

# Metabolomic Data Analysis with MetaboAnalyst 5.0

Name: guest5553748766599075063

May 24, 2021

## 1 Background

MSEA or Metabolite Set Enrichment Analysis is a way to identify biologically meaningful patterns that are significantly enriched in quantitative metabolomic data. In conventional approaches, metabolites are evaluated individually for their significance under conditions of study. Those compounds that have passed certain significance level are then combined to see if any meaningful patterns can be discerned. In contrast, MSEA directly investigates if a set of functionally related metabolites without the need to preselect compounds based on some arbitrary cut-off threshold. It has the potential to identify subtle but consistent changes among a group of related compounds, which may go undetected with the conventional approaches.

Essentially, MSEA is a metabolomic version of the popular GSEA (Gene Set Enrichment Analysis) software with its own collection of metabolite set libraries as well as an implementation of user-friendly web-interfaces. GSEA is widely used in genomics data analysis and has proven to be a powerful alternative to conventional approaches. For more information, please refer to the original paper by Subramanian A, and a nice review paper by Nam D, Kim SY.<sup>1, 2</sup>

## 2 MSEA Overview

Metabolite set enrichment analysis consists of four steps - data input, data processing, data analysis, and results download. Different analysis procedures are performed based on different input types. In addition, users can also browse and search the metabolite set libraries as well as upload their self-defined metabolite sets for enrichment analysis. Users can also perform metabolite name mapping between a variety of compound names, synonyms, and major database identifiers.

## 3 Data Input

There are three enrichment analysis algorithms offered by MSEA. Accordingly, three different types of data inputs are required by these three approaches:

- A list of important compound names - entered as a one column data (*Over Representation Analysis (ORA)*);
- A single measured biofluid (urine, blood, CSF) sample- entered as tab separated two-column data with the first column for compound name, and the second for concentration values (*Single Sample Profiling (SSP)*);

---

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

<sup>2</sup>Nam D, Kim SY. *Gene-set approach for expression pattern analysis*, Briefings in Bioinformatics. 2008 9(3): 189-197.

- A compound concentration table - entered as a comma separated (.csv) file with the each sample per row and each metabolite concentration per column. The first column is sample names and the second column for sample phenotype labels (*Quantitative Enrichment Analysis (QEA)*)

You selected Over Representation Analysis (ORA) which requires a list of compound names as input.

## 4 Data Process

The first step is to standardize the compound labels. It is an essential step since the compound labels will be subsequently compared with compounds contained in the metabolite set library. MSEA has a built-in tool to convert between compound common names, synonyms, identifiers used in HMDB ID, PubChem, ChEBI, BiGG, METLIN, KEGG, or Reactome. **Table 1** shows the conversion results. Note: *1* indicates exact match, *2* indicates approximate match, and *0* indicates no match. A text file contain the result can be found the downloaded file *name\_map.csv*

	Query	Match	HMDB
1	HMDB0000123	Glycine	HMDB0000123
2	HMDB0014691	Acetohydroxamic Acid	HMDB0014691
3	HMDB00031239	Ethyl nitrite	HMDB00031239
4	HMDB0161401	NA	NA
5	HMDB0000925	Trimethylamine N-oxide	HMDB0000925
6	HMDB0142449	NA	NA
7	HMDB0140038	NA	NA
8	HMDB0012136	1-Amino-propan-2-ol	HMDB0012136
9	HMDB0062143	NA	NA
10	HMDB0031558	Methyloxirane	HMDB0031558
11	HMDB0031652	Allyl alcohol	HMDB0031652
12	HMDB0003366	Propanal	HMDB0003366
13	HMDB0001659	Acetone	HMDB0001659
14	HMDB0000246	Tetrahydrofuran	HMDB0000246
15	HMDB0171202	NA	NA
16	HMDB0000474	Butanone	HMDB0000474
17	HMDB0003543	Butanal	HMDB0003543
18	HMDB0034431	2,2-Dimethyloxirane	HMDB0034431
19	HMDB0031324	3-Buten-1-ol	HMDB0031324
20	HMDB0033858	2-Buten-1-ol	HMDB0033858
21	HMDB0031243	2-Methylpropanal	HMDB0031243
22	HMDB0171604	NA	NA
23	HMDB0171603	NA	NA
24	HMDB0032231	Dimethylethanolamine	HMDB0032231
25	HMDB0031404	Cyclohexylamine	HMDB0031404
26	HMDB0032416	2-Methylpiperidine	HMDB0032416
27	HMDB0031544	3-Methylcyclopentene	HMDB0031544
28	HMDB0062716	NA	NA
29	HMDB0033971	2-Diethylaminoethanol	HMDB0033971
30	HMDB0000630	Cytosine	HMDB0000630
31	HMDB0031335	2-Chloro-1-propanol	HMDB0031335
32	HMDB0182885	NA	NA
33	HMDB0039786	NA	NA
34	HMDB0173815	NA	NA
35	HMDB0173816	NA	NA
36	HMDB0171081	NA	NA
37	HMDB0032576	2-Methoxy-1,4-benzoquinone	HMDB0032576
38	HMDB0033812	Sesamol	HMDB0033812
39	HMDB0059965	NA	NA
40	HMDB0032920	alpha-Furyl methyl diketone	HMDB0032920
41	HMDB0171080	NA	NA
42	HMDB0062484	NA	NA
43	HMDB0004062	Gentisate aldehyde	HMDB0004062
44	HMDB0002466	3-Hydroxybenzoic acid	HMDB0002466
45	HMDB0000500	4-Hydroxybenzoic acid	HMDB0000500
46	HMDB0001895	Salicylic acid	HMDB0001895
47	HMDB0035646	Methyl 2-(methylthio)acetate	HMDB0035646
48	HMDB0001527	3-Methylthiopropionic acid	HMDB0001527
49	HMDB0112255	NA	NA
50	HMDB0126388	NA	NA
51	HMDB0166105	NA	NA
52	HMDB0125590	NA	NA
53	HMDB0168417	NA	NA
54	HMDB0168448	NA	NA
55	HMDB0041607	NA	NA
56	HMDB0004284	Tyrosol	HMDB0004284
57	HMDB0032137	2,6-Dimethyl-1,4-benzenediol	HMDB0032137
58	HMDB0040174	NA	NA
59	HMDB0040177	NA	NA

60	HMDB0032139	1,2-Dimethoxybenzene	HMDB0032139
61	HMDB0032036	4-Ethoxyphenol	HMDB0032036
62	HMDB0039802	NA	NA
63	HMDB0029671	1,4-Dimethoxybenzene	HMDB0029671
64	HMDB0029672	1,3-Dimethoxybenzene	HMDB0029672
65	HMDB0032290	1-(2-Furyl)butan-3-one	HMDB0032290
66	HMDB0168418	NA	NA
67	HMDB0032159	2-Acetyl-3,5-dimethylfuran	HMDB0032159
68	HMDB0029563	3-Acetyl-2,5-dimethylfuran	HMDB0029563
69	HMDB0032136	2-Methoxy-4-methylphenol	HMDB0032136
70	HMDB0034241	4-Methoxybenzyl alcohol	HMDB0034241
71	HMDB0029638	4-Methylbenzaldehyde	HMDB0029638
72	HMDB0006236	Phenylacetaldehyde	HMDB0006236
73	HMDB0013815	2,3-Dihydrobenzofuran	HMDB0013815
74	HMDB0029637	3-Methylbenzaldehyde	HMDB0029637
75	HMDB0172088	NA	NA
76	HMDB0029636	2-Methylbenzaldehyde	HMDB0029636
77	HMDB0038997	NA	NA
78	HMDB0062765	Styrene Oxide	HMDB0062765
79	HMDB0004072	4-Hydroxystyrene	HMDB0004072
80	HMDB0124943	NA	NA
81	HMDB0033910	Acetophenone	HMDB0033910
82	HMDB0167775	NA	NA
83	HMDB0167776	NA	NA
84	HMDB0039781	NA	NA
85	HMDB0041476	NA	NA
86	HMDB0041562	NA	NA
87	HMDB0032373	3-Mercapto-2-methyl-1-butanol	HMDB0032373
88	HMDB0036149	NA	NA
89	HMDB0000251	Taurine	HMDB0000251
90	HMDB0011601	3-Methylcytosine	HMDB0011601
91	HMDB0004339	2-O-Methylcytosine	HMDB0004339
92	HMDB0002894	5-Methylcytosine	HMDB0002894
93	HMDB0041922	NA	NA
94	HMDB0171225	NA	NA
95	HMDB0164607	NA	NA
96	HMDB0166218	NA	NA
97	HMDB0164608	NA	NA
98	HMDB0171213	NA	NA
99	HMDB0166253	NA	NA
100	HMDB0171212	NA	NA
101	HMDB0166254	NA	NA
102	HMDB0166217	NA	NA
103	HMDB0172056	NA	NA
104	HMDB0172059	NA	NA
105	HMDB0172058	NA	NA
106	HMDB0172057	NA	NA
107	HMDB0159225	NA	NA
108	HMDB0159223	NA	NA
109	HMDB0159222	NA	NA
110	HMDB0005785	Indole-3-carbinol	HMDB0005785
111	HMDB0030204	1-(2-Furanylmethyl)-1H-pyrrole	HMDB0030204
112	HMDB0040009	NA	NA
113	HMDB0040011	NA	NA
114	HMDB0159224	NA	NA
115	HMDB0011664	3-Methylene-indolenine	HMDB0011664
116	HMDB0033731	Quinoline	HMDB0033731
117	HMDB0034244	Isoquinoline	HMDB0034244
118	HMDB0032980	3,4-Dimethylthiophene	HMDB0032980
119	HMDB0032979	2,5-Dimethylthiophene	HMDB0032979
120	HMDB0032977	2,3-Dimethylthiophene	HMDB0032977
121	HMDB0032978	2,4-Dimethylthiophene	HMDB0032978
122	HMDB0035385	3-Ethylthiophene	HMDB0035385
123	HMDB0035384	2-Ethylthiophene	HMDB0035384
124	HMDB0038973	NA	NA
125	HMDB0038433	NA	NA
126	HMDB0032341	Isoamyl isothiocyanate	HMDB0032341
127	HMDB0179339	NA	NA
128	HMDB0187593	NA	NA
129	HMDB0179338	NA	NA
130	HMDB0179340	NA	NA
131	HMDB0179337	NA	NA
132	HMDB0031543	3-Methyl-1,2-cyclopentanedione	HMDB0031543
133	HMDB0032233	2,5-Dimethyl-3(2H)-furanone	HMDB0032233
134	HMDB0034247	2-(Methoxymethyl)furan	HMDB0034247
135	HMDB0039778	NA	NA
136	HMDB0029581	(2E,4E)-2,4-Hexadienoic acid	HMDB0029581
137	HMDB0031344	1,2-Cyclohexanedione	HMDB0031344
138	HMDB0031759	(E)-4-Oxo-2-hexen-1-al	HMDB0031759
139	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-diol	HMDB0001164
140	HMDB0040260	NA	NA
141	HMDB0033569	Syoyualdehyde	HMDB0033569
142	HMDB0029444	2-Pyrrolidineacetic acid	HMDB0029444
143	HMDB0094697	NA	NA
144	HMDB0059649	NA	NA
145	HMDB0015212	Vigabatrin	HMDB0015212
146	HMDB0062225	NA	NA

147	HMDB0000070	Pipecolic acid	HMDB0000070
148	HMDB0062767	NA	NA
149	HMDB0004226	N4-Acetylaminobutanal	HMDB0004226
150	HMDB0005960	D-Pipecolic acid	HMDB0005960
151	HMDB0000716	L-Pipecolic acid	HMDB0000716
152	HMDB0029435	L-trans-4-Methyl-2-pyrrolidinecarboxylic acid	HMDB0029435
153	HMDB0094696	N-Methyl-proline	HMDB0094696
154	HMDB0033453	Fagomine	HMDB0033453
155	HMDB0142963	NA	NA
156	HMDB0168724	NA	NA
157	HMDB0168723	NA	NA
158	HMDB0061157	NA	NA
159	HMDB0029449	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	HMDB0029449
160	HMDB0031537	3-Methylcyclohexanethiol	HMDB0031537
161	HMDB0040153	NA	NA
162	HMDB0128943	NA	NA
163	HMDB0132477	NA	NA
164	HMDB0129097	NA	NA
165	HMDB0168839	NA	NA
166	HMDB0128916	NA	NA
167	HMDB0012233	Glutarate semialdehyde	HMDB0012233
168	HMDB0029172	3-keto-2-Methylbutyrate	HMDB0029172
169	HMDB0001865	2-Oxovaleric acid	HMDB0001865
170	HMDB0000310	Methylacetoacetic acid	HMDB0000310
171	HMDB0031643	Ethyl pyruvate	HMDB0031643
172	HMDB0000019	Alpha-ketoisovaleric acid	HMDB0000019
173	HMDB0003771	2-Methylacetoacetic acid	HMDB0003771
174	HMDB0000720	Levulinic acid	HMDB0000720
175	HMDB0034466	Acetoxyacetone	HMDB0034466
176	HMDB0128917	NA	NA
177	HMDB0129096	NA	NA
178	HMDB0129098	NA	NA
179	HMDB0168838	NA	NA
180	HMDB0177210	NA	NA
181	HMDB0169666	NA	NA
182	HMDB0177209	NA	NA
183	HMDB0171727	NA	NA
184	HMDB0032356	N-Lactoyl ethanolamine	HMDB0032356
185	HMDB0039499	NA	NA
186	HMDB0031658	L-2-Amino-5-hydroxypentanoic acid	HMDB0031658
187	HMDB0002108	Methylcysteine	HMDB0002108
188	HMDB0000742	Homocysteine	HMDB0000742
189	HMDB0038949	NA	NA
190	HMDB0030410	L-2-Amino-3-methylenehexanoic acid	HMDB0030410
191	HMDB0004827	Proline betaine	HMDB0004827
192	HMDB0034080	3-Methyl-1,2-cyclohexanedione	HMDB0034080
193	HMDB0033629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	HMDB0033629
194	HMDB0041474	NA	NA
195	HMDB0034835	3-(3-Ethylloxiranyl)-2-propenal	HMDB0034835
196	HMDB0031223	Enol-3-Ethyl-1,2-cyclopentanedione	HMDB0031223
197	HMDB0040445	NA	NA
198	HMDB0037026	NA	NA
199	HMDB0031222	3-Ethyl-1,2-cyclopentanedione	HMDB0031222
200	HMDB0037027	NA	NA
201	HMDB0029582	Methyl sorbate	HMDB0029582
202	HMDB0032067	Allyl crotonate	HMDB0032067
203	HMDB0032333	4-Hydroxy-4-methyl-5-hexenoic acid gamma lactone	HMDB0032333
204	HMDB0145126	NA	NA
205	HMDB0000062	L-Carnitine	HMDB0000062
206	HMDB0062496	Malonyl-Carnitin	HMDB0062496
207	HMDB0062634	NA	NA
208	HMDB0155786	NA	NA
209	HMDB0032380	(S1)-Methoxy-3-heptanethiol	HMDB0032380
210	HMDB0172136	NA	NA
211	HMDB0165770	NA	NA
212	HMDB0165771	NA	NA
213	HMDB0165773	NA	NA
214	HMDB0172134	NA	NA
215	HMDB0172135	NA	NA
216	HMDB0240308	NA	NA
217	HMDB0165772	NA	NA
218	HMDB0029737	1H-Indole-3-carboxaldehyde	HMDB0029737
219	HMDB0004186	3-Methyldioxyindole	HMDB0004186
220	HMDB0001424	4-(3-Pyridyl)-3-butenic acid	HMDB0001424
221	HMDB0062406	NA	NA
222	HMDB0029300	p-Anisidine	HMDB0029300
223	HMDB0167379	NA	NA
224	HMDB0032578	4-Hydroxybenzylamine	HMDB0032578
225	HMDB0040360	NA	NA
226	HMDB0036058	NA	NA
227	HMDB0167378	NA	NA
228	HMDB0032492	2-Propionylpyrrole	HMDB0032492
229	HMDB0166738	NA	NA
230	HMDB0164724	NA	NA
231	HMDB0165094	NA	NA
232	HMDB0165096	NA	NA
233	HMDB0165095	NA	NA

