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	HMDB0000925	Trimethylamine N-oxide	HMDB0000925
2	HMDB0142449	NA	NA
3	HMDB0140038	NA	NA
4	HMDB0012136	1-Amino-propan-2-ol	HMDB0012136
5	HMDB0062143	NA	NA
6	HMDB0031558	Methyloxirane	HMDB0031558
7	HMDB0031652	Allyl alcohol	HMDB0031652
8	HMDB0003366	Propanal	HMDB0003366
9	HMDB0001659	Acetone	HMDB0001659

10	HMDB0060253	1-Methylpyrrolinium	HMDB0060253
11	HMDB0172632	NA	NA
12	HMDB0062600	NA	NA
13	HMDB0012815	5-Aminopentanal	HMDB0012815
14	HMDB0033529	(+)-2,3-Dihydro-3-methyl-1H-pyrrole	HMDB0033529
15	HMDB0040173	NA	NA
16	HMDB0061878	NA	NA
17	HMDB0001252	Betaine aldehyde	HMDB0001252
18	HMDB0031404	Cyclohexylamine	HMDB0031404
19	HMDB0032416	2-Methylpiperidine	HMDB0032416
20	HMDB0031544	3-Methylcyclopentene	HMDB0031544
21	HMDB0062716	NA	NA
22	HMDB0033971	2-Diethylaminoethanol	HMDB0033971
23	HMDB0059844	NA	NA
24	HMDB0000642	Erythronilic acid	HMDB0000642
25	HMDB0041603	NA	NA
26	HMDB0040735	NA	NA
27	HMDB0002011	4-Hydroxyisovaleric acid	HMDB0002011
28	HMDB0001863	2-Hydroxyvaleric acid	HMDB0001863
29	HMDB0000754	3-Hydroxyisovaleric acid	HMDB0000754
30	HMDB0000531	3-Hydroxyvaleric acid	HMDB0000531
31	HMDB0000410	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	HMDB0000410
32	HMDB0000407	2-Hydroxy-3-methylbutyric acid	HMDB0000407
33	HMDB0000396	2-Ethylhydracrylic acid	HMDB0000396
34	HMDB0000354	2-Methyl-3-hydroxybutyric acid	HMDB0000354
35	HMDB0000351	3-Hydroxy-2-methyl-[R-(R,S)]-butanoic acid	HMDB0000351
36	HMDB0172069	NA	NA
37	HMDB0172068	NA	NA
38	HMDB0172067	NA	NA
39	HMDB0161206	NA	NA
40	HMDB0161204	NA	NA
41	HMDB0161205	NA	NA
42	HMDB0062584	NA	NA
43	HMDB0062057	NA	NA
44	HMDB0061927	NA	NA
45	HMDB0001987	2-Hydroxy-2-methylbutyric acid	HMDB0001987
46	HMDB0130836	NA	NA
47	HMDB0029599	Glutaral	HMDB0029599
48	HMDB0031648	2,4-Pentanedione	HMDB0031648
49	HMDB0031602	4-Pentenoic acid	HMDB0031602
50	HMDB0029608	Angelic acid	HMDB0029608
51	HMDB0035143	Dihydro-3-methyl-2(3H)-furanone	HMDB0035143
52	HMDB0032385	Methyl methacrylate	HMDB0032385
53	HMDB0032351	Isopropenyl acetate	HMDB0032351
54	HMDB0032459	2-Pentenoic acid	HMDB0032459
55	HMDB0031178	Dihydro-2-methyl-3(2H)-furanone	HMDB0031178
56	HMDB0033840	Dihydro-5-methyl-2(3H)-furanone	HMDB0033840
57	HMDB0031598	2,3-Pentanedione	HMDB0031598
58	HMDB0033978	Ethyl acrylate	HMDB0033978
59	HMDB0002167	3-Methylbutyrolactone	HMDB0002167
60	HMDB0001862	2-Ethylacrylic acid	HMDB0001862
61	HMDB0000509	Senecioic acid	HMDB0000509
62	HMDB0001470	Tiglic acid	HMDB0001470
63	HMDB0129418	NA	NA
64	HMDB0163713	NA	NA
65	HMDB0163714	NA	NA
66	HMDB0163712	NA	NA
67	HMDB0130837	NA	NA
68	HMDB0170858	NA	NA
69	HMDB0180166	NA	NA
70	HMDB0132474	NA	NA
71	HMDB0149276	NA	NA
72	HMDB0182885	NA	NA
73	HMDB0039786	NA	NA
74	HMDB0173815	NA	NA
75	HMDB0173816	NA	NA
76	HMDB0171081	NA	NA
77	HMDB0032576	2-Methoxy-1,4-benzoquinone	HMDB0032576
78	HMDB0033812	Sesamol	HMDB0033812
79	HMDB0059965	NA	NA
80	HMDB0032920	alpha-Furyl methyl diketone	HMDB0032920
81	HMDB0171080	NA	NA
82	HMDB0062484	NA	NA
83	HMDB0004062	Gentisate aldehyde	HMDB0004062
84	HMDB0002466	3-Hydroxybenzoic acid	HMDB0002466
85	HMDB0000500	4-Hydroxybenzoic acid	HMDB0000500
86	HMDB0001895	Salicylic acid	HMDB0001895
87	HMDB0035646	Methyl 2-(methylthio)acetate	HMDB0035646
88	HMDB0001527	3-Methylthiopropionic acid	HMDB0001527
89	HMDB0112255	NA	NA
90	HMDB0041801	NA	NA
91	HMDB0041799	NA	NA
92	HMDB0041571	NA	NA
93	HMDB0041568	NA	NA
94	HMDB0041569	NA	NA
95	HMDB0041570	NA	NA
96	HMDB0041254	NA	NA

97	HMDB0031844	Trimethylpyrazine	HMDB0031844
98	HMDB0000251	Taurine	HMDB0000251
99	HMDB0041922	NA	NA
100	HMDB0171225	NA	NA
101	HMDB0164607	NA	NA
102	HMDB0166218	NA	NA
103	HMDB0164608	NA	NA
104	HMDB0171213	NA	NA
105	HMDB0166253	NA	NA
106	HMDB0171212	NA	NA
107	HMDB0166254	NA	NA
108	HMDB0166217	NA	NA
109	HMDB0062781	NA	NA
110	HMDB0059784	NA	NA
111	HMDB0161317	NA	NA
112	HMDB0160653	NA	NA
113	HMDB0160654	NA	NA
114	HMDB0000208	Oxoglutaric acid	HMDB0000208
115	HMDB0013701	3-Oxoglutaric acid	HMDB0013701
116	HMDB0164700	NA	NA
117	HMDB0161318	NA	NA
118	HMDB0041390	NA	NA
119	HMDB0041393	NA	NA
120	HMDB0033966	Di-2-propenyl disulfide, 9CI	HMDB0033966
121	HMDB0000139	Glyceric acid	HMDB0000139
122	HMDB0031818	D-2,3-Dihydroxypropanoic acid	HMDB0031818
123	HMDB0006372	L-Glyceric acid	HMDB0006372
124	HMDB0172056	NA	NA
125	HMDB0172059	NA	NA
126	HMDB0172058	NA	NA
127	HMDB0172057	NA	NA
128	HMDB0159225	NA	NA
129	HMDB0159223	NA	NA
130	HMDB0159222	NA	NA
131	HMDB0005785	Indole-3-carbinol	HMDB0005785
132	HMDB0030204	1-(2-Furanylmethyl)-1H-pyrrole	HMDB0030204
133	HMDB0040009	NA	NA
134	HMDB0040011	NA	NA
135	HMDB0159224	NA	NA
136	HMDB0011664	3-Methylene-indolenine	HMDB0011664
137	HMDB0033731	Quinoline	HMDB0033731
138	HMDB0034244	Isoquinoline	HMDB0034244
139	HMDB0032980	3,4-Dimethylthiophene	HMDB0032980
140	HMDB0032979	2,5-Dimethylthiophene	HMDB0032979
141	HMDB0032977	2,3-Dimethylthiophene	HMDB0032977
142	HMDB0032978	2,4-Dimethylthiophene	HMDB0032978
143	HMDB0035385	3-Ethylthiophene	HMDB0035385
144	HMDB0035384	2-Ethylthiophene	HMDB0035384
145	HMDB0038973	NA	NA
146	HMDB0038433	NA	NA
147	HMDB0032341	Isoamyl isothiocyanate	HMDB0032341
148	HMDB0179339	NA	NA
149	HMDB0187593	NA	NA
150	HMDB0179338	NA	NA
151	HMDB0179340	NA	NA
152	HMDB0179337	NA	NA
153	HMDB0031543	3-Methyl-1,2-cyclopentanedione	HMDB0031543
154	HMDB0032233	2,5-Dimethyl-3(2H)-furanone	HMDB0032233
155	HMDB0034247	2-(Methoxymethyl)furan	HMDB0034247
156	HMDB0039778	NA	NA
157	HMDB0029581	(2E,4E)-2,4-Hexadienoic acid	HMDB0029581
158	HMDB0031344	1,2-Cyclohexanedione	HMDB0031344
159	HMDB0031759	(E)-4-Oxo-2-hexen-1-al	HMDB0031759
160	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-diol	HMDB0001164
161	HMDB0040260	NA	NA
162	HMDB0033569	Syoyualdehyde	HMDB0033569
163	HMDB0029444	2-Pyrrolidineacetic acid	HMDB0029444
164	HMDB0094697	NA	NA
165	HMDB0059649	NA	NA
166	HMDB0015212	Vigabatrin	HMDB0015212
167	HMDB0062225	NA	NA
168	HMDB0000070	Pipecolic acid	HMDB0000070
169	HMDB0062767	NA	NA
170	HMDB0004226	N4-Acetylaminobutanal	HMDB0004226
171	HMDB0005960	D-Pipecolic acid	HMDB0005960
172	HMDB0000716	L-Pipecolic acid	HMDB0000716
173	HMDB0029435	L-trans-4-Methyl-2-pyrrolidinecarboxylic acid	HMDB0029435
174	HMDB0094696	N-Methyl-proline	HMDB0094696
175	HMDB0033453	Fagomine	HMDB0033453
176	HMDB0142963	NA	NA
177	HMDB0168724	NA	NA
178	HMDB0168723	NA	NA
179	HMDB0061157	NA	NA
180	HMDB0029449	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	HMDB0029449
181	HMDB0031537	3-Methylcyclohexanethiol	HMDB0031537
182	HMDB0040153	NA	NA
183	HMDB0002108	Methylcysteine	HMDB0002108

184	HMDB0000742	Homocysteine	HMDB0000742
185	HMDB0004812	2,5-Furandicarboxylic acid	HMDB0004812
186	HMDB0040939	NA	NA
187	HMDB0187641	NA	NA
188	HMDB0000134	Fumaric acid	HMDB0000134
189	HMDB0000176	Maleic acid	HMDB0000176
190	HMDB0172136	NA	NA
191	HMDB0165770	NA	NA
192	HMDB0165771	NA	NA
193	HMDB0165773	NA	NA
194	HMDB0172134	NA	NA
195	HMDB0172135	NA	NA
196	HMDB0240308	NA	NA
197	HMDB0165772	NA	NA
198	HMDB0029737	1H-Indole-3-carboxaldehyde	HMDB0029737
199	HMDB0004186	3-Methyldioxyindole	HMDB0004186
200	HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	HMDB0001424
201	HMDB0062406	NA	NA
202	HMDB0029300	p-Anisidine	HMDB0029300
203	HMDB0167379	NA	NA
204	HMDB0032578	4-Hydroxybenzylamine	HMDB0032578
205	HMDB0040360	NA	NA
206	HMDB0036058	NA	NA
207	HMDB0167378	NA	NA
208	HMDB0032492	2-Propionylpyrrole	HMDB0032492
209	HMDB0167848	NA	NA
210	HMDB0167849	NA	NA
211	HMDB0167850	NA	NA
212	HMDB0032748	R-1-Propenyl 1-propanesulfinothioate	HMDB0032748
213	HMDB0032741	S-2-Propenyl 1-propanesulfinothioate	HMDB0032741
214	HMDB0032749	R-Propyl 1-propenesulfinothioate	HMDB0032749
215	HMDB0039965	NA	NA
216	HMDB0240327	NA	NA
217	HMDB0159478	NA	NA
218	HMDB0159477	NA	NA
219	HMDB0158747	NA	NA
220	HMDB0158748	NA	NA
221	HMDB0158745	NA	NA
222	HMDB0158746	NA	NA
223	HMDB0159480	NA	NA
224	HMDB0159479	NA	NA
225	HMDB0161124	NA	NA
226	HMDB0161123	NA	NA
227	HMDB0161125	NA	NA
228	HMDB0155922	NA	NA
229	HMDB0061930	NA	NA
230	HMDB0033837	Dimethyl succinate	HMDB0033837
231	HMDB0006900	(S)-2-Aceto-2-hydroxybutanoic acid	HMDB0006900
232	HMDB0002173	Solerol	HMDB0002173
233	HMDB0002074	2,2-Dimethylsuccinic acid	HMDB0002074
234	HMDB0000858	Monomethyl glutaric acid	HMDB0000858
235	HMDB0000752	Methylglutaric acid	HMDB0000752
236	HMDB0000422	2-Methylglutaric acid	HMDB0000422
237	HMDB0000448	Adipic acid	HMDB0000448
238	HMDB0062489	NA	NA
239	HMDB0010207	L-Rhamnulose	HMDB0010207
240	HMDB0033821	2-O-Methyl-D-xylose	HMDB0033821
241	HMDB0062477	NA	NA
242	HMDB0062498	NA	NA
243	HMDB0062499	NA	NA
244	HMDB0060267	L-Fuculose	HMDB0060267
245	HMDB0005876	3-Deoxyfructose	HMDB0005876
246	HMDB0012327	2-Deoxygalactopyranose	HMDB0012327
247	HMDB0002712	1,5-Anhydrosorbitol	HMDB0002712
248	HMDB0059625	NA	NA
249	HMDB0029196	D-Fucose	HMDB0029196
250	HMDB0003081	Beta-D-Fucose	HMDB0003081
251	HMDB0000174	L-Fucose	HMDB0000174
252	HMDB0059624	NA	NA
253	HMDB0000849	Rhamnose	HMDB0000849
254	HMDB0124735	NA	NA
255	HMDB0240304	NA	NA
256	HMDB0041477	NA	NA
257	HMDB0031660	Dibutyl sulfide	HMDB0031660
258	HMDB0168717	NA	NA
259	HMDB0168715	NA	NA
260	HMDB0168716	NA	NA
261	HMDB0168718	NA	NA
262	HMDB0062061	NA	NA
263	HMDB0030302	2,3,4-Trimethylhexane	HMDB0030302
264	HMDB0029595	Nonane	HMDB0029595
265	HMDB0030301	2,2,3,4-Tetramethylpentane	HMDB0030301
266	HMDB0031556	Isononane	HMDB0031556
267	HMDB0031416	3,4-Dimethylheptane	HMDB0031416
268	HMDB0062017	NA	NA
269	HMDB0062013	NA	NA
270	HMDB0000072	cis-Aconitic acid	HMDB0000072

