	HMDB0059967	NA	NA
537	HMDB0061117	NA	NA
538	HMDB0011719	Homovanillic acid sulfate	HMDB0011719
539	HMDB0002899	Ellagic acid	HMDB0002899
540	HMDB0015039	Ethacrynic acid	HMDB0015039
541	HMDB0060626	NA	NA
542	HMDB0171728	NA	NA
543	HMDB0000230	N-Acetylneuraminic acid	HMDB0000230
544	HMDB0000773	N-Acetyl-a-neuraminic acid	HMDB0000773
545	HMDB0161436	NA	NA
546	HMDB0167290	NA	NA
547	HMDB0167291	NA	NA
548	HMDB0167294	NA	NA
549	HMDB0167293	NA	NA
550	HMDB0167296	NA	NA
551	HMDB0167297	NA	NA
552	HMDB0179979	NA	NA
553	HMDB0179980	NA	NA
554	HMDB0153318	NA	NA
555	HMDB0172140	NA	NA
556	HMDB0028880	Histidinyl-Asparagine	HMDB0028880
557	HMDB0028733	Asparaginy-Histidine	HMDB0028733
558	HMDB0061039	NA	NA
559	HMDB0031766	Alachlor	HMDB0031766
560	HMDB0038584	NA	NA
561	HMDB0170783	NA	NA
562	HMDB0170784	NA	NA
563	HMDB0170785	NA	NA
564	HMDB0170788	NA	NA
565	HMDB0170786	NA	NA
566	HMDB0170787	NA	NA
567	HMDB0033359	Cryptodrine	HMDB0033359
568	HMDB0039096	NA	NA
569	HMDB0173636	NA	NA
570	HMDB0041314	NA	NA
571	HMDB0130350	NA	NA
572	HMDB0130347	NA	NA
573	HMDB0175079	NA	NA
574	HMDB0178312	NA	NA
575	HMDB0141160	NA	NA
576	HMDB0141105	NA	NA
577	HMDB0141099	NA	NA
578	HMDB0141080	NA	NA
579	HMDB0141122	NA	NA
580	HMDB0141079	NA	NA
581	HMDB0141126	NA	NA
582	HMDB0141149	NA	NA
583	HMDB0141119	NA	NA
584	HMDB0040889	NA	NA
585	HMDB0129039	NA	NA
586	HMDB0138953	NA	NA
587	HMDB0141045	NA	NA
588	HMDB0138954	NA	NA
589	HMDB0138952	NA	NA
590	HMDB0138951	NA	NA
591	HMDB0138956	NA	NA
592	HMDB0140994	NA	NA
593	HMDB0138959	NA	NA
594	HMDB0138955	NA	NA
595	HMDB0138957	NA	NA
596	HMDB0138958	NA	NA
597	HMDB0141056	NA	NA
598	HMDB0141150	NA	NA
599	HMDB0141152	NA	NA
600	HMDB0141153	NA	NA
601	HMDB0141164	NA	NA
602	HMDB0146848	NA	NA
603	HMDB0146849	NA	NA
604	HMDB0141181	NA	NA
605	HMDB0141151	NA	NA
606	HMDB0141180	NA	NA
607	HMDB0141162	NA	NA
608	HMDB0141161	NA	NA
609	HMDB0141169	NA	NA
610	HMDB0141163	NA	NA
611	HMDB0141145	NA	NA
612	HMDB0141146	NA	NA
613	HMDB0141057	NA	NA
614	HMDB0141101	NA	NA
615	HMDB0141102	NA	NA
616	HMDB0141100	NA	NA
617	HMDB0141103	NA	NA
618	HMDB0141106	NA	NA

619	HMDB0141107	NA	NA
620	HMDB0141120	NA	NA
621	HMDB0141121	NA	NA
622	HMDB0141130	NA	NA
623	HMDB0141129	NA	NA
624	HMDB0141128	NA	NA
625	HMDB0141127	NA	NA
626	HMDB0141139	NA	NA
627	HMDB0141140	NA	NA
628	HMDB0141170	NA	NA
629	HMDB0036635	NA	NA
630	HMDB0041298	NA	NA
631	HMDB0033310	Moracin C	HMDB0033310
632	HMDB0031744	Artocarbene	HMDB0031744
633	HMDB0141044	NA	NA
634	HMDB0138682	NA	NA
635	HMDB0011741	gamma-Glutamyltyrosine	HMDB0011741
636	HMDB0029161	NA	NA
637	HMDB0029104	Tyrosyl-Glutamate	HMDB0029104
638	HMDB0028831	Glutamyltyrosine	HMDB0028831
639	HMDB0062553	NA	NA
640	HMDB0041309	NA	NA
641	HMDB0000839	Pentaporphyrin I	HMDB0000839
642	HMDB0029428	Hypoglycin B	HMDB0029428
643	HMDB0061318	NA	NA
644	HMDB0015102	Desloratadine	HMDB0015102
645	HMDB0062434	NA	NA
646	HMDB0062637	NA	NA
647	HMDB0062281	11-HpODE	HMDB0062281
648	HMDB0003871	13-L-Hydroperoxylinoleic acid	HMDB0003871
649	HMDB0040900	NA	NA
650	HMDB0010208	15,16-DiHODE	HMDB0010208
651	HMDB0010221	9,10-DiHODE	HMDB0010221
652	HMDB0004706	8(R)-Hydroperoxylinoleic acid	HMDB0004706
653	HMDB0010201	12,13-DiHODE	HMDB0010201
654	HMDB0006940	9(S)-HPODE	HMDB0006940
655	HMDB0155886	NA	NA
656	HMDB0010734	(R)-3-Hydroxy-hexadecanoic acid	HMDB0010734
657	HMDB0006294	16-Hydroxy hexadecanoic acid	HMDB0006294
658	HMDB0155887	NA	NA
659	HMDB0112188	NA	NA
660	HMDB0112186	NA	NA
661	HMDB0112189	NA	NA
662	HMDB0112185	NA	NA
663	HMDB0061658	NA	NA
664	HMDB0112187	NA	NA
665	HMDB0112191	NA	NA
666	HMDB0112184	NA	NA
667	HMDB0112190	NA	NA
668	HMDB0112192	NA	NA
669	HMDB0184174	NA	NA
670	HMDB0184176	NA	NA
671	HMDB0184175	NA	NA
672	HMDB0184180	NA	NA
673	HMDB0031057	(R)-2-Hydroxyhexadecanoic acid	HMDB0031057
674	HMDB0184177	NA	NA
675	HMDB0184178	NA	NA
676	HMDB0184328	NA	NA
677	HMDB0062548	NA	NA
678	HMDB0038580	NA	NA
679	HMDB0033631	Lactapiperanol D	HMDB0033631
680	HMDB0180021	NA	NA
681	HMDB0180098	NA	NA
682	HMDB0180100	NA	NA
683	HMDB0180099	NA	NA
684	HMDB0180102	NA	NA
685	HMDB0034780	Capsiate	HMDB0034780
686	HMDB0180103	NA	NA
687	HMDB0184951	NA	NA
688	HMDB0184949	NA	NA
689	HMDB0184953	NA	NA
690	HMDB0012799	5'-Carboxy-gamma-chromanol	HMDB0012799
691	HMDB0184954	NA	NA
692	HMDB0184950	NA	NA
693	HMDB0061677	NA	NA
694	HMDB0000552	3-Methylglutaryl carnitine	HMDB0000552
695	HMDB0039044	NA	NA
696	HMDB0131544	NA	NA
697	HMDB0153683	NA	NA
698	HMDB0134716	NA	NA
699	HMDB0131577	NA	NA
700	HMDB0140842	NA	NA
701	HMDB0039858	NA	NA
702	HMDB0150310	NA	NA
703	HMDB0150311	NA	NA
704	HMDB0030019	4'-Methoxymucidin	HMDB0030019
705	HMDB0125543	NA	NA