234	HMDB0165097	NA	NA
235	HMDB0166737	NA	NA
236	HMDB0031484	2-Heptenoic acid	HMDB0031484
237	HMDB0038962	NA	NA
238	HMDB0031500	Methyl 2E-hexenoate	HMDB0031500
239	HMDB0166739	NA	NA
240	HMDB0029314	Isopentenyl acetate	HMDB0029314
241	HMDB0031477	3,4-Heptanedione	HMDB0031477
242	HMDB0031476	2,3-Heptanedione	HMDB0031476
243	HMDB0031504	Methyl (Z)-3-hexenoate	HMDB0031504
244	HMDB0031603	Ethyl 4-pentenoate	HMDB0031603
245	HMDB0040214	NA	NA
246	HMDB0031342	Cyclohexanecarboxylic acid	HMDB0031342
247	HMDB0038271	NA	NA
248	HMDB0031174	4-Methyl-5-hexanolide	HMDB0031174
249	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	HMDB0031681
250	HMDB0033793	4-Heptenoic acid	HMDB0033793
251	HMDB0031593	5-Methyl-2,3-hexanedione	HMDB0031593
252	HMDB0039819	NA	NA
253	HMDB0166736	NA	NA
254	HMDB0173760	NA	NA
255	HMDB0173761	NA	NA
256	HMDB0173762	NA	NA
257	HMDB0173763	NA	NA
258	HMDB0180322	NA	NA
259	HMDB0180323	NA	NA
260	HMDB0029165	1,3-Diacetylpropane	HMDB0029165
261	HMDB0031351	Cyclohexyl formate	HMDB0031351
262	HMDB0032460	4-Pentenyl acetate	HMDB0032460
263	HMDB0032391	3-Methyl-3-butenyl acetate	HMDB0032391
264	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	HMDB0030330
265	HMDB0059876	NA	NA
266	HMDB0040591	NA	NA
267	HMDB0145113	NA	NA
268	HMDB0145114	NA	NA
269	HMDB0145115	NA	NA
270	HMDB0145125	NA	NA
271	HMDB0145116	NA	NA
272	HMDB0094649	2-Amino-heptanoic acid	HMDB0094649
273	HMDB0001161	4-Trimethylammoniobutanoic acid	HMDB0001161
274	HMDB0006831	3-Dehydroxycarnitine	HMDB0006831
275	HMDB0000895	Acetylcholine	HMDB0000895
276	HMDB0013811	1-Nitroheptane	HMDB0013811
277	HMDB0240327	NA	NA
278	HMDB0159478	NA	NA
279	HMDB0159477	NA	NA
280	HMDB0158747	NA	NA
281	HMDB0158748	NA	NA
282	HMDB0158745	NA	NA
283	HMDB0158746	NA	NA
284	HMDB0159480	NA	NA
285	HMDB0159479	NA	NA
286	HMDB0161124	NA	NA
287	HMDB0161123	NA	NA
288	HMDB0161125	NA	NA
289	HMDB0155922	NA	NA
290	HMDB0061930	NA	NA
291	HMDB0033837	Dimethyl succinate	HMDB0033837
292	HMDB0006900	(S)-2-Aceto-2-hydroxybutanoic acid	HMDB0006900
293	HMDB0002173	Solerol	HMDB0002173
294	HMDB0002074	2,2-Dimethylsuccinic acid	HMDB0002074
295	HMDB0000858	Monomethyl glutaric acid	HMDB0000858
296	HMDB0000752	Methylglutaric acid	HMDB0000752
297	HMDB0000422	2-Methylglutaric acid	HMDB0000422
298	HMDB0000448	Adipic acid	HMDB0000448
299	HMDB0062489	NA	NA
300	HMDB0010207	L-Rhamnulose	HMDB0010207
301	HMDB0033821	2-O-Methyl-D-xylose	HMDB0033821
302	HMDB0062477	NA	NA
303	HMDB0062498	NA	NA
304	HMDB0062499	NA	NA
305	HMDB0060267	L-Fuculose	HMDB0060267
306	HMDB0005876	3-Deoxyfructose	HMDB0005876
307	HMDB0012327	2-Deoxygalactopyranose	HMDB0012327
308	HMDB0002712	1,5-Anhydrosorbitol	HMDB0002712
309	HMDB0059625	NA	NA
310	HMDB0029196	D-Fucose	HMDB0029196
311	HMDB0003081	Beta-D-Fucose	HMDB0003081
312	HMDB0000174	L-Fucose	HMDB0000174
313	HMDB0059624	NA	NA
314	HMDB0000849	Rhamnose	HMDB0000849
315	HMDB0124735	NA	NA
316	HMDB0240304	NA	NA
317	HMDB0041477	NA	NA
318	HMDB0031660	Dibutyl sulfide	HMDB0031660
319	HMDB0168717	NA	NA
320	HMDB0168715	NA	NA

321	HMDB0168716	NA	NA
322	HMDB0168718	NA	NA
323	HMDB0062061	NA	NA
324	HMDB0030302	2,3,4-Trimethylhexane	HMDB0030302
325	HMDB0029595	Nonane	HMDB0029595
326	HMDB0030301	2,2,3,4-Tetramethylpentane	HMDB0030301
327	HMDB0031556	Isononane	HMDB0031556
328	HMDB0031416	3,4-Dimethylheptane	HMDB0031416
329	HMDB0062017	NA	NA
330	HMDB0062013	NA	NA
331	HMDB0240251	NA	NA
332	HMDB0061880	NA	NA
333	HMDB0060460	cis-4-Hydroxy-D-proline	HMDB0060460
334	HMDB0000725	4-Hydroxyproline	HMDB0000725
335	HMDB0036576	NA	NA
336	HMDB0000766	N-Acetyl-L-alanine	HMDB0000766
337	HMDB0000783	Propionylglycine	HMDB0000783
338	HMDB0002104	L-Glutamic gamma-semialdehyde	HMDB0002104
339	HMDB0002113	3-Hydroxy-L-proline	HMDB0002113
340	HMDB0006055	4-Hydroxy-L-proline	HMDB0006055
341	HMDB0059659	Trans-3-hydroxy-L-proline	HMDB0059659
342	HMDB0001149	5-Aminolevulinic acid	HMDB0001149
343	HMDB0006272	5-Amino-2-oxopentanoic acid	HMDB0006272
344	HMDB0177404	NA	NA
345	HMDB0164041	NA	NA
346	HMDB0014389	Mesalazine	HMDB0014389
347	HMDB0001972	3-Aminosalicylic acid	HMDB0001972
348	HMDB0059749	NA	NA
349	HMDB0001476	3-Hydroxyanthranilic acid	HMDB0001476
350	HMDB0059811	NA	NA
351	HMDB0014378	Aminosalicylic Acid	HMDB0014378
352	HMDB0001280	2-Aminomuconic acid semialdehyde	HMDB0001280
353	HMDB0031670	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	HMDB0031670
354	HMDB0028696	Alanyl-Serine	HMDB0028696
355	HMDB0029032	Serylalanine	HMDB0029032
356	HMDB0145395	NA	NA
357	HMDB0029061	Threoninyl-Glycine	HMDB0029061
358	HMDB0028851	Glycyl-Threonine	HMDB0028851
359	HMDB0169117	NA	NA
360	HMDB0125105	NA	NA
361	HMDB0038987	NA	NA
362	HMDB0032029	2-Isopropylphenol	HMDB0032029
363	HMDB0032149	1-Methoxy-2,4-dimethylbenzene	HMDB0032149
364	HMDB0032625	4-Propylphenol	HMDB0032625
365	HMDB0029667	2,3,6-Trimethylphenol	HMDB0029667
366	HMDB0039782	NA	NA
367	HMDB0038986	NA	NA
368	HMDB0032624	2-Propylphenol	HMDB0032624
369	HMDB0038988	NA	NA
370	HMDB0032621	(2-Methoxyethyl)benzene	HMDB0032621
371	HMDB0038985	NA	NA
372	HMDB0031312	Benzyl ethyl ether	HMDB0031312
373	HMDB0033962	3-Phenyl-1-propanol	HMDB0033962
374	HMDB0031627	1-Phenyl-1-propanol	HMDB0031627
375	HMDB0034378	(Áś)-1-(4-Methylphenyl)ethanol	HMDB0034378
376	HMDB0031628	2-Phenyl-1-propanol	HMDB0031628
377	HMDB0038984	NA	NA
378	HMDB0032544	2,4,6-Trimethylphenol	HMDB0032544
379	HMDB0031446	p-Isopropylphenol	HMDB0031446
380	HMDB0032441	Nona-2,4,6-trienal	HMDB0032441
381	HMDB0059896	NA	NA
382	HMDB0169118	NA	NA
383	HMDB0163404	NA	NA
384	HMDB0164725	NA	NA
385	HMDB0164726	NA	NA
386	HMDB0165787	NA	NA
387	HMDB0172015	NA	NA
388	HMDB0180325	NA	NA
389	HMDB0180324	NA	NA
390	HMDB0034230	Mesifurane	HMDB0034230
391	HMDB0164727	NA	NA
392	HMDB0041426	NA	NA
393	HMDB0041427	NA	NA
394	HMDB0033551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	HMDB0033551
395	HMDB0033736	Homofureanol	HMDB0033736
396	HMDB0038593	NA	NA
397	HMDB0029412	Betonicine	HMDB0029412
398	HMDB0011757	N-Acetylvaline	HMDB0011757
399	HMDB0031345	Calystegine A6	HMDB0031345
400	HMDB0000339	2-Methylbutyrylglycine	HMDB0000339
401	HMDB0000678	Isovalerylglycine	HMDB0000678
402	HMDB0000927	Valerylglycine	HMDB0000927
403	HMDB0012154	3-Dehydrocarnitine	HMDB0012154
404	HMDB0012175	5-Acetamidovalerate	HMDB0012175
405	HMDB0036384	NA	NA
406	HMDB0029409	Turicine	HMDB0029409
407	HMDB0038625	NA	NA