271	HMDB0001264	Dehydroascorbic acid	HMDB0001264
272	HMDB0000958	trans-Aconitic acid	HMDB0000958
273	HMDB0062706	NA	NA
274	HMDB0040200	NA	NA
275	HMDB0039789	NA	NA
276	HMDB0038974	NA	NA
277	HMDB0039790	NA	NA
278	HMDB0031518	D-Malic acid	HMDB0031518
279	HMDB0000744	Malic acid	HMDB0000744
280	HMDB0032872	Velcorin	HMDB0032872
281	HMDB0000156	L-Malic acid	HMDB0000156
282	HMDB0166840	NA	NA
283	HMDB0166841	NA	NA
284	HMDB0166843	NA	NA
285	HMDB0013004	NA	NA
286	HMDB0004110	Phosphonoacetate	HMDB0004110
287	HMDB0001494	Acetylphosphate	HMDB0001494
288	HMDB0002285	2-Indolecarboxylic acid	HMDB0002285
289	HMDB0240311	NA	NA
290	HMDB0060289	Quinoline-4,8-diol	HMDB0060289
291	HMDB0003320	Indole-3-carboxylic acid	HMDB0003320
292	HMDB0031172	3-Formyl-6-hydroxyindole	HMDB0031172
293	HMDB0004077	4,6-Dihydroxyquinoline	HMDB0004077
294	HMDB0032398	Methyl n-formylanthranilate	HMDB0032398
295	HMDB0000992	3-Succinoylpyridine	HMDB0000992
296	HMDB0000714	Hippuric acid	HMDB0000714
297	HMDB0062583	NA	NA
298	HMDB0032595	1-(4-Methoxyphenyl)-2-nitroethylene	HMDB0032595
299	HMDB0184242	NA	NA
300	HMDB0012884	Adrenochrome	HMDB0012884
301	HMDB0038174	NA	NA
302	HMDB0033388	NA	NA
303	HMDB0185632	NA	NA
304	HMDB0059856	NA	NA
305	HMDB0012153	3,4-Dihydroxybenzylamine	HMDB0012153
306	HMDB0030410	L-2-Amino-3-methylenehexanoic acid	HMDB0030410
307	HMDB0004827	Proline betaine	HMDB0004827
308	HMDB0038949	NA	NA
309	HMDB0032332	Hydroxylated lecithin	HMDB0032332
310	HMDB0145430	NA	NA
311	HMDB0128078	NA	NA
312	HMDB0134039	NA	NA
313	HMDB0135273	NA	NA
314	HMDB0135648	NA	NA
315	HMDB0135274	NA	NA
316	HMDB0135275	NA	NA
317	HMDB0035243	1-Phenyl-1,2-propanedione	HMDB0035243
318	HMDB0000930	trans-Cinnamic acid	HMDB0000930
319	HMDB0000567	Cinnamic acid	HMDB0000567
320	HMDB0036626	NA	NA
321	HMDB0040986	(E)-3-(4-Hydroxyphenyl)-2-propenal	HMDB0040986
322	HMDB0031725	(E)-3-(2-Hydroxyphenyl)-2-propenal	HMDB0031725
323	HMDB0032947	Di-2-furanylmethane	HMDB0032947
324	HMDB0062407	NA	NA
325	HMDB0004992	Benzocaine	HMDB0004992
326	HMDB0001007	3-Pyridinebutanoic acid	HMDB0001007
327	HMDB0059934	NA	NA
328	HMDB0033589	Ethyl 2-aminobenzoate	HMDB0033589
329	HMDB0033485	Gentiatibetine	HMDB0033485
330	HMDB0034169	Methyl N-methylanthranilate	HMDB0034169
331	HMDB0006044	Norsalsolinol	HMDB0006044
332	HMDB0000159	L-Phenylalanine	HMDB0000159
333	HMDB0159744	NA	NA
334	HMDB0062402	NA	NA
335	HMDB0155168	NA	NA
336	HMDB0029455	Ginkgotoxin	HMDB0029455
337	HMDB0000068	Epinephrine	HMDB0000068
338	HMDB0000819	Normetanephrine	HMDB0000819
339	HMDB0002832	Methylnoradrenaline	HMDB0002832
340	HMDB0015652	Levonordefrin	HMDB0015652
341	HMDB0062515	NA	NA
342	HMDB0061679	NA	NA
343	HMDB0154785	NA	NA
344	HMDB0000232	Quinolinic acid	HMDB0000232
345	HMDB0033161	2,6-Pyridinedicarboxylic acid	HMDB0033161
346	HMDB0001330	2-Amino-3-carboxymuconic acid semialdehyde	HMDB0001330
347	HMDB0062578	NA	NA
348	HMDB0185628	NA	NA
349	HMDB0060260	NA	NA
350	HMDB0001552	2-Keto-glutaramic acid	HMDB0001552
351	HMDB0003584	Taurocyamine	HMDB0003584
352	HMDB0015320	Desflurane	HMDB0015320
353	HMDB0060648	NA	NA
354	HMDB0060371	3-Fumarylpyruvate	HMDB0060371
355	HMDB0153544	NA	NA
356	HMDB0130404	NA	NA
357	HMDB0125352	NA	NA

358	HMDB0062183	NA	NA
359	HMDB0006556	L-4-Hydroxyglutamate semialdehyde	HMDB0006556
360	HMDB0002393	N-Methyl-D-aspartic acid	HMDB0002393
361	HMDB0002931	N-Acetylserine	HMDB0002931
362	HMDB0003011	O-Acetylserine	HMDB0003011
363	HMDB0003339	D-Glutamic acid	HMDB0003339
364	HMDB0000148	L-Glutamic acid	HMDB0000148
365	HMDB0060475	DL-Glutamate	HMDB0060475
366	HMDB0033550	3-(Carboxymethylamino)propanoic acid	HMDB0033550
367	HMDB0156263	NA	NA
368	HMDB0185619	NA	NA
369	HMDB0012247	L-2,3-Dihydrodipicolinate	HMDB0012247
370	HMDB0000439	2-Furoylglycine	HMDB0000439
371	HMDB0031700	1-(Malonylamino)cyclopropanecarboxylic acid	HMDB0031700
372	HMDB0166108	NA	NA
373	HMDB0171094	NA	NA
374	HMDB0172092	NA	NA
375	HMDB0062005	NA	NA
376	HMDB0124926	NA	NA
377	HMDB0168664	NA	NA
378	HMDB0150437	NA	NA
379	HMDB0125528	NA	NA
380	HMDB0137457	NA	NA
381	HMDB0146870	NA	NA
382	HMDB0146889	NA	NA
383	HMDB0166106	NA	NA
384	HMDB0166109	NA	NA
385	HMDB0182861	NA	NA
386	HMDB0166107	NA	NA
387	HMDB0183905	NA	NA
388	HMDB0183904	NA	NA
389	HMDB0036907	NA	NA
390	HMDB0029660	2',6'-Dihydroxyacetophenone	HMDB0029660
391	HMDB0029657	2,4'-Dihydroxyacetophenone	HMDB0029657
392	HMDB0029659	2',4'-Dihydroxyacetophenone	HMDB0029659
393	HMDB0029658	2',3'-Dihydroxyacetophenone	HMDB0029658
394	HMDB0032594	2-(Hydroxymethyl)benzoic acid	HMDB0032594
395	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	HMDB0033003
396	HMDB0032629	2',5'-Dihydroxyacetophenone	HMDB0032629
397	HMDB0032572	Methylparaben	HMDB0032572
398	HMDB0029662	3',5'-Dihydroxyacetophenone	HMDB0029662
399	HMDB0029661	3',4'-Dihydroxyacetophenone	HMDB0029661
400	HMDB0032604	2-Methoxybenzoic acid	HMDB0032604
401	HMDB0034172	Methyl 2-hydroxybenzoate	HMDB0034172
402	HMDB0032606	3-Methoxybenzoic acid	HMDB0032606
403	HMDB0041283	NA	NA
404	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	HMDB0004815
405	HMDB0012308	Vanillin	HMDB0012308
406	HMDB0032919	Ethyl 2-furanyl diketone	HMDB0032919
407	HMDB0172091	NA	NA
408	HMDB0032399	Methyl furfuracrylate	HMDB0032399
409	HMDB0000703	Mandelic acid	HMDB0000703
410	HMDB0000669	Ortho-Hydroxyphenylacetic acid	HMDB0000669
411	HMDB0060390	NA	NA
412	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	HMDB0003791
413	HMDB0062635	NA	NA
414	HMDB0031609	Phenoxyacetic acid	HMDB0031609
415	HMDB0000440	3-Hydroxyphenylacetic acid	HMDB0000440
416	HMDB0001101	p-Anisic acid	HMDB0001101
417	HMDB0000020	p-Hydroxyphenylacetic acid	HMDB0000020
418	HMDB0002390	3-Cresotinic acid	HMDB0002390
419	HMDB0000216	Norepinephrine	HMDB0000216
420	HMDB0035178	6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	HMDB0035178
421	HMDB0037685	NA	NA
422	HMDB0155164	NA	NA
423	HMDB0001537	6-Hydroxydopamine	HMDB0001537
424	HMDB0000239	Pyridoxine	HMDB0000239
425	HMDB0004817	5-Hydroxydopamine	HMDB0004817
426	HMDB0012150	2-Keto-6-acetamidocaproate	HMDB0012150
427	HMDB0032945	1-Phenyl-2,4-pentadiyn-1-one	HMDB0032945
428	HMDB0029738	Indole-3-methyl acetate	HMDB0029738
429	HMDB0002302	Indole-3-propionic acid	HMDB0002302
430	HMDB0014970	Phensuximide	HMDB0014970
431	HMDB0163575	NA	NA
432	HMDB0161234	NA	NA
433	HMDB0012209	Diethylphosphate	HMDB0012209
434	HMDB0040050	NA	NA
435	HMDB0040051	NA	NA
436	HMDB0040043	NA	NA
437	HMDB0039662	NA	NA
438	HMDB0040029	NA	NA
439	HMDB0040047	NA	NA
440	HMDB0040016	NA	NA
441	HMDB0030175	Venoterpine	HMDB0030175
442	HMDB0032935	1-(2-Thienyl)-1-butanone	HMDB0032935
443	HMDB0040231	NA	NA
444	HMDB0040589	NA	NA

445	HMDB0175069	NA	NA
446	HMDB0175071	NA	NA
447	HMDB0175067	NA	NA
448	HMDB0000292	Xanthine	HMDB0000292
449	HMDB0000786	Oxypurinol	HMDB0000786
450	HMDB0001182	6,8-Dihydroxypurine	HMDB0001182
451	HMDB0168872	NA	NA
452	HMDB0180803	NA	NA
453	HMDB0033845	(Z)-5-[(5-Methyl-2-thienyl)methylene]-2(5H)-furanone	HMDB0033845
454	HMDB0062803	NA	NA
455	HMDB0149524	NA	NA
456	HMDB0033717	(1R,2R)-Isocitric acid	HMDB0033717
457	HMDB0000094	Citric acid	HMDB0000094
458	HMDB0000193	Isocitric acid	HMDB0000193
459	HMDB0001874	D-threo-Isocitric acid	HMDB0001874
460	HMDB0005971	Diketogulonic acid	HMDB0005971
461	HMDB0006511	2,3-Diketo-L-gulonate	HMDB0006511
462	HMDB0041862	NA	NA
463	HMDB0162021	NA	NA
464	HMDB0038628	NA	NA
465	HMDB0040972	NA	NA
466	HMDB0004073	5-Hydroxyindoleacetaldehyde	HMDB0004073
467	HMDB0000197	Indoleacetic acid	HMDB0000197
468	HMDB0166095	NA	NA
469	HMDB0060758	NA	NA
470	HMDB0240317	NA	NA
471	HMDB0162020	NA	NA
472	HMDB0162023	NA	NA
473	HMDB0162022	NA	NA
474	HMDB0013292	p-Methylhippuric acid	HMDB0013292
475	HMDB0013245	m-Methylhippuric acid	HMDB0013245
476	HMDB0000821	Phenylacetylglycine	HMDB0000821
477	HMDB0000859	Methyl hippurate	HMDB0000859
478	HMDB0011723	2-Methylhippuric acid	HMDB0011723
479	HMDB0060366	3-Carbamoyl-2-phenylpropionaldehyde	HMDB0060366
480	HMDB0060389	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	HMDB0060389
481	HMDB0034250	Betamipron	HMDB0034250
482	HMDB0032388	Methyl n-acetylanthranilate	HMDB0032388
483	HMDB0000073	Dopamine	HMDB0000073
484	HMDB0060277	NA	NA
485	HMDB0012309	Vanillylamine	HMDB0012309
486	HMDB0004825	p-Octopamine	HMDB0004825
487	HMDB0156498	NA	NA
488	HMDB0037786	NA	NA
489	HMDB0172919	NA	NA
490	HMDB0000401	2,8-Dihydroxyadenine	HMDB0000401
491	HMDB0160079	NA	NA
492	HMDB0158555	NA	NA
493	HMDB0002032	8-Hydroxyguanine	HMDB0002032
494	HMDB0059918	NA	NA
495	HMDB0033532	Dimethicone	HMDB0033532
496	HMDB0042002	NA	NA
497	HMDB0131235	NA	NA
498	HMDB0131234	NA	NA
499	HMDB0131233	NA	NA
500	HMDB0151526	NA	NA
501	HMDB0151525	NA	NA
502	HMDB0180894	NA	NA
503	HMDB0126620	NA	NA
504	HMDB0240350	NA	NA
505	HMDB0001490	Vanylglycol	HMDB0001490
506	HMDB0040603	NA	NA
507	HMDB0035056	1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol	HMDB0035056
508	HMDB0036072	NA	NA
509	HMDB0039650	NA	NA
510	HMDB0059730	NA	NA
511	HMDB0180032	NA	NA
512	HMDB0125593	NA	NA
513	HMDB0125597	NA	NA
514	HMDB0126618	NA	NA
515	HMDB0126619	NA	NA
516	HMDB0033092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	HMDB0033092
517	HMDB0032306	4-Heptenal diethyl acetal	HMDB0032306
518	HMDB0038791	NA	NA
519	HMDB0033584	Diethyl tartrate	HMDB0033584
520	HMDB0059767	NA	NA
521	HMDB0157322	NA	NA
522	HMDB0157321	NA	NA
523	HMDB0157320	NA	NA
524	HMDB0157323	NA	NA
525	HMDB0157324	NA	NA
526	HMDB0029416	L-Targinine	HMDB0029416
527	HMDB0000670	Homo-L-arginine	HMDB0000670
528	HMDB0015454	Rasagiline	HMDB0015454
529	HMDB0032926	Polycartine B	HMDB0032926
530	HMDB0005973	Dimethyltryptamine	HMDB0005973
531	HMDB0033961	2-(3-Methylbutyl)-1H-pyrrolo[2,3-b]pyridine	HMDB0033961

532	HMDB0061284	NA	NA
533	HMDB0001892	Menadione	HMDB0001892
534	HMDB0033765	Methyl (Z)-2-decene-4,6,8-triynoate	HMDB0033765
535	HMDB0061682	NA	NA
536	HMDB0060608	NA	NA
537	HMDB0163574	NA	NA
538	HMDB0163573	NA	NA
539	HMDB0162439	NA	NA
540	HMDB0165489	NA	NA
541	HMDB0002042	3-Phenylpropionylglycine	HMDB0002042
542	HMDB0000860	Phenylpropionylglycine	HMDB0000860
543	HMDB0000512	N-Acetyl-L-phenylalanine	HMDB0000512
544	HMDB0165491	NA	NA
545	HMDB0015165	Ethinamate	HMDB0015165
546	HMDB0167325	NA	NA
547	HMDB0002182	Phenylephrine	HMDB0002182
548	HMDB0062266	NA	NA
549	HMDB0014748	Metaraminol	HMDB0014748
550	HMDB0060592	NA	NA
551	HMDB0060807	NA	NA
552	HMDB0032020	4-(beta-Methylaminoethyl)catechol	HMDB0032020
553	HMDB0041888	NA	NA
554	HMDB0062811	NA	NA
555	HMDB0039837	NA	NA
556	HMDB0038869	NA	NA
557	HMDB0000022	3-Methoxytyramine	HMDB0000022
558	HMDB0004826	p-Synephrine	HMDB0004826
559	HMDB0012162	4-Methoxytyramine	HMDB0012162
560	HMDB0094703	Propanoic acid, 2-(methoxyimino)-, trimethylsilyl ester	HMDB0094703
561	HMDB0012286	S-Prenyl-L-cysteine	HMDB0012286
562	HMDB0151316	NA	NA
563	HMDB0151313	NA	NA
564	HMDB0166861	NA	NA
565	HMDB0157325	NA	NA
566	HMDB0157326	NA	NA
567	HMDB0000325	3-Hydroxysuberic acid	HMDB0000325
568	HMDB0040220	NA	NA
569	HMDB0061681	NA	NA
570	HMDB0029968	Ethyl beta-D-glucopyranoside	HMDB0029968
571	HMDB0033942	Dambonitol	HMDB0033942
572	HMDB0032329	2-Hexylthiophene	HMDB0032329
573	HMDB0060323	NA	NA
574	HMDB0003066	Chalcone	HMDB0003066
575	HMDB0135598	NA	NA
576	HMDB0031016	10-Undecen-1-ol	HMDB0031016
577	HMDB0032371	1-Menthyl methyl ether	HMDB0032371
578	HMDB0030943	6-Undecanone	HMDB0030943
579	HMDB0032379	trans- and cis-1-Methoxy-1-decene	HMDB0032379
580	HMDB0163244	NA	NA
581	HMDB0030941	Undecanal	HMDB0030941
582	HMDB0031065	(Âś)-(E)-3-Methyl-4-decen-1-ol	HMDB0031065
583	HMDB0031064	(Z)-3-Methyl-3-decen-1-ol	HMDB0031064
584	HMDB0033713	2-Undecanone	HMDB0033713
585	HMDB0034856	2-Undecen-1-ol	HMDB0034856
586	HMDB0014631	Altretamine	HMDB0014631
587	HMDB0041615	NA	NA
588	HMDB0035753	(R)-(E)-4,7-Megastigmadien-9-one	HMDB0035753
589	HMDB0034959	Edulan I	HMDB0034959
590	HMDB0036818	NA	NA
591	HMDB0036144	NA	NA
592	HMDB0151804	NA	NA
593	HMDB0034979	gamma-Ionone	HMDB0034979
594	HMDB0029822	2,5-Diisopropyl-3-methylphenol	HMDB0029822
595	HMDB0029824	2,4-Diisopropyl-3-methylphenol	HMDB0029824
596	HMDB0032541	4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one	HMDB0032541
597	HMDB0029821	2,5-Diisopropyl-4-methylphenol	HMDB0029821
598	HMDB0036565	NA	NA
599	HMDB0033545	(2E,4Z,7Z)-2,4,7-Tridecatrienal	HMDB0033545
600	HMDB0035682	delta-Damascone	HMDB0035682
601	HMDB0034671	(E)-5,8-Megastigmadien-4-one	HMDB0034671
602	HMDB0036027	alpha-Damascone	HMDB0036027
603	HMDB0037139	NA	NA
604	HMDB0032498	Pseudoionone	HMDB0032498
605	HMDB0036022	Isospirene	HMDB0036022
606	HMDB0031733	4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde	HMDB0031733
607	HMDB0029823	2,4-Diisopropyl-5-methylphenol	HMDB0029823
608	HMDB0036684	NA	NA
609	HMDB0029825	2,3-Diisopropyl-5-methylphenol	HMDB0029825
610	HMDB0059883	NA	NA
611	HMDB0029820	2,6-Diisopropyl-3-methylphenol	HMDB0029820
612	HMDB0014018	4-Hydroxypropofol	HMDB0014018
613	HMDB0037389	NA	NA
614	HMDB0038292	NA	NA
615	HMDB0040439	NA	NA
616	HMDB0039685	NA	NA
617	HMDB0041497	NA	NA
618	HMDB0031840	(S,Z)-Lyratol acetate	HMDB0031840