706	HMDB0125544	NA	NA
707	HMDB0125545	NA	NA
708	HMDB0125547	NA	NA
709	HMDB0125546	NA	NA
710	HMDB0125548	NA	NA
711	HMDB0129031	NA	NA
712	HMDB0129032	NA	NA
713	HMDB0141104	NA	NA
714	HMDB0141131	NA	NA
715	HMDB0141141	NA	NA
716	HMDB0141165	NA	NA
717	HMDB0141171	NA	NA
718	HMDB0129034	NA	NA
719	HMDB0149106	NA	NA
720	HMDB0140204	NA	NA
721	HMDB0140116	NA	NA
722	HMDB0129033	NA	NA
723	HMDB0129035	NA	NA
724	HMDB0129037	NA	NA
725	HMDB0129036	NA	NA
726	HMDB0129038	NA	NA
727	HMDB0140114	NA	NA
728	HMDB0140118	NA	NA
729	HMDB0140117	NA	NA
730	HMDB0140115	NA	NA
731	HMDB0146850	NA	NA
732	HMDB0040670	NA	NA
733	HMDB0176556	NA	NA
734	HMDB0030936	5,8,12-Trihydroxy-9-octadecenoic acid	HMDB0030936
735	HMDB0004710	9,10,13-TriHOME	HMDB0004710
736	HMDB0038555	NA	NA
737	HMDB0172549	NA	NA
738	HMDB0004708	9,12,13-TriHOME	HMDB0004708
739	HMDB0037839	NA	NA
740	HMDB0029089	Tryptophyl-Methionine	HMDB0029089
741	HMDB0028984	Methionyl-Tryptophan	HMDB0028984
742	HMDB0000489	Aspartylglycosamine	HMDB0000489
743	HMDB0136315	NA	NA
744	HMDB0136311	NA	NA
745	HMDB0136314	NA	NA
746	HMDB0136313	NA	NA
747	HMDB0136316	NA	NA
748	HMDB0005037	Sumatriptan	HMDB0005037
749	HMDB0153675	NA	NA
750	HMDB0153676	NA	NA
751	HMDB0151629	NA	NA
752	HMDB0151909	NA	NA
753	HMDB0153670	NA	NA
754	HMDB0153672	NA	NA
755	HMDB0153671	NA	NA
756	HMDB0153674	NA	NA
757	HMDB0146373	NA	NA
758	HMDB0140280	NA	NA
759	HMDB0136509	NA	NA
760	HMDB0130773	NA	NA
761	HMDB0130772	NA	NA
762	HMDB0130769	NA	NA
763	HMDB0130768	NA	NA
764	HMDB0130580	NA	NA
765	HMDB0138454	NA	NA
766	HMDB0130574	NA	NA
767	HMDB0130573	NA	NA
768	HMDB0130576	NA	NA
769	HMDB0130899	NA	NA
770	HMDB0132853	NA	NA
771	HMDB0134815	NA	NA
772	HMDB0133983	NA	NA
773	HMDB0133985	NA	NA
774	HMDB0133980	NA	NA
775	HMDB0133300	NA	NA
776	HMDB0133299	NA	NA
777	HMDB0132915	NA	NA
778	HMDB0132911	NA	NA
779	HMDB0132909	NA	NA
780	HMDB0130569	NA	NA
781	HMDB0130570	NA	NA
782	HMDB0130578	NA	NA
783	HMDB0146408	NA	NA
784	HMDB0146435	NA	NA
785	HMDB0147284	NA	NA
786	HMDB0147288	NA	NA
787	HMDB0150246	NA	NA
788	HMDB0150244	NA	NA
789	HMDB0151165	NA	NA
790	HMDB0146372	NA	NA
791	HMDB0130397	NA	NA
792	HMDB0130393	NA	NA

793	HMDB0130373	NA	NA
794	HMDB0130370	NA	NA
795	HMDB0130369	NA	NA
796	HMDB0128539	NA	NA
797	HMDB0126073	NA	NA
798	HMDB0140838	NA	NA
799	HMDB0140839	NA	NA
800	HMDB0151166	NA	NA
801	HMDB0130571	NA	NA
802	HMDB0030875	2',4-Dihydroxy-4',6'-dimethoxychalcone	HMDB0030875
803	HMDB0033861	3-Hydroxy-2,9-dimethoxypterocarpan	HMDB0033861
804	HMDB0034116	Homopisatin	HMDB0034116
805	HMDB0033142	Melilotocarpan A	HMDB0033142
806	HMDB0041321	NA	NA
807	HMDB0038812	NA	NA
808	HMDB0033292	8-Hydroxy-3,9-dimethoxypterocarpan	HMDB0033292
809	HMDB0031421	Heliannone B	HMDB0031421
810	HMDB0038110	NA	NA
811	HMDB0034008	Methylnissolin	HMDB0034008
812	HMDB0031705	Heliannone A	HMDB0031705
813	HMDB0041322	NA	NA
814	HMDB0034001	3-Hydroxy-4,9-dimethoxypterocarpan	HMDB0034001
815	HMDB0130378	NA	NA
816	HMDB0140279	NA	NA
817	HMDB0130568	NA	NA
818	HMDB0140278	NA	NA
819	HMDB0030341	Piplartine	HMDB0030341
820	HMDB0137020	NA	NA
821	HMDB0137023	NA	NA
822	HMDB0137024	NA	NA
823	HMDB0137022	NA	NA
824	HMDB0137025	NA	NA
825	HMDB0137027	NA	NA
826	HMDB0137026	NA	NA
827	HMDB0137021	NA	NA
828	HMDB0136330	NA	NA
829	HMDB0136329	NA	NA
830	HMDB0136327	NA	NA
831	HMDB0136328	NA	NA
832	HMDB0136326	NA	NA
833	HMDB0136325	NA	NA
834	HMDB0013220	Beta-Citryl-L-glutamic acid	HMDB0013220
835	HMDB0155333	NA	NA
836	HMDB0187538	NA	NA
837	HMDB0002044	8-Hydroxyguanosine	HMDB0002044
838	HMDB0141391	NA	NA
839	HMDB0141389	NA	NA
840	HMDB0135622	NA	NA
841	HMDB0135448	NA	NA
842	HMDB0001570	Thymidine 3',5'-cyclic monophosphate	HMDB0001570
843	HMDB0154811	NA	NA
844	HMDB0154812	NA	NA
845	HMDB0178281	NA	NA
846	HMDB0154815	NA	NA
847	HMDB0154816	NA	NA
848	HMDB0014618	Chlordiazepoxide	HMDB0014618
849	HMDB0173604	NA	NA
850	HMDB0173603	NA	NA
851	HMDB0173602	NA	NA
852	HMDB0173601	NA	NA
853	HMDB0173600	NA	NA
854	HMDB0173596	NA	NA
855	HMDB0173594	NA	NA
856	HMDB0173595	NA	NA
857	HMDB0173598	NA	NA
858	HMDB0173597	NA	NA
859	HMDB0015536	Imipenem	HMDB0015536
860	HMDB0146077	NA	NA
861	HMDB0060088	NA	NA
862	HMDB0169559	NA	NA
863	HMDB0137378	NA	NA
864	HMDB0015031	Testolactone	HMDB0015031
865	HMDB0038684	NA	NA
866	HMDB0000010	2-Methoxyestrone	HMDB0000010
867	HMDB0006768	19-Oxoandrost-4-ene-3,17-dione	HMDB0006768
868	HMDB0006772	Adrenosterone	HMDB0006772
869	HMDB0011195	2-Hydroxy-3-methoxyestrone	HMDB0011195
870	HMDB0039569	NA	NA
871	HMDB0015097	Zaleplon	HMDB0015097
872	HMDB0133470	NA	NA
873	HMDB0125851	NA	NA
874	HMDB0124921	NA	NA
875	HMDB0124820	NA	NA
876	HMDB0030799	5-Deoxymyricanone	HMDB0030799
877	HMDB0036401	NA	NA
878	HMDB0036399	NA	NA
879	HMDB0034010	4',7-Dihydroxy-2'-methoxy-3'-prenylisoflavan	HMDB0034010

880	HMDB0032737	2,2-Bis[4-(2,3-epoxypropoxy)phenyl]propane	HMDB0032737
881	HMDB0031929	Zanthodioline	HMDB0031929
882	HMDB0015607	Lucanthone	HMDB0015607
883	HMDB0014915	Propiomazine	HMDB0014915
884	HMDB0015204	Mequitazine	HMDB0015204
885	HMDB0041906	NA	NA
886	HMDB0147295	NA	NA
887	HMDB0141110	NA	NA
888	HMDB0141111	NA	NA
889	HMDB0141134	NA	NA
890	HMDB0141135	NA	NA
891	HMDB0141142	NA	NA
892	HMDB0141168	NA	NA
893	HMDB0141174	NA	NA
894	HMDB0141173	NA	NA
895	HMDB0147032	NA	NA
896	HMDB0147293	NA	NA
897	HMDB0147294	NA	NA
898	HMDB0147297	NA	NA
899	HMDB0147298	NA	NA
900	HMDB0147299	NA	NA
901	HMDB0147300	NA	NA
902	HMDB0141074	NA	NA
903	HMDB0141073	NA	NA
904	HMDB0128989	NA	NA
905	HMDB0128988	NA	NA
906	HMDB0128986	NA	NA
907	HMDB0128987	NA	NA
908	HMDB0128991	NA	NA
909	HMDB0128990	NA	NA
910	HMDB0128992	NA	NA
911	HMDB0141065	NA	NA
912	HMDB0141066	NA	NA
913	HMDB0147302	NA	NA
914	HMDB0141087	NA	NA
915	HMDB0146924	NA	NA
916	HMDB0033535	Honyudisin	HMDB0033535
917	HMDB0030600	4-(3-Methyl-1-butenyl)-3,3',4',5-tetrahydroxystilbene	HMDB0030600
918	HMDB0037586	NA	NA
919	HMDB0035478	2',3,4',5-Tetrahydroxy-4-prenylstilbene	HMDB0035478
920	HMDB0173719	NA	NA
921	HMDB0038724	NA	NA
922	HMDB0003601	(S)-Reticuline	HMDB0003601
923	HMDB0177097	NA	NA
924	HMDB0173722	NA	NA
925	HMDB0173723	NA	NA
926	HMDB0173724	NA	NA
927	HMDB0173726	NA	NA
928	HMDB0177092	NA	NA
929	HMDB0173721	NA	NA
930	HMDB0173720	NA	NA
931	HMDB0149429	NA	NA
932	HMDB0177099	NA	NA
933	HMDB0177098	NA	NA
934	HMDB0177111	NA	NA
935	HMDB0177112	NA	NA
936	HMDB0170226	NA	NA
937	HMDB0170229	NA	NA
938	HMDB0170228	NA	NA
939	HMDB0170227	NA	NA
940	HMDB0170230	NA	NA
941	HMDB0004704	9,10-DHOME	HMDB0004704
942	HMDB0004705	12,13-DHOME	HMDB0004705
943	HMDB0041220	NA	NA
944	HMDB0061650	9,10-Epoxy stearic acid	HMDB0061650
945	HMDB0031679	(9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid	HMDB0031679
946	HMDB0000782	Octadecanedioic acid	HMDB0000782
947	HMDB0062756	NA	NA
948	HMDB0169430	NA	NA
949	HMDB0184817	NA	NA
950	HMDB0185025	NA	NA
951	HMDB0062684	NA	NA
952	HMDB0164511	NA	NA
953	HMDB0062749	NA	NA
954	HMDB0062688	NA	NA
955	HMDB0062409	NA	NA
956	HMDB0062479	NA	NA
957	HMDB0062615	NA	NA
958	HMDB0062614	NA	NA
959	HMDB0062619	NA	NA
960	HMDB0062687	NA	NA
961	HMDB0012498	10,11-dihydro-12-oxo-LTB4	HMDB0012498
962	HMDB0012839	6,7-dihydro-5-oxo-12-epi-LTB4	HMDB0012839
963	HMDB0060103	NA	NA
964	HMDB0060105	NA	NA
965	HMDB0060104	NA	NA
966	HMDB0001085	Leukotriene B4	HMDB0001085