408	HMDB0029230	4-Hydroxystachydrine	HMDB0029230
409	HMDB0061678	NA	NA
410	HMDB0035360	N-Methyl-1-deoxynojirimycin	HMDB0035360
411	HMDB0163316	NA	NA
412	HMDB0163318	NA	NA
413	HMDB0163317	NA	NA
414	HMDB0163315	NA	NA
415	HMDB0163319	NA	NA
416	HMDB0062166	NA	NA
417	HMDB0032164	Allyl valerate	HMDB0032164
418	HMDB0037624	NA	NA
419	HMDB0029761	Ethyl (E)-2-methyl-4-pentenoate	HMDB0029761
420	HMDB0031403	Cyclohexanecetic acid	HMDB0031403
421	HMDB0035422	4-Butyl-gamma-butyrolactone	HMDB0035422
422	HMDB0031352	Cyclohexyl acetate	HMDB0031352
423	HMDB0031343	Methyl cyclohexanecarboxylate	HMDB0031343
424	HMDB0036212	NA	NA
425	HMDB0032533	trans-3-Hexenyl acetate	HMDB0032533
426	HMDB0240301	NA	NA
427	HMDB0032266	Ethyl (E)-3-hexenoate	HMDB0032266
428	HMDB0036236	NA	NA
429	HMDB0032268	Ethyl 2E-hexenoate	HMDB0032268
430	HMDB0000392	2-Octenoic acid	HMDB0000392
431	HMDB0001568	trans-2-Octenoic acid	HMDB0001568
432	HMDB0038036	NA	NA
433	HMDB0039793	NA	NA
434	HMDB0037630	NA	NA
435	HMDB0038310	NA	NA
436	HMDB0039872	NA	NA
437	HMDB0037622	NA	NA
438	HMDB0040215	cis-3-Hexenyl acetate	HMDB0040215
439	HMDB0040212	NA	NA
440	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate	HMDB0032278
441	HMDB0031293	2,3-Octanedione	HMDB0031293
442	HMDB0013904	(3E)-2-Propylpent-3-enoic acid	HMDB0013904
443	HMDB0059908	NA	NA
444	HMDB0013902	2-ene-Valproic acid	HMDB0013902
445	HMDB0013897	4-ene-Valproic acid	HMDB0013897
446	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid	HMDB0013903
447	HMDB0061342	NA	NA
448	HMDB0032267	Ethyl 5-hexenoate	HMDB0032267
449	HMDB0032207	cis-5-Octenoic acid	HMDB0032207
450	HMDB0062077	NA	NA
451	HMDB0240571	NA	NA
452	HMDB0000991	DL-2-Aminooctanoic acid	HMDB0000991
453	HMDB0240732	NA	NA
454	HMDB0014375	Pregabalin	HMDB0014375
455	HMDB0013305	Propionylcholine	HMDB0013305
456	HMDB0015654	Methacholine	HMDB0015654
457	HMDB0002285	2-Indolecarboxylic acid	HMDB0002285
458	HMDB0240311	NA	NA
459	HMDB0060289	Quinoline-4,8-diol	HMDB0060289
460	HMDB0003320	Indole-3-carboxylic acid	HMDB0003320
461	HMDB0031172	3-Formyl-6-hydroxyindole	HMDB0031172
462	HMDB0004077	4,6-Dihydroxyquinoline	HMDB0004077
463	HMDB0032398	Methyl n-formylanthranilate	HMDB0032398
464	HMDB0000992	3-Succinoylpyridine	HMDB0000992
465	HMDB0000714	Hippuric acid	HMDB0000714
466	HMDB0062583	NA	NA
467	HMDB0032595	1-(4-Methoxyphenyl)-2-nitroethylene	HMDB0032595
468	HMDB0184242	NA	NA
469	HMDB0012884	Adrenochrome	HMDB0012884
470	HMDB0038174	NA	NA
471	HMDB0033388	NA	NA
472	HMDB0185632	NA	NA
473	HMDB0059856	NA	NA
474	HMDB0012153	3,4-Dihydroxybenzylamine	HMDB0012153
475	HMDB0032332	Hydroxylated lecithin	HMDB0032332
476	HMDB0145430	NA	NA
477	HMDB0128078	NA	NA
478	HMDB0134039	NA	NA
479	HMDB0135273	NA	NA
480	HMDB0135648	NA	NA
481	HMDB0135274	NA	NA
482	HMDB0135275	NA	NA
483	HMDB0035243	1-Phenyl-1,2-propanedione	HMDB0035243
484	HMDB0000930	trans-Cinnamic acid	HMDB0000930
485	HMDB0000567	Cinnamic acid	HMDB0000567
486	HMDB0036626	NA	NA
487	HMDB0040986	(E)-3-(4-Hydroxyphenyl)-2-propenal	HMDB0040986
488	HMDB0031725	(E)-3-(2-Hydroxyphenyl)-2-propenal	HMDB0031725
489	HMDB0032947	Di-2-furanylmethane	HMDB0032947
490	HMDB0062407	NA	NA
491	HMDB0004992	Benzocaine	HMDB0004992
492	HMDB0001007	3-Pyridinebutanoic acid	HMDB0001007
493	HMDB0059934	NA	NA
494	HMDB0033589	Ethyl 2-aminobenzoate	HMDB0033589

495	HMDB0033485	Gentiatibetine	HMDB0033485
496	HMDB0034169	Methyl N-methylanthranilate	HMDB0034169
497	HMDB0006044	Norsalsolinol	HMDB0006044
498	HMDB0000159	L-Phenylalanine	HMDB0000159
499	HMDB0159744	NA	NA
500	HMDB0062402	NA	NA
501	HMDB0155168	NA	NA
502	HMDB0029455	Ginkgotoxin	HMDB0029455
503	HMDB0000068	Epinephrine	HMDB0000068
504	HMDB0000819	Normetanephine	HMDB0000819
505	HMDB0002832	Methylnoradrenaline	HMDB0002832
506	HMDB0015652	Levonordefrin	HMDB0015652
507	HMDB0062515	NA	NA
508	HMDB0061679	NA	NA
509	HMDB0154785	NA	NA
510	HMDB0000232	Quinolinic acid	HMDB0000232
511	HMDB0033161	2,6-Pyridinedicarboxylic acid	HMDB0033161
512	HMDB0185628	NA	NA
513	HMDB0001330	2-Amino-3-carboxymuconic acid semialdehyde	HMDB0001330
514	HMDB0062578	NA	NA
515	HMDB0060260	NA	NA
516	HMDB0001552	2-Keto-glutaramic acid	HMDB0001552
517	HMDB0003584	Taurocyamine	HMDB0003584
518	HMDB0000289	Uric acid	HMDB0000289
519	HMDB0033249	6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine	HMDB0033249
520	HMDB0000734	Indoleacrylic acid	HMDB0000734
521	HMDB0040768	NA	NA
522	HMDB0060244	Phosphodimethylethanolamine	HMDB0060244
523	HMDB0166108	NA	NA
524	HMDB0171094	NA	NA
525	HMDB0172092	NA	NA
526	HMDB0062005	NA	NA
527	HMDB0124926	NA	NA
528	HMDB0168664	NA	NA
529	HMDB0150437	NA	NA
530	HMDB0125528	NA	NA
531	HMDB0137457	NA	NA
532	HMDB0146870	NA	NA
533	HMDB0146889	NA	NA
534	HMDB0166106	NA	NA
535	HMDB0166109	NA	NA
536	HMDB0182861	NA	NA
537	HMDB0166107	NA	NA
538	HMDB0183905	NA	NA
539	HMDB0183904	NA	NA
540	HMDB0036907	NA	NA
541	HMDB0029660	2',6'-Dihydroxyacetophenone	HMDB0029660
542	HMDB0029657	2,4'-Dihydroxyacetophenone	HMDB0029657
543	HMDB0029659	2',4'-Dihydroxyacetophenone	HMDB0029659
544	HMDB0029658	2',3'-Dihydroxyacetophenone	HMDB0029658
545	HMDB0032594	2-(Hydroxymethyl)benzoic acid	HMDB0032594
546	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	HMDB0033003
547	HMDB0032629	2',5'-Dihydroxyacetophenone	HMDB0032629
548	HMDB0032572	Methylparaben	HMDB0032572
549	HMDB0029662	3',5'-Dihydroxyacetophenone	HMDB0029662
550	HMDB0029661	3',4'-Dihydroxyacetophenone	HMDB0029661
551	HMDB0032604	2-Methoxybenzoic acid	HMDB0032604
552	HMDB0034172	Methyl 2-hydroxybenzoate	HMDB0034172
553	HMDB0032606	3-Methoxybenzoic acid	HMDB0032606
554	HMDB0041283	NA	NA
555	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	HMDB0004815
556	HMDB0012308	Vanillin	HMDB0012308
557	HMDB0032919	Ethyl 2-furanyl diketone	HMDB0032919
558	HMDB0172091	NA	NA
559	HMDB0032399	Methyl furfuracrylate	HMDB0032399
560	HMDB0000703	Mandelic acid	HMDB0000703
561	HMDB0000669	Ortho-Hydroxyphenylacetic acid	HMDB0000669
562	HMDB0060390	NA	NA
563	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	HMDB0003791
564	HMDB0062635	NA	NA
565	HMDB0031609	Phenoxyacetic acid	HMDB0031609
566	HMDB0000440	3-Hydroxyphenylacetic acid	HMDB0000440
567	HMDB0001101	p-Anisic acid	HMDB0001101
568	HMDB0000020	p-Hydroxyphenylacetic acid	HMDB0000020
569	HMDB0002390	3-Cresotinic acid	HMDB0002390
570	HMDB0000216	Norepinephrine	HMDB0000216
571	HMDB0035178	6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	HMDB0035178
572	HMDB0037685	NA	NA
573	HMDB0155164	NA	NA
574	HMDB0001537	6-Hydroxydopamine	HMDB0001537
575	HMDB0000239	Pyridoxine	HMDB0000239
576	HMDB0004817	5-Hydroxydopamine	HMDB0004817
577	HMDB0012150	2-Keto-6-acetamidocaproate	HMDB0012150
578	HMDB0032945	1-Phenyl-2,4-pentadiyn-1-one	HMDB0032945
579	HMDB0029738	Indole-3-methyl acetate	HMDB0029738
580	HMDB0002302	Indole-3-propionic acid	HMDB0002302
581	HMDB0014970	Phensuximide	HMDB0014970



582	HMDB0163575	NA	NA
583	HMDB0161234	NA	NA
584	HMDB0012209	Diethylphosphate	HMDB0012209
585	HMDB0040050	NA	NA
586	HMDB0040051	NA	NA
587	HMDB0040043	NA	NA
588	HMDB0039662	NA	NA
589	HMDB0040029	NA	NA
590	HMDB0040047	NA	NA
591	HMDB0040016	NA	NA
592	HMDB0030175	Venoterpine	HMDB0030175
593	HMDB0032935	1-(2-Thienyl)-1-butanone	HMDB0032935
594	HMDB0040231	NA	NA
595	HMDB0040589	NA	NA
596	HMDB0175069	NA	NA
597	HMDB0175071	NA	NA
598	HMDB0175067	NA	NA
599	HMDB0162021	NA	NA
600	HMDB0038628	NA	NA
601	HMDB0040972	NA	NA
602	HMDB0004073	5-Hydroxyindoleacetaldehyde	HMDB0004073
603	HMDB0000197	Indoleacetic acid	HMDB0000197
604	HMDB0166095	NA	NA
605	HMDB0060758	NA	NA
606	HMDB0240317	NA	NA
607	HMDB0162020	NA	NA
608	HMDB0162023	NA	NA
609	HMDB0162022	NA	NA
610	HMDB0013292	p-Methylhippuric acid	HMDB0013292
611	HMDB0013245	m-Methylhippuric acid	HMDB0013245
612	HMDB0000821	Phenylacetylglycine	HMDB0000821
613	HMDB0000859	Methyl hippurate	HMDB0000859
614	HMDB0011723	2-Methylhippuric acid	HMDB0011723
615	HMDB0060366	3-Carbamoyl-2-phenylpropionaldehyde	HMDB0060366
616	HMDB0060389	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	HMDB0060389
617	HMDB0034250	Betamipron	HMDB0034250
618	HMDB0032388	Methyl n-acetylanthranilate	HMDB0032388
619	HMDB0000073	Dopamine	HMDB0000073
620	HMDB0060277	NA	NA
621	HMDB0012309	Vanillylamine	HMDB0012309
622	HMDB0004825	p-Octopamine	HMDB0004825
623	HMDB0156498	NA	NA
624	HMDB0037786	NA	NA
625	HMDB0172919	NA	NA
626	HMDB0177509	NA	NA
627	HMDB0141046	NA	NA
628	HMDB0133751	NA	NA
629	HMDB0133750	NA	NA
630	HMDB0133749	NA	NA
631	HMDB0133752	NA	NA
632	HMDB0146627	NA	NA
633	HMDB0157134	NA	NA
634	HMDB0151225	NA	NA
635	HMDB0141158	NA	NA
636	HMDB0135643	NA	NA
637	HMDB0133755	NA	NA
638	HMDB0133594	NA	NA
639	HMDB0133595	NA	NA
640	HMDB0133504	NA	NA
641	HMDB0133598	NA	NA
642	HMDB0133599	NA	NA
643	HMDB0133596	NA	NA
644	HMDB0133747	NA	NA
645	HMDB0133748	NA	NA
646	HMDB0133597	NA	NA
647	HMDB0060335	1,2-Dihydronaphthalene-1,2-diol	HMDB0060335
648	HMDB0033830	Cassiastearoptene	HMDB0033830
649	HMDB0040577	NA	NA
650	HMDB0029714	4,5-Dihydro-1-benzoxepin-3(2H)-one	HMDB0029714
651	HMDB0033591	Safrole	HMDB0033591
652	HMDB0033833	Methyl cinnamate	HMDB0033833
653	HMDB0032611	3-(4-Methoxyphenyl)-2-propenal	HMDB0032611
654	HMDB0040592	NA	NA
655	HMDB0038893	NA	NA
656	HMDB0039655	NA	NA
657	HMDB0033763	Ethyl N-methylanthranilate	HMDB0033763
658	HMDB0040021	NA	NA
659	HMDB0030372	Maltotaxine	HMDB0030372
660	HMDB0041931	NA	NA
661	HMDB0001189	2(N)-Methyl-norsalsolinol	HMDB0001189
662	HMDB0005199	(R)-Salsolinol	HMDB0005199
663	HMDB0031811	3,5-Dimethylphenyl methylcarbamate	HMDB0031811
664	HMDB0042012	NA	NA
665	HMDB0029224	N-methylphenylalanine	HMDB0029224
666	HMDB0029223	alpha-Methylphenylalanine	HMDB0029223
667	HMDB0094790	NA	NA
668	HMDB0094799	NA	NA