619	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	HMDB0035801
620	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate	HMDB0035375
621	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate	HMDB0035376
622	HMDB0132986	NA	NA
623	HMDB0034450	Neocnidilide	HMDB0034450
624	HMDB0032567	Hexylresorcinol	HMDB0032567
625	HMDB0035126	(Âś)-Myrtenyl acetate	HMDB0035126
626	HMDB0041610	NA	NA
627	HMDB0038046	NA	NA
628	HMDB0037018	NA	NA
629	HMDB0037231	NA	NA
630	HMDB0035085	Vulgarole	HMDB0035085
631	HMDB0041572	NA	NA
632	HMDB0029388	Cucurbic acid	HMDB0029388
633	HMDB0037326	NA	NA
634	HMDB0033601	Dihydrojasmonic acid	HMDB0033601
635	HMDB0040195	NA	NA
636	HMDB0035723	(1R,2S,3S,4R)-p-Menthane-2,3-diol	HMDB0035723
637	HMDB0034457	Propyl heptanoate	HMDB0034457
638	HMDB0061987	NA	NA
639	HMDB0062146	NA	NA
640	HMDB0038038	NA	NA
641	HMDB0036228	2-Methylpropyl hexanoate	HMDB0036228
642	HMDB0040167	NA	NA
643	HMDB0036136	NA	NA
644	HMDB0187563	NA	NA
645	HMDB0037387	NA	NA
646	HMDB0000511	Capric acid	HMDB0000511
647	HMDB0031264	Methyl nonanoate	HMDB0031264
648	HMDB0094654	1-Methylethyl heptanoic acid	HMDB0094654
649	HMDB0171179	NA	NA
650	HMDB0171178	NA	NA
651	HMDB0171177	NA	NA
652	HMDB0171176	NA	NA
653	HMDB0179213	NA	NA
654	HMDB0179212	NA	NA
655	HMDB0179927	NA	NA
656	HMDB0180500	NA	NA
657	HMDB0180498	NA	NA
658	HMDB0180499	NA	NA
659	HMDB0180497	NA	NA
660	HMDB0180502	NA	NA
661	HMDB0180501	NA	NA
662	HMDB0180503	NA	NA
663	HMDB0180504	NA	NA
664	HMDB0171175	NA	NA
665	HMDB0061805	NA	NA
666	HMDB0180097	NA	NA
667	HMDB0032302	Heptanal propyleneglycol acetal	HMDB0032302
668	HMDB0032155	Acetaldehyde 1,3-octanediol acetal	HMDB0032155
669	HMDB0032264	Ethyl 2-ethylhexanoate	HMDB0032264
670	HMDB0032315	Hexanal butane-2,3-diol acetal	HMDB0032315
671	HMDB0032045	Pentyl 3-methylbutanoate	HMDB0032045
672	HMDB0041216	NA	NA
673	HMDB0034849	4-Methylnonanoic acid	HMDB0034849
674	HMDB0037849	Hexyl 2-methylpropanoate	HMDB0037849
675	HMDB0040157	NA	NA
676	HMDB0033620	Hexyl butyrate	HMDB0033620
677	HMDB0035595	trans-p-Menthane-1,8-diol	HMDB0035595
678	HMDB0029760	1,1-Diethoxy-2-hexene	HMDB0029760
679	HMDB0032070	Isooctyl acetate	HMDB0032070
680	HMDB0040211	NA	NA
681	HMDB0040529	NA	NA
682	HMDB0038783	NA	NA
683	HMDB0036145	NA	NA
684	HMDB0039218	NA	NA
685	HMDB0038602	Octyl acetate	HMDB0038602
686	HMDB0030029	Isopentyl isopentanoate	HMDB0030029
687	HMDB0031739	7-Hydroxy-3,7-dimethyloctanal	HMDB0031739
688	HMDB0035360	N-Methyl-1-deoxynojirimycin	HMDB0035360
689	HMDB0014362	Bethanidine	HMDB0014362
690	HMDB0155301	NA	NA
691	HMDB0060602	N-acetyl-5-aminosalicylic acid	HMDB0060602
692	HMDB0030726	2-Hydroxy-6,7-dimethoxybenzoxazole	HMDB0030726
693	HMDB0004067	Leucodopachrome	HMDB0004067
694	HMDB0002404	Alpha-Hydroxyhippuric acid	HMDB0002404
695	HMDB0002016	4-Carboxyphenylglycine	HMDB0002016
696	HMDB0001229	Dopaquinone	HMDB0001229
697	HMDB0000840	Salicyluric acid	HMDB0000840
698	HMDB0183407	NA	NA
699	HMDB0184100	NA	NA
700	HMDB0006116	3-Hydroxyhippuric acid	HMDB0006116
701	HMDB0166076	NA	NA
702	HMDB0038055	NA	NA
703	HMDB0039119	NA	NA
704	HMDB0013678	4-Hydroxyhippuric acid	HMDB0013678
705	HMDB0166113	NA	NA

706	HMDB0141198	NA	NA
707	HMDB0136739	NA	NA
708	HMDB0030819	Aesculetin	HMDB0030819
709	HMDB0141200	NA	NA
710	HMDB0141199	NA	NA
711	HMDB0032951	4,7-Dihydroxy-2H-1-benzopyran-2-one	HMDB0032951
712	HMDB0032950	5,7-Dihydroxy-4H-1-benzopyran-4-one	HMDB0032950
713	HMDB0130547	NA	NA
714	HMDB0141201	NA	NA
715	HMDB0136740	NA	NA
716	HMDB0015627	Droxidopa	HMDB0015627
717	HMDB0159157	NA	NA
718	HMDB0159158	NA	NA
719	HMDB0159159	NA	NA
720	HMDB0006488	N-Acetyl-L-glutamate 5-semialdehyde	HMDB0006488
721	HMDB0031162	3,3'-Thiobispropanoic acid	HMDB0031162
722	HMDB0179354	NA	NA
723	HMDB0240388	NA	NA
724	HMDB0165618	NA	NA
725	HMDB0030216	Mukonal	HMDB0030216
726	HMDB0161787	NA	NA
727	HMDB0030195	gamma-Fagarine	HMDB0030195
728	HMDB0037614	NA	NA
729	HMDB0029419	Glycylglycylglycine	HMDB0029419
730	HMDB0028836	Glycyl-Asparagine	HMDB0028836
731	HMDB0028731	Asparaginyl-Glycine	HMDB0028731
732	HMDB0035145	Chrycolide	HMDB0035145
733	HMDB0000832	Capryloylglycine	HMDB0000832
734	HMDB0013116	Valproylglycine	HMDB0013116
735	HMDB0041540	NA	NA
736	HMDB0059745	NA	NA
737	HMDB0036172	NA	NA
738	HMDB0032247	(Z)-4-Dodecenal	HMDB0032247
739	HMDB0041404	NA	NA
740	HMDB0037275	NA	NA
741	HMDB0041490	NA	NA
742	HMDB0163217	NA	NA
743	HMDB0134122	NA	NA
744	HMDB0134121	NA	NA
745	HMDB0094674	NA	NA
746	HMDB0035643	beta-Sinensal	HMDB0035643
747	HMDB0038164	NA	NA
748	HMDB0036201	NA	NA
749	HMDB0038187	NA	NA
750	HMDB0036797	NA	NA
751	HMDB0036733	NA	NA
752	HMDB0036667	NA	NA
753	HMDB0036813	NA	NA
754	HMDB0035081	(5alpha,10alpha)-3,7(11)-Eudesmadien-2-one	HMDB0035081
755	HMDB0036718	NA	NA
756	HMDB0036109	NA	NA
757	HMDB0035747	Patchoulenone	HMDB0035747
758	HMDB0040686	NA	NA
759	HMDB0037000	NA	NA
760	HMDB0038195	NA	NA
761	HMDB0038201	NA	NA
762	HMDB0038215	NA	NA
763	HMDB0038200	NA	NA
764	HMDB0038511	NA	NA
765	HMDB0013687	Nookatone	HMDB0013687
766	HMDB0035657	Solavetivone	HMDB0035657
767	HMDB0035786	Valerenal	HMDB0035786
768	HMDB0037061	NA	NA
769	HMDB0035835	Furanoeremophilane	HMDB0035835
770	HMDB0037068	NA	NA
771	HMDB0039637	NA	NA
772	HMDB0036071	NA	NA
773	HMDB0036443	NA	NA
774	HMDB0035082	(5beta,7beta,10beta)-3,11-Eudesmadien-2-one	HMDB0035082
775	HMDB0013693	Sinensal	HMDB0013693
776	HMDB0001539	Asymmetric dimethylarginine	HMDB0001539
777	HMDB0003334	Symmetric dimethylarginine	HMDB0003334
778	HMDB0039274	NA	NA
779	HMDB0030838	Feniculin	HMDB0030838
780	HMDB0030572	(Âś)-Anisoxide	HMDB0030572
781	HMDB0039356	NA	NA
782	HMDB0031313	2-Pentyl-3-phenyl-2-propenal	HMDB0031313
783	HMDB0061830	NA	NA
784	HMDB0035593	Rishitin	HMDB0035593
785	HMDB0037605	NA	NA
786	HMDB0036790	NA	NA
787	HMDB0036791	NA	NA
788	HMDB0037820	NA	NA
789	HMDB0040178	NA	NA
790	HMDB0160293	NA	NA
791	HMDB0160295	NA	NA
792	HMDB0160291	NA	NA

793	HMDB0160290	NA	NA
794	HMDB0160289	NA	NA
795	HMDB0160292	NA	NA
796	HMDB0160296	NA	NA
797	HMDB0160294	NA	NA
798	HMDB0160298	NA	NA
799	HMDB0160297	NA	NA
800	HMDB0032369	L-Menthyl acetoacetate	HMDB0032369
801	HMDB0033619	Hexyl hexanoate	HMDB0033619
802	HMDB0059868	NA	NA
803	HMDB0032440	Nonanal propyleneglycol acetal	HMDB0032440
804	HMDB0061988	NA	NA
805	HMDB0035410	(R)-Dihydrocitronellol acetate	HMDB0035410
806	HMDB0000638	Dodecanoic acid	HMDB0000638
807	HMDB0040166	NA	NA
808	HMDB0030998	Ethyl decanoate	HMDB0030998
809	HMDB0034137	Octyl 2-methylpropanoate	HMDB0034137
810	HMDB0036225	NA	NA
811	HMDB0034136	Octyl butanoate	HMDB0034136
812	HMDB0034128	Isopropyl nonanoate	HMDB0034128
813	HMDB0032310	2-Heptyl butyrate	HMDB0032310
814	HMDB0168119	NA	NA
815	HMDB0168120	NA	NA
816	HMDB0168121	NA	NA
817	HMDB0015050	Phenformin	HMDB0015050
818	HMDB0004231	Pantothenol	HMDB0004231
819	HMDB0014917	Nalidixic Acid	HMDB0014917
820	HMDB0240661	NA	NA
821	HMDB0015305	Phenobarbital	HMDB0015305
822	HMDB0061316	NA	NA
823	HMDB0183400	NA	NA
824	HMDB0240342	NA	NA
825	HMDB0183397	NA	NA
826	HMDB0183398	NA	NA
827	HMDB0032041	1,3-Diphenyl-1-propanone	HMDB0032041
828	HMDB0035896	Lactaroviolin	HMDB0035896
829	HMDB0032561	1,3-Diphenyl-2-propanone	HMDB0032561
830	HMDB0059660	NA	NA
831	HMDB0000114	Glycerylphosphorylethanolamine	HMDB0000114
832	HMDB0015441	Aprobarbital	HMDB0015441
833	HMDB0028983	Methionyl-Threonine	HMDB0028983
834	HMDB0029067	Threoninyl-Methionine	HMDB0029067
835	HMDB0060324	NA	NA
836	HMDB0013279	N-Nonanoylglycine	HMDB0013279
837	HMDB0032526	(Z)-8-Tetradecenal	HMDB0032526
838	HMDB0032525	Tetradec-2-enal	HMDB0032525
839	HMDB0029704	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadien-3-one	HMDB0029704
840	HMDB0159344	NA	NA
841	HMDB0240361	NA	NA
842	HMDB0061952	NA	NA
843	HMDB0035293	Norambreinolide	HMDB0035293
844	HMDB0037631	NA	NA
845	HMDB0037712	NA	NA
846	HMDB0142471	NA	NA
847	HMDB0140099	NA	NA
848	HMDB0003254	Muramic acid	HMDB0003254
849	HMDB0038662	NA	NA
850	HMDB0168958	NA	NA
851	HMDB0035923	Hirsutin	HMDB0035923
852	HMDB0168517	NA	NA
853	HMDB0000101	Deoxyadenosine	HMDB0000101
854	HMDB0001983	5'-Deoxyadenosine	HMDB0001983
855	HMDB0060974	NA	NA
856	HMDB0060618	NA	NA
857	HMDB0004821	Bisnorbiotin	HMDB0004821
858	HMDB0035232	Rotundine B	HMDB0035232
859	HMDB0162810	NA	NA
860	HMDB0036589	NA	NA
861	HMDB0035965	5beta-1,3,7(11)-Eudesmatrien-8-one	HMDB0035965
862	HMDB0038147	NA	NA
863	HMDB0031736	2-Hexyl-3-phenyl-2-propenal	HMDB0031736
864	HMDB0036769	NA	NA
865	HMDB0035612	(R)-ar-Turmerone	HMDB0035612
866	HMDB0036108	NA	NA
867	HMDB0059863	NA	NA
868	HMDB0059946	NA	NA
869	HMDB0041618	NA	NA
870	HMDB0176325	NA	NA
871	HMDB0059947	NA	NA
872	HMDB0176328	NA	NA
873	HMDB0000872	Tetradecanedioic acid	HMDB0000872
874	HMDB0176327	NA	NA
875	HMDB0040429	NA	NA
876	HMDB0176326	NA	NA
877	HMDB0040219	NA	NA
878	HMDB0028744	Asparaginyl-Valine	HMDB0028744
879	HMDB0029122	Valyl-Asparagine	HMDB0029122