967	HMDB0039171	NA	NA
968	HMDB0034686	(14S)-14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid	HMDB0034686
969	HMDB0039441	NA	NA
970	HMDB0011135	5-HPETE	HMDB0011135
971	HMDB0010219	8,15-DiHETE	HMDB0010219
972	HMDB0004690	Hepoxilin B3	HMDB0004690
973	HMDB0004688	Hepoxilin A3	HMDB0004688
974	HMDB0004243	12(S)-HPETE	HMDB0004243
975	HMDB0004244	15(S)-HPETE	HMDB0004244
976	HMDB0002982	Prostaglandin B1	HMDB0002982
977	HMDB0002656	Prostaglandin A1	HMDB0002656
978	HMDB0002236	8-iso-PGA1	HMDB0002236
979	HMDB0001193	5(S)-Hydroperoxyeicosatetraenoic acid	HMDB0001193
980	HMDB0004696	11(R)-HPETE	HMDB0004696
981	HMDB0004693	11H-14,15-EETA	HMDB0004693
982	HMDB0010216	5,15-DiHETE	HMDB0010216
983	HMDB0010211	17,18-DiHETE	HMDB0010211
984	HMDB0010204	14,15-DiHETE	HMDB0010204
985	HMDB0005089	12(S)-Leukotriene B4	HMDB0005089
986	HMDB0005088	6-trans-12-epi-Leukotriene B4	HMDB0005088
987	HMDB0005087	6-trans-Leukotriene B4	HMDB0005087
988	HMDB0005050	15H-11,12-EETA	HMDB0005050
989	HMDB0004699	8(S)-HPETE	HMDB0004699
990	HMDB0004692	12(R)-HPETE	HMDB0004692
991	HMDB0001442	Prostaglandin E1	HMDB0001442
992	HMDB0184338	NA	NA
993	HMDB0183703	NA	NA
994	HMDB0062278	NA	NA
995	HMDB0012563	13,14-Dihydro- lipoxin A4	HMDB0012563
996	HMDB0013041	Prostaglandin H1	HMDB0013041
997	HMDB0060045	NA	NA
998	HMDB0060107	NA	NA
999	HMDB0035380	Sterebin G	HMDB0035380
1000	HMDB0001139	Prostaglandin F2a	HMDB0001139
1001	HMDB0001483	Prostaglandin F2b	HMDB0001483
1002	HMDB0001965	Troxilin B3	HMDB0001965
1003	HMDB0001977	Trioxilin A3	HMDB0001977
1004	HMDB0002115	8-isoprostaglandin PGF2b	HMDB0002115
1005	HMDB0004684	11,12,15-THETA	HMDB0004684
1006	HMDB0004686	8-Isoprostaglandin E1	HMDB0004686
1007	HMDB0004685	13,14-Dihydro-15-keto PGF2a	HMDB0004685
1008	HMDB0004694	11,14,15-THETA	HMDB0004694
1009	HMDB0005083	8-Isoprostaglandin F2a	HMDB0005083
1010	HMDB0005102	Prostaglandin D1	HMDB0005102
1011	HMDB0006562	8-iso-13,14-dihydro-15-keto-PGF2a	HMDB0006562
1012	HMDB0010170	11,12,15-TriHETRE	HMDB0010170
1013	HMDB0010199	11b-PGF2a	HMDB0010199
1014	HMDB0011137	11-Epi-PGF2a	HMDB0011137
1015	HMDB0240240	NA	NA
1016	HMDB0154672	NA	NA
1017	HMDB0154674	NA	NA
1018	HMDB0154675	NA	NA
1019	HMDB0154673	NA	NA
1020	HMDB0154671	NA	NA
1021	HMDB0154670	NA	NA
1022	HMDB0029566	Isopulegone caffeate	HMDB0029566
1023	HMDB0154668	NA	NA
1024	HMDB0134704	NA	NA
1025	HMDB0147915	NA	NA
1026	HMDB0154665	NA	NA
1027	HMDB0154669	NA	NA
1028	HMDB0154666	NA	NA
1029	HMDB0154667	NA	NA
1030	HMDB0148183	NA	NA
1031	HMDB0153649	NA	NA
1032	HMDB0125854	NA	NA
1033	HMDB0141256	NA	NA
1034	HMDB0124819	NA	NA
1035	HMDB0125836	NA	NA
1036	HMDB0125842	NA	NA
1037	HMDB0133467	NA	NA
1038	HMDB0041386	NA	NA
1039	HMDB0034412	2'-O-Methylphaseollinisoflavan	HMDB0034412
1040	HMDB0039439	NA	NA
1041	HMDB0033672	4'-O-Methylglabridin	HMDB0033672
1042	HMDB0029514	Licochalcone A	HMDB0029514
1043	HMDB0033782	Bergamottin	HMDB0033782
1044	HMDB0039309	NA	NA
1045	HMDB0030846	Archangelin	HMDB0030846
1046	HMDB0039438	NA	NA
1047	HMDB0033671	2'-O-Methylglabridin	HMDB0033671
1048	HMDB0032665	Licoagrocarpin	HMDB0032665
1049	HMDB0031633	Orientanol B	HMDB0031633
1050	HMDB0001272	Nicotine glucuronide	HMDB0001272
1051	HMDB0032808	Niazirinin	HMDB0032808
1052	HMDB0131864	NA	NA
1053	HMDB0124924	NA	NA

1054	HMDB0131867	NA	NA
1055	HMDB0133539	NA	NA
1056	HMDB0124927	NA	NA
1057	HMDB0125807	NA	NA
1058	HMDB0131075	NA	NA
1059	HMDB0133516	NA	NA
1060	HMDB0133495	NA	NA
1061	HMDB0133485	NA	NA
1062	HMDB0133468	NA	NA
1063	HMDB0131866	NA	NA
1064	HMDB0131865	NA	NA
1065	HMDB0124928	NA	NA
1066	HMDB0124929	NA	NA
1067	HMDB0124838	NA	NA
1068	HMDB0124800	NA	NA
1069	HMDB0124826	NA	NA
1070	HMDB0124829	NA	NA
1071	HMDB0124835	NA	NA
1072	HMDB0124837	NA	NA
1073	HMDB0124922	NA	NA
1074	HMDB0130876	NA	NA
1075	HMDB0138809	NA	NA
1076	HMDB0150217	NA	NA
1077	HMDB0150219	NA	NA
1078	HMDB0124822	NA	NA
1079	HMDB0150216	NA	NA
1080	HMDB0150218	NA	NA
1081	HMDB0150215	NA	NA
1082	HMDB0147761	NA	NA
1083	HMDB0147762	NA	NA
1084	HMDB0147765	NA	NA
1085	HMDB0147767	NA	NA
1086	HMDB0147766	NA	NA
1087	HMDB0147764	NA	NA
1088	HMDB0147768	NA	NA
1089	HMDB0147769	NA	NA
1090	HMDB0149836	NA	NA
1091	HMDB0150181	NA	NA
1092	HMDB0150186	NA	NA
1093	HMDB0150185	NA	NA
1094	HMDB0150182	NA	NA
1095	HMDB0150184	NA	NA
1096	HMDB0150187	NA	NA
1097	HMDB0150214	NA	NA
1098	HMDB0035440	alpha,beta-Dihydroxanthohumol	HMDB0035440
1099	HMDB0030666	Chalepin acetate	HMDB0030666
1100	HMDB0035403	Gingerenone A	HMDB0035403
1101	HMDB0030798	Myricanone	HMDB0030798
1102	HMDB0033880	Mammea B/AC cyclo D	HMDB0033880
1103	HMDB0033879	Mammea B/AD cyclo D	HMDB0033879
1104	HMDB0030333	Fragransol C	HMDB0030333
1105	HMDB0041401	NA	NA
1106	HMDB0138808	NA	NA
1107	HMDB0184970	NA	NA
1108	HMDB0184809	NA	NA
1109	HMDB0114763	NA	NA
1110	HMDB0062319	NA	NA
1111	HMDB0176802	NA	NA
1112	HMDB0176822	NA	NA
1113	HMDB0031877	Acetylsalvipisone	HMDB0031877
1114	HMDB0161644	NA	NA
1115	HMDB0161632	NA	NA
1116	HMDB0161627	NA	NA
1117	HMDB0161628	NA	NA
1118	HMDB0161629	NA	NA
1119	HMDB0161622	NA	NA
1120	HMDB0161624	NA	NA
1121	HMDB0161626	NA	NA
1122	HMDB0161623	NA	NA
1123	HMDB0161625	NA	NA
1124	HMDB0185679	NA	NA
1125	HMDB0185658	NA	NA
1126	HMDB0185694	NA	NA
1127	HMDB0185682	NA	NA
1128	HMDB0185676	NA	NA
1129	HMDB0185661	NA	NA
1130	HMDB0185673	NA	NA
1131	HMDB0185698	NA	NA
1132	HMDB0185670	NA	NA
1133	HMDB0185667	NA	NA
1134	HMDB0185664	NA	NA
1135	HMDB0179611	NA	NA
1136	HMDB0179614	NA	NA
1137	HMDB0179608	NA	NA
1138	HMDB0179615	NA	NA
1139	HMDB0179605	NA	NA
1140	HMDB0179606	NA	NA