669	HMDB0094784	NA	NA
670	HMDB0094786	NA	NA
671	HMDB0094787	NA	NA
672	HMDB0094793	NA	NA
673	HMDB0094785	NA	NA
674	HMDB0094782	NA	NA
675	HMDB0094780	NA	NA
676	HMDB0094783	NA	NA
677	HMDB0094788	NA	NA
678	HMDB0094789	NA	NA
679	HMDB0094791	NA	NA
680	HMDB0167323	NA	NA
681	HMDB0094800	NA	NA
682	HMDB0094796	NA	NA
683	HMDB0094797	NA	NA
684	HMDB0094798	NA	NA
685	HMDB0094794	NA	NA
686	HMDB0094792	NA	NA
687	HMDB0094795	NA	NA
688	HMDB0185183	NA	NA
689	HMDB0004063	Metanephrine	HMDB0004063
690	HMDB0036074	NA	NA
691	HMDB0060558	NA	NA
692	HMDB0154796	NA	NA
693	HMDB0062493	NA	NA
694	HMDB0094781	NA	NA
695	HMDB0033433	(S)-Homostachydrine	HMDB0033433
696	HMDB0014447	Tranexamic Acid	HMDB0014447
697	HMDB0000462	Allantoin	HMDB0000462
698	HMDB0170210	NA	NA
699	HMDB0170209	NA	NA
700	HMDB0038896	NA	NA
701	HMDB0033556	2,5-Dimethyl-1,4-dithiane-2,5-diol	HMDB0033556
702	HMDB0013858	3-Dechloroethylfosfamide	HMDB0013858
703	HMDB0060881	NA	NA
704	HMDB0013859	2-Dechloroethylfosfamide	HMDB0013859
705	HMDB0014480	Nitrofurazone	HMDB0014480
706	HMDB0062605	NA	NA
707	HMDB0134031	NA	NA
708	HMDB0141768	NA	NA
709	HMDB0141767	NA	NA
710	HMDB0134029	NA	NA
711	HMDB0134030	NA	NA
712	HMDB0126545	NA	NA
713	HMDB0128076	NA	NA
714	HMDB0062774	NA	NA
715	HMDB0125104	NA	NA
716	HMDB0129375	NA	NA
717	HMDB0166606	NA	NA
718	HMDB0163003	NA	NA
719	HMDB0041592	Coumaric acid	HMDB0041592
720	HMDB0030677	cis-p-Coumaric acid	HMDB0030677
721	HMDB0012225	Enol-phenylpyruvate	HMDB0012225
722	HMDB0001713	m-Coumaric acid	HMDB0001713
723	HMDB0002035	4-Hydroxycinnamic acid	HMDB0002035
724	HMDB0000205	Phenylpyruvic acid	HMDB0000205
725	HMDB0031629	NA	NA
726	HMDB0002641	2-Hydroxycinnamic acid	HMDB0002641
727	HMDB0062148	NA	NA
728	HMDB0062655	Cis-2-coumarate	HMDB0062655
729	HMDB0134028	NA	NA
730	HMDB0150719	NA	NA
731	HMDB0150717	NA	NA
732	HMDB0150718	NA	NA
733	HMDB0150716	NA	NA
734	HMDB0150720	NA	NA
735	HMDB0150715	NA	NA
736	HMDB0162085	NA	NA
737	HMDB0162086	NA	NA
738	HMDB0164039	NA	NA
739	HMDB0164040	NA	NA
740	HMDB0185178	NA	NA
741	HMDB0059720	NA	NA
742	HMDB0001119	4-Hydroxy-4-(3-pyridyl)-butanoic acid	HMDB0001119
743	HMDB0002184	L-Threo-3-Phenylserine	HMDB0002184
744	HMDB0003831	Beta-Tyrosine	HMDB0003831
745	HMDB0006050	o-Tyrosine	HMDB0006050
746	HMDB0060280	NA	NA
747	HMDB0000158	L-Tyrosine	HMDB0000158
748	HMDB0164171	NA	NA
749	HMDB0035177	2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepine-4-one	HMDB0035177
750	HMDB0155114	NA	NA
751	HMDB0155115	NA	NA
752	HMDB0155853	NA	NA
753	HMDB0185174	NA	NA
754	HMDB0185175	NA	NA
755	HMDB0185176	NA	NA

756	HMDB0185177	NA	NA
757	HMDB0155116	NA	NA
758	HMDB0000401	2,8-Dihydroxyadenine	HMDB0000401
759	HMDB0160079	NA	NA
760	HMDB0158555	NA	NA
761	HMDB0002032	8-Hydroxyguanine	HMDB0002032
762	HMDB0059918	NA	NA
763	HMDB0033532	Dimethicone	HMDB0033532
764	HMDB0042002	NA	NA
765	HMDB0131235	NA	NA
766	HMDB0131234	NA	NA
767	HMDB0131233	NA	NA
768	HMDB0151526	NA	NA
769	HMDB0151525	NA	NA
770	HMDB0180894	NA	NA
771	HMDB0126620	NA	NA
772	HMDB0240350	NA	NA
773	HMDB0001490	Vanylglycol	HMDB0001490
774	HMDB0040603	NA	NA
775	HMDB0035056	1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol	HMDB0035056
776	HMDB0036072	NA	NA
777	HMDB0039650	NA	NA
778	HMDB0059730	NA	NA
779	HMDB0180032	NA	NA
780	HMDB0125593	NA	NA
781	HMDB0125597	NA	NA
782	HMDB0126618	NA	NA
783	HMDB0126619	NA	NA
784	HMDB0033092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	HMDB0033092
785	HMDB0032306	4-Heptenal diethyl acetal	HMDB0032306
786	HMDB0041611	NA	NA
787	HMDB0180875	NA	NA
788	HMDB0062348	NA	NA
789	HMDB0168681	NA	NA
790	HMDB0168656	NA	NA
791	HMDB0168684	NA	NA
792	HMDB0168682	NA	NA
793	HMDB0168683	NA	NA
794	HMDB0171689	NA	NA
795	HMDB0177510	NA	NA
796	HMDB0180873	NA	NA
797	HMDB0180874	NA	NA
798	HMDB0180872	NA	NA
799	HMDB0240325	NA	NA
800	HMDB0124925	NA	NA
801	HMDB0167324	NA	NA
802	HMDB0166615	NA	NA
803	HMDB0166610	NA	NA
804	HMDB0125519	NA	NA
805	HMDB0125525	NA	NA
806	HMDB0125539	NA	NA
807	HMDB0134035	NA	NA
808	HMDB0134033	NA	NA
809	HMDB0134034	NA	NA
810	HMDB0134032	NA	NA
811	HMDB0134038	NA	NA
812	HMDB0134037	NA	NA
813	HMDB0134036	NA	NA
814	HMDB0137472	NA	NA
815	HMDB0141765	NA	NA
816	HMDB0141766	NA	NA
817	HMDB0142136	NA	NA
818	HMDB0166065	NA	NA
819	HMDB0032605	Methyl 2-methoxybenzoate	HMDB0032605
820	HMDB0033752	3-(2-Hydroxyphenyl)propanoic acid	HMDB0033752
821	HMDB0034243	Ipomeanine	HMDB0034243
822	HMDB0040645	NA	NA
823	HMDB0032030	Guaicyl acetate	HMDB0032030
824	HMDB0029665	Ethyl vanillin	HMDB0029665
825	HMDB0034993	4-Methoxybenzyl formate	HMDB0034993
826	HMDB0029817	Ethyl salicylate	HMDB0029817
827	HMDB0005175	Homovanillin	HMDB0005175
828	HMDB0032573	Ethylparaben	HMDB0032573
829	HMDB0032639	Methyl 4-methoxybenzoate	HMDB0032639
830	HMDB0031132	3,4-Dihydroxyphenylacetone	HMDB0031132
831	HMDB0062026	NA	NA
832	HMDB0059969	NA	NA
833	HMDB0062590	NA	NA
834	HMDB0041683	NA	NA
835	HMDB0142137	NA	NA
836	HMDB0032138	3,4-Dimethoxybenzaldehyde	HMDB0032138
837	HMDB0002229	3-Phenoxypropionic acid	HMDB0002229
838	HMDB0168657	NA	NA
839	HMDB0000375	3-(3-Hydroxyphenyl)propanoic acid	HMDB0000375
840	HMDB0000563	D-Phenyllactic acid	HMDB0000563
841	HMDB0002199	Desaminotyrosine	HMDB0002199
842	HMDB0000779	Phenyllactic acid	HMDB0000779

843	HMDB0002072	4-Methoxyphenylacetic acid	HMDB0002072
844	HMDB0000748	L-3-Phenyllactic acid	HMDB0000748
845	HMDB0185611	NA	NA
846	HMDB0185616	NA	NA
847	HMDB0185609	NA	NA
848	HMDB0185610	NA	NA
849	HMDB0185613	NA	NA
850	HMDB0035291	Isoplumbagin	HMDB0035291
851	HMDB0166096	NA	NA
852	HMDB0029472	Isoeugenitol	HMDB0029472
853	HMDB0029466	Eugenitol	HMDB0029466
854	HMDB0032952	Citropten	HMDB0032952
855	HMDB0036627	NA	NA
856	HMDB0030818	Scoparone	HMDB0030818
857	HMDB0136785	NA	NA
858	HMDB0136786	NA	NA
859	HMDB0181531	NA	NA
860	HMDB0136784	NA	NA
861	HMDB0035303	3-Methoxy-4,5-methylenedioxycinnamaldehyde	HMDB0035303
862	HMDB0029775	Vinyl caffeate	HMDB0029775
863	HMDB0181534	NA	NA
864	HMDB0181532	NA	NA
865	HMDB0181533	NA	NA
866	HMDB0129368	NA	NA
867	HMDB0036187	NA	NA
868	HMDB0032414	2-Methyl-3 or 5 or 6-(furfurylthio)pyrazine (mixture of isomers)	HMDB0032414
869	HMDB0038791	NA	NA
870	HMDB0033584	Diethyl tartrate	HMDB0033584
871	HMDB0059767	NA	NA
872	HMDB0157322	NA	NA
873	HMDB0157321	NA	NA
874	HMDB0157320	NA	NA
875	HMDB0157323	NA	NA
876	HMDB0157324	NA	NA
877	HMDB0029416	L-Targinine	HMDB0029416
878	HMDB0000670	Homo-L-arginine	HMDB0000670
879	HMDB0015454	Rasagiline	HMDB0015454
880	HMDB0032926	Polycartine B	HMDB0032926
881	HMDB0005973	Dimethyltryptamine	HMDB0005973
882	HMDB0033961	2-(3-Methylbutyl)-1H-pyrrolo[2,3-b]pyridine	HMDB0033961
883	HMDB0061284	NA	NA
884	HMDB0001892	Menadione	HMDB0001892
885	HMDB0033765	Methyl (Z)-2-decene-4,6,8-trienoate	HMDB0033765
886	HMDB0061682	NA	NA
887	HMDB0060608	NA	NA
888	HMDB0163574	NA	NA
889	HMDB0163573	NA	NA
890	HMDB0162439	NA	NA
891	HMDB0165489	NA	NA
892	HMDB0002042	3-Phenylpropionylglycine	HMDB0002042
893	HMDB0000860	Phenylpropionylglycine	HMDB0000860
894	HMDB0000512	N-Acetyl-L-phenylalanine	HMDB0000512
895	HMDB0165491	NA	NA
896	HMDB0015165	Ethinamate	HMDB0015165
897	HMDB0167325	NA	NA
898	HMDB0002182	Phenylephrine	HMDB0002182
899	HMDB0062266	NA	NA
900	HMDB0014748	Metaraminol	HMDB0014748
901	HMDB0060592	NA	NA
902	HMDB0060807	NA	NA
903	HMDB0032020	4-(beta-Methylaminoethyl)catechol	HMDB0032020
904	HMDB0041888	NA	NA
905	HMDB0062811	NA	NA
906	HMDB0039837	NA	NA
907	HMDB0038869	NA	NA
908	HMDB0000022	3-Methoxytyramine	HMDB0000022
909	HMDB0004826	p-Syneprine	HMDB0004826
910	HMDB0012162	4-Methoxytyramine	HMDB0012162
911	HMDB0094703	Propanoic acid, 2-(methoxyimino)-, trimethylsilyl ester	HMDB0094703
912	HMDB0012286	S-Prenyl-L-cysteine	HMDB0012286
913	HMDB0169421	NA	NA
914	HMDB0163468	NA	NA
915	HMDB0163469	NA	NA
916	HMDB0179168	NA	NA
917	HMDB0163465	NA	NA
918	HMDB0163466	NA	NA
919	HMDB0094711	NA	NA
920	HMDB0059936	NA	NA
921	HMDB0062081	NA	NA
922	HMDB0060287	NA	NA
923	HMDB0059937	NA	NA
924	HMDB0036396	NA	NA
925	HMDB0040165	NA	NA
926	HMDB0036188	NA	NA
927	HMDB0036213	NA	NA
928	HMDB0040203	NA	NA
929	HMDB0040202	NA	NA