880	HMDB0015322	Dexfenfluramine	HMDB0015322
881	HMDB0168125	NA	NA
882	HMDB0178271	NA	NA
883	HMDB0178272	NA	NA
884	HMDB0038839	NA	NA
885	HMDB0015095	Pindolol	HMDB0015095
886	HMDB0170615	NA	NA
887	HMDB0139570	NA	NA
888	HMDB0015411	Practolol	HMDB0015411
889	HMDB0001924	Atenolol	HMDB0001924
890	HMDB0240369	NA	NA
891	HMDB0175189	NA	NA
892	HMDB0175187	NA	NA
893	HMDB0175188	NA	NA
894	HMDB0162484	NA	NA
895	HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	HMDB0033197
896	HMDB0036047	NA	NA
897	HMDB0059661	NA	NA
898	HMDB0015088	Rizatriptan	HMDB0015088
899	HMDB0014873	Naftifine	HMDB0014873
900	HMDB0014578	Cyproheptadine	HMDB0014578
901	HMDB0186509	NA	NA
902	HMDB0184957	NA	NA
903	HMDB0184936	NA	NA
904	HMDB0062677	NA	NA
905	HMDB0004590	19-Nor-5-androstenediol	HMDB0004590
906	HMDB0032464	Phenethyl decanoate	HMDB0032464
907	HMDB0002697	19-Norandrosterone	HMDB0002697
908	HMDB0032672	4,8,12,15-Octadecatetraenoic acid	HMDB0032672
909	HMDB0005886	19-Noretiocholanolone	HMDB0005886
910	HMDB0034382	(E,E)-11,13-Octadecadien-9-ynoic acid	HMDB0034382
911	HMDB0006547	Stearidonic acid	HMDB0006547
912	HMDB0186501	NA	NA
913	HMDB0186507	NA	NA
914	HMDB0186508	NA	NA
915	HMDB0062288	NA	NA
916	HMDB0186510	NA	NA
917	HMDB0186500	NA	NA
918	HMDB0186506	NA	NA
919	HMDB0186505	NA	NA
920	HMDB0186504	NA	NA
921	HMDB0186502	NA	NA
922	HMDB0186497	NA	NA
923	HMDB0186499	NA	NA
924	HMDB0186498	NA	NA
925	HMDB0112093	NA	NA
926	HMDB0112099	NA	NA
927	HMDB0112102	NA	NA
928	HMDB0112103	NA	NA
929	HMDB0186503	NA	NA
930	HMDB0034586	(9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid	HMDB0034586
931	HMDB0031088	12,13-Epoxy-9,15-octadecadienoic acid	HMDB0031088
932	HMDB0029969	Squamostanal A	HMDB0029969
933	HMDB0031103	2-Hydroxylinolenic acid	HMDB0031103
934	HMDB0036832	NA	NA
935	HMDB0030950	15,16-Epoxy-9,12-octadecadienoic acid	HMDB0030950
936	HMDB0029786	10-Oxo-11-octadecen-13-olide	HMDB0029786
937	HMDB0011108	17-Hydroxylinolenic acid	HMDB0011108
938	HMDB0010224	9-HOTE	HMDB0010224
939	HMDB0010220	9(10)-EpODE	HMDB0010220
940	HMDB0010206	15(16)-EpODE	HMDB0010206
941	HMDB0010200	A-12(13)-EpODE	HMDB0010200
942	HMDB0010203	13-HOTE	HMDB0010203
943	HMDB0004669	9-OxoODE	HMDB0004669
944	HMDB0004668	13-OxoODE	HMDB0004668
945	HMDB0031934	(9S,10E,12Z,15Z)-9-Hydroxy-10,12,15-octadecatrienoic acid	HMDB0031934
946	HMDB0030995	(2'E,4'Z,8E)-Colneleic acid	HMDB0030995
947	HMDB0061644	NA	NA
948	HMDB0039603	NA	NA
949	HMDB0061979	NA	NA
950	HMDB0033791	(E)-3-Hexadecenoic acid	HMDB0033791
951	HMDB0038958	NA	NA
952	HMDB0031711	15-Hexadecanolide	HMDB0031711
953	HMDB0003229	Palmitoleic acid	HMDB0003229
954	HMDB0010735	Trans-Hexa-dec-2-enoic acid	HMDB0010735
955	HMDB0037647	NA	NA
956	HMDB0041422	NA	NA
957	HMDB0032638	(Z)-5-Hexadecenoic acid	HMDB0032638
958	HMDB0031053	(E)-6-Hexadecenoic acid	HMDB0031053
959	HMDB0035877	(Z)-13-Hexadecenoic acid	HMDB0035877
960	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	HMDB0031145
961	HMDB0002186	Hypogeic acid	HMDB0002186
962	HMDB0171478	NA	NA
963	HMDB0171479	NA	NA
964	HMDB0171477	NA	NA
965	HMDB0012328	Palmitelaidic acid	HMDB0012328
966	HMDB0171476	NA	NA

967	HMDB0000756	L-Hexanoylcarnitine	HMDB0000756
968	HMDB0000705	Hexanoylcarnitine	HMDB0000705
969	HMDB0014413	Ropinirole	HMDB0014413
970	HMDB0015070	Oxymetazoline	HMDB0015070
971	HMDB0061189	NA	NA
972	HMDB0062555	hydroxyisovaleroyl carnitine	HMDB0062555
973	HMDB0240421	NA	NA
974	HMDB0040904	NA	NA
975	HMDB0168550	NA	NA
976	HMDB0168551	NA	NA
977	HMDB0168552	NA	NA
978	HMDB0168553	NA	NA
979	HMDB0168554	NA	NA
980	HMDB0168549	NA	NA
981	HMDB0137260	NA	NA
982	HMDB0137271	NA	NA
983	HMDB0030974	8-Acetoxy-4-acoren-3-one	HMDB0030974
984	HMDB0031928	Panaxytriol	HMDB0031928
985	HMDB0030801	1-(4-Hydroxy-3-methoxyphenyl)-3-decanone	HMDB0030801
986	HMDB0039251	NA	NA
987	HMDB0134775	NA	NA
988	HMDB0038798	NA	NA
989	HMDB0035075	Tanacetol B	HMDB0035075
990	HMDB0060952	NA	NA
991	HMDB0014521	Palonosetron	HMDB0014521
992	HMDB0030283	Hydrocinchonine	HMDB0030283
993	HMDB0175409	NA	NA
994	HMDB0175412	NA	NA
995	HMDB0175413	NA	NA
996	HMDB0175414	NA	NA
997	HMDB0175415	NA	NA
998	HMDB0175408	NA	NA
999	HMDB0175410	NA	NA
1000	HMDB0175411	NA	NA
1001	HMDB0160594	NA	NA
1002	HMDB0173892	NA	NA
1003	HMDB0175402	NA	NA
1004	HMDB0175403	NA	NA
1005	HMDB0175404	NA	NA
1006	HMDB0175405	NA	NA
1007	HMDB0175406	NA	NA
1008	HMDB0175407	NA	NA
1009	HMDB0030964	Linolenelaidic acid	HMDB0030964
1010	HMDB0001388	Alpha-Linolenic acid	HMDB0001388
1011	HMDB0003073	Gamma-Linolenic acid	HMDB0003073
1012	HMDB0030962	Calendic acid	HMDB0030962
1013	HMDB0030963	Punicic acid	HMDB0030963
1014	HMDB0160589	NA	NA
1015	HMDB0160588	NA	NA
1016	HMDB0112194	NA	NA
1017	HMDB0062652	NA	NA
1018	HMDB0173890	NA	NA
1019	HMDB0160590	NA	NA
1020	HMDB0160592	NA	NA
1021	HMDB0160591	NA	NA
1022	HMDB0160593	NA	NA
1023	HMDB0160595	NA	NA
1024	HMDB0173886	NA	NA
1025	HMDB0173885	NA	NA
1026	HMDB0173887	NA	NA
1027	HMDB0173889	NA	NA
1028	HMDB0173891	NA	NA
1029	HMDB0173888	NA	NA
1030	HMDB0173893	NA	NA
1031	HMDB0004667	13S-hydroxyoctadecadienoic acid	HMDB0004667
1032	HMDB0061708	NA	NA
1033	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	HMDB0029796
1034	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid	HMDB0029998
1035	HMDB0029978	Avenoleic acid	HMDB0029978
1036	HMDB0010223	9-HODE	HMDB0010223
1037	HMDB0004701	9,10-Epoxyoctadecenoic acid	HMDB0004701
1038	HMDB0004702	12,13-EpOME	HMDB0004702
1039	HMDB0004670	Alpha-dimorphecolic acid	HMDB0004670
1040	HMDB0000220	Palmitic acid	HMDB0000220
1041	HMDB0060083	NA	NA
1042	HMDB0061373	NA	NA
1043	HMDB0032324	Hexyl decanoate	HMDB0032324
1044	HMDB0032249	Dodecyl butyrate	HMDB0032249
1045	HMDB0033166	Octyl octanoate	HMDB0033166
1046	HMDB0032065	Butyl dodecanoate	HMDB0032065
1047	HMDB0036210	NA	NA
1048	HMDB0034153	Ethyl tetradecanoate	HMDB0034153
1049	HMDB0031068	Isopalmitic acid	HMDB0031068
1050	HMDB0002396	Trimethyltridecanoic acid	HMDB0002396
1051	HMDB0040367	NA	NA
1052	HMDB0037521	NA	NA
1053	HMDB0014883	Modafinil	HMDB0014883

1054	HMDB0160041	NA	NA
1055	HMDB0163698	NA	NA
1056	HMDB0165052	NA	NA
1057	HMDB0165051	NA	NA
1058	HMDB0165056	NA	NA
1059	HMDB0165053	NA	NA
1060	HMDB0165054	NA	NA
1061	HMDB0165057	NA	NA
1062	HMDB0165060	NA	NA
1063	HMDB0165059	NA	NA
1064	HMDB0171223	NA	NA
1065	HMDB0163699	NA	NA
1066	HMDB0163695	NA	NA
1067	HMDB0160042	NA	NA
1068	HMDB0160039	NA	NA
1069	HMDB0160038	NA	NA
1070	HMDB0158762	NA	NA
1071	HMDB0158761	NA	NA
1072	HMDB0156882	NA	NA
1073	HMDB0156881	NA	NA
1074	HMDB0160699	NA	NA
1075	HMDB0160700	NA	NA
1076	HMDB0163691	NA	NA
1077	HMDB0163694	NA	NA
1078	HMDB0163687	NA	NA
1079	HMDB0163686	NA	NA
1080	HMDB0163690	NA	NA
1081	HMDB0161121	NA	NA
1082	HMDB0161119	NA	NA
1083	HMDB0161120	NA	NA
1084	HMDB0161118	NA	NA
1085	HMDB0167299	NA	NA
1086	HMDB0012267	N-Succinyl-L,L-2,6-diaminopimelate	HMDB0012267
1087	HMDB0032992	Furaneol 4-glucoside	HMDB0032992
1088	HMDB0179393	NA	NA
1089	HMDB0179378	NA	NA
1090	HMDB0179374	NA	NA
1091	HMDB0179371	NA	NA
1092	HMDB0179368	NA	NA
1093	HMDB0179370	NA	NA
1094	HMDB0179366	NA	NA
1095	HMDB0031304	Osmundalin	HMDB0031304
1096	HMDB0179364	NA	NA
1097	HMDB0163718	NA	NA
1098	HMDB0169674	NA	NA
1099	HMDB0169701	NA	NA
1100	HMDB0163365	NA	NA
1101	HMDB0163366	NA	NA
1102	HMDB0163368	NA	NA
1103	HMDB0163372	NA	NA
1104	HMDB0165598	NA	NA
1105	HMDB0165599	NA	NA
1106	HMDB0165602	NA	NA
1107	HMDB0165606	NA	NA
1108	HMDB0039096	NA	NA
1109	HMDB0173636	NA	NA
1110	HMDB0041314	NA	NA
1111	HMDB0130350	NA	NA
1112	HMDB0130347	NA	NA
1113	HMDB0175079	NA	NA
1114	HMDB0178312	NA	NA
1115	HMDB0141160	NA	NA
1116	HMDB0141105	NA	NA
1117	HMDB0141099	NA	NA
1118	HMDB0141080	NA	NA
1119	HMDB0141122	NA	NA
1120	HMDB0141079	NA	NA
1121	HMDB0141126	NA	NA
1122	HMDB0141149	NA	NA
1123	HMDB0141119	NA	NA
1124	HMDB0040889	NA	NA
1125	HMDB0129039	NA	NA
1126	HMDB0138953	NA	NA
1127	HMDB0141045	NA	NA
1128	HMDB0138954	NA	NA
1129	HMDB0138952	NA	NA
1130	HMDB0138951	NA	NA
1131	HMDB0138956	NA	NA
1132	HMDB0140994	NA	NA
1133	HMDB0138959	NA	NA
1134	HMDB0138955	NA	NA
1135	HMDB0138957	NA	NA
1136	HMDB0138958	NA	NA
1137	HMDB0141056	NA	NA
1138	HMDB0141150	NA	NA
1139	HMDB0141152	NA	NA
1140	HMDB0141153	NA	NA

1141	HMDB0141164	NA	NA
1142	HMDB0146848	NA	NA
1143	HMDB0146849	NA	NA
1144	HMDB0141181	NA	NA
1145	HMDB0141151	NA	NA
1146	HMDB0141180	NA	NA
1147	HMDB0141162	NA	NA
1148	HMDB0141161	NA	NA
1149	HMDB0141169	NA	NA
1150	HMDB0141163	NA	NA
1151	HMDB0141145	NA	NA
1152	HMDB0141146	NA	NA
1153	HMDB0141057	NA	NA
1154	HMDB0141101	NA	NA
1155	HMDB0141102	NA	NA
1156	HMDB0141100	NA	NA
1157	HMDB0141103	NA	NA
1158	HMDB0141106	NA	NA
1159	HMDB0141107	NA	NA
1160	HMDB0141120	NA	NA
1161	HMDB0141121	NA	NA
1162	HMDB0141130	NA	NA
1163	HMDB0141129	NA	NA
1164	HMDB0141128	NA	NA
1165	HMDB0141127	NA	NA
1166	HMDB0141139	NA	NA
1167	HMDB0141140	NA	NA
1168	HMDB0141170	NA	NA
1169	HMDB0036635	NA	NA
1170	HMDB0041298	NA	NA
1171	HMDB0033310	Moracin C	HMDB0033310
1172	HMDB0031744	Artocarbene	HMDB0031744
1173	HMDB0141044	NA	NA
1174	HMDB0138682	NA	NA
1175	HMDB0011741	gamma-Glutamyltyrosine	HMDB0011741
1176	HMDB0029161	NA	NA
1177	HMDB0029104	Tyrosyl-Glutamate	HMDB0029104
1178	HMDB0028831	Glutamyltyrosine	HMDB0028831
1179	HMDB0062553	NA	NA
1180	HMDB0041309	NA	NA
1181	HMDB0000839	Pentaporphyrin I	HMDB0000839
1182	HMDB0029428	Hypoglycin B	HMDB0029428
1183	HMDB0061318	NA	NA
1184	HMDB0015102	Desloratadine	HMDB0015102
1185	HMDB0170226	NA	NA
1186	HMDB0170229	NA	NA
1187	HMDB0170227	NA	NA
1188	HMDB0170230	NA	NA
1189	HMDB0170228	NA	NA
1190	HMDB0004704	9,10-DHOME	HMDB0004704
1191	HMDB0061650	9,10-Epoxystearic acid	HMDB0061650
1192	HMDB0004705	12,13-DHOME	HMDB0004705
1193	HMDB0041220	NA	NA
1194	HMDB0031679	(9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid	HMDB0031679
1195	HMDB0000782	Octadecanedioic acid	HMDB0000782
1196	HMDB0183795	NA	NA
1197	HMDB0183794	NA	NA
1198	HMDB0183797	NA	NA
1199	HMDB0183799	NA	NA
1200	HMDB0183798	NA	NA
1201	HMDB0183796	NA	NA
1202	HMDB0183800	NA	NA
1203	HMDB0183802	NA	NA
1204	HMDB0183801	NA	NA
1205	HMDB0186752	NA	NA
1206	HMDB0186756	NA	NA
1207	HMDB0186754	NA	NA
1208	HMDB0183792	NA	NA
1209	HMDB0183793	NA	NA
1210	HMDB0137406	NA	NA
1211	HMDB0157378	NA	NA
1212	HMDB0183791	NA	NA
1213	HMDB0183790	NA	NA
1214	HMDB0186755	NA	NA
1215	HMDB0186753	NA	NA
1216	HMDB0186758	NA	NA
1217	HMDB0186759	NA	NA
1218	HMDB0186757	NA	NA
1219	HMDB0062411	NA	NA
1220	HMDB0062412	NA	NA
1221	HMDB0039484	Gibberellin A12 7-aldehyde	HMDB0039484
1222	HMDB0179080	NA	NA
1223	HMDB0041057	NA	NA
1224	HMDB0034630	(4Z,9a)-9-(3-Methyl-2-butenoyloxy)-4,10(14)-oplopadien-3-one	HMDB0034630
1225	HMDB0036725	NA	NA
1226	HMDB0036747	NA	NA
1227	HMDB0038885	NA	NA