1141	HMDB0179618	NA	NA
1142	HMDB0179619	NA	NA
1143	HMDB0179623	NA	NA
1144	HMDB0179626	NA	NA
1145	HMDB0182175	NA	NA
1146	HMDB0179627	NA	NA
1147	HMDB0182176	NA	NA
1148	HMDB0014334	Bortezomib	HMDB0014334
1149	HMDB0061005	NA	NA
1150	HMDB0060583	NA	NA
1151	HMDB0030868	Citreoviridin A	HMDB0030868
1152	HMDB0030523	Citreoviridin C	HMDB0030523
1153	HMDB0036462	NA	NA
1154	HMDB0035027	Melleolide F	HMDB0035027
1155	HMDB0035774	Armillyl orsellinate	HMDB0035774
1156	HMDB0015459	Cortisone acetate	HMDB0015459
1157	HMDB0038917	NA	NA
1158	HMDB0031380	(6beta,7alpha,12beta,13beta)-7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide	HMDB0031380
1159	HMDB0179899	NA	NA
1160	HMDB0179900	NA	NA
1161	HMDB0179898	NA	NA
1162	HMDB0179897	NA	NA
1163	HMDB0179895	NA	NA
1164	HMDB0179894	NA	NA
1165	HMDB0179893	NA	NA
1166	HMDB0179896	NA	NA
1167	HMDB0015227	Fluvastatin	HMDB0015227
1168	HMDB0185383	NA	NA
1169	HMDB0158037	NA	NA
1170	HMDB0015439	Tasosartan	HMDB0015439
1171	HMDB0153809	NA	NA
1172	HMDB0033906	2'-Hydroxy-3',4',5',7,8-pentamethoxyflavan	HMDB0033906
1173	HMDB0039032	NA	NA
1174	HMDB0032731	(1E,4Z,6a,8b,10a)-8-Angeloyloxy-10,15-dihydroxy-3-oxo-1,4,11(13)-germacratrien-12,6-olide	HMDB0032731
1175	HMDB0035108	Diosbulbin A	HMDB0035108
1176	HMDB0036780	NA	NA
1177	HMDB0032105	1,2-Anhydridoniveusin	HMDB0032105
1178	HMDB0030081	Carissanol	HMDB0030081
1179	HMDB0039575	NA	NA
1180	HMDB0178288	NA	NA
1181	HMDB0038581	NA	NA
1182	HMDB0014671	Erlotinib	HMDB0014671
1183	HMDB0038643	NA	NA
1184	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol	HMDB0011644
1185	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al	HMDB0006894
1186	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one	HMDB0006887
1187	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one	HMDB0006886
1188	HMDB0006764	17a,20a-Dihydroxycholesterol	HMDB0006764
1189	HMDB0006763	20a,22b-Dihydroxycholesterol	HMDB0006763
1190	HMDB0006281	7-a,27-Dihydroxycholesterol	HMDB0006281
1191	HMDB0060136	7alpha,24S-Dihydroxycholesterol	HMDB0060136
1192	HMDB0006280	7-a,25-Dihydroxycholesterol	HMDB0006280
1193	HMDB0159657	NA	NA
1194	HMDB0172272	NA	NA
1195	HMDB0172271	NA	NA
1196	HMDB0172269	NA	NA
1197	HMDB0172270	NA	NA
1198	HMDB0172267	NA	NA
1199	HMDB0172265	NA	NA
1200	HMDB0172268	NA	NA
1201	HMDB0172266	NA	NA
1202	HMDB0185566	NA	NA
1203	HMDB0185568	NA	NA
1204	HMDB0185575	NA	NA
1205	HMDB0185573	NA	NA
1206	HMDB0185574	NA	NA
1207	HMDB0185571	NA	NA
1208	HMDB0185572	NA	NA
1209	HMDB0185569	NA	NA
1210	HMDB0185567	NA	NA
1211	HMDB0185570	NA	NA
1212	HMDB0172262	NA	NA
1213	HMDB0172264	NA	NA
1214	HMDB0062675	NA	NA
1215	HMDB0062664	NA	NA
1216	HMDB0062607	NA	NA
1217	HMDB0062420	NA	NA
1218	HMDB0062419	NA	NA
1219	HMDB0159652	NA	NA
1220	HMDB0159656	NA	NA
1221	HMDB0172263	NA	NA
1222	HMDB0159658	NA	NA
1223	HMDB0159655	NA	NA
1224	HMDB0159654	NA	NA
1225	HMDB0159653	NA	NA
1226	HMDB0159651	NA	NA
1227	HMDB0184845	NA	NA

1228	HMDB0184846	NA	NA
1229	HMDB0155084	NA	NA
1230	HMDB0184842	NA	NA
1231	HMDB0184843	NA	NA
1232	HMDB0184841	NA	NA
1233	HMDB0184844	NA	NA
1234	HMDB0184848	NA	NA
1235	HMDB0184847	NA	NA
1236	HMDB0184849	NA	NA
1237	HMDB0184851	NA	NA
1238	HMDB0184850	NA	NA
1239	HMDB0185576	NA	NA
1240	HMDB0185577	NA	NA
1241	HMDB0185578	NA	NA
1242	HMDB0184168	NA	NA
1243	HMDB0003550	Calcidiol	HMDB0003550
1244	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	HMDB0036012
1245	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	HMDB0034328
1246	HMDB0035585	1-Phenyl-1,3-heneicosanedione	HMDB0035585
1247	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	HMDB0006721
1248	HMDB0006722	25-Hydroxytachysterol3	HMDB0006722
1249	HMDB0001993	7a-Hydroxy-cholestene-3-one	HMDB0001993
1250	HMDB0000501	7-Ketocholesterol	HMDB0000501
1251	HMDB0015504	Alfacalcidol	HMDB0015504
1252	HMDB0039871	NA	NA
1253	HMDB0060132	NA	NA
1254	HMDB0060131	NA	NA
1255	HMDB0184149	NA	NA
1256	HMDB0174260	NA	NA
1257	HMDB0174261	NA	NA
1258	HMDB0172274	NA	NA
1259	HMDB0172275	NA	NA
1260	HMDB0172273	NA	NA
1261	HMDB0155085	NA	NA
1262	HMDB0155087	NA	NA
1263	HMDB0155086	NA	NA
1264	HMDB0155081	NA	NA
1265	HMDB0155082	NA	NA
1266	HMDB0174265	NA	NA
1267	HMDB0174262	NA	NA
1268	HMDB0174263	NA	NA
1269	HMDB0184150	NA	NA
1270	HMDB0184148	NA	NA
1271	HMDB0184147	NA	NA
1272	HMDB0184145	NA	NA
1273	HMDB0184146	NA	NA
1274	HMDB0184144	NA	NA
1275	HMDB0174268	NA	NA
1276	HMDB0174267	NA	NA
1277	HMDB0174266	NA	NA
1278	HMDB0174264	NA	NA
1279	HMDB0155083	NA	NA
1280	HMDB0155080	NA	NA
1281	HMDB0184143	NA	NA
1282	HMDB0154867	NA	NA
1283	HMDB0154866	NA	NA
1284	HMDB0035951	Erucoylacetone	HMDB0035951
1285	HMDB0164879	NA	NA
1286	HMDB0002126	27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	HMDB0002126
1287	HMDB0036883	NA	NA
1288	HMDB0159770	NA	NA
1289	HMDB0159769	NA	NA
1290	HMDB0159767	NA	NA
1291	HMDB0159766	NA	NA
1292	HMDB0159765	NA	NA
1293	HMDB0159768	NA	NA
1294	HMDB0062421	NA	NA
1295	HMDB0062416	NA	NA
1296	HMDB0159772	NA	NA
1297	HMDB0159774	NA	NA
1298	HMDB0159773	NA	NA
1299	HMDB0159897	NA	NA
1300	HMDB0159894	NA	NA
1301	HMDB0159896	NA	NA
1302	HMDB0159893	NA	NA
1303	HMDB0159889	NA	NA
1304	HMDB0159890	NA	NA
1305	HMDB0159892	NA	NA
1306	HMDB0159891	NA	NA
1307	HMDB0000558	5a-Cholestane-3a,7a,12a,23,25-pentol	HMDB0000558
1308	HMDB0002208	Cholestane-3,7,12,24,25-pentol	HMDB0002208
1309	HMDB0000483	5b-Cholestane-3a,7a,12a,23S,25-pentol	HMDB0000483
1310	HMDB0000556	5b-Cholestane-3a,7a,12a,24,25-pentol	HMDB0000556
1311	HMDB0000513	5b-Cholestane-3a,7a,12a,23R,25-pentol	HMDB0000513
1312	HMDB0002180	5b-Cholestane-3a,7a,12a,25,26-pentol	HMDB0002180
1313	HMDB0011187	TG(8:0/8:0/8:0)	HMDB0011187
1314	HMDB0059930	NA	NA