930	HMDB0163470	NA	NA
931	HMDB0151316	NA	NA
932	HMDB0151313	NA	NA
933	HMDB0166861	NA	NA
934	HMDB0157325	NA	NA
935	HMDB0157326	NA	NA
936	HMDB0000325	3-Hydroxysuberlic acid	HMDB0000325
937	HMDB0040220	NA	NA
938	HMDB0061681	NA	NA
939	HMDB0029968	Ethyl beta-D-glucopyranoside	HMDB0029968
940	HMDB0033942	Dambonitol	HMDB0033942
941	HMDB0032329	2-Hexylthiophene	HMDB0032329
942	HMDB0060323	NA	NA
943	HMDB0003066	Chalcone	HMDB0003066
944	HMDB0135598	NA	NA
945	HMDB0031016	10-Undecen-1-ol	HMDB0031016
946	HMDB0032371	1-Menthyl methyl ether	HMDB0032371
947	HMDB0030943	6-Undecanone	HMDB0030943
948	HMDB0032379	trans- and cis-1-Methoxy-1-decene	HMDB0032379
949	HMDB0163244	NA	NA
950	HMDB0030941	Undecanal	HMDB0030941
951	HMDB0031065	( <i>Á</i> )-( <i>E</i> )-3-Methyl-4-decen-1-ol	HMDB0031065
952	HMDB0031064	( <i>Z</i> )-3-Methyl-3-decen-1-ol	HMDB0031064
953	HMDB0033713	2-Undecanone	HMDB0033713
954	HMDB0034856	2-Undecen-1-ol	HMDB0034856
955	HMDB0014631	Altretamine	HMDB0014631
956	HMDB0041615	NA	NA
957	HMDB0035753	( <i>R</i> )-( <i>E</i> )-4,7-Megastigmadien-9-one	HMDB0035753
958	HMDB0034959	Egulan I	HMDB0034959
959	HMDB0036818	NA	NA
960	HMDB0036144	NA	NA
961	HMDB0151804	NA	NA
962	HMDB0034979	gamma-Ionone	HMDB0034979
963	HMDB0029822	2,5-Diisopropyl-3-methylphenol	HMDB0029822
964	HMDB0029824	2,4-Diisopropyl-3-methylphenol	HMDB0029824
965	HMDB0032541	4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one	HMDB0032541
966	HMDB0029821	2,5-Diisopropyl-4-methylphenol	HMDB0029821
967	HMDB0036565	NA	NA
968	HMDB0033545	(2 <i>E</i> ,4 <i>Z</i> ,7 <i>Z</i> )-2,4,7-Tridecatrienal	HMDB0033545
969	HMDB0035682	delta-Damascone	HMDB0035682
970	HMDB0034671	( <i>E</i> )-5,8-Megastigmadien-4-one	HMDB0034671
971	HMDB0036027	alpha-Damascone	HMDB0036027
972	HMDB0037139	NA	NA
973	HMDB0032498	Pseudoionone	HMDB0032498
974	HMDB0036022	Isopiprene	HMDB0036022
975	HMDB0031733	4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde	HMDB0031733
976	HMDB0029823	2,4-Diisopropyl-5-methylphenol	HMDB0029823
977	HMDB0036684	NA	NA
978	HMDB0029825	2,3-Diisopropyl-5-methylphenol	HMDB0029825
979	HMDB0059883	NA	NA
980	HMDB0029820	2,6-Diisopropyl-3-methylphenol	HMDB0029820
981	HMDB0014018	4-Hydroxypropofol	HMDB0014018
982	HMDB0037389	NA	NA
983	HMDB0038292	NA	NA
984	HMDB0040439	NA	NA
985	HMDB0039685	NA	NA
986	HMDB0041497	NA	NA
987	HMDB0031840	( <i>S,Z</i> )-Lyratol acetate	HMDB0031840
988	HMDB0035801	(2 <i>S</i> ,4 <i>R</i> )- <i>p</i> -Mentha-1(7),5-dien-2-ol acetate	HMDB0035801
989	HMDB0035375	Ethyl (2 <i>E</i> ,4 <i>E</i> ,7 <i>Z</i> )-Decatrienoate	HMDB0035375
990	HMDB0035376	Ethyl (2 <i>E</i> ,4 <i>Z</i> ,7 <i>Z</i> )-Decatrienoate	HMDB0035376
991	HMDB0132986	NA	NA
992	HMDB0034450	Neocnidilide	HMDB0034450
993	HMDB0032567	Hexylresorcinol	HMDB0032567
994	HMDB0035126	( <i>Á</i> )-Myrtenyl acetate	HMDB0035126
995	HMDB0041610	NA	NA
996	HMDB0038046	NA	NA
997	HMDB0037018	NA	NA
998	HMDB0037231	NA	NA
999	HMDB0035085	Vulgarole	HMDB0035085
1000	HMDB0041572	NA	NA
1001	HMDB0029388	Cucurbitic acid	HMDB0029388
1002	HMDB0037326	NA	NA
1003	HMDB0033601	Dihydrojasmonic acid	HMDB0033601
1004	HMDB0040195	NA	NA
1005	HMDB0035723	(1 <i>R</i> ,2 <i>S</i> ,3 <i>S</i> ,4 <i>R</i> )- <i>p</i> -Menthane-2,3-diol	HMDB0035723
1006	HMDB0034457	Propyl heptanoate	HMDB0034457
1007	HMDB0061987	NA	NA
1008	HMDB0062146	NA	NA
1009	HMDB0038038	NA	NA
1010	HMDB0036228	2-Methylpropyl hexanoate	HMDB0036228
1011	HMDB0040167	NA	NA
1012	HMDB0036136	NA	NA
1013	HMDB0187563	NA	NA
1014	HMDB0037387	NA	NA
1015	HMDB0000511	Capric acid	HMDB0000511
1016	HMDB0031264	Methyl nonanoate	HMDB0031264

1017	HMDB0094654	1-Methylethyl heptanoic acid	HMDB0094654
1018	HMDB0171179	NA	NA
1019	HMDB0171178	NA	NA
1020	HMDB0171177	NA	NA
1021	HMDB0171176	NA	NA
1022	HMDB0179213	NA	NA
1023	HMDB0179212	NA	NA
1024	HMDB0179927	NA	NA
1025	HMDB0180500	NA	NA
1026	HMDB0180498	NA	NA
1027	HMDB0180499	NA	NA
1028	HMDB0180497	NA	NA
1029	HMDB0180502	NA	NA
1030	HMDB0180501	NA	NA
1031	HMDB0180503	NA	NA
1032	HMDB0180504	NA	NA
1033	HMDB0171175	NA	NA
1034	HMDB0061805	NA	NA
1035	HMDB0180097	NA	NA
1036	HMDB0032302	Heptanal propyleneglycol acetal	HMDB0032302
1037	HMDB0032155	Acetaldehyde 1,3-octanediol acetal	HMDB0032155
1038	HMDB0032264	Ethyl 2-ethylhexanoate	HMDB0032264
1039	HMDB0032315	Hexanal butane-2,3-diol acetal	HMDB0032315
1040	HMDB0032045	Pentyl 3-methylbutanoate	HMDB0032045
1041	HMDB0041216	NA	NA
1042	HMDB0034849	4-Methylnonanoic acid	HMDB0034849
1043	HMDB0037849	Hexyl 2-methylpropanoate	HMDB0037849
1044	HMDB0040157	NA	NA
1045	HMDB0033620	Hexyl butyrate	HMDB0033620
1046	HMDB0035595	trans-p-Menthane-1,8-diol	HMDB0035595
1047	HMDB0029760	1,1-Diethoxy-2-hexene	HMDB0029760
1048	HMDB0032070	Isooctyl acetate	HMDB0032070
1049	HMDB0040211	NA	NA
1050	HMDB0040529	NA	NA
1051	HMDB0038783	NA	NA
1052	HMDB0036145	NA	NA
1053	HMDB0039218	NA	NA
1054	HMDB0038602	Octyl acetate	HMDB0038602
1055	HMDB0030029	Isopentyl isopentanoate	HMDB0030029
1056	HMDB0031739	7-Hydroxy-3,7-dimethyloctanal	HMDB0031739
1057	HMDB0014362	Bethanidine	HMDB0014362
1058	HMDB0155301	NA	NA
1059	HMDB0060602	N-acetyl-5-aminosalicylic acid	HMDB0060602
1060	HMDB0030726	2-Hydroxy-6,7-dimethoxybenzoxazole	HMDB0030726
1061	HMDB0004067	Leucodopachrome	HMDB0004067
1062	HMDB0002404	Alpha-Hydroxyhippuric acid	HMDB0002404
1063	HMDB0002016	4-Carboxyphenylglycine	HMDB0002016
1064	HMDB0001229	Dopaquinone	HMDB0001229
1065	HMDB0000840	Salicyluric acid	HMDB0000840
1066	HMDB0183407	NA	NA
1067	HMDB0184100	NA	NA
1068	HMDB0006116	3-Hydroxyhippuric acid	HMDB0006116
1069	HMDB0166076	NA	NA
1070	HMDB0038055	NA	NA
1071	HMDB0039119	NA	NA
1072	HMDB0013678	4-Hydroxyhippuric acid	HMDB0013678
1073	HMDB0166113	NA	NA
1074	HMDB0141198	NA	NA
1075	HMDB0136739	NA	NA
1076	HMDB0030819	Aesculetin	HMDB0030819
1077	HMDB0141200	NA	NA
1078	HMDB0141199	NA	NA
1079	HMDB0032951	4,7-Dihydroxy-2H-1-benzopyran-2-one	HMDB0032951
1080	HMDB0032950	5,7-Dihydroxy-4H-1-benzopyran-4-one	HMDB0032950
1081	HMDB0130547	NA	NA
1082	HMDB0141201	NA	NA
1083	HMDB0136740	NA	NA
1084	HMDB0015627	Droxidopa	HMDB0015627
1085	HMDB0159157	NA	NA
1086	HMDB0159158	NA	NA
1087	HMDB0159159	NA	NA
1088	HMDB0006488	N-Acetyl-L-glutamate 5-semialdehyde	HMDB0006488
1089	HMDB0031162	3,3'-Thiobispropanoic acid	HMDB0031162
1090	HMDB0179354	NA	NA
1091	HMDB0240388	NA	NA
1092	HMDB0165618	NA	NA
1093	HMDB0000904	Citrulline	HMDB0000904
1094	HMDB0003148	Argininic acid	HMDB0003148
1095	HMDB0003269	Nicotinuric acid	HMDB0003269
1096	HMDB0164043	NA	NA
1097	HMDB0176142	NA	NA
1098	HMDB0041912	NA	NA
1099	HMDB0059766	NA	NA
1100	HMDB0032055	N-Acetylhistidine	HMDB0032055
1101	HMDB0162075	NA	NA
1102	HMDB0094728	NA	NA
1103	HMDB0094729	NA	NA

1104	HMDB0006348	Pseudoecgonine	HMDB0006348
1105	HMDB0006548	Ecgonine	HMDB0006548
1106	HMDB0094730	NA	NA
1107	HMDB0094731	NA	NA
1108	HMDB0163437	NA	NA
1109	HMDB0028691	Alanyl-Leucine	HMDB0028691
1110	HMDB0028922	Leucyl-Alanine	HMDB0028922
1111	HMDB0028690	Alanyl-Isoleucine	HMDB0028690
1112	HMDB0163436	NA	NA
1113	HMDB0094713	NA	NA
1114	HMDB0163435	NA	NA
1115	HMDB0163440	NA	NA
1116	HMDB0028900	Isoleucyl-Alanine	HMDB0028900
1117	HMDB0039590	NA	NA
1118	HMDB0039339	NA	NA
1119	HMDB0032531	2-trans-6-cis-Dodecadienal	HMDB0032531
1120	HMDB0038108	NA	NA
1121	HMDB0031181	Homodihydrojasmane	HMDB0031181
1122	HMDB0014410	Crotamiton	HMDB0014410
1123	HMDB0151779	NA	NA
1124	HMDB0030931	(E)-2-Tridecene-4,6,8-triyn-1-ol	HMDB0030931
1125	HMDB0038526	NA	NA
1126	HMDB0060850	NA	NA
1127	HMDB0030305	Dioscorine	HMDB0030305
1128	HMDB0037896	NA	NA
1129	HMDB0032273	N-Ethyl trans-2-cis-6-nonadienamide	HMDB0032273
1130	HMDB0037889	NA	NA
1131	HMDB0037897	NA	NA
1132	HMDB0037890	NA	NA
1133	HMDB0037895	NA	NA
1134	HMDB0037894	NA	NA
1135	HMDB0037891	NA	NA
1136	HMDB0032205	cis- and trans-L-Mercapto-p-menthan-3-one	HMDB0032205
1137	HMDB0037385	NA	NA
1138	HMDB0030216	Mukonal	HMDB0030216
1139	HMDB0161787	NA	NA
1140	HMDB0030195	gamma-Fagarine	HMDB0030195
1141	HMDB0037614	NA	NA
1142	HMDB0029419	Glycylglycylglycine	HMDB0029419
1143	HMDB0028836	Glycyl-Asparagine	HMDB0028836
1144	HMDB0028731	Asparaginylnl-Glycine	HMDB0028731
1145	HMDB0041613	NA	NA
1146	HMDB0041614	NA	NA
1147	HMDB0030143	Talaromycin A	HMDB0030143
1148	HMDB0000623	Dodecanedioic acid	HMDB0000623
1149	HMDB0240291	NA	NA
1150	HMDB0000832	Capryloylglycine	HMDB0000832
1151	HMDB0013116	Valproylglycine	HMDB0013116
1152	HMDB0041540	NA	NA
1153	HMDB0059745	NA	NA
1154	HMDB0036172	NA	NA
1155	HMDB0032247	(Z)-4-Dodecenal	HMDB0032247
1156	HMDB0041404	NA	NA
1157	HMDB0037275	NA	NA
1158	HMDB0041490	NA	NA
1159	HMDB0163217	NA	NA
1160	HMDB0134122	NA	NA
1161	HMDB0134121	NA	NA
1162	HMDB0094674	NA	NA
1163	HMDB0035643	beta-Sinensal	HMDB0035643
1164	HMDB0038164	NA	NA
1165	HMDB0036201	NA	NA
1166	HMDB0038187	NA	NA
1167	HMDB0036797	NA	NA
1168	HMDB0036733	NA	NA
1169	HMDB0036667	NA	NA
1170	HMDB0036813	NA	NA
1171	HMDB0035081	(5alpha,10alpha)-3,7(11)-Eudesmadien-2-one	HMDB0035081
1172	HMDB0036718	NA	NA
1173	HMDB0036109	NA	NA
1174	HMDB0035747	Patchoulenone	HMDB0035747
1175	HMDB0040686	NA	NA
1176	HMDB0037000	NA	NA
1177	HMDB0038195	NA	NA
1178	HMDB0038201	NA	NA
1179	HMDB0038215	NA	NA
1180	HMDB0038200	NA	NA
1181	HMDB0038511	NA	NA
1182	HMDB0013687	Nookatone	HMDB0013687
1183	HMDB0035657	Solavetivone	HMDB0035657
1184	HMDB0035786	Valerenal	HMDB0035786
1185	HMDB0037061	NA	NA
1186	HMDB0035835	Furanoeremophilane	HMDB0035835
1187	HMDB0037068	NA	NA
1188	HMDB0039637	NA	NA
1189	HMDB0036071	NA	NA
1190	HMDB0036443	NA	NA