1228	HMDB0036812	NA	NA
1229	HMDB0012452	all-trans-18-Hydroxyretinoic acid	HMDB0012452
1230	HMDB0061095	NA	NA
1231	HMDB0012451	all-trans-5,6-Epoxyretinoic acid	HMDB0012451
1232	HMDB0060093	NA	NA
1233	HMDB0006254	4-Hydroxyretinoic acid	HMDB0006254
1234	HMDB0005832	6b-Hydroxymethandienone	HMDB0005832
1235	HMDB0005079	15-Deoxy-d-12,14-PGJ2	HMDB0005079
1236	HMDB0000344	2-Methoxyestradiol-3-methylether	HMDB0000344
1237	HMDB0156417	NA	NA
1238	HMDB0031773	Phytocassane E	HMDB0031773
1239	HMDB0039442	NA	NA
1240	HMDB0034691	Yucalexin B9	HMDB0034691
1241	HMDB0034631	(4Z,9a)-9-Angeloyloxy-4,10(14)-oplopadien-3-one	HMDB0034631
1242	HMDB0037233	NA	NA
1243	HMDB0036147	NA	NA
1244	HMDB0036750	NA	NA
1245	HMDB0035710	Cafestol	HMDB0035710
1246	HMDB0036762	NA	NA
1247	HMDB0041056	NA	NA
1248	HMDB0014855	Norethindrone	HMDB0014855
1249	HMDB0012794	4-Oxoretinal	HMDB0012794
1250	HMDB0060092	NA	NA
1251	HMDB0138135	NA	NA
1252	HMDB0040644	NA	NA
1253	HMDB0179595	NA	NA
1254	HMDB0062408	NA	NA
1255	HMDB0062296	NA	NA
1256	HMDB0062293	NA	NA
1257	HMDB0062222	NA	NA
1258	HMDB0183807	NA	NA
1259	HMDB0183804	NA	NA
1260	HMDB0183803	NA	NA
1261	HMDB0179598	NA	NA
1262	HMDB0179596	NA	NA
1263	HMDB0179597	NA	NA
1264	HMDB0179593	NA	NA
1265	HMDB0179594	NA	NA
1266	HMDB0137428	NA	NA
1267	HMDB0183806	NA	NA
1268	HMDB0183808	NA	NA
1269	HMDB0183816	NA	NA
1270	HMDB0183815	NA	NA
1271	HMDB0183814	NA	NA
1272	HMDB0183812	NA	NA
1273	HMDB0183813	NA	NA
1274	HMDB0183811	NA	NA
1275	HMDB0183810	NA	NA
1276	HMDB0183809	NA	NA
1277	HMDB0137419	NA	NA
1278	HMDB0012611	18R-HEPE	HMDB0012611
1279	HMDB0012534	11R-HEPE	HMDB0012534
1280	HMDB0013633	12-KETE	HMDB0013633
1281	HMDB0060053	NA	NA
1282	HMDB0061114	NA	NA
1283	HMDB0037523	NA	NA
1284	HMDB0036706	NA	NA
1285	HMDB0038521	NA	NA
1286	HMDB0036712	NA	NA
1287	HMDB0041058	NA	NA
1288	HMDB0010217	5-KETE	HMDB0010217
1289	HMDB0010212	17,18-EpETE	HMDB0010212
1290	HMDB0010209	15-HEPE	HMDB0010209
1291	HMDB0010210	15-KETE	HMDB0010210
1292	HMDB0010205	14,15-EpETE	HMDB0010205
1293	HMDB0010202	12-HEPE	HMDB0010202
1294	HMDB0006027	Oxymesterone	HMDB0006027
1295	HMDB0005081	5-HEPE	HMDB0005081
1296	HMDB0001337	Leukotriene A4	HMDB0001337
1297	HMDB0036752	NA	NA
1298	HMDB0036713	NA	NA
1299	HMDB0036698	NA	NA
1300	HMDB0039012	NA	NA
1301	HMDB0035311	Galanal A	HMDB0035311
1302	HMDB0036724	NA	NA
1303	HMDB0036930	NA	NA
1304	HMDB0030101	Methyl [8]-Shogaol	HMDB0030101
1305	HMDB0036839	NA	NA
1306	HMDB0036776	NA	NA
1307	HMDB0036806	NA	NA
1308	HMDB0035116	(ent-7alpha)-7-Hydroxy-8(14),15-pimaradien-19-oic acid	HMDB0035116
1309	HMDB0039716	NA	NA
1310	HMDB0179600	NA	NA
1311	HMDB0002369	9-cis-Retinoic acid	HMDB0002369
1312	HMDB0036710	NA	NA
1313	HMDB0061925	NA	NA
1314	HMDB0012788	4-OH-Retinal	HMDB0012788

1315	HMDB0036564	NA	NA
1316	HMDB0006219	13-cis-Retinoic acid	HMDB0006219
1317	HMDB0012329	4-Oxoretinol	HMDB0012329
1318	HMDB0038702	NA	NA
1319	HMDB0036711	NA	NA
1320	HMDB0036697	NA	NA
1321	HMDB0012874	9,13-cis-Retinoate	HMDB0012874
1322	HMDB0041925	NA	NA
1323	HMDB0156407	NA	NA
1324	HMDB0156406	NA	NA
1325	HMDB0156405	NA	NA
1326	HMDB0156404	NA	NA
1327	HMDB0156409	NA	NA
1328	HMDB0156408	NA	NA
1329	HMDB0156411	NA	NA
1330	HMDB0156410	NA	NA
1331	HMDB0156413	NA	NA
1332	HMDB0156418	NA	NA
1333	HMDB0156401	NA	NA
1334	HMDB0156403	NA	NA
1335	HMDB0156402	NA	NA
1336	HMDB0001852	All-trans-retinoic acid	HMDB0001852
1337	HMDB0156412	NA	NA
1338	HMDB0183805	NA	NA
1339	HMDB0060994	NA	NA
1340	HMDB0038580	NA	NA
1341	HMDB0033631	Lactapiperanol D	HMDB0033631
1342	HMDB0180021	NA	NA
1343	HMDB0180098	NA	NA
1344	HMDB0180100	NA	NA
1345	HMDB0180099	NA	NA
1346	HMDB0180102	NA	NA
1347	HMDB0034780	Capsiate	HMDB0034780
1348	HMDB0180103	NA	NA
1349	HMDB0184951	NA	NA
1350	HMDB0184949	NA	NA
1351	HMDB0184953	NA	NA
1352	HMDB0012799	5'-Carboxy-gamma-chromanol	HMDB0012799
1353	HMDB0184954	NA	NA
1354	HMDB0184950	NA	NA
1355	HMDB0061677	NA	NA
1356	HMDB0000552	3-Methylglutarylcarnitine	HMDB0000552
1357	HMDB0039044	NA	NA
1358	HMDB0131544	NA	NA
1359	HMDB0153683	NA	NA
1360	HMDB0134716	NA	NA
1361	HMDB0131577	NA	NA
1362	HMDB0140842	NA	NA
1363	HMDB0039858	NA	NA
1364	HMDB0150310	NA	NA
1365	HMDB0150311	NA	NA
1366	HMDB0030019	4'-Methoxymucidin	HMDB0030019
1367	HMDB0125543	NA	NA
1368	HMDB0125544	NA	NA
1369	HMDB0125545	NA	NA
1370	HMDB0125547	NA	NA
1371	HMDB0125546	NA	NA
1372	HMDB0125548	NA	NA
1373	HMDB0129031	NA	NA
1374	HMDB0129032	NA	NA
1375	HMDB0141104	NA	NA
1376	HMDB0141131	NA	NA
1377	HMDB0141141	NA	NA
1378	HMDB0141165	NA	NA
1379	HMDB0141171	NA	NA
1380	HMDB0129034	NA	NA
1381	HMDB0149106	NA	NA
1382	HMDB0140204	NA	NA
1383	HMDB0140116	NA	NA
1384	HMDB0129033	NA	NA
1385	HMDB0129035	NA	NA
1386	HMDB0129037	NA	NA
1387	HMDB0129036	NA	NA
1388	HMDB0129038	NA	NA
1389	HMDB0140114	NA	NA
1390	HMDB0140118	NA	NA
1391	HMDB0140117	NA	NA
1392	HMDB0140115	NA	NA
1393	HMDB0146850	NA	NA
1394	HMDB0040670	NA	NA
1395	HMDB0176556	NA	NA
1396	HMDB0134938	NA	NA
1397	HMDB0013189	3-Indole carboxylic acid glucuronide	HMDB0013189
1398	HMDB0011658	2,8-Dihydroxyquinoline-beta-D-glucuronide	HMDB0011658
1399	HMDB0131931	NA	NA
1400	HMDB0131929	NA	NA
1401	HMDB0137816	NA	NA

1402	HMDB0137819	NA	NA
1403	HMDB0137821	NA	NA
1404	HMDB0140538	NA	NA
1405	HMDB0126563	NA	NA
1406	HMDB0125037	NA	NA
1407	HMDB0126566	NA	NA
1408	HMDB0131932	NA	NA
1409	HMDB0126564	NA	NA
1410	HMDB0126567	NA	NA
1411	HMDB0126570	NA	NA
1412	HMDB0125219	NA	NA
1413	HMDB0125216	NA	NA
1414	HMDB0125207	NA	NA
1415	HMDB0125079	NA	NA
1416	HMDB0125067	NA	NA
1417	HMDB0125052	NA	NA
1418	HMDB0126569	NA	NA
1419	HMDB0128213	NA	NA
1420	HMDB0131759	NA	NA
1421	HMDB0131760	NA	NA
1422	HMDB0131925	NA	NA
1423	HMDB0131928	NA	NA
1424	HMDB0140542	NA	NA
1425	HMDB0140556	NA	NA
1426	HMDB0167579	NA	NA
1427	HMDB0152484	NA	NA
1428	HMDB0167582	NA	NA
1429	HMDB0167580	NA	NA
1430	HMDB0167581	NA	NA
1431	HMDB0030835	trans-3,3',4',5,5',7-Hexahydroxyflavanone	HMDB0030835
1432	HMDB0152029	NA	NA
1433	HMDB0152031	NA	NA
1434	HMDB0152038	NA	NA
1435	HMDB0152035	NA	NA
1436	HMDB0152036	NA	NA
1437	HMDB0152037	NA	NA
1438	HMDB0152402	NA	NA
1439	HMDB0152479	NA	NA
1440	HMDB0039815	NA	NA
1441	HMDB0127839	NA	NA
1442	HMDB0128709	NA	NA
1443	HMDB0125826	NA	NA
1444	HMDB0125820	NA	NA
1445	HMDB0127778	NA	NA
1446	HMDB0127840	NA	NA
1447	HMDB0127779	NA	NA
1448	HMDB0125825	NA	NA
1449	HMDB0172923	NA	NA
1450	HMDB0172926	NA	NA
1451	HMDB0141622	NA	NA
1452	HMDB0034767	(1R*,3R*,3'S*)-1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-beta-carboline-3-carboxylic acid	HMDB0034767
1453	HMDB0142252	NA	NA
1454	HMDB0172514	NA	NA
1455	HMDB0172522	NA	NA
1456	HMDB0158878	NA	NA
1457	HMDB0166871	NA	NA
1458	HMDB0166874	NA	NA
1459	HMDB0166876	NA	NA
1460	HMDB0166877	NA	NA
1461	HMDB0158883	NA	NA
1462	HMDB0158879	NA	NA
1463	HMDB0166873	NA	NA
1464	HMDB0158880	NA	NA
1465	HMDB0158886	NA	NA
1466	HMDB0158885	NA	NA
1467	HMDB0160786	NA	NA
1468	HMDB0160787	NA	NA
1469	HMDB0166859	NA	NA
1470	HMDB0166870	NA	NA
1471	HMDB0158882	NA	NA
1472	HMDB0158881	NA	NA
1473	HMDB0158887	NA	NA
1474	HMDB0157435	NA	NA
1475	HMDB0157434	NA	NA
1476	HMDB0156934	NA	NA
1477	HMDB0156933	NA	NA
1478	HMDB0157433	NA	NA
1479	HMDB0156932	NA	NA
1480	HMDB0152126	NA	NA
1481	HMDB0152125	NA	NA
1482	HMDB0160788	NA	NA
1483	HMDB0039724	NA	NA
1484	HMDB0039726	NA	NA
1485	HMDB0029938	Acaciabiuronic acid	HMDB0029938
1486	HMDB0039722	NA	NA
1487	HMDB0155824	NA	NA
1488	HMDB0156218	NA	NA

1489	HMDB0157438	NA	NA
1490	HMDB0157437	NA	NA
1491	HMDB0157439	NA	NA
1492	HMDB0157441	NA	NA
1493	HMDB0157440	NA	NA
1494	HMDB0166391	NA	NA
1495	HMDB0166390	NA	NA
1496	HMDB0166392	NA	NA
1497	HMDB0156220	NA	NA
1498	HMDB0156219	NA	NA
1499	HMDB0155322	NA	NA
1500	HMDB0125610	NA	NA
1501	HMDB0125611	NA	NA
1502	HMDB0125612	NA	NA
1503	HMDB0125609	NA	NA
1504	HMDB0156221	NA	NA
1505	HMDB0155320	NA	NA
1506	HMDB0155318	NA	NA
1507	HMDB0155319	NA	NA
1508	HMDB0155321	NA	NA
1509	HMDB0166393	NA	NA
1510	HMDB0005011	Clopidogrel	HMDB0005011
1511	HMDB0175192	NA	NA
1512	HMDB0128893	NA	NA
1513	HMDB0062467	NA	NA
1514	HMDB0128890	NA	NA
1515	HMDB0128891	NA	NA
1516	HMDB0149084	NA	NA
1517	HMDB0164007	NA	NA
1518	HMDB0149086	NA	NA
1519	HMDB0033659	Dihydrohydroxy-O-methylsterigmatocystin	HMDB0033659
1520	HMDB0030589	O-Methylsterigmatocystin	HMDB0030589
1521	HMDB0148696	NA	NA
1522	HMDB0148232	NA	NA
1523	HMDB0030619	Ovalitenone	HMDB0030619
1524	HMDB0163589	NA	NA
1525	HMDB0014743	Sulindac	HMDB0014743
1526	HMDB0147815	NA	NA
1527	HMDB0147744	NA	NA
1528	HMDB0147742	NA	NA
1529	HMDB0147651	NA	NA
1530	HMDB0150253	NA	NA
1531	HMDB0147649	NA	NA
1532	HMDB0150255	NA	NA
1533	HMDB0147648	NA	NA
1534	HMDB0033298	3-(3,4-Dihydroxybenzyl)-7-hydroxy-5-methoxy-4-chromanone	HMDB0033298
1535	HMDB0148509	NA	NA
1536	HMDB0148510	NA	NA
1537	HMDB0148508	NA	NA
1538	HMDB0148507	NA	NA
1539	HMDB0148512	NA	NA
1540	HMDB0147889	NA	NA
1541	HMDB0148511	NA	NA
1542	HMDB0147535	NA	NA
1543	HMDB0147529	NA	NA
1544	HMDB0138112	NA	NA
1545	HMDB0137444	NA	NA
1546	HMDB0137443	NA	NA
1547	HMDB0137442	NA	NA
1548	HMDB0135788	NA	NA
1549	HMDB0133961	NA	NA
1550	HMDB0133962	NA	NA
1551	HMDB0133959	NA	NA
1552	HMDB0133957	NA	NA
1553	HMDB0133958	NA	NA
1554	HMDB0133295	NA	NA
1555	HMDB0138110	NA	NA
1556	HMDB0138111	NA	NA
1557	HMDB0146399	NA	NA
1558	HMDB0146753	NA	NA
1559	HMDB0146751	NA	NA
1560	HMDB0146573	NA	NA
1561	HMDB0146572	NA	NA
1562	HMDB0146426	NA	NA
1563	HMDB0146422	NA	NA
1564	HMDB0146412	NA	NA
1565	HMDB0140872	NA	NA
1566	HMDB0138632	NA	NA
1567	HMDB0133294	NA	NA
1568	HMDB0151836	NA	NA
1569	HMDB0037749	NA	NA
1570	HMDB0033797	Olivin	HMDB0033797
1571	HMDB0033924	Cajanol	HMDB0033924
1572	HMDB0030111	Homoferreirin	HMDB0030111
1573	HMDB0041790	NA	NA
1574	HMDB0037481	NA	NA
1575	HMDB0033692	Melilotocarpan D	HMDB0033692