1315	HMDB0167285	NA	NA
1316	HMDB0179976	NA	NA
1317	HMDB0179977	NA	NA
1318	HMDB0179975	NA	NA
1319	HMDB0167287	NA	NA
1320	HMDB0179974	NA	NA
1321	HMDB0167288	NA	NA
1322	HMDB0167286	NA	NA
1323	HMDB0036131	NA	NA
1324	HMDB0168857	NA	NA
1325	HMDB0062445	NA	NA
1326	HMDB0145193	NA	NA
1327	HMDB0161711	NA	NA
1328	HMDB0145200	NA	NA
1329	HMDB0161709	NA	NA
1330	HMDB0161720	NA	NA
1331	HMDB0145201	NA	NA
1332	HMDB0145177	NA	NA
1333	HMDB0145180	NA	NA
1334	HMDB0145185	NA	NA
1335	HMDB0145187	NA	NA
1336	HMDB0145189	NA	NA
1337	HMDB0145196	NA	NA
1338	HMDB0145197	NA	NA
1339	HMDB0145190	NA	NA
1340	HMDB0145192	NA	NA
1341	HMDB0145181	NA	NA
1342	HMDB0165633	NA	NA
1343	HMDB0163398	NA	NA
1344	HMDB0169690	NA	NA
1345	HMDB0169689	NA	NA
1346	HMDB0163397	NA	NA
1347	HMDB0163729	NA	NA
1348	HMDB0163728	NA	NA
1349	HMDB0240233	NA	NA
1350	HMDB0035144	(3beta,17alpha,23S,24S)-17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-15-one	HMDB0035144
1351	HMDB0170385	NA	NA
1352	HMDB0035221	(3beta,17alpha,23S)-17,23-Epoxy-3,28,29-trihydroxy-27-norlanost-8-en-24-one	HMDB0035221
1353	HMDB0170384	NA	NA
1354	HMDB0167563	NA	NA
1355	HMDB0167569	NA	NA
1356	HMDB0167571	NA	NA
1357	HMDB0167565	NA	NA
1358	HMDB0172392	NA	NA
1359	HMDB0172390	NA	NA
1360	HMDB0167567	NA	NA
1361	HMDB0062208	NA	NA
1362	HMDB0159763	NA	NA
1363	HMDB0159762	NA	NA
1364	HMDB0000359	3a,7a-Dihydroxycoprostanic acid	HMDB0000359
1365	HMDB0159775	NA	NA
1366	HMDB0159887	NA	NA
1367	HMDB0003533	3a,7a,12a-Trihydroxy-5b-cholestan-26-al	HMDB0003533
1368	HMDB0159898	NA	NA
1369	HMDB0159886	NA	NA
1370	HMDB0133638	NA	NA
1371	HMDB0133618	NA	NA
1372	HMDB0011475	LysoPE(0:0/18:1(11Z))	HMDB0011475
1373	HMDB0011476	LysoPE(0:0/18:1(9Z))	HMDB0011476
1374	HMDB0011506	LysoPE(18:1(9Z)/0:0)	HMDB0011506
1375	HMDB0011505	LysoPE(18:1(11Z)/0:0)	HMDB0011505
1376	HMDB0114758	NA	NA
1377	HMDB0062303	NA	NA
1378	HMDB0172575	NA	NA
1379	HMDB0175472	NA	NA
1380	HMDB0170465	NA	NA
1381	HMDB0167392	NA	NA
1382	HMDB0170466	NA	NA
1383	HMDB0030180	Crustecdysone	HMDB0030180
1384	HMDB0170469	NA	NA
1385	HMDB0170467	NA	NA
1386	HMDB0170468	NA	NA
1387	HMDB0240232	NA	NA
1388	HMDB0171796	NA	NA
1389	HMDB0171795	NA	NA
1390	HMDB0171797	NA	NA
1391	HMDB0171798	NA	NA
1392	HMDB0170648	NA	NA
1393	HMDB0170654	NA	NA
1394	HMDB0170645	NA	NA
1395	HMDB0170653	NA	NA
1396	HMDB0170658	NA	NA
1397	HMDB0170657	NA	NA
1398	HMDB0170656	NA	NA
1399	HMDB0170649	NA	NA
1400	HMDB0170652	NA	NA
1401	HMDB0170647	NA	NA

1402	HMDB0170646	NA	NA
1403	HMDB0170655	NA	NA
1404	HMDB0184654	NA	NA
1405	HMDB0184468	NA	NA
1406	HMDB0139941	NA	NA
1407	HMDB0139958	NA	NA
1408	HMDB0035635	Kanokoside A	HMDB0035635
1409	HMDB0004482	2-Methoxyestrone 3-glucuronide	HMDB0004482
1410	HMDB0154676	NA	NA
1411	HMDB0169584	NA	NA
1412	HMDB0146115	NA	NA
1413	HMDB0161563	NA	NA
1414	HMDB0161564	NA	NA
1415	HMDB0161602	NA	NA
1416	HMDB0161603	NA	NA
1417	HMDB0158633	NA	NA
1418	HMDB0158234	NA	NA
1419	HMDB0158235	NA	NA
1420	HMDB0158642	NA	NA
1421	HMDB0158238	NA	NA
1422	HMDB0158621	NA	NA
1423	HMDB0158636	NA	NA
1424	HMDB0158629	NA	NA
1425	HMDB0158625	NA	NA
1426	HMDB0158226	NA	NA
1427	HMDB0158231	NA	NA
1428	HMDB0158228	NA	NA
1429	HMDB0157580	NA	NA
1430	HMDB0158210	NA	NA
1431	HMDB0158213	NA	NA
1432	HMDB0158219	NA	NA
1433	HMDB0158216	NA	NA
1434	HMDB0158221	NA	NA
1435	HMDB0158223	NA	NA
1436	HMDB0158225	NA	NA
1437	HMDB0158639	NA	NA
1438	HMDB0158646	NA	NA
1439	HMDB0158643	NA	NA
1440	HMDB0169111	NA	NA
1441	HMDB0171254	NA	NA
1442	HMDB0171269	NA	NA
1443	HMDB0171253	NA	NA
1444	HMDB0171257	NA	NA
1445	HMDB0171258	NA	NA
1446	HMDB0171264	NA	NA
1447	HMDB0171268	NA	NA
1448	HMDB0171273	NA	NA
1449	HMDB0171272	NA	NA
1450	HMDB0169110	NA	NA
1451	HMDB0169105	NA	NA
1452	HMDB0169108	NA	NA
1453	HMDB0158650	NA	NA
1454	HMDB0158654	NA	NA
1455	HMDB0158656	NA	NA
1456	HMDB0158660	NA	NA
1457	HMDB0169095	NA	NA
1458	HMDB0169099	NA	NA
1459	HMDB0169097	NA	NA
1460	HMDB0169101	NA	NA
1461	HMDB0169103	NA	NA
1462	HMDB0169107	NA	NA
1463	HMDB0033412	Gibberellin A20 13-glucoside	HMDB0033412
1464	HMDB0037084	NA	NA
1465	HMDB0038610	NA	NA
1466	HMDB0171261	NA	NA
1467	HMDB0015181	Fluocinonide	HMDB0015181
1468	HMDB0140090	NA	NA
1469	HMDB0033177	Sapiol	HMDB0033177
1470	HMDB0038738	NA	NA
1471	HMDB0157582	NA	NA
1472	HMDB0179952	NA	NA
1473	HMDB0179953	NA	NA
1474	HMDB0174900	NA	NA
1475	HMDB0167227	NA	NA
1476	HMDB0167180	NA	NA
1477	HMDB0035700	Lucidenic acid J	HMDB0035700
1478	HMDB0167212	NA	NA
1479	HMDB0167174	NA	NA
1480	HMDB0167200	NA	NA
1481	HMDB0167223	NA	NA
1482	HMDB0167220	NA	NA
1483	HMDB0167217	NA	NA
1484	HMDB0167216	NA	NA
1485	HMDB0167195	NA	NA
1486	HMDB0167213	NA	NA
1487	HMDB0167206	NA	NA
1488	HMDB0167209	NA	NA