1191	HMDB0035082	(5beta,7beta,10beta)-3,11-Eudesmadien-2-one	HMDB0035082
1192	HMDB0013693	Sinensal	HMDB0013693
1193	HMDB0000210	Pantothenic acid	HMDB0000210
1194	HMDB0062717	NA	NA
1195	HMDB0062766	4-ethylamino-6-isopropylamino-1,3,5-triazin-2-ol	HMDB0062766
1196	HMDB0035175	2-Amino-1,6-dimethylfuro[3,2-e]imidazo[4,5-b]pyridine	HMDB0035175
1197	HMDB0012204	Cis-zeatin	HMDB0012204
1198	HMDB0040032	NA	NA
1199	HMDB0001539	Asymmetric dimethylarginine	HMDB0001539
1200	HMDB0003334	Symmetric dimethylarginine	HMDB0003334
1201	HMDB0039274	NA	NA
1202	HMDB0030838	Feniculn	HMDB0030838
1203	HMDB0030572	(Âš)-Anisoxide	HMDB0030572
1204	HMDB0039356	NA	NA
1205	HMDB0031313	2-Pentyl-3-phenyl-2-propenal	HMDB0031313
1206	HMDB0061830	NA	NA
1207	HMDB0181581	NA	NA
1208	HMDB0028797	Glutaminyglycine	HMDB0028797
1209	HMDB0028682	Alanyl-Asparagine	HMDB0028682
1210	HMDB0028724	Asparaginy-Alanine	HMDB0028724
1211	HMDB0028855	Glycyl-Gamma-glutamate	HMDB0028855
1212	HMDB0028839	Glycyl-Glutamine	HMDB0028839
1213	HMDB0033191	2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	HMDB0033191
1214	HMDB0150426	NA	NA
1215	HMDB0034046	1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene	HMDB0034046
1216	HMDB0037492	NA	NA
1217	HMDB0040424	NA	NA
1218	HMDB0061823	NA	NA
1219	HMDB0061942	NA	NA
1220	HMDB0032589	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	HMDB0032589
1221	HMDB0132937	NA	NA
1222	HMDB0132935	NA	NA
1223	HMDB0132936	NA	NA
1224	HMDB0132939	NA	NA
1225	HMDB0132948	NA	NA
1226	HMDB0151796	NA	NA
1227	HMDB0151797	NA	NA
1228	HMDB0151800	NA	NA
1229	HMDB0151798	NA	NA
1230	HMDB0151799	NA	NA
1231	HMDB0151801	NA	NA
1232	HMDB0132933	NA	NA
1233	HMDB0151802	NA	NA
1234	HMDB0035593	Rishitin	HMDB0035593
1235	HMDB0037605	NA	NA
1236	HMDB0036790	NA	NA
1237	HMDB0036791	NA	NA
1238	HMDB0037820	NA	NA
1239	HMDB0040178	NA	NA
1240	HMDB0160293	NA	NA
1241	HMDB0160295	NA	NA
1242	HMDB0160291	NA	NA
1243	HMDB0160290	NA	NA
1244	HMDB0160289	NA	NA
1245	HMDB0160292	NA	NA
1246	HMDB0160296	NA	NA
1247	HMDB0160294	NA	NA
1248	HMDB0160298	NA	NA
1249	HMDB0160297	NA	NA
1250	HMDB0032369	L-Menthyl acetoacetate	HMDB0032369
1251	HMDB0033619	Hexyl hexanoate	HMDB0033619
1252	HMDB0059868	NA	NA
1253	HMDB0032440	Nonanal propyleneglycol acetal	HMDB0032440
1254	HMDB0061988	NA	NA
1255	HMDB0035410	(R)-Dihydrocitronellol acetate	HMDB0035410
1256	HMDB0000638	Dodecanoic acid	HMDB0000638
1257	HMDB0040166	NA	NA
1258	HMDB0030998	Ethyl decanoate	HMDB0030998
1259	HMDB0034137	Octyl 2-methylpropanoate	HMDB0034137
1260	HMDB0036225	NA	NA
1261	HMDB0034136	Octyl butanoate	HMDB0034136
1262	HMDB0034128	Isopropyl nonanoate	HMDB0034128
1263	HMDB0032310	2-Heptyl butyrate	HMDB0032310
1264	HMDB0168119	NA	NA
1265	HMDB0168120	NA	NA
1266	HMDB0168121	NA	NA
1267	HMDB0015050	Phenformin	HMDB0015050
1268	HMDB0004231	Pantothenol	HMDB0004231
1269	HMDB0061683	NA	NA
1270	HMDB0031813	N-Carbamoyl-2-amino-2-(4-hydroxyphenyl)acetic acid	HMDB0031813
1271	HMDB0000014	Deoxycytidine	HMDB0000014
1272	HMDB0028732	Asparaginy-Hydroxyproline	HMDB0028732
1273	HMDB0028858	Hydroxypropyl-Asparagine	HMDB0028858
1274	HMDB0040046	NA	NA
1275	HMDB0161863	NA	NA
1276	HMDB0161860	NA	NA
1277	HMDB0041444	NA	NA



1278	HMDB0033452	Koenoline	HMDB0033452
1279	HMDB0161862	NA	NA
1280	HMDB0161861	NA	NA
1281	HMDB0161859	NA	NA
1282	HMDB0161858	NA	NA
1283	HMDB0161857	NA	NA
1284	HMDB0015614	Ibudilast	HMDB0015614
1285	HMDB0060531	NA	NA
1286	HMDB0015493	Aminophenazone	HMDB0015493
1287	HMDB0030310	Harmaline	HMDB0030310
1288	HMDB0042058	NA	NA
1289	HMDB0060963	NA	NA
1290	HMDB0014917	Nalidixic Acid	HMDB0014917
1291	HMDB0240661	NA	NA
1292	HMDB0015305	Phenobarbital	HMDB0015305
1293	HMDB0061316	NA	NA
1294	HMDB0183400	NA	NA
1295	HMDB0240342	NA	NA
1296	HMDB0183397	NA	NA
1297	HMDB0183398	NA	NA
1298	HMDB0032041	1,3-Diphenyl-1-propanone	HMDB0032041
1299	HMDB0035896	Lactarviolin	HMDB0035896
1300	HMDB0032561	1,3-Diphenyl-2-propanone	HMDB0032561
1301	HMDB0059660	NA	NA
1302	HMDB0000114	Glycerylphosphorylethanolamine	HMDB0000114
1303	HMDB0015441	Aprobarbital	HMDB0015441
1304	HMDB0028983	Methionyl-Threonine	HMDB0028983
1305	HMDB0029067	Threoninyl-Methionine	HMDB0029067
1306	HMDB0060324	NA	NA
1307	HMDB0013279	N-Nonanoylglycine	HMDB0013279
1308	HMDB0032526	(Z)-8-Tetradecenal	HMDB0032526
1309	HMDB0032525	Tetradec-2-enal	HMDB0032525
1310	HMDB0029704	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadien-3-one	HMDB0029704
1311	HMDB0159344	NA	NA
1312	HMDB0240361	NA	NA
1313	HMDB0061952	NA	NA
1314	HMDB0035293	Norambreinolide	HMDB0035293
1315	HMDB0037631	NA	NA
1316	HMDB0037712	NA	NA
1317	HMDB0142471	NA	NA
1318	HMDB0140099	NA	NA
1319	HMDB0003254	Muramic acid	HMDB0003254
1320	HMDB0038662	NA	NA
1321	HMDB0168958	NA	NA
1322	HMDB0035923	Hirsutin	HMDB0035923
1323	HMDB0168517	NA	NA
1324	HMDB0000101	Deoxyadenosine	HMDB0000101
1325	HMDB0001983	5'-Deoxyadenosine	HMDB0001983
1326	HMDB0060974	NA	NA
1327	HMDB0060618	NA	NA
1328	HMDB0004821	Bisnorbiotin	HMDB0004821
1329	HMDB0035232	Rotundine B	HMDB0035232
1330	HMDB0162810	NA	NA
1331	HMDB0036589	NA	NA
1332	HMDB0035965	5beta-1,3,7(11)-Eudesmatrien-8-one	HMDB0035965
1333	HMDB0038147	NA	NA
1334	HMDB0031736	2-Hexyl-3-phenyl-2-propenal	HMDB0031736
1335	HMDB0036769	NA	NA
1336	HMDB0035612	(R)-ar-Turmerone	HMDB0035612
1337	HMDB0036108	NA	NA
1338	HMDB0059863	NA	NA
1339	HMDB0240643	NA	NA
1340	HMDB0134142	NA	NA
1341	HMDB0134140	NA	NA
1342	HMDB0134141	NA	NA
1343	HMDB0134143	NA	NA
1344	HMDB0134153	NA	NA
1345	HMDB0150675	NA	NA
1346	HMDB0177624	NA	NA
1347	HMDB0177700	NA	NA
1348	HMDB0183493	NA	NA
1349	HMDB0134137	NA	NA
1350	HMDB0134139	NA	NA
1351	HMDB0134131	NA	NA
1352	HMDB0134135	NA	NA
1353	HMDB0134132	NA	NA
1354	HMDB0134134	NA	NA
1355	HMDB0134133	NA	NA
1356	HMDB0134136	NA	NA
1357	HMDB0134138	NA	NA
1358	HMDB0036466	NA	NA
1359	HMDB0036647	NA	NA
1360	HMDB0038698	NA	NA
1361	HMDB0037710	NA	NA
1362	HMDB0035639	Petasalbin	HMDB0035639
1363	HMDB0037391	NA	NA
1364	HMDB0038190	NA	NA

1365	HMDB0038795	NA	NA
1366	HMDB0036390	NA	NA
1367	HMDB0033252	Curcumanolide A	HMDB0033252
1368	HMDB0035408	1,10-Epoxygermacrone	HMDB0035408
1369	HMDB0039621	NA	NA
1370	HMDB0034562	9-Pentadecene-12,14-diyne-1,11-diol	HMDB0034562
1371	HMDB0036449	NA	NA
1372	HMDB0033960	Curcumenol	HMDB0033960
1373	HMDB0035935	Dihydroisoalantolactone	HMDB0035935
1374	HMDB0031349	Epiacoronene	HMDB0031349
1375	HMDB0035413	(4alpha,5alpha)-11-Eremophilene-2,9-dione	HMDB0035413
1376	HMDB0036392	NA	NA
1377	HMDB0034956	Oxysolavetivone	HMDB0034956
1378	HMDB0035869	alpha-Rotunol	HMDB0035869
1379	HMDB0038914	NA	NA
1380	HMDB0041036	NA	NA
1381	HMDB0037739	NA	NA
1382	HMDB0036427	NA	NA
1383	HMDB0035794	beta-Costic acid	HMDB0035794
1384	HMDB0035889	Germacrone 4,5-epoxide	HMDB0035889
1385	HMDB0036035	Marasmene	HMDB0036035
1386	HMDB0038796	NA	NA
1387	HMDB0034742	Saussurea lactone	HMDB0034742
1388	HMDB0033253	Curcumenone	HMDB0033253
1389	HMDB0030016	Valerenic acid	HMDB0030016
1390	HMDB0037640	NA	NA
1391	HMDB0035202	7-Hydroxycostal	HMDB0035202
1392	HMDB0038198	NA	NA
1393	HMDB0037038	NA	NA
1394	HMDB0035407	Dehydrocurdione	HMDB0035407
1395	HMDB0032081	4,10-Longipinanedione	HMDB0032081
1396	HMDB0179139	NA	NA
1397	HMDB0112094	NA	NA
1398	HMDB0179145	NA	NA
1399	HMDB0179147	NA	NA
1400	HMDB0179146	NA	NA
1401	HMDB0179257	NA	NA
1402	HMDB0179258	NA	NA
1403	HMDB0179268	NA	NA
1404	HMDB0179269	NA	NA
1405	HMDB0179266	NA	NA
1406	HMDB0179267	NA	NA
1407	HMDB0179272	NA	NA
1408	HMDB0179271	NA	NA
1409	HMDB0179148	NA	NA
1410	HMDB0179143	NA	NA
1411	HMDB0112086	NA	NA
1412	HMDB0168751	NA	NA
1413	HMDB0177221	NA	NA
1414	HMDB0179140	NA	NA
1415	HMDB0179142	NA	NA
1416	HMDB0179141	NA	NA
1417	HMDB0179273	NA	NA
1418	HMDB0179270	NA	NA
1419	HMDB0183498	NA	NA
1420	HMDB0183500	NA	NA
1421	HMDB0184273	NA	NA
1422	HMDB0184275	NA	NA
1423	HMDB0183495	NA	NA
1424	HMDB0183496	NA	NA
1425	HMDB0182315	NA	NA
1426	HMDB0182313	NA	NA
1427	HMDB0182314	NA	NA
1428	HMDB0182312	NA	NA
1429	HMDB0182319	NA	NA
1430	HMDB0182316	NA	NA
1431	HMDB0182318	NA	NA
1432	HMDB0182317	NA	NA
1433	HMDB0182321	NA	NA
1434	HMDB0182320	NA	NA
1435	HMDB0040685	NA	NA
1436	HMDB0035597	alpha-Carissanol	HMDB0035597
1437	HMDB0030918	1-Hydroxyepiacorone	HMDB0030918
1438	HMDB0030919	Acorusdiol	HMDB0030919
1439	HMDB0036663	NA	NA
1440	HMDB0038502	NA	NA
1441	HMDB0035309	6alpha-Carissanol	HMDB0035309
1442	HMDB0033149	(4R,5S,7R,11R)-11,12-Dihydroxy-1(10)-spirovetiven-2-one	HMDB0033149
1443	HMDB0036448	NA	NA
1444	HMDB0035767	Piperalol	HMDB0035767
1445	HMDB0034574	Apotrichodiol	HMDB0034574
1446	HMDB0035613	Epioxylubimin	HMDB0035613
1447	HMDB0037063	NA	NA
1448	HMDB0032122	3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol	HMDB0032122
1449	HMDB0037969	NA	NA
1450	HMDB0035729	Dihydromyoporone	HMDB0035729
1451	HMDB0179144	NA	NA