1576	HMDB0037477	NA	NA
1577	HMDB0152003	NA	NA
1578	HMDB0152002	NA	NA
1579	HMDB0033683	Melilotocarpan E	HMDB0033683
1580	HMDB0151832	NA	NA
1581	HMDB0151833	NA	NA
1582	HMDB0151834	NA	NA
1583	HMDB0151632	NA	NA
1584	HMDB0151630	NA	NA
1585	HMDB0151631	NA	NA
1586	HMDB0152601	NA	NA
1587	HMDB0153237	NA	NA
1588	HMDB0037251	NA	NA
1589	HMDB0154307	NA	NA
1590	HMDB0153788	NA	NA
1591	HMDB0041234	NA	NA
1592	HMDB0153512	NA	NA
1593	HMDB0153415	NA	NA
1594	HMDB0151417	NA	NA
1595	HMDB0146221	NA	NA
1596	HMDB0146754	NA	NA
1597	HMDB0147650	NA	NA
1598	HMDB0138109	NA	NA
1599	HMDB0147743	NA	NA
1600	HMDB0132897	NA	NA
1601	HMDB0128591	NA	NA
1602	HMDB0128590	NA	NA
1603	HMDB0128197	NA	NA
1604	HMDB0126060	NA	NA
1605	HMDB0124872	NA	NA
1606	HMDB0130367	NA	NA
1607	HMDB0132894	NA	NA
1608	HMDB0132895	NA	NA
1609	HMDB0132890	NA	NA
1610	HMDB0132891	NA	NA
1611	HMDB0132883	NA	NA
1612	HMDB0132866	NA	NA
1613	HMDB0131742	NA	NA
1614	HMDB0131738	NA	NA
1615	HMDB0130897	NA	NA
1616	HMDB0130669	NA	NA
1617	HMDB0130668	NA	NA
1618	HMDB0130395	NA	NA
1619	HMDB0130391	NA	NA
1620	HMDB0146752	NA	NA
1621	HMDB0154672	NA	NA
1622	HMDB0154674	NA	NA
1623	HMDB0154675	NA	NA
1624	HMDB0154673	NA	NA
1625	HMDB0154671	NA	NA
1626	HMDB0154670	NA	NA
1627	HMDB0029566	Isopulegone caffeate	HMDB0029566
1628	HMDB0154668	NA	NA
1629	HMDB0134704	NA	NA
1630	HMDB0147915	NA	NA
1631	HMDB0154665	NA	NA
1632	HMDB0154669	NA	NA
1633	HMDB0154666	NA	NA
1634	HMDB0154667	NA	NA
1635	HMDB0148183	NA	NA
1636	HMDB0153649	NA	NA
1637	HMDB0125854	NA	NA
1638	HMDB0141256	NA	NA
1639	HMDB0124819	NA	NA
1640	HMDB0125836	NA	NA
1641	HMDB0125842	NA	NA
1642	HMDB0133467	NA	NA
1643	HMDB0041386	NA	NA
1644	HMDB0034412	2'-O-Methylphaseollinisoflavan	HMDB0034412
1645	HMDB0039439	NA	NA
1646	HMDB0033672	4'-O-Methylglabridin	HMDB0033672
1647	HMDB0029514	Licochalcone A	HMDB0029514
1648	HMDB0033782	Bergamottin	HMDB0033782
1649	HMDB0039309	NA	NA
1650	HMDB0030846	Archangelin	HMDB0030846
1651	HMDB0039438	NA	NA
1652	HMDB0033671	2'-O-Methylglabridin	HMDB0033671
1653	HMDB0032665	Licoagrocarpin	HMDB0032665
1654	HMDB0031633	Orientanol B	HMDB0031633
1655	HMDB0001272	Nicotine glucuronide	HMDB0001272
1656	HMDB0032808	Niazirinin	HMDB0032808
1657	HMDB0131864	NA	NA
1658	HMDB0124924	NA	NA
1659	HMDB0131867	NA	NA
1660	HMDB0133539	NA	NA
1661	HMDB0124927	NA	NA
1662	HMDB0125807	NA	NA

1663	HMDB0131075	NA	NA
1664	HMDB0133516	NA	NA
1665	HMDB0133495	NA	NA
1666	HMDB0133485	NA	NA
1667	HMDB0133468	NA	NA
1668	HMDB0131866	NA	NA
1669	HMDB0131865	NA	NA
1670	HMDB0124928	NA	NA
1671	HMDB0124929	NA	NA
1672	HMDB0124838	NA	NA
1673	HMDB0124800	NA	NA
1674	HMDB0124826	NA	NA
1675	HMDB0124829	NA	NA
1676	HMDB0124835	NA	NA
1677	HMDB0124837	NA	NA
1678	HMDB0124922	NA	NA
1679	HMDB0130876	NA	NA
1680	HMDB0138809	NA	NA
1681	HMDB0150217	NA	NA
1682	HMDB0150219	NA	NA
1683	HMDB0124822	NA	NA
1684	HMDB0150216	NA	NA
1685	HMDB0150218	NA	NA
1686	HMDB0150215	NA	NA
1687	HMDB0147761	NA	NA
1688	HMDB0147762	NA	NA
1689	HMDB0147765	NA	NA
1690	HMDB0147767	NA	NA
1691	HMDB0147766	NA	NA
1692	HMDB0147764	NA	NA
1693	HMDB0147768	NA	NA
1694	HMDB0147769	NA	NA
1695	HMDB0149836	NA	NA
1696	HMDB0150181	NA	NA
1697	HMDB0150186	NA	NA
1698	HMDB0150185	NA	NA
1699	HMDB0150182	NA	NA
1700	HMDB0150184	NA	NA
1701	HMDB0150187	NA	NA
1702	HMDB0150214	NA	NA
1703	HMDB0035440	alpha,beta-Dihydroxanthohumol	HMDB0035440
1704	HMDB0030666	Chalepin acetate	HMDB0030666
1705	HMDB0035403	Gingerenone A	HMDB0035403
1706	HMDB0030798	Myricanone	HMDB0030798
1707	HMDB0033880	Mammea B/AC cyclo D	HMDB0033880
1708	HMDB0033879	Mammea B/AD cyclo D	HMDB0033879
1709	HMDB0030333	Fragransol C	HMDB0030333
1710	HMDB0041401	NA	NA
1711	HMDB0138808	NA	NA
1712	HMDB0184970	NA	NA
1713	HMDB0184809	NA	NA
1714	HMDB0162087	NA	NA
1715	HMDB0164047	NA	NA
1716	HMDB0162089	NA	NA
1717	HMDB0185204	NA	NA
1718	HMDB0185205	NA	NA
1719	HMDB0155721	NA	NA
1720	HMDB0240402	NA	NA
1721	HMDB0240215	NA	NA
1722	HMDB0037263	NA	NA
1723	HMDB0029833	Cyclodopa glucoside	HMDB0029833
1724	HMDB0164046	NA	NA
1725	HMDB0010362	6-Hydroxy-5-methoxyindole glucuronide	HMDB0010362
1726	HMDB0010363	5-Hydroxy-6-methoxyindole glucuronide	HMDB0010363
1727	HMDB0183679	NA	NA
1728	HMDB0152039	NA	NA
1729	HMDB0137817	NA	NA
1730	HMDB0137820	NA	NA
1731	HMDB0137822	NA	NA
1732	HMDB0140545	NA	NA
1733	HMDB0150750	NA	NA
1734	HMDB0150752	NA	NA
1735	HMDB0150751	NA	NA
1736	HMDB0136090	NA	NA
1737	HMDB0181157	NA	NA
1738	HMDB0181159	NA	NA
1739	HMDB0040829	NA	NA
1740	HMDB0005034	Topiramate	HMDB0005034
1741	HMDB0038515	NA	NA
1742	HMDB0141625	NA	NA
1743	HMDB0142281	NA	NA
1744	HMDB0128445	NA	NA
1745	HMDB0128454	NA	NA
1746	HMDB0128439	NA	NA
1747	HMDB0128457	NA	NA
1748	HMDB0128441	NA	NA
1749	HMDB0128456	NA	NA

1750	HMDB0128453	NA	NA
1751	HMDB0128449	NA	NA
1752	HMDB0128450	NA	NA
1753	HMDB0128452	NA	NA
1754	HMDB0128448	NA	NA
1755	HMDB0128446	NA	NA
1756	HMDB0128442	NA	NA
1757	HMDB0128444	NA	NA
1758	HMDB0128438	NA	NA
1759	HMDB0128437	NA	NA
1760	HMDB0128458	NA	NA
1761	HMDB0177036	NA	NA
1762	HMDB0059612	NA	NA
1763	HMDB0177043	NA	NA
1764	HMDB0147189	NA	NA
1765	HMDB0147188	NA	NA
1766	HMDB0148992	NA	NA
1767	HMDB0177490	NA	NA
1768	HMDB0147184	NA	NA
1769	HMDB0140356	NA	NA
1770	HMDB0138063	NA	NA
1771	HMDB0128976	NA	NA
1772	HMDB0128981	NA	NA
1773	HMDB0128983	NA	NA
1774	HMDB0131634	NA	NA
1775	HMDB0131637	NA	NA
1776	HMDB0138062	NA	NA
1777	HMDB0147185	NA	NA
1778	HMDB0159333	NA	NA
1779	HMDB0030730	3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin	HMDB0030730
1780	HMDB0144961	NA	NA
1781	HMDB0144931	NA	NA
1782	HMDB0033084	7-Hydroxydehydroglaucine	HMDB0033084
1783	HMDB0061331	NA	NA
1784	HMDB0036765	NA	NA
1785	HMDB0176548	NA	NA
1786	HMDB0035212	Sonchuionoside C	HMDB0035212
1787	HMDB0182762	NA	NA
1788	HMDB0030370	Citroside A	HMDB0030370
1789	HMDB0182758	NA	NA
1790	HMDB0182757	NA	NA
1791	HMDB0182755	NA	NA
1792	HMDB0182753	NA	NA
1793	HMDB0178171	NA	NA
1794	HMDB0178167	NA	NA
1795	HMDB0178165	NA	NA
1796	HMDB0178164	NA	NA
1797	HMDB0178162	NA	NA
1798	HMDB0178160	NA	NA
1799	HMDB0029772	Corchoionol C 9-glucoside	HMDB0029772
1800	HMDB0182760	NA	NA
1801	HMDB0000222	L-Palmitoylcarnitine	HMDB0000222
1802	HMDB0011574	MG(20:2(11Z,14Z)/0:0/0:0)	HMDB0011574
1803	HMDB0011544	MG(0:0/20:2(11Z,14Z)/0:0)	HMDB0011544
1804	HMDB0036865	NA	NA
1805	HMDB0035959	Persenone B	HMDB0035959
1806	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol	HMDB0011644
1807	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al	HMDB0006894
1808	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one	HMDB0006887
1809	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one	HMDB0006886
1810	HMDB0006764	17a,20a-Dihydroxycholesterol	HMDB0006764
1811	HMDB0006763	20a,22b-Dihydroxycholesterol	HMDB0006763
1812	HMDB0006281	7-a,27-Dihydroxycholesterol	HMDB0006281
1813	HMDB0060136	7alpha,24S-Dihydroxycholesterol	HMDB0060136
1814	HMDB0006280	7-a,25-Dihydroxycholesterol	HMDB0006280
1815	HMDB0159657	NA	NA
1816	HMDB0172272	NA	NA
1817	HMDB0172271	NA	NA
1818	HMDB0172269	NA	NA
1819	HMDB0172270	NA	NA
1820	HMDB0172267	NA	NA
1821	HMDB0172265	NA	NA
1822	HMDB0172268	NA	NA
1823	HMDB0172266	NA	NA
1824	HMDB0185566	NA	NA
1825	HMDB0185568	NA	NA
1826	HMDB0185575	NA	NA
1827	HMDB0185573	NA	NA
1828	HMDB0185574	NA	NA
1829	HMDB0185571	NA	NA
1830	HMDB0185572	NA	NA
1831	HMDB0185569	NA	NA
1832	HMDB0185567	NA	NA
1833	HMDB0185570	NA	NA
1834	HMDB0172262	NA	NA
1835	HMDB0172264	NA	NA
1836	HMDB0062675	NA	NA

1837	HMDB0062664	NA	NA
1838	HMDB0062607	NA	NA
1839	HMDB0062420	NA	NA
1840	HMDB0062419	NA	NA
1841	HMDB0159652	NA	NA
1842	HMDB0159656	NA	NA
1843	HMDB0172263	NA	NA
1844	HMDB0159658	NA	NA
1845	HMDB0159655	NA	NA
1846	HMDB0159654	NA	NA
1847	HMDB0159653	NA	NA
1848	HMDB0159651	NA	NA
1849	HMDB0184845	NA	NA
1850	HMDB0184846	NA	NA
1851	HMDB0155084	NA	NA
1852	HMDB0184842	NA	NA
1853	HMDB0184843	NA	NA
1854	HMDB0184841	NA	NA
1855	HMDB0184844	NA	NA
1856	HMDB0184848	NA	NA
1857	HMDB0184847	NA	NA
1858	HMDB0184849	NA	NA
1859	HMDB0184851	NA	NA
1860	HMDB0184850	NA	NA
1861	HMDB0185576	NA	NA
1862	HMDB0185577	NA	NA
1863	HMDB0185578	NA	NA
1864	HMDB0184168	NA	NA
1865	HMDB0003550	Calcidiol	HMDB0003550
1866	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	HMDB0036012
1867	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	HMDB0034328
1868	HMDB0035585	1-Phenyl-1,3-heneicosanedione	HMDB0035585
1869	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	HMDB0006721
1870	HMDB0006722	25-Hydroxytachysterol3	HMDB0006722
1871	HMDB0001993	7a-Hydroxy-cholestene-3-one	HMDB0001993
1872	HMDB0000501	7-Ketocholesterol	HMDB0000501
1873	HMDB0015504	Alfacalcidol	HMDB0015504
1874	HMDB0039871	NA	NA
1875	HMDB0060132	NA	NA
1876	HMDB0060131	NA	NA
1877	HMDB0184149	NA	NA
1878	HMDB0174260	NA	NA
1879	HMDB0174261	NA	NA
1880	HMDB0172274	NA	NA
1881	HMDB0172275	NA	NA
1882	HMDB0172273	NA	NA
1883	HMDB0155085	NA	NA
1884	HMDB0155087	NA	NA
1885	HMDB0155086	NA	NA
1886	HMDB0155081	NA	NA
1887	HMDB0155082	NA	NA
1888	HMDB0174265	NA	NA
1889	HMDB0174262	NA	NA
1890	HMDB0174263	NA	NA
1891	HMDB0184150	NA	NA
1892	HMDB0184148	NA	NA
1893	HMDB0184147	NA	NA
1894	HMDB0184145	NA	NA
1895	HMDB0184146	NA	NA
1896	HMDB0184144	NA	NA
1897	HMDB0174268	NA	NA
1898	HMDB0174267	NA	NA
1899	HMDB0174266	NA	NA
1900	HMDB0174264	NA	NA
1901	HMDB0155083	NA	NA
1902	HMDB0155080	NA	NA
1903	HMDB0184143	NA	NA
1904	HMDB0154867	NA	NA
1905	HMDB0154866	NA	NA
1906	HMDB0035951	Erucoylacetone	HMDB0035951
1907	HMDB0164879	NA	NA
1908	HMDB0038793	NA	NA
1909	HMDB0038787	NA	NA
1910	HMDB0175541	NA	NA
1911	HMDB0175538	NA	NA
1912	HMDB0175530	NA	NA
1913	HMDB0175535	NA	NA
1914	HMDB0147021	NA	NA
1915	HMDB0147024	NA	NA
1916	HMDB0147025	NA	NA
1917	HMDB0147019	NA	NA
1918	HMDB0147020	NA	NA
1919	HMDB0148764	NA	NA
1920	HMDB0147022	NA	NA
1921	HMDB0147023	NA	NA
1922	HMDB0148762	NA	NA
1923	HMDB0168741	NA	NA

1924	HMDB0148763	NA	NA
1925	HMDB0148761	NA	NA
1926	HMDB0148760	NA	NA
1927	HMDB0148765	NA	NA
1928	HMDB0148759	NA	NA
1929	HMDB0147026	NA	NA
1930	HMDB0147018	NA	NA
1931	HMDB0168749	NA	NA
1932	HMDB0168747	NA	NA
1933	HMDB0168748	NA	NA
1934	HMDB0168750	NA	NA
1935	HMDB0168746	NA	NA
1936	HMDB0168744	NA	NA
1937	HMDB0168740	NA	NA
1938	HMDB0168742	NA	NA
1939	HMDB0168743	NA	NA
1940	HMDB0168739	NA	NA
1941	HMDB0168745	NA	NA
1942	HMDB0041407	NA	NA
1943	HMDB0014838	Eplerenone	HMDB0014838
1944	HMDB0037039	NA	NA
1945	HMDB0030404	Armillaripin	HMDB0030404
1946	HMDB0039380	NA	NA
1947	HMDB0173691	NA	NA
1948	HMDB0173689	NA	NA
1949	HMDB0173685	NA	NA
1950	HMDB0173687	NA	NA
1951	HMDB0173683	NA	NA
1952	HMDB0062274	NA	NA
1953	HMDB0062282	NA	NA
1954	HMDB0062292	NA	NA
1955	HMDB0034662	Dihydrofukinolide	HMDB0034662
1956	HMDB0164538	NA	NA
1957	HMDB0164537	NA	NA
1958	HMDB0164536	NA	NA
1959	HMDB0240233	NA	NA
1960	HMDB0139759	NA	NA
1961	HMDB0139773	NA	NA
1962	HMDB0139772	NA	NA
1963	HMDB0139774	NA	NA
1964	HMDB0139775	NA	NA
1965	HMDB0139761	NA	NA
1966	HMDB0139764	NA	NA
1967	HMDB0139762	NA	NA
1968	HMDB0139760	NA	NA
1969	HMDB0139763	NA	NA
1970	HMDB0139766	NA	NA
1971	HMDB0139767	NA	NA
1972	HMDB0139765	NA	NA
1973	HMDB0139768	NA	NA
1974	HMDB0139769	NA	NA
1975	HMDB0139771	NA	NA
1976	HMDB0139770	NA	NA
1977	HMDB0139778	NA	NA
1978	HMDB0139776	NA	NA
1979	HMDB0139777	NA	NA
1980	HMDB0038618	NA	NA
1981	HMDB0183867	NA	NA
1982	HMDB0183864	NA	NA
1983	HMDB0183876	NA	NA
1984	HMDB0183860	NA	NA
1985	HMDB0183873	NA	NA
1986	HMDB0183891	NA	NA
1987	HMDB0183870	NA	NA
1988	HMDB0183894	NA	NA
1989	HMDB0036548	NA	NA
1990	HMDB0006226	24R,25-Dihydroxyvitamin D3	HMDB0006226
1991	HMDB0062401	NA	NA
1992	HMDB0062610	NA	NA
1993	HMDB0062736	NA	NA
1994	HMDB0159642	NA	NA
1995	HMDB0159643	NA	NA
1996	HMDB0159645	NA	NA
1997	HMDB0159644	NA	NA
1998	HMDB0174275	NA	NA
1999	HMDB0174276	NA	NA
2000	HMDB0174277	NA	NA
2001	HMDB0174278	NA	NA
2002	HMDB0174280	NA	NA
2003	HMDB0174279	NA	NA
2004	HMDB0174281	NA	NA
2005	HMDB0174282	NA	NA
2006	HMDB0174283	NA	NA
2007	HMDB0174274	NA	NA
2008	HMDB0174272	NA	NA
2009	HMDB0159649	NA	NA
2010	HMDB0159646	NA	NA