1489	HMDB0167203	NA	NA
1490	HMDB0167186	NA	NA
1491	HMDB0167183	NA	NA
1492	HMDB0167177	NA	NA
1493	HMDB0167189	NA	NA
1494	HMDB0167192	NA	NA
1495	HMDB0167196	NA	NA
1496	HMDB0167197	NA	NA
1497	HMDB0173045	NA	NA
1498	HMDB0033471	N1,N10-Diferuloylspermidine	HMDB0033471
1499	HMDB0158489	NA	NA
1500	HMDB0158490	NA	NA
1501	HMDB0158494	NA	NA
1502	HMDB0158485	NA	NA
1503	HMDB0158502	NA	NA
1504	HMDB0158497	NA	NA
1505	HMDB0158498	NA	NA
1506	HMDB0158486	NA	NA
1507	HMDB0158501	NA	NA
1508	HMDB0158493	NA	NA
1509	HMDB0030685	Cycloheterophyllin	HMDB0030685
1510	HMDB0034665	Artonin A	HMDB0034665
1511	HMDB0029471	Isocycloheterophyllin	HMDB0029471
1512	HMDB0035187	Artonin F	HMDB0035187
1513	HMDB0034667	Artonin B	HMDB0034667
1514	HMDB0187390	NA	NA
1515	HMDB0187391	NA	NA
1516	HMDB0187182	NA	NA
1517	HMDB0187392	NA	NA
1518	HMDB0035167	Cinn cassiol C1 19-glucoside	HMDB0035167
1519	HMDB0168850	NA	NA
1520	HMDB0183642	NA	NA
1521	HMDB0177911	NA	NA
1522	HMDB0168858	NA	NA
1523	HMDB0168859	NA	NA
1524	HMDB0177908	NA	NA
1525	HMDB0183653	NA	NA
1526	HMDB0183640	NA	NA
1527	HMDB0183646	NA	NA
1528	HMDB0183661	NA	NA
1529	HMDB0183660	NA	NA
1530	HMDB0183664	NA	NA
1531	HMDB0183663	NA	NA
1532	HMDB0183666	NA	NA
1533	HMDB0183667	NA	NA
1534	HMDB0183668	NA	NA
1535	HMDB0183671	NA	NA
1536	HMDB0183670	NA	NA
1537	HMDB0183659	NA	NA
1538	HMDB0183662	NA	NA
1539	HMDB0183655	NA	NA
1540	HMDB0183644	NA	NA
1541	HMDB0183645	NA	NA
1542	HMDB0183656	NA	NA
1543	HMDB0183647	NA	NA
1544	HMDB0183648	NA	NA
1545	HMDB0183649	NA	NA
1546	HMDB0183651	NA	NA
1547	HMDB0183652	NA	NA
1548	HMDB0183657	NA	NA
1549	HMDB0183672	NA	NA
1550	HMDB0035603	Mascaroside	HMDB0035603
1551	HMDB0183641	NA	NA
1552	HMDB0037083	NA	NA
1553	HMDB0036903	NA	NA
1554	HMDB0040672	NA	NA
1555	HMDB0162428	NA	NA
1556	HMDB0162427	NA	NA
1557	HMDB0038028	NA	NA
1558	HMDB0145256	NA	NA
1559	HMDB0145259	NA	NA
1560	HMDB0145255	NA	NA
1561	HMDB0145268	NA	NA
1562	HMDB0145246	NA	NA
1563	HMDB0145249	NA	NA
1564	HMDB0145247	NA	NA
1565	HMDB0145253	NA	NA
1566	HMDB0145260	NA	NA
1567	HMDB0145261	NA	NA
1568	HMDB0145267	NA	NA
1569	HMDB0145263	NA	NA
1570	HMDB0145250	NA	NA
1571	HMDB0145262	NA	NA
1572	HMDB0145264	NA	NA
1573	HMDB0145265	NA	NA
1574	HMDB0145258	NA	NA
1575	HMDB0145252	NA	NA

1576	HMDB0145270	NA	NA
1577	HMDB0014433	Amcinonide	HMDB0014433
1578	HMDB0034339	Ixocarpalactone B	HMDB0034339
1579	HMDB0034059	4beta-Hydroxywithanolide E	HMDB0034059
1580	HMDB0034400	Withaperuvin F	HMDB0034400
1581	HMDB0034191	Withaperuvin B	HMDB0034191
1582	HMDB0031355	28-Hydroxywithanolide E	HMDB0031355
1583	HMDB0033943	Withaperuvin G	HMDB0033943
1584	HMDB0030362	Cavipetin B	HMDB0030362
1585	HMDB0170358	NA	NA
1586	HMDB0187402	NA	NA
1587	HMDB0185457	NA	NA
1588	HMDB0015393	Darunavir	HMDB0015393
1589	HMDB0168629	NA	NA
1590	HMDB0168628	NA	NA
1591	HMDB0161739	NA	NA
1592	HMDB0161740	NA	NA
1593	HMDB0031388	23-Hydroxyphysalolactone	HMDB0031388
1594	HMDB0173080	NA	NA
1595	HMDB0015101	Telmisartan	HMDB0015101
1596	HMDB0164474	NA	NA
1597	HMDB0164482	NA	NA
1598	HMDB0164483	NA	NA
1599	HMDB0164491	NA	NA
1600	HMDB0164495	NA	NA
1601	HMDB0164506	NA	NA
1602	HMDB0164502	NA	NA
1603	HMDB0140666	NA	NA
1604	HMDB0140667	NA	NA
1605	HMDB0140668	NA	NA
1606	HMDB0032648	Muridienin 1	HMDB0032648
1607	HMDB0032850	Muricadienin	HMDB0032850
1608	HMDB0072546	NA	NA
1609	HMDB0072531	NA	NA
1610	HMDB0072529	NA	NA
1611	HMDB0072338	NA	NA
1612	HMDB0072333	NA	NA
1613	HMDB0072245	NA	NA
1614	HMDB0072206	NA	NA
1615	HMDB0071968	NA	NA
1616	HMDB0071738	NA	NA
1617	HMDB0100886	NA	NA
1618	HMDB0100885	NA	NA
1619	HMDB0100884	NA	NA
1620	HMDB0096650	NA	NA
1621	HMDB0096651	NA	NA
1622	HMDB0096564	NA	NA
1623	HMDB0096562	NA	NA
1624	HMDB0096563	NA	NA
1625	HMDB0071685	NA	NA
1626	HMDB0071676	NA	NA
1627	HMDB0071663	NA	NA
1628	HMDB0096649	NA	NA
1629	HMDB0071443	NA	NA
1630	HMDB0071222	NA	NA
1631	HMDB0071165	NA	NA
1632	HMDB0034194	Jurubine	HMDB0034194
1633	HMDB0164367	NA	NA
1634	HMDB0164368	NA	NA
1635	HMDB0164358	NA	NA
1636	HMDB0164359	NA	NA
1637	HMDB0164350	NA	NA
1638	HMDB0164349	NA	NA
1639	HMDB0164341	NA	NA
1640	HMDB0164340	NA	NA
1641	HMDB0033477	NA	NA
1642	HMDB0184827	NA	NA
1643	HMDB0062478	NA	NA
1644	HMDB0060155	NA	NA
1645	HMDB0013061	S-(PGA1)-glutathione	HMDB0013061
1646	HMDB0013060	S-(9-hydroxy-PGA2)-glutathione	HMDB0013060
1647	HMDB0013057	S-(9-deoxy-delta12-PGD2)-glutathione	HMDB0013057
1648	HMDB0013056	S-(11-OH-9-deoxy-delta9,12-PGD2)-glutathione	HMDB0013056
1649	HMDB0183885	NA	NA
1650	HMDB0183879	NA	NA
1651	HMDB0183878	NA	NA
1652	HMDB0183884	NA	NA
1653	HMDB0001198	Leukotriene C4	HMDB0001198
1654	HMDB0183882	NA	NA
1655	HMDB0005095	11-trans-Leukotriene C4	HMDB0005095
1656	HMDB0183888	NA	NA
1657	HMDB0183887	NA	NA
1658	HMDB0183881	NA	NA
1659	HMDB0178719	NA	NA
1660	HMDB0178728	NA	NA
1661	HMDB0178720	NA	NA
1662	HMDB0178718	NA	NA

1663	HMDB0178717	NA	NA
1664	HMDB0178729	NA	NA
1665	HMDB0178730	NA	NA
1666	HMDB0178727	NA	NA
1667	HMDB0160619	NA	NA
1668	HMDB0160620	NA	NA
1669	HMDB0160617	NA	NA
1670	HMDB0160616	NA	NA
1671	HMDB0173931	NA	NA
1672	HMDB0173932	NA	NA
1673	HMDB0014351	Reserpine	HMDB0014351
1674	HMDB0030172	Oxyacanthine	HMDB0030172
1675	HMDB0015330	Tubocurarine	HMDB0015330
1676	HMDB0015129	Neomycin	HMDB0015129
1677	HMDB0002160	Harderoporpyrinogen	HMDB0002160
1678	HMDB0039454	NA	NA
1679	HMDB0173693	NA	NA
1680	HMDB0173692	NA	NA
1681	HMDB0173699	NA	NA
1682	HMDB0173698	NA	NA
1683	HMDB0142988	NA	NA
1684	HMDB0142998	NA	NA
1685	HMDB0142997	NA	NA
1686	HMDB0143001	NA	NA
1687	HMDB0142987	NA	NA
1688	HMDB0142978	NA	NA
1689	HMDB0142977	NA	NA
1690	HMDB0142917	NA	NA
1691	HMDB0142918	NA	NA
1692	HMDB0142919	NA	NA
1693	HMDB0142921	NA	NA
1694	HMDB0142920	NA	NA
1695	HMDB0142926	NA	NA
1696	HMDB0142929	NA	NA
1697	HMDB0142928	NA	NA
1698	HMDB0142927	NA	NA
1699	HMDB0143002	NA	NA
1700	HMDB0143007	NA	NA
1701	HMDB0143006	NA	NA
1702	HMDB0143108	NA	NA
1703	HMDB0143104	NA	NA
1704	HMDB0143098	NA	NA
1705	HMDB0143093	NA	NA
1706	HMDB0143086	NA	NA
1707	HMDB0143085	NA	NA
1708	HMDB0143076	NA	NA
1709	HMDB0143075	NA	NA
1710	HMDB0143066	NA	NA
1711	HMDB0143065	NA	NA
1712	HMDB0143061	NA	NA
1713	HMDB0143060	NA	NA
1714	HMDB0143022	NA	NA
1715	HMDB0143012	NA	NA
1716	HMDB0143011	NA	NA
1717	HMDB0143021	NA	NA
1718	HMDB0142916	NA	NA
1719	HMDB0142915	NA	NA
1720	HMDB0142901	NA	NA
1721	HMDB0142899	NA	NA
1722	HMDB0142902	NA	NA
1723	HMDB0142900	NA	NA
1724	HMDB0142905	NA	NA
1725	HMDB0142904	NA	NA
1726	HMDB0142903	NA	NA
1727	HMDB0142908	NA	NA
1728	HMDB0142911	NA	NA
1729	HMDB0142913	NA	NA
1730	HMDB0142914	NA	NA
1731	HMDB0142912	NA	NA
1732	HMDB0142930	NA	NA
1733	HMDB0165936	NA	NA
1734	HMDB0165918	NA	NA
1735	HMDB0173230	NA	NA
1736	HMDB0173229	NA	NA
1737	HMDB0165966	NA	NA
1738	HMDB0164809	NA	NA
1739	HMDB0034433	Riboflavine 2',3',4',5'-tetrabutanoate	HMDB0034433
1740	HMDB0157944	NA	NA
1741	HMDB0157945	NA	NA
1742	HMDB0157949	NA	NA
1743	HMDB0157950	NA	NA
1744	HMDB0157951	NA	NA
1745	HMDB0157955	NA	NA
1746	HMDB0157956	NA	NA
1747	HMDB0157943	NA	NA
1748	HMDB0157938	NA	NA
1749	HMDB0157939	NA	NA