1452	HMDB0032792	(Ás)-(E)-3-Methyl-4-decen-1-yl acetate	HMDB0032792
1453	HMDB0031028	Methyl (E)-2-dodecenoate	HMDB0031028
1454	HMDB0038078	NA	NA
1455	HMDB0037626	NA	NA
1456	HMDB0031017	10-Undecenyl acetate	HMDB0031017
1457	HMDB0034286	Ethyl 10-undecenoate	HMDB0034286
1458	HMDB0040451	NA	NA
1459	HMDB0037907	NA	NA
1460	HMDB0037226	NA	NA
1461	HMDB0039805	NA	NA
1462	HMDB0037187	NA	NA
1463	HMDB0031741	Coniferan	HMDB0031741
1464	HMDB0000824	Propionylcarnitine	HMDB0000824
1465	HMDB0062514	NA	NA
1466	HMDB0240784	NA	NA
1467	HMDB0059946	NA	NA
1468	HMDB0041618	NA	NA
1469	HMDB0176325	NA	NA
1470	HMDB0059947	NA	NA
1471	HMDB0176328	NA	NA
1472	HMDB0000872	Tetradecanedioic acid	HMDB0000872
1473	HMDB0176327	NA	NA
1474	HMDB0040429	NA	NA
1475	HMDB0176326	NA	NA
1476	HMDB0040219	NA	NA
1477	HMDB0060002	NA	NA
1478	HMDB0240658	NA	NA
1479	HMDB0240657	NA	NA
1480	HMDB0006512	3-Mercaptolactate-cysteine disulfide	HMDB0006512
1481	HMDB0169467	NA	NA
1482	HMDB0169468	NA	NA
1483	HMDB0169469	NA	NA
1484	HMDB0172924	NA	NA
1485	HMDB0172927	NA	NA
1486	HMDB0040349	NA	NA
1487	HMDB0152315	NA	NA
1488	HMDB0142172	NA	NA
1489	HMDB0142174	NA	NA
1490	HMDB0146404	NA	NA
1491	HMDB0146402	NA	NA
1492	HMDB0149145	NA	NA
1493	HMDB0146405	NA	NA
1494	HMDB0146406	NA	NA
1495	HMDB0146407	NA	NA
1496	HMDB0149144	NA	NA
1497	HMDB0149143	NA	NA
1498	HMDB0142171	NA	NA
1499	HMDB0142170	NA	NA
1500	HMDB0128183	NA	NA
1501	HMDB0128665	NA	NA
1502	HMDB0128667	NA	NA
1503	HMDB0128668	NA	NA
1504	HMDB0128674	NA	NA
1505	HMDB0128673	NA	NA
1506	HMDB0137280	NA	NA
1507	HMDB0137283	NA	NA
1508	HMDB0137284	NA	NA
1509	HMDB0137291	NA	NA
1510	HMDB0137290	NA	NA
1511	HMDB0141325	NA	NA
1512	HMDB0142075	NA	NA
1513	HMDB0142076	NA	NA
1514	HMDB0142169	NA	NA
1515	HMDB0179746	NA	NA
1516	HMDB0142173	NA	NA
1517	HMDB0041691	NA	NA
1518	HMDB0030018	Elenolide	HMDB0030018
1519	HMDB0140920	NA	NA
1520	HMDB0032616	Sinapic acid	HMDB0032616
1521	HMDB0034069	cis-Sinapic acid	HMDB0034069
1522	HMDB0127488	NA	NA
1523	HMDB0014567	Methocarbamol	HMDB0014567
1524	HMDB0013134	Fumaryl carnitine	HMDB0013134
1525	HMDB0032769	Osmaronin	HMDB0032769
1526	HMDB0029397	L-Nicotianine	HMDB0029397
1527	HMDB0000732	Hydroxykynurenine	HMDB0000732
1528	HMDB0012819	5-Hydroxykynurenine	HMDB0012819
1529	HMDB0014787	Stavudine	HMDB0014787
1530	HMDB0011631	L-3-Hydroxykynurenine	HMDB0011631
1531	HMDB0060750	NA	NA
1532	HMDB0002224	5-Methyldeoxycytidine	HMDB0002224
1533	HMDB0028861	Hydroxypropyl-Glutamine	HMDB0028861
1534	HMDB0038516	NA	NA
1535	HMDB0028798	Glutaminyhydroxyproline	HMDB0028798
1536	HMDB0028877	Hydroxypropyl-Gamma-glutamate	HMDB0028877
1537	HMDB0178266	NA	NA
1538	HMDB0037694	NA	NA

1539	HMDB0040006	NA	NA
1540	HMDB0037695	NA	NA
1541	HMDB0042008	NA	NA
1542	HMDB0033430	Tanakine	HMDB0033430
1543	HMDB0033429	Tanakamine	HMDB0033429
1544	HMDB0142966	NA	NA
1545	HMDB0029448	DL-Ornithino-L-alanine	HMDB0029448
1546	HMDB0041858	NA	NA
1547	HMDB0135607	NA	NA
1548	HMDB0141386	NA	NA
1549	HMDB0135600	NA	NA
1550	HMDB0135404	NA	NA
1551	HMDB0135599	NA	NA
1552	HMDB0141385	NA	NA
1553	HMDB0141387	NA	NA
1554	HMDB0135604	NA	NA
1555	HMDB0135603	NA	NA
1556	HMDB0135602	NA	NA
1557	HMDB0032584	4-Hydroxychalcone	HMDB0032584
1558	HMDB0037696	NA	NA
1559	HMDB0014922	Mefenamic acid	HMDB0014922
1560	HMDB0040380	NA	NA
1561	HMDB0029366	N-[2-(4-Hydroxyphenyl)ethyl]benzamide	HMDB0029366
1562	HMDB0147191	NA	NA
1563	HMDB0131062	NA	NA
1564	HMDB0131065	NA	NA
1565	HMDB0036050	NA	NA
1566	HMDB0033771	Cyperine	HMDB0033771
1567	HMDB0030690	(E)-Suberenol	HMDB0030690
1568	HMDB0039592	NA	NA
1569	HMDB0030788	Citrusal	HMDB0030788
1570	HMDB0135759	NA	NA
1571	HMDB0135760	NA	NA
1572	HMDB0135761	NA	NA
1573	HMDB0141827	NA	NA
1574	HMDB0151855	NA	NA
1575	HMDB0153660	NA	NA
1576	HMDB0135757	NA	NA
1577	HMDB0135758	NA	NA
1578	HMDB0129916	NA	NA
1579	HMDB0129917	NA	NA
1580	HMDB0129919	NA	NA
1581	HMDB0129920	NA	NA
1582	HMDB0129922	NA	NA
1583	HMDB0131064	NA	NA
1584	HMDB0131066	NA	NA
1585	HMDB0131067	NA	NA
1586	HMDB0132269	NA	NA
1587	HMDB0129918	NA	NA
1588	HMDB0030854	(S)-Auraptenol	HMDB0030854
1589	HMDB0030110	Celerin	HMDB0030110
1590	HMDB0030948	Dihydrowyerone	HMDB0030948
1591	HMDB0039142	NA	NA
1592	HMDB0041192	NA	NA
1593	HMDB0034133	3-(1,1-Dimethylallyl)scopoletin	HMDB0034133
1594	HMDB0030853	(R)-Meranzin	HMDB0030853
1595	HMDB0033015	5,6-Dihydroyangonin	HMDB0033015
1596	HMDB0035254	7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone	HMDB0035254
1597	HMDB0033016	7,8-Dihydroyangonin	HMDB0033016
1598	HMDB0030578	Apigravin	HMDB0030578
1599	HMDB0032953	7-Methoxy-5-prenyloxycoumarin	HMDB0032953
1600	HMDB0061290	NA	NA
1601	HMDB0061303	NA	NA
1602	HMDB0039146	NA	NA
1603	HMDB0037679	NA	NA
1604	HMDB0035019	Phenethyl salicylate	HMDB0035019
1605	HMDB0029302	1-Phenyl-6,7-dihydroxy-isochroman	HMDB0029302
1606	HMDB0036347	NA	NA
1607	HMDB0002209	Equol	HMDB0002209
1608	HMDB0130495	NA	NA
1609	HMDB0014713	Fenoprofen	HMDB0014713
1610	HMDB0135409	NA	NA
1611	HMDB0135406	NA	NA
1612	HMDB0135408	NA	NA
1613	HMDB0135407	NA	NA
1614	HMDB0135593	NA	NA
1615	HMDB0135594	NA	NA
1616	HMDB0135405	NA	NA
1617	HMDB0130496	NA	NA
1618	HMDB0135355	NA	NA
1619	HMDB0135397	NA	NA
1620	HMDB0135595	NA	NA
1621	HMDB0151857	NA	NA
1622	HMDB0130497	NA	NA
1623	HMDB0168444	NA	NA
1624	HMDB0135601	NA	NA
1625	HMDB0168447	NA	NA

1626	HMDB0148520	NA	NA
1627	HMDB0168443	NA	NA
1628	HMDB0182848	NA	NA
1629	HMDB0168445	NA	NA
1630	HMDB0168442	NA	NA
1631	HMDB0135596	NA	NA
1632	HMDB0168446	NA	NA
1633	HMDB0029953	D-erythro-D-galacto-octitol	HMDB0029953
1634	HMDB0060478	gamma-Glutamyl-beta-cyanoalanine	HMDB0060478
1635	HMDB0000089	Cytidine	HMDB0000089
1636	HMDB0015122	Cytarabine	HMDB0015122
1637	HMDB0155273	NA	NA
1638	HMDB0001904	3-Nitrotyrosine	HMDB0001904
1639	HMDB0028751	Aspartyl-Glutamine	HMDB0028751
1640	HMDB0028793	Glutaminylaspartic acid	HMDB0028793
1641	HMDB0029144	gamma-Glutamylasparagine	HMDB0029144
1642	HMDB0028814	Glutamylasparagine	HMDB0028814
1643	HMDB0028730	Asparaginy-Glutamate	HMDB0028730
1644	HMDB0028767	Aspartyl-Gamma-glutamate	HMDB0028767
1645	HMDB0033701	Hydrocotarnine	HMDB0033701
1646	HMDB0031770	Carbofuran	HMDB0031770
1647	HMDB0014798	Metaxalone	HMDB0014798
1648	HMDB0139892	NA	NA
1649	HMDB0138550	NA	NA
1650	HMDB0033925	Oroselone	HMDB0033925
1651	HMDB0032998	2-Methoxyxanthone	HMDB0032998
1652	HMDB0161779	NA	NA
1653	HMDB0161778	NA	NA
1654	HMDB0161783	NA	NA
1655	HMDB0161782	NA	NA
1656	HMDB0161780	NA	NA
1657	HMDB0162111	NA	NA
1658	HMDB0162103	NA	NA
1659	HMDB0162104	NA	NA
1660	HMDB0162105	NA	NA
1661	HMDB0162108	NA	NA
1662	HMDB0162109	NA	NA
1663	HMDB0162106	NA	NA
1664	HMDB0162107	NA	NA
1665	HMDB0162110	NA	NA
1666	HMDB0162112	NA	NA
1667	HMDB0161832	NA	NA
1668	HMDB0161833	NA	NA
1669	HMDB0161834	NA	NA
1670	HMDB0149051	NA	NA
1671	HMDB0149050	NA	NA
1672	HMDB0149006	NA	NA
1673	HMDB0148541	NA	NA
1674	HMDB0148540	NA	NA
1675	HMDB0148786	NA	NA
1676	HMDB0148785	NA	NA
1677	HMDB0148998	NA	NA
1678	HMDB0149048	NA	NA
1679	HMDB0147226	NA	NA
1680	HMDB0148542	NA	NA
1681	HMDB0128505	NA	NA
1682	HMDB0148539	NA	NA
1683	HMDB0145646	NA	NA
1684	HMDB0145647	NA	NA
1685	HMDB0145645	NA	NA
1686	HMDB0135172	NA	NA
1687	HMDB0149007	NA	NA
1688	HMDB0128506	NA	NA
1689	HMDB0128503	NA	NA
1690	HMDB0128504	NA	NA
1691	HMDB0040876	NA	NA
1692	HMDB0030946	(2E,11Z)-Wyerone acid	HMDB0030946
1693	HMDB0041016	NA	NA
1694	HMDB0030595	Suberenone	HMDB0030595
1695	HMDB0033735	Graveolone	HMDB0033735
1696	HMDB0039430	NA	NA
1697	HMDB0004215	3,3',4'5-Tetrahydroxystilbene	HMDB0004215
1698	HMDB0170845	NA	NA
1699	HMDB0164057	NA	NA
1700	HMDB0135900	NA	NA
1701	HMDB0135902	NA	NA
1702	HMDB0135904	NA	NA
1703	HMDB0164055	NA	NA
1704	HMDB0164056	NA	NA
1705	HMDB0164058	NA	NA
1706	HMDB0170846	NA	NA
1707	HMDB0170974	NA	NA
1708	HMDB0170976	NA	NA
1709	HMDB0170979	NA	NA
1710	HMDB0170978	NA	NA
1711	HMDB0131284	NA	NA
1712	HMDB0131285	NA	NA