2011	HMDB0159647	NA	NA
2012	HMDB0159648	NA	NA
2013	HMDB0159650	NA	NA
2014	HMDB0172935	NA	NA
2015	HMDB0172936	NA	NA
2016	HMDB0174269	NA	NA
2017	HMDB0174271	NA	NA
2018	HMDB0174270	NA	NA
2019	HMDB0174273	NA	NA
2020	HMDB0012453	3 beta-Hydroxy-5-cholestenoate	HMDB0012453
2021	HMDB0001903	Calcitriol	HMDB0001903
2022	HMDB0030024	Sarsasapogenin	HMDB0030024
2023	HMDB0060133	NA	NA
2024	HMDB0060425	7alpha,25-Dihydroxy-4-cholesten-3-one	HMDB0060425
2025	HMDB0060508	NA	NA
2026	HMDB0030048	Smilagenin	HMDB0030048
2027	HMDB0030047	Neotigogenin	HMDB0030047
2028	HMDB0015046	Paricalcitol	HMDB0015046
2029	HMDB0000430	24,25-Dihydroxyvitamin D	HMDB0000430
2030	HMDB0001420	25,26-dihydroxyvitamin D	HMDB0001420
2031	HMDB0002197	7a,12a-Dihydroxy-cholestene-3-one	HMDB0002197
2032	HMDB0006720	23S,25-dihydroxyvitamin D3	HMDB0006720
2033	HMDB0012459	7 alpha,26-Dihydroxy-4-cholesten-3-one	HMDB0012459
2034	HMDB0012457	7 alpha,24-Dihydroxy-4-cholesten-3-one	HMDB0012457
2035	HMDB0035300	Octadecyl cis-p-coumarate	HMDB0035300
2036	HMDB0162231	NA	NA
2037	HMDB0159898	NA	NA
2038	HMDB0159886	NA	NA
2039	HMDB0159887	NA	NA
2040	HMDB0159775	NA	NA
2041	HMDB0159762	NA	NA
2042	HMDB0159763	NA	NA
2043	HMDB0062208	NA	NA
2044	HMDB0000359	3a,7a-Dihydroxycoprostanic acid	HMDB0000359
2045	HMDB0003533	3a,7a,12a-Trihydroxy-5b-cholestan-26-al	HMDB0003533
2046	HMDB0172392	NA	NA
2047	HMDB0172390	NA	NA
2048	HMDB0167571	NA	NA
2049	HMDB0167569	NA	NA
2050	HMDB0167567	NA	NA
2051	HMDB0167565	NA	NA
2052	HMDB0167563	NA	NA
2053	HMDB0159764	NA	NA
2054	HMDB0159888	NA	NA
2055	HMDB0005814	Testosterone enanthate	HMDB0005814
2056	HMDB0062613	NA	NA
2057	HMDB0012458	7alpha-Hydroxy-3-oxo-4-cholestenoate	HMDB0012458
2058	HMDB0060128	NA	NA
2059	HMDB0060127	NA	NA
2060	HMDB0030066	Australigenin	HMDB0030066
2061	HMDB0036249	NA	NA
2062	HMDB0034403	Barogenin	HMDB0034403
2063	HMDB0011590	MG(24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0/0:0)	HMDB0011590
2064	HMDB0166149	NA	NA
2065	HMDB0174217	NA	NA
2066	HMDB0157634	NA	NA
2067	HMDB0157631	NA	NA
2068	HMDB0157632	NA	NA
2069	HMDB0157633	NA	NA
2070	HMDB0157635	NA	NA
2071	HMDB0157638	NA	NA
2072	HMDB0164013	NA	NA
2073	HMDB0160505	NA	NA
2074	HMDB0160504	NA	NA
2075	HMDB0157644	NA	NA
2076	HMDB0157646	NA	NA
2077	HMDB0157643	NA	NA
2078	HMDB0157645	NA	NA
2079	HMDB0157640	NA	NA
2080	HMDB0157641	NA	NA
2081	HMDB0157639	NA	NA
2082	HMDB0157642	NA	NA
2083	HMDB0157637	NA	NA
2084	HMDB0157636	NA	NA
2085	HMDB0034293	Asperagenin	HMDB0034293
2086	HMDB0032783	Porrigenin A	HMDB0032783
2087	HMDB0157653	NA	NA
2088	HMDB0157650	NA	NA
2089	HMDB0157649	NA	NA
2090	HMDB0157652	NA	NA
2091	HMDB0157654	NA	NA
2092	HMDB0157651	NA	NA
2093	HMDB0157648	NA	NA
2094	HMDB0160506	NA	NA
2095	HMDB0157647	NA	NA
2096	HMDB0161140	NA	NA
2097	HMDB0000708	Glycoursodeoxycholic acid	HMDB0000708

2098	HMDB0161141	NA	NA
2099	HMDB0006898	Chenodeoxyglycocholic acid	HMDB0006898
2100	HMDB0000631	Deoxycholic acid glycine conjugate	HMDB0000631
2101	HMDB0000637	Chenodeoxycholic acid glycine conjugate	HMDB0000637
2102	HMDB0184641	NA	NA
2103	HMDB0161139	NA	NA
2104	HMDB0173226	NA	NA
2105	HMDB0173227	NA	NA
2106	HMDB0173228	NA	NA
2107	HMDB0173225	NA	NA
2108	HMDB0173223	NA	NA
2109	HMDB0173224	NA	NA
2110	HMDB0012516	11'-Carboxy-alpha-tocotrienol	HMDB0012516
2111	HMDB0030140	Adlupulone	HMDB0030140
2112	HMDB0030041	Lupulone	HMDB0030041
2113	HMDB0037823	NA	NA
2114	HMDB0014498	Buclizine	HMDB0014498
2115	HMDB0172607	NA	NA
2116	HMDB0170224	NA	NA
2117	HMDB0041212	NA	NA
2118	HMDB0033806	2'-O-Methylcajanone	HMDB0033806
2119	HMDB0030849	Artocarpin	HMDB0030849
2120	HMDB0140394	NA	NA
2121	HMDB0129645	NA	NA
2122	HMDB0134743	NA	NA
2123	HMDB0162013	NA	NA
2124	HMDB0162016	NA	NA
2125	HMDB0162004	NA	NA
2126	HMDB0142798	NA	NA
2127	HMDB0142979	NA	NA
2128	HMDB0142983	NA	NA
2129	HMDB0142989	NA	NA
2130	HMDB0142992	NA	NA
2131	HMDB0142993	NA	NA
2132	HMDB0143013	NA	NA
2133	HMDB0143016	NA	NA
2134	HMDB0142982	NA	NA
2135	HMDB0142838	NA	NA
2136	HMDB0142799	NA	NA
2137	HMDB0142805	NA	NA
2138	HMDB0142795	NA	NA
2139	HMDB0142808	NA	NA
2140	HMDB0142824	NA	NA
2141	HMDB0142822	NA	NA
2142	HMDB0142828	NA	NA
2143	HMDB0142834	NA	NA
2144	HMDB0142809	NA	NA
2145	HMDB0143017	NA	NA
2146	HMDB0143090	NA	NA
2147	HMDB0143094	NA	NA
2148	HMDB0143096	NA	NA
2149	HMDB0143100	NA	NA
2150	HMDB0143110	NA	NA
2151	HMDB0143964	NA	NA
2152	HMDB0143966	NA	NA
2153	HMDB0143091	NA	NA
2154	HMDB0143087	NA	NA
2155	HMDB0143080	NA	NA
2156	HMDB0143023	NA	NA
2157	HMDB0143026	NA	NA
2158	HMDB0143027	NA	NA
2159	HMDB0143067	NA	NA
2160	HMDB0143070	NA	NA
2161	HMDB0143071	NA	NA
2162	HMDB0143106	NA	NA
2163	HMDB0143081	NA	NA
2164	HMDB0142788	NA	NA
2165	HMDB0142729	NA	NA
2166	HMDB0142725	NA	NA
2167	HMDB0142719	NA	NA
2168	HMDB0142718	NA	NA
2169	HMDB0142715	NA	NA
2170	HMDB0142739	NA	NA
2171	HMDB0143077	NA	NA
2172	HMDB0142728	NA	NA
2173	HMDB0142735	NA	NA
2174	HMDB0142738	NA	NA
2175	HMDB0142789	NA	NA
2176	HMDB0142785	NA	NA
2177	HMDB0142758	NA	NA
2178	HMDB0142759	NA	NA
2179	HMDB0142755	NA	NA
2180	HMDB0142748	NA	NA
2181	HMDB0142749	NA	NA
2182	HMDB0142745	NA	NA
2183	HMDB0035858	Obacunone	HMDB0035858
2184	HMDB0035031	Desoxylimonin	HMDB0035031

2185	HMDB0039920	NA	NA
2186	HMDB0039918	NA	NA
2187	HMDB0039919	NA	NA
2188	HMDB0015013	Flupenthixol	HMDB0015013
2189	HMDB0184201	NA	NA
2190	HMDB0183261	NA	NA
2191	HMDB0183260	NA	NA
2192	HMDB0183262	NA	NA
2193	HMDB0183264	NA	NA
2194	HMDB0183267	NA	NA
2195	HMDB0183269	NA	NA
2196	HMDB0184206	NA	NA
2197	HMDB0184207	NA	NA
2198	HMDB0183254	NA	NA
2199	HMDB0183258	NA	NA
2200	HMDB0183250	NA	NA
2201	HMDB0183251	NA	NA
2202	HMDB0039214	NA	NA
2203	HMDB0036631	NA	NA
2204	HMDB0030688	Cyclomulberrin	HMDB0030688
2205	HMDB0040480	NA	NA
2206	HMDB0029506	Kuwanon B	HMDB0029506
2207	HMDB0029505	Kuwanon A	HMDB0029505
2208	HMDB0131612	NA	NA
2209	HMDB0131610	NA	NA
2210	HMDB0131607	NA	NA
2211	HMDB0131606	NA	NA
2212	HMDB0131608	NA	NA
2213	HMDB0131609	NA	NA
2214	HMDB0131611	NA	NA
2215	HMDB0166772	NA	NA
2216	HMDB0166773	NA	NA
2217	HMDB0185408	NA	NA
2218	HMDB0185426	NA	NA
2219	HMDB0155347	NA	NA
2220	HMDB0155348	NA	NA
2221	HMDB0034064	2-Angeloyl-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one	HMDB0034064
2222	HMDB0012936	Dynorphin B (10-13)	HMDB0012936
2223	HMDB0035068	Melleolide M	HMDB0035068
2224	HMDB0179387	NA	NA
2225	HMDB0179386	NA	NA
2226	HMDB0179390	NA	NA
2227	HMDB0179389	NA	NA
2228	HMDB0061104	NA	NA
2229	HMDB0139815	NA	NA
2230	HMDB0144973	NA	NA
2231	HMDB0144948	NA	NA
2232	HMDB0144943	NA	NA
2233	HMDB0144938	NA	NA
2234	HMDB0139798	NA	NA
2235	HMDB0139801	NA	NA
2236	HMDB0139799	NA	NA
2237	HMDB0139800	NA	NA
2238	HMDB0139797	NA	NA
2239	HMDB0144978	NA	NA
2240	HMDB0139796	NA	NA
2241	HMDB0139795	NA	NA
2242	HMDB0144983	NA	NA
2243	HMDB0144998	NA	NA
2244	HMDB0144988	NA	NA
2245	HMDB0144933	NA	NA
2246	HMDB0144918	NA	NA
2247	HMDB0139811	NA	NA
2248	HMDB0139813	NA	NA
2249	HMDB0139809	NA	NA
2250	HMDB0139806	NA	NA
2251	HMDB0139807	NA	NA
2252	HMDB0139808	NA	NA
2253	HMDB0139814	NA	NA
2254	HMDB0139816	NA	NA
2255	HMDB0139805	NA	NA
2256	HMDB0139817	NA	NA
2257	HMDB0139812	NA	NA
2258	HMDB0139818	NA	NA
2259	HMDB0139804	NA	NA
2260	HMDB0139820	NA	NA
2261	HMDB0139819	NA	NA
2262	HMDB0139803	NA	NA
2263	HMDB0144913	NA	NA
2264	HMDB0139802	NA	NA
2265	HMDB0145003	NA	NA
2266	HMDB0144993	NA	NA
2267	HMDB0145038	NA	NA
2268	HMDB0145034	NA	NA
2269	HMDB0145032	NA	NA
2270	HMDB0139810	NA	NA
2271	HMDB0145018	NA	NA

2272	HMDB0145013	NA	NA
2273	HMDB0145008	NA	NA
2274	HMDB0032622	Phenethyl rutinoside	HMDB0032622
2275	HMDB0094682	5alpha-Androstan-3alpha,17beta-diol disulfate	HMDB0094682
2276	HMDB0240625	NA	NA
2277	HMDB0172330	NA	NA
2278	HMDB0138981	NA	NA
2279	HMDB0138985	NA	NA
2280	HMDB0138983	NA	NA
2281	HMDB0138982	NA	NA
2282	HMDB0138963	NA	NA
2283	HMDB0138657	NA	NA
2284	HMDB0138986	NA	NA
2285	HMDB0138990	NA	NA
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2289	HMDB0138976	NA	NA
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2291	HMDB0138977	NA	NA
2292	HMDB0138656	NA	NA
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2310	HMDB0138697	NA	NA
2311	HMDB0138984	NA	NA
2312	HMDB0138989	NA	NA
2313	HMDB0138973	NA	NA
2314	HMDB0129052	NA	NA
2315	HMDB0125560	NA	NA
2316	HMDB0125552	NA	NA
2317	HMDB0125562	NA	NA
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2319	HMDB0125558	NA	NA
2320	HMDB0125554	NA	NA
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2322	HMDB0125553	NA	NA
2323	HMDB0125556	NA	NA
2324	HMDB0125555	NA	NA
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2327	HMDB0125563	NA	NA
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2329	HMDB0129073	NA	NA
2330	HMDB0129066	NA	NA
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2332	HMDB0129067	NA	NA
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2334	HMDB0129064	NA	NA
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2336	HMDB0129061	NA	NA
2337	HMDB0129074	NA	NA
2338	HMDB0129081	NA	NA
2339	HMDB0140238	NA	NA
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2341	HMDB0140130	NA	NA
2342	HMDB0140124	NA	NA
2343	HMDB0140122	NA	NA
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2345	HMDB0129082	NA	NA
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2347	HMDB0129059	NA	NA
2348	HMDB0129058	NA	NA
2349	HMDB0129054	NA	NA
2350	HMDB0125577	NA	NA
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2353	HMDB0125566	NA	NA
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2356	HMDB0125571	NA	NA
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2364	HMDB0129048	NA	NA
2365	HMDB0129049	NA	NA
2366	HMDB0129046	NA	NA
2367	HMDB0129047	NA	NA
2368	HMDB0129045	NA	NA
2369	HMDB0129042	NA	NA
2370	HMDB0125567	NA	NA
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2372	HMDB0150323	NA	NA
2373	HMDB0131587	NA	NA
2374	HMDB0131586	NA	NA
2375	HMDB0131555	NA	NA
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2377	HMDB0034608	PSF-A	HMDB0034608
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2379	HMDB0187161	NA	NA
2380	HMDB0187164	NA	NA
2381	HMDB0187169	NA	NA
2382	HMDB0187172	NA	NA
2383	HMDB0187181	NA	NA
2384	HMDB0176585	NA	NA
2385	HMDB0176586	NA	NA
2386	HMDB0176925	NA	NA
2387	HMDB0176921	NA	NA
2388	HMDB0039706	NA	NA
2389	HMDB0034072	Gentianose	HMDB0034072
2390	HMDB0006599	3-Galactosyllactose	HMDB0006599
2391	HMDB0001262	Maltotriose	HMDB0001262
2392	HMDB0033748	Umbelliferose	HMDB0033748
2393	HMDB0040984	NA	NA
2394	HMDB0029930	beta-D-Fructofuranosyl alpha-D-glucopyranosyl-(1->4)-D-glucopyranoside	HMDB0029930
2395	HMDB0040181	NA	NA
2396	HMDB0039708	NA	NA
2397	HMDB0029929	6-O-Glucosylmaltose	HMDB0029929
2398	HMDB0033673	6-Kestose	HMDB0033673
2399	HMDB0038853	NA	NA
2400	HMDB0003213	Raffinose	HMDB0003213
2401	HMDB0039704	NA	NA
2402	HMDB0039707	NA	NA
2403	HMDB0029921	Neokestose	HMDB0029921
2404	HMDB0060468	D-Gal alpha 1->6D-Gal alpha 1->6D-Glucose	HMDB0060468
2405	HMDB0041948	NA	NA
2406	HMDB0003539	Levan	HMDB0003539
2407	HMDB0038852	NA	NA
2408	HMDB0029910	Gentiotriose	HMDB0029910
2409	HMDB0006857	Dextrin	HMDB0006857
2410	HMDB0011729	1-Kestose	HMDB0011729
2411	HMDB0011730	Melezitose	HMDB0011730
2412	HMDB0038851	NA	NA
2413	HMDB0035322	Fagopyritol B2	HMDB0035322
2414	HMDB0029922	Galactotriose	HMDB0029922
2415	HMDB0029937	Panose	HMDB0029937
2416	HMDB0039703	NA	NA
2417	HMDB0142726	NA	NA
2418	HMDB0142746	NA	NA
2419	HMDB0144455	NA	NA
2420	HMDB0142823	NA	NA
2421	HMDB0144467	NA	NA
2422	HMDB0143965	NA	NA
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2424	HMDB0144463	NA	NA
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2431	HMDB0142796	NA	NA
2432	HMDB0144443	NA	NA
2433	HMDB0142736	NA	NA
2434	HMDB0142716	NA	NA
2435	HMDB0142756	NA	NA
2436	HMDB0142786	NA	NA
2437	HMDB0031674	Armillarinin	HMDB0031674
2438	HMDB0015129	Neomycin	HMDB0015129
2439	HMDB0002160	Harderoporphyrinogen	HMDB0002160
2440	HMDB0039454	NA	NA
2441	HMDB0173693	NA	NA
2442	HMDB0173692	NA	NA
2443	HMDB0173699	NA	NA
2444	HMDB0173698	NA	NA
2445	HMDB0142988	NA	NA