1750	HMDB0157937	NA	NA
1751	HMDB0157933	NA	NA
1752	HMDB0157932	NA	NA
1753	HMDB0157931	NA	NA
1754	HMDB0157898	NA	NA
1755	HMDB0157896	NA	NA
1756	HMDB0157957	NA	NA
1757	HMDB0158932	NA	NA
1758	HMDB0158968	NA	NA
1759	HMDB0158964	NA	NA
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1762	HMDB0158959	NA	NA
1763	HMDB0158953	NA	NA
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1765	HMDB0158949	NA	NA
1766	HMDB0158948	NA	NA
1767	HMDB0158944	NA	NA
1768	HMDB0158943	NA	NA
1769	HMDB0158937	NA	NA
1770	HMDB0158938	NA	NA
1771	HMDB0158939	NA	NA
1772	HMDB0158933	NA	NA
1773	HMDB0158969	NA	NA
1774	HMDB0157897	NA	NA
1775	HMDB0157050	NA	NA
1776	HMDB0157221	NA	NA
1777	HMDB0157842	NA	NA
1778	HMDB0157841	NA	NA
1779	HMDB0157843	NA	NA
1780	HMDB0157847	NA	NA
1781	HMDB0157846	NA	NA
1782	HMDB0157851	NA	NA
1783	HMDB0157848	NA	NA
1784	HMDB0157853	NA	NA
1785	HMDB0157215	NA	NA
1786	HMDB0157218	NA	NA
1787	HMDB0157212	NA	NA
1788	HMDB0157051	NA	NA
1789	HMDB0157054	NA	NA
1790	HMDB0157057	NA	NA
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1792	HMDB0157066	NA	NA
1793	HMDB0157063	NA	NA
1794	HMDB0157206	NA	NA
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1797	HMDB0157852	NA	NA
1798	HMDB0157856	NA	NA
1799	HMDB0157857	NA	NA
1800	HMDB0157876	NA	NA
1801	HMDB0157881	NA	NA
1802	HMDB0157882	NA	NA
1803	HMDB0157883	NA	NA
1804	HMDB0157886	NA	NA
1805	HMDB0157887	NA	NA
1806	HMDB0157888	NA	NA
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1811	HMDB0157877	NA	NA
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1814	HMDB0157862	NA	NA
1815	HMDB0157863	NA	NA
1816	HMDB0157866	NA	NA
1817	HMDB0157867	NA	NA
1818	HMDB0157868	NA	NA
1819	HMDB0157871	NA	NA
1820	HMDB0157873	NA	NA
1821	HMDB0157872	NA	NA
1822	HMDB0185009	NA	NA
1823	HMDB0185010	NA	NA
1824	HMDB0014964	Natamycin	HMDB0014964
1825	HMDB0040917	NA	NA
1826	HMDB0015032	Benzylpenicilloyl Polylysine	HMDB0015032
1827	HMDB0184092	NA	NA
1828	HMDB0184087	NA	NA
1829	HMDB0015183	Ergoloid mesylate	HMDB0015183
1830	HMDB0168627	NA	NA
1831	HMDB0161735	NA	NA
1832	HMDB0161734	NA	NA
1833	HMDB0161733	NA	NA
1834	HMDB0168626	NA	NA
1835	HMDB0161736	NA	NA
1836	HMDB0184371	NA	NA

1837	HMDB0184657	NA	NA
1838	HMDB0184663	NA	NA
1839	HMDB0168002	NA	NA
1840	HMDB0168000	NA	NA
1841	HMDB0167999	NA	NA
1842	HMDB0168001	NA	NA
1843	HMDB0167998	NA	NA
1844	HMDB0167996	NA	NA
1845	HMDB0167997	NA	NA
1846	HMDB0168003	NA	NA
1847	HMDB0168005	NA	NA
1848	HMDB0168009	NA	NA
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2461	HMDB0095263	NA	NA
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2499	HMDB0095925	NA	NA
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2550	HMDB0007716	DG(22:5(4Z,7Z,10Z,13Z,16Z)/20:0/0:0)	HMDB0007716
2551	HMDB0007745	DG(22:5(7Z,10Z,13Z,16Z,19Z)/20:0/0:0)	HMDB0007745
2552	HMDB0007831	DG(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	HMDB0007831
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2555	HMDB0007381	DG(20:0/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	HMDB0007381
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2557	HMDB0007408	DG(20:1(11Z)/22:4(7Z,10Z,13Z,16Z)/0:0)	HMDB0007408
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2804	HMDB0054482	NA	NA
2805	HMDB0052244	NA	NA
2806	HMDB0054403	NA	NA
2807	HMDB0004889	Ganglioside GA2 (d18:1/9Z-18:1)	HMDB0004889
2808	HMDB0001543	Diguanosine hexaphosphate	HMDB0001543
2809	HMDB0006563	Hexaglutamyl folate	HMDB0006563
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2811	HMDB0032781	Acetyljuguboside B	HMDB0032781
2812	HMDB0015601	Vapreotide	HMDB0015601
2813	HMDB0112241	NA	NA
2814	HMDB0031372	Ceposide D	HMDB0031372
2815	HMDB0039829	NA	NA
2816	HMDB0038616	NA	NA
2817	HMDB0110936	NA	NA
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2820	HMDB0057518	NA	NA
2821	HMDB0057482	NA	NA
2822	HMDB0110858	NA	NA

4 Pathway Analysis

In this step, users are asked to select a pathway library, as well as specify the algorithms for pathway enrichment analysis and pathway topology analysis.

4.1 Pathway Library

There are 15 pathway libraries currently supported, with a total of 1173 pathways :

- Homo sapiens (human) [80]
- Mus musculus (mouse) [82]
- Rattus norvegicus (rat) [81]
- Bos taurus (cow) [81]
- Danio rerio (zebrafish) [81]
- Drosophila melanogaster (fruit fly) [79]
- Caenorhabditis elegans (nematode) [78]
- Saccharomyces cerevisiae (yeast) [65]
- Oryza sativa japonica (Japanese rice) [83]
- Arabidopsis thaliana (thale cress) [87]
- Escherichia coli K-12 MG1655 [87]
- Bacillus subtilis [80]
- Pseudomonas putida KT2440 [89]
- Staphylococcus aureus N315 (MRSA/VSSA)[73]
- Thermotoga maritima [57]

Your selected pathway library code is **hsa** (KEGG organisms abbreviation).

4.2 Over Representation Analysis

Over-representation analysis tests if a particular group of compounds is represented more than expected by chance within the user uploaded compound list. In the context of pathway analysis, we are testing if compounds involved in a particular pathway are enriched compared to random hits. MetPA offers two of the most commonly used methods for over-representation analysis:

- Fishers'Exact test
- Hypergeometric Test

Please note, MetPA uses one-tailed Fisher's exact test which will give essentially the same result as the result calculated by the hypergeometric test.

The selected over-representation analysis method is **Hypergeometric test**.

4.3 Pathway Topology Analysis

The structure of biological pathways represent our knowledge about the complex relationships among molecules within a cell or a living organism. However, most pathway analysis algorithms fail to take structural information into consideration when estimating which pathways are significantly changed under conditions of study. It is well-known that changes in more important positions of a network will trigger a more severe impact on the pathway than changes occurred in marginal or relatively isolated positions.

The pathway topology analysis uses two well-established node centrality measures to estimate node importance - **degree centrality** and **betweenness centrality**. Degree centrality is defined as the number of links occurred upon a node. For a directed graph there are two types of degree: in-degree for links come from other nodes, and out-degree for links initiated from the current node. Metabolic networks are directed graph. Here we only consider the out-degree for node importance measure. It is assumed that nodes upstream will have regulatory roles for the downstream nodes, not vice versa. The betweenness centrality measures the number of shortest paths going through the node. Since the metabolic network is directed, we use the relative betweenness centrality for a metabolite as the importance measure. The degree centrality measure focuses more on local connectivities, while the betweenness centrality measure focuses more on global network topology. For more detailed discussions on various graph-based methods for analyzing biological networks, please refer to the article by Tero Aittokallio, T. et al. ¹

Please note, for comparison among different pathways, the node importance values calculated from centrality measures are further normalized by the sum of the importance of the pathway. Therefore, the total/maximum importance of each pathway is 1; the importance measure of each metabolite node is actually the percentage w.r.t the total pathway importance, and the pathway impact value is the cumulative percentage from the matched metabolite nodes.

Your selected node importance measure for topological analysis is **relative betweenness centrality**.

5 Pathway Analysis Result

The results from pathway analysis are presented graphically as well as in a detailed table.

A Google-map style interactive visualization system was implemented to facilitate data exploration. The graphical output contains three levels of view: **metabolome view**, **pathway view**, and **compound view**. Only the metabolome view is shown below. Pathway views and compound views are generated dynamically based on your interactions with the visualization system. They are available in your downloaded files.