1713	HMDB0127824	NA	NA
1714	HMDB0131281	NA	NA
1715	HMDB0131283	NA	NA
1716	HMDB0170977	NA	NA
1717	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	HMDB0031668
1718	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	HMDB0034056
1719	HMDB0037681	NA	NA
1720	HMDB0029470	Isodillapiole	HMDB0029470
1721	HMDB0041379	NA	NA
1722	HMDB0135906	NA	NA
1723	HMDB0038563	NA	NA
1724	HMDB0037130	NA	NA
1725	HMDB0094660	Diethyl phthalic acid	HMDB0094660
1726	HMDB0033776	Apiole	HMDB0033776
1727	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	HMDB0029226
1728	HMDB0135689	NA	NA
1729	HMDB0013247	Monobutylphthalate	HMDB0013247
1730	HMDB0030725	Dillapiol	HMDB0030725
1731	HMDB0002056	Monoisobutyl phthalic acid	HMDB0002056
1732	HMDB0147179	NA	NA
1733	HMDB0140340	NA	NA
1734	HMDB0173973	NA	NA
1735	HMDB0173971	NA	NA
1736	HMDB0173972	NA	NA
1737	HMDB0173975	NA	NA
1738	HMDB0173976	NA	NA
1739	HMDB0177472	NA	NA
1740	HMDB0177470	NA	NA
1741	HMDB0173974	NA	NA
1742	HMDB0128944	NA	NA
1743	HMDB0131630	NA	NA
1744	HMDB0128958	NA	NA
1745	HMDB0039027	NA	NA
1746	HMDB0128963	NA	NA
1747	HMDB0138052	NA	NA
1748	HMDB0128962	NA	NA
1749	HMDB0030882	(S)-Rutaretin	HMDB0030882
1750	HMDB0128960	NA	NA
1751	HMDB0128961	NA	NA
1752	HMDB0032838	Dorsteniol	HMDB0032838
1753	HMDB0131653	NA	NA
1754	HMDB0147178	NA	NA
1755	HMDB0131691	NA	NA
1756	HMDB0131700	NA	NA
1757	HMDB0167944	NA	NA
1758	HMDB0163475	NA	NA
1759	HMDB0171044	NA	NA
1760	HMDB0167134	NA	NA
1761	HMDB0028752	Aspartyl-Glutamate	HMDB0028752
1762	HMDB0029145	NA	NA
1763	HMDB0030419	gamma-Glutamylaspartic acid	HMDB0030419
1764	HMDB0062501	NA	NA
1765	HMDB0028815	Glutamylaspartic acid	HMDB0028815
1766	HMDB0030413	NA	NA
1767	HMDB0011164	L-beta-aspartyl-L-glutamic acid	HMDB0011164
1768	HMDB0000767	Pseudouridine	HMDB0000767
1769	HMDB0000296	Uridine	HMDB0000296
1770	HMDB0156330	NA	NA
1771	HMDB0126635	NA	NA
1772	HMDB0130466	NA	NA
1773	HMDB0130477	NA	NA
1774	HMDB0006794	5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate	HMDB0006794
1775	HMDB0157260	NA	NA
1776	HMDB0157259	NA	NA
1777	HMDB0125157	NA	NA
1778	HMDB0166885	NA	NA
1779	HMDB0155302	NA	NA
1780	HMDB0180914	NA	NA
1781	HMDB0177249	NA	NA
1782	HMDB0163614	NA	NA
1783	HMDB0040734	NA	NA
1784	HMDB0006005	Indolylacryloylglycine	HMDB0006005
1785	HMDB0030218	Lansine	HMDB0030218
1786	HMDB0030319	Mukeic acid	HMDB0030319
1787	HMDB0031360	L-cis-Cyclo(aspartylphenylalanyl)	HMDB0031360
1788	HMDB0161891	NA	NA
1789	HMDB0161893	NA	NA
1790	HMDB0028848	Glycyl-Phenylalanine	HMDB0028848
1791	HMDB0028995	Phenylalanyl-Glycine	HMDB0028995
1792	HMDB0061722	NA	NA
1793	HMDB0000030	Biotin	HMDB0000030
1794	HMDB0028974	Methionyl-Hydroxyproline	HMDB0028974
1795	HMDB0028869	Hydroxypropyl-Methionine	HMDB0028869
1796	HMDB0015063	Azacitidine	HMDB0015063
1797	HMDB0014949	Ribavirin	HMDB0014949
1798	HMDB0060337	NA	NA
1799	HMDB0240369	NA	NA

1800	HMDB0034885	Imazamethabenz	HMDB0034885
1801	HMDB0035193	1-(9H-Pyrido[3,4-b]indol-1-yl)-1,4-butanediol	HMDB0035193
1802	HMDB0033519	N-Ornithyl-L-aurine	HMDB0033519
1803	HMDB0033461	4-Coumaroylputrescine	HMDB0033461
1804	HMDB0139874	NA	NA
1805	HMDB0062429	7,12-Dimethylbenz[a]anthracene	HMDB0062429
1806	HMDB0028811	Glutaminy-Gamma-glutamate	HMDB0028811
1807	HMDB0029163	Gamma-glutamyl-Gamma-glutamate	HMDB0029163
1808	HMDB0032764	N2-Succinoylarginine	HMDB0032764
1809	HMDB0028795	Glutaminyglutamine	HMDB0028795
1810	HMDB0011655	2-(3-Carboxy-3-aminopropyl)-L-histidine	HMDB0011655
1811	HMDB0029063	Threoninyl-Histidine	HMDB0029063
1812	HMDB0028895	Histidinyl-Threonine	HMDB0028895
1813	HMDB0028833	Glutamyl-Gamma-glutamate	HMDB0028833
1814	HMDB0028796	Glutaminyglutamic acid	HMDB0028796
1815	HMDB0029147	N-gamma-Glutamylglutamine	HMDB0029147
1816	HMDB0028817	Glutamylglutamine	HMDB0028817
1817	HMDB0011738	N2-gamma-Glutamylglutamine	HMDB0011738
1818	HMDB0005766	Norophthalmic acid	HMDB0005766
1819	HMDB0240577	NA	NA
1820	HMDB0000982	5-Methylcytidine	HMDB0000982
1821	HMDB0039229	Pyro-L-glutaminy-L-glutamine	HMDB0039229
1822	HMDB0032559	(Ás)-2-(1-Methylpropyl)-4,6-dinitrophenol	HMDB0032559
1823	HMDB0033610	Pandamarilactam 3x	HMDB0033610
1824	HMDB0139906	NA	NA
1825	HMDB0164387	NA	NA
1826	HMDB0000086	Glycerophosphocholine	HMDB0000086
1827	HMDB0142996	NA	NA
1828	HMDB0143005	NA	NA
1829	HMDB0151865	NA	NA
1830	HMDB0137520	NA	NA
1831	HMDB0130494	NA	NA
1832	HMDB0135588	NA	NA
1833	HMDB0135591	NA	NA
1834	HMDB0135592	NA	NA
1835	HMDB0137534	NA	NA
1836	HMDB0135587	NA	NA
1837	HMDB0135590	NA	NA
1838	HMDB0151856	NA	NA
1839	HMDB0032130	3',4'-Dihydroxychalcone	HMDB0032130
1840	HMDB0135586	NA	NA
1841	HMDB0153774	NA	NA
1842	HMDB0036738	NA	NA
1843	HMDB0039612	NA	NA
1844	HMDB0032129	2',5'-Dihydroxychalcone	HMDB0032129
1845	HMDB0014643	Tolmetin	HMDB0014643
1846	HMDB0033345	(Ás)-Ribaline	HMDB0033345
1847	HMDB0041329	NA	NA
1848	HMDB0015568	Vorinostat	HMDB0015568
1849	HMDB0029134	Valyl-Phenylalanine	HMDB0029134
1850	HMDB0029008	Phenylalanyl-Valine	HMDB0029008
1851	HMDB0139553	NA	NA
1852	HMDB0139638	NA	NA
1853	HMDB0033463	Subaphylline	HMDB0033463
1854	HMDB0139620	NA	NA
1855	HMDB0139619	NA	NA
1856	HMDB0139617	NA	NA
1857	HMDB0139618	NA	NA
1858	HMDB0139605	NA	NA
1859	HMDB0032674	(Z,Z)-2,9,16-Heptadecatriene-4,6-diyn-8-ol	HMDB0032674
1860	HMDB0033693	Falcarinone	HMDB0033693
1861	HMDB0040893	NA	NA
1862	HMDB0031873	1,7-Diphenyl-4-hepten-3-one	HMDB0031873
1863	HMDB0133902	NA	NA
1864	HMDB0029059	Threoninyl-Glutamine	HMDB0029059
1865	HMDB0029075	Threoninyl-Gamma-glutamate	HMDB0029075
1866	HMDB0028807	Glutaminylthreonine	HMDB0028807
1867	HMDB0134633	NA	NA
1868	HMDB0138211	NA	NA
1869	HMDB0134631	NA	NA
1870	HMDB0134626	NA	NA
1871	HMDB0134634	NA	NA
1872	HMDB0134632	NA	NA
1873	HMDB0134629	NA	NA
1874	HMDB0134624	NA	NA
1875	HMDB0134630	NA	NA
1876	HMDB0134627	NA	NA
1877	HMDB0134628	NA	NA
1878	HMDB0035080	Miltirone	HMDB0035080
1879	HMDB0134623	NA	NA
1880	HMDB0134625	NA	NA
1881	HMDB0041090	NA	NA
1882	HMDB0060663	NA	NA
1883	HMDB0177722	NA	NA
1884	HMDB0033064	(E)-2-Methyl-2-buten-1-ol O-beta-D-Glucopyranoside	HMDB0033064
1885	HMDB0031876	Prenyl glucoside	HMDB0031876
1886	HMDB0177064	NA	NA

1887	HMDB0033483	6,7-Dihydro-4-(hydroxymethyl)-2-(p-hydroxyphenethyl)-7-methyl-5H-2-pyridinium	HMDB0033483
1888	HMDB0002053	Histidylproline diketopiperazine	HMDB0002053
1889	HMDB0014257	E-10-Hydroxydesmethylnortriptyline	HMDB0014257
1890	HMDB0040785	NA	NA
1891	HMDB0038838	NA	NA
1892	HMDB0060840	NA	NA
1893	HMDB0028953	Lysyl-Histidine	HMDB0028953
1894	HMDB0028890	HistidinyL-Lysine	HMDB0028890
1895	HMDB0041845	NA	NA
1896	HMDB0015415	Oxtriphyllyne	HMDB0015415
1897	HMDB0029133	Valyl-Methionine	HMDB0029133
1898	HMDB0028986	Methionyl-Valine	HMDB0028986
1899	HMDB0175189	NA	NA
1900	HMDB0175187	NA	NA
1901	HMDB0175188	NA	NA
1902	HMDB0162484	NA	NA
1903	HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	HMDB0033197
1904	HMDB0036047	NA	NA
1905	HMDB0059661	NA	NA
1906	HMDB0015088	Rizatriptan	HMDB0015088
1907	HMDB0014873	Naftifine	HMDB0014873
1908	HMDB0014578	Cyproheptadine	HMDB0014578
1909	HMDB0011687	Phenylbutyrylglutamine	HMDB0011687
1910	HMDB0033514	Fusarochromanone	HMDB0033514
1911	HMDB0181167	NA	NA
1912	HMDB0139531	NA	NA
1913	HMDB0139533	NA	NA
1914	HMDB0139532	NA	NA
1915	HMDB0139535	NA	NA
1916	HMDB0139993	NA	NA
1917	HMDB0014451	Talbutal	HMDB0014451
1918	HMDB0139534	NA	NA
1919	HMDB0059959	NA	NA
1920	HMDB0186509	NA	NA
1921	HMDB0184957	NA	NA
1922	HMDB0184936	NA	NA
1923	HMDB0062677	NA	NA
1924	HMDB0004590	19-Nor-5-androstenediol	HMDB0004590
1925	HMDB0032464	Phenethyl decanoate	HMDB0032464
1926	HMDB0002697	19-Norandrosterone	HMDB0002697
1927	HMDB0032672	4,8,12,15-Octadecatetraenoic acid	HMDB0032672
1928	HMDB0005886	19-Noretiocholanolone	HMDB0005886
1929	HMDB0034382	(E,E)-11,13-Octadecadien-9-ynoic acid	HMDB0034382
1930	HMDB0006547	Stearidonic acid	HMDB0006547
1931	HMDB0186501	NA	NA
1932	HMDB0186507	NA	NA
1933	HMDB0186508	NA	NA
1934	HMDB0062288	NA	NA
1935	HMDB0186510	NA	NA
1936	HMDB0186500	NA	NA
1937	HMDB0186506	NA	NA
1938	HMDB0186505	NA	NA
1939	HMDB0186504	NA	NA
1940	HMDB0186502	NA	NA
1941	HMDB0186497	NA	NA
1942	HMDB0186499	NA	NA
1943	HMDB0186498	NA	NA
1944	HMDB0112093	NA	NA
1945	HMDB0112099	NA	NA
1946	HMDB0112102	NA	NA
1947	HMDB0112103	NA	NA
1948	HMDB0186503	NA	NA
1949	HMDB0034586	(9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid	HMDB0034586
1950	HMDB0031088	12,13-Epoxy-9,15-octadecadienoic acid	HMDB0031088
1951	HMDB0029969	Squamostanal A	HMDB0029969
1952	HMDB0031103	2-Hydroxylinolenic acid	HMDB0031103
1953	HMDB0036832	NA	NA
1954	HMDB0030950	15,16-Epoxy-9,12-octadecadienoic acid	HMDB0030950
1955	HMDB0029786	10-Oxo-11-octadecen-13-olide	HMDB0029786
1956	HMDB0011108	17-Hydroxylinolenic acid	HMDB0011108
1957	HMDB0010224	9-HOTE	HMDB0010224
1958	HMDB0010220	9(10)-EpODE	HMDB0010220
1959	HMDB0010206	15(16)-EpODE	HMDB0010206
1960	HMDB0010200	A-12(13)-EpODE	HMDB0010200
1961	HMDB0010203	13-HOTE	HMDB0010203
1962	HMDB0004669	9-OxoODE	HMDB0004669
1963	HMDB0004668	13-OxoODE	HMDB0004668
1964	HMDB0031934	(9S,10E,12Z,15Z)-9-Hydroxy-10,12,15-octadecatrienoic acid	HMDB0031934
1965	HMDB0030995	(2'E,4'Z,8E)-Colneleic acid	HMDB0030995
1966	HMDB0061644	NA	NA
1967	HMDB0039603	NA	NA
1968	HMDB0061979	NA	NA
1969	HMDB0033791	(E)-3-Hexadecenoic acid	HMDB0033791
1970	HMDB0038958	NA	NA
1971	HMDB0031711	15-Hexadecanolide	HMDB0031711
1972	HMDB0003229	Palmitoleic acid	HMDB0003229
1973	HMDB0010735	Trans-Hexa-dec-2-enoic acid	HMDB0010735



1974	HMDB0037647	NA	NA
1975	HMDB0041422	NA	NA
1976	HMDB0032638	(Z)-5-Hexadecenoic acid	HMDB0032638
1977	HMDB0031053	(E)-6-Hexadecenoic acid	HMDB0031053
1978	HMDB0035877	(Z)-13-Hexadecenoic acid	HMDB0035877
1979	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	HMDB0031145
1980	HMDB0002186	Hypogeic acid	HMDB0002186
1981	HMDB0171478	NA	NA
1982	HMDB0171479	NA	NA
1983	HMDB0171477	NA	NA
1984	HMDB0012328	Palmitelaidic acid	HMDB