2446	HMDB0142998	NA	NA
2447	HMDB0142997	NA	NA
2448	HMDB0143001	NA	NA
2449	HMDB0142987	NA	NA
2450	HMDB0142978	NA	NA
2451	HMDB0142977	NA	NA
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2459	HMDB0142928	NA	NA
2460	HMDB0142927	NA	NA
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2462	HMDB0143007	NA	NA
2463	HMDB0143006	NA	NA
2464	HMDB0143108	NA	NA
2465	HMDB0143104	NA	NA
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2467	HMDB0143093	NA	NA
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2478	HMDB0143011	NA	NA
2479	HMDB0143021	NA	NA
2480	HMDB0142916	NA	NA
2481	HMDB0142915	NA	NA
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2483	HMDB0142899	NA	NA
2484	HMDB0142902	NA	NA
2485	HMDB0142900	NA	NA
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2494	HMDB0142930	NA	NA
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2497	HMDB0173230	NA	NA
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2507	HMDB0157955	NA	NA
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2528	HMDB0158948	NA	NA
2529	HMDB0158944	NA	NA
2530	HMDB0158943	NA	NA
2531	HMDB0158937	NA	NA
2532	HMDB0158938	NA	NA

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2534	HMDB0158933	NA	NA
2535	HMDB0158969	NA	NA
2536	HMDB0157897	NA	NA
2537	HMDB0157050	NA	NA
2538	HMDB0157221	NA	NA
2539	HMDB0157842	NA	NA
2540	HMDB0157841	NA	NA
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2542	HMDB0157847	NA	NA
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2544	HMDB0157851	NA	NA
2545	HMDB0157848	NA	NA
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2555	HMDB0157063	NA	NA
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2557	HMDB0157205	NA	NA
2558	HMDB0157209	NA	NA
2559	HMDB0157852	NA	NA
2560	HMDB0157856	NA	NA
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2563	HMDB0157881	NA	NA
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2565	HMDB0157883	NA	NA
2566	HMDB0157886	NA	NA
2567	HMDB0157887	NA	NA
2568	HMDB0157888	NA	NA
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2573	HMDB0157877	NA	NA
2574	HMDB0157858	NA	NA
2575	HMDB0157861	NA	NA
2576	HMDB0157862	NA	NA
2577	HMDB0157863	NA	NA
2578	HMDB0157866	NA	NA
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2587	HMDB0166013	NA	NA
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2589	HMDB0166007	NA	NA
2590	HMDB0170721	NA	NA
2591	HMDB0166009	NA	NA
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2599	HMDB0168064	NA	NA
2600	HMDB0170719	NA	NA
2601	HMDB0170718	NA	NA
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2603	HMDB0168080	NA	NA
2604	HMDB0168077	NA	NA
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2606	HMDB0168068	NA	NA
2607	HMDB0168067	NA	NA
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2614	HMDB0165879	NA	NA
2615	HMDB0165880	NA	NA
2616	HMDB0170735	NA	NA
2617	HMDB0170737	NA	NA
2618	HMDB0166008	NA	NA
2619	HMDB0165977	NA	NA

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2621	HMDB0165999	NA	NA
2622	HMDB0165985	NA	NA
2623	HMDB0165984	NA	NA
2624	HMDB0165976	NA	NA
2625	HMDB0165983	NA	NA
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2694	HMDB0165930	NA	NA
2695	HMDB0165929	NA	NA
2696	HMDB0165927	NA	NA
2697	HMDB0165924	NA	NA
2698	HMDB0165926	NA	NA
2699	HMDB0165925	NA	NA
2700	HMDB0165922	NA	NA
2701	HMDB0181031	NA	NA
2702	HMDB0177742	NA	NA
2703	HMDB0177531	NA	NA
2704	HMDB0177529	NA	NA
2705	HMDB0177530	NA	NA
2706	HMDB0164570	NA	NA

2707	HMDB0040745	NA	NA
2708	HMDB0164979	NA	NA
2709	HMDB0164980	NA	NA
2710	HMDB0164978	NA	NA
2711	HMDB0164977	NA	NA
2712	HMDB0061054	NA	NA
2713	HMDB0061057	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.

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

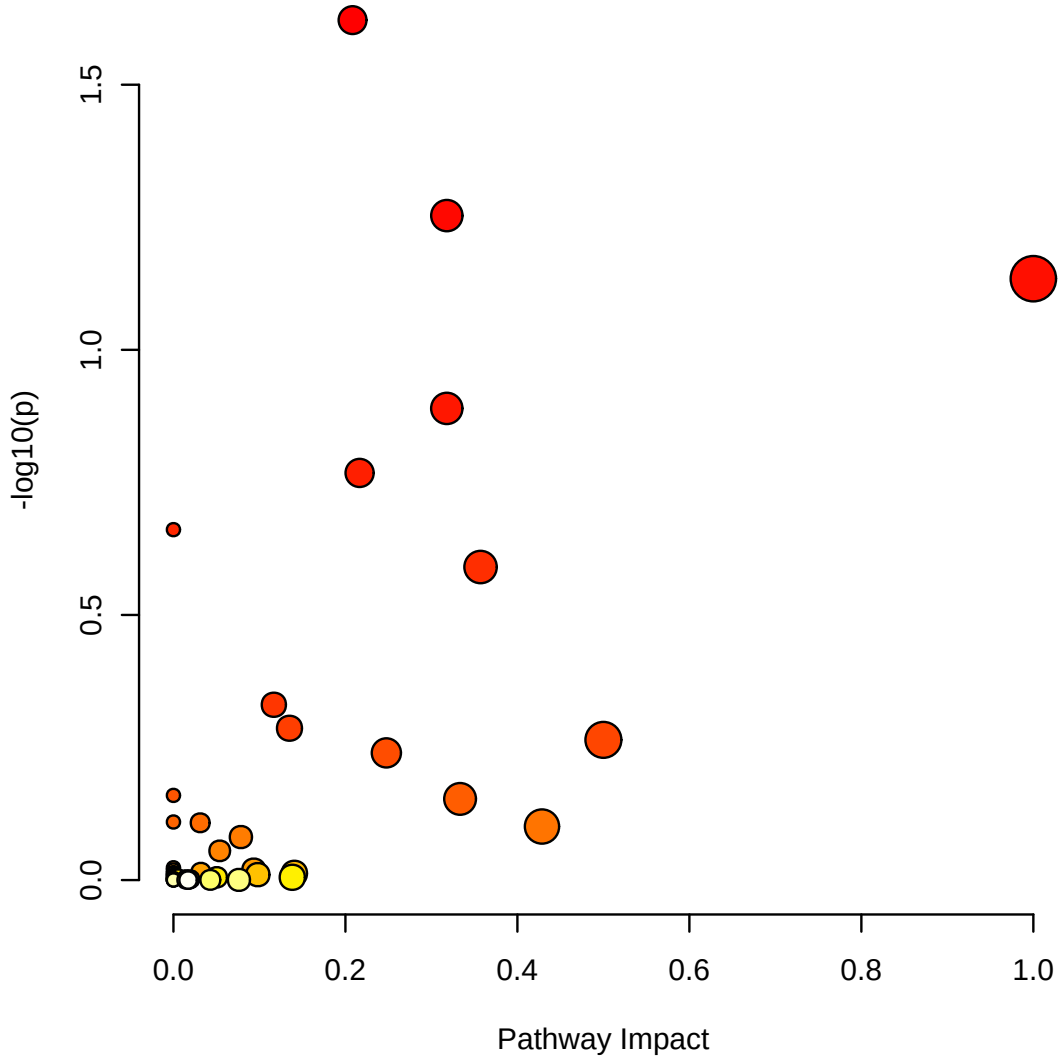

Figure 1: Summary of Pathway Analysis

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
Primary bile acid biosynthesis	46	8.19	14	2.39E-02	1.62E+00	1.00E+00	1.00E+00	0.21
Tyrosine metabolism	42	7.48	12	5.58E-02	1.25E+00	1.00E+00	1.00E+00	0.32
D-Glutamine and D-glutamate metabolism	6	1.07	3	7.34E-02	1.13E+00	1.00E+00	1.00E+00	1.00
Citrate cycle (TCA cycle)	20	3.56	6	1.29E-01	8.90E-01	1.00E+00	1.00E+00	0.32
Retinol metabolism	17	3.03	5	1.71E-01	7.68E-01	1.00E+00	1.00E+00	0.22
Linoleic acid metabolism	5	0.89	2	2.18E-01	6.61E-01	1.00E+00	1.00E+00	0.00
Phenylalanine metabolism	10	1.78	3	2.57E-01	5.90E-01	1.00E+00	1.00E+00	0.36
Arginine biosynthesis	14	2.49	3	4.67E-01	3.31E-01	1.00E+00	1.00E+00	0.12
Glyoxylate and dicarboxylate metabolism	32	5.70	6	5.17E-01	2.86E-01	1.00E+00	1.00E+00	0.13
Phenylalanine, tyrosine and tryptophan biosynthesis	4	0.71	1	5.44E-01	2.64E-01	1.00E+00	1.00E+00	0.50
Alanine, aspartate and glutamate metabolism	28	4.99	5	5.76E-01	2.40E-01	1.00E+00	1.00E+00	0.25
Nitrogen metabolism	6	1.07	1	6.92E-01	1.60E-01	1.00E+00	1.00E+00	0.00
alpha-Linolenic acid metabolism	13	2.31	2	7.03E-01	1.53E-01	1.00E+00	1.00E+00	0.33
Butanoate metabolism	15	2.67	2	7.77E-01	1.10E-01	1.00E+00	1.00E+00	0.00
Pyruvate metabolism	22	3.92	3	7.80E-01	1.08E-01	1.00E+00	1.00E+00	0.03
Taurine and hypotaurine metabolism	8	1.42	1	7.93E-01	1.01E-01	1.00E+00	1.00E+00	0.43
Vitamin B6 metabolism	9	1.60	1	8.30E-01	8.11E-02	1.00E+00	1.00E+00	0.08
Tryptophan metabolism	41	7.30	5	8.81E-01	5.51E-02	1.00E+00	1.00E+00	0.05
Nicotinate and nicotinamide metabolism	15	2.67	1	9.48E-01	2.32E-02	1.00E+00	1.00E+00	0.00
Histidine metabolism	16	2.85	1	9.57E-01	1.89E-02	1.00E+00	1.00E+00	0.00
Glycerolipid metabolism	16	2.85	1	9.57E-01	1.89E-02	1.00E+00	1.00E+00	0.09
Galactose metabolism	27	4.81	2	9.67E-01	1.47E-02	1.00E+00	1.00E+00	0.03
Biosynthesis of unsaturated fatty acids	36	6.41	3	9.68E-01	1.39E-02	1.00E+00	1.00E+00	0.00
Starch and sucrose metabolism	18	3.21	1	9.71E-01	1.26E-02	1.00E+00	1.00E+00	0.00
Pentose and glucuronate interconversions	18	3.21	1	9.71E-01	1.26E-02	1.00E+00	1.00E+00	0.14
Arginine and proline metabolism	38	6.77	3	9.77E-01	1.02E-02	1.00E+00	1.00E+00	0.10
Fructose and mannose metabolism	20	3.56	1	9.81E-01	8.46E-03	1.00E+00	1.00E+00	0.00
Ether lipid metabolism	20	3.56	1	9.81E-01	8.46E-03	1.00E+00	1.00E+00	0.00
Pentose phosphate pathway	22	3.92	1	9.87E-01	5.66E-03	1.00E+00	1.00E+00	0.00
Steroid biosynthesis	42	7.48	3	9.88E-01	5.46E-03	1.00E+00	1.00E+00	0.01
Glycine, serine and threonine metabolism	33	5.88	2	9.88E-01	5.23E-03	1.00E+00	1.00E+00	0.05
Cysteine and methionine metabolism	33	5.88	2	9.88E-01	5.23E-03	1.00E+00	1.00E+00	0.14
Lysine degradation	25	4.45	1	9.93E-01	3.10E-03	1.00E+00	1.00E+00	0.00
Fatty acid biosynthesis	47	8.37	3	9.94E-01	2.45E-03	1.00E+00	1.00E+00	0.01
Fatty acid degradation	39	6.94	2	9.96E-01	1.81E-03	1.00E+00	1.00E+00	0.00
Glutathione metabolism	28	4.99	1	9.96E-01	1.70E-03	1.00E+00	1.00E+00	0.02
Porphyrin and chlorophyll metabolism	30	5.34	1	9.97E-01	1.14E-03	1.00E+00	1.00E+00	0.00
Aminoacyl-tRNA biosynthesis	48	8.55	2	9.99E-01	3.56E-04	1.00E+00	1.00E+00	0.00
Glycerophospholipid metabolism	36	6.41	1	9.99E-01	3.41E-04	1.00E+00	1.00E+00	0.04
Arachidonic acid metabolism	36	6.41	1	9.99E-01	3.41E-04	1.00E+00	1.00E+00	0.08
Amino sugar and nucleotide sugar metabolism	37	6.59	1	9.99E-01	2.79E-04	1.00E+00	1.00E+00	0.00
Fatty acid elongation	39	6.94	1	1.00E+00	1.87E-04	1.00E+00	1.00E+00	0.00
Drug metabolism - cytochrome P450	55	9.79	2	1.00E+00	9.77E-05	1.00E+00	1.00E+00	0.01
Purine metabolism	65	11.57	2	1.00E+00	1.48E-05	1.00E+00	1.00E+00	0.02
Steroid hormone biosynthesis	85	15.13	2	1.00E+00	3.09E-07	1.00E+00	1.00E+00	0.02

6 Appendix: R Command History

```
 [1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
 [2] "cmpd.vec<-c(\"HMDB0000925\",\"HMDB0142449\",\"HMDB0140038\",\"HMDB0012136\",\"HMDB0062143\",\"
 [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] "mSet<-PreparePDFReport(mSet, \"guest19989929154535238 34\")\n"
```

The report was generated on Mon May 24 14:58:17 2021 with R version 4.0.2 (2020-06-22).