¹Tero Aittokallio and Benno Schwikowski. *Graph-based methods for analyzing networks in cell biology*, Briefings in Bioinformatics 2006 7(3):243-255

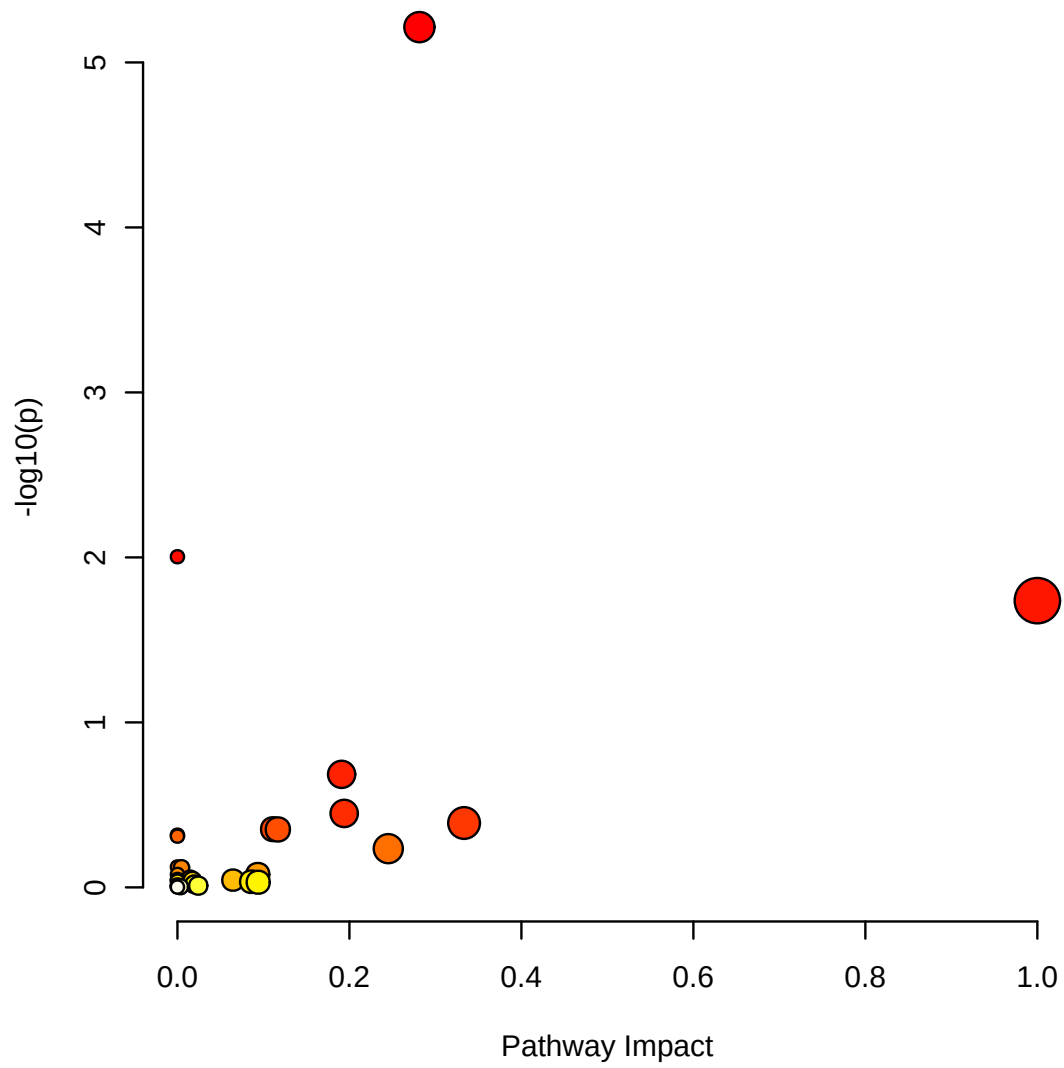


Figure 1: Summary of Pathway Analysis

The table below shows the detailed results from the pathway analysis. Since we are testing many pathways at the same time, the statistical p values from enrichment analysis are further adjusted for multiple testings. In particular, the **Total** is the total number of compounds in the pathway; the **Hits** is the actually matched number from the user uploaded data; the **Raw p** is the original p value calculated from the enrichment analysis; the **Holm p** is the p value adjusted by Holm-Bonferroni method; the **FDR p** is the p value adjusted using False Discovery Rate; the **Impact** is the pathway impact value calculated from pathway topology analysis.

Table 2: Result from Pathway Analysis

	Total	Expected	Hits	Raw p	-log10(p)	Holm adjust	FDR	Impact
Arachidonic acid metabolism	36	3.81	14	6.11E-06	5.21E+00	5.13E-04	5.13E-04	0.28
Linoleic acid metabolism	5	0.53	3	9.91E-03	2.00E+00	8.22E-01	4.16E-01	0.00
D-Glutamine and D-glutamate metabolism	6	0.63	3	1.83E-02	1.74E+00	1.00E+00	5.12E-01	1.00
Primary bile acid biosynthesis	46	4.87	7	2.07E-01	6.85E-01	1.00E+00	1.00E+00	0.19
Citrate cycle (TCA cycle)	20	2.12	3	3.56E-01	4.48E-01	1.00E+00	1.00E+00	0.19
alpha-Linolenic acid metabolism	13	1.38	2	4.07E-01	3.90E-01	1.00E+00	1.00E+00	0.33
Glyoxylate and dicarboxylate metabolism	32	3.39	4	4.44E-01	3.53E-01	1.00E+00	1.00E+00	0.11
Arginine biosynthesis	14	1.48	2	4.46E-01	3.51E-01	1.00E+00	1.00E+00	0.12
Butanoate metabolism	15	1.59	2	4.82E-01	3.17E-01	1.00E+00	1.00E+00	0.00
Nitrogen metabolism	6	0.63	1	4.89E-01	3.10E-01	1.00E+00	1.00E+00	0.00
Alanine, aspartate and glutamate metabolism	28	2.96	3	5.83E-01	2.35E-01	1.00E+00	1.00E+00	0.25
Biosynthesis of unsaturated fatty acids	36	3.81	3	7.52E-01	1.24E-01	1.00E+00	1.00E+00	0.00
Lysine degradation	25	2.65	2	7.61E-01	1.19E-01	1.00E+00	1.00E+00	0.00
Histidine metabolism	16	1.69	1	8.34E-01	7.86E-02	1.00E+00	1.00E+00	0.00
Glycerolipid metabolism	16	1.69	1	8.34E-01	7.86E-02	1.00E+00	1.00E+00	0.09
Fatty acid biosynthesis	47	4.97	3	8.91E-01	5.03E-02	1.00E+00	1.00E+00	0.01
Fructose and mannose metabolism	20	2.12	1	8.95E-01	4.83E-02	1.00E+00	1.00E+00	0.00
Steroid hormone biosynthesis	85	8.99	6	9.04E-01	4.40E-02	1.00E+00	1.00E+00	0.06
Sphingolipid metabolism	21	2.22	1	9.06E-01	4.29E-02	1.00E+00	1.00E+00	0.00
Glycerophospholipid metabolism	36	3.81	2	9.09E-01	4.16E-02	1.00E+00	1.00E+00	0.02
Pentose phosphate pathway	22	2.33	1	9.16E-01	3.81E-02	1.00E+00	1.00E+00	0.00
Arginine and proline metabolism	38	4.02	2	9.24E-01	3.43E-02	1.00E+00	1.00E+00	0.09
Pyrimidine metabolism	39	4.13	2	9.31E-01	3.11E-02	1.00E+00	1.00E+00	0.09
Glutathione metabolism	28	2.96	1	9.58E-01	1.88E-02	1.00E+00	1.00E+00	0.02
Porphyrin and chlorophyll metabolism	30	3.17	1	9.66E-01	1.49E-02	1.00E+00	1.00E+00	0.00
Glycine, serine and threonine metabolism	33	3.49	1	9.76E-01	1.05E-02	1.00E+00	1.00E+00	0.02
Amino sugar and nucleotide sugar metabolism	37	3.91	1	9.85E-01	6.63E-03	1.00E+00	1.00E+00	0.00
Fatty acid elongation	39	4.13	1	9.88E-01	5.26E-03	1.00E+00	1.00E+00	0.00
Fatty acid degradation	39	4.13	1	9.88E-01	5.26E-03	1.00E+00	1.00E+00	0.00
Steroid biosynthesis	42	4.44	1	9.91E-01	3.72E-03	1.00E+00	1.00E+00	0.00
Aminoacyl-tRNA biosynthesis	48	5.08	1	9.96E-01	1.86E-03	1.00E+00	1.00E+00	0.00

6 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "compd.vec<-c(\"HMDB0000973\", \"HMDB0001429\", \"HMDB0002105\", \"HMDB0002142\", \"HMDB0031404\", \"I"
[3] "mSet<-Setup.MapData(mSet, compd.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<-PlotKEGGPath(mSet, \"D-Glutamine and D-glutamate metabolism\", 528, 480, \"png\", NULL)"
[11] "mSet<-RenderMetPAGraph(mSet, \"zoom1621874111494.png\", 528.0, 480.0, 100.0)"
[12] "mSet<-PlotKEGGPath(mSet, \"Arachidonic acid metabolism\", 528, 480, \"png\", NULL)"
[13] "mSet<-SaveTransformedData(mSet)"
[14] "mSet<-PreparePDFReport(mSet, \"guest6846586895463805941\")\n"
```

The report was generated on Mon May 24 12:35:19 2021 with R version 4.0.2 (2020-06-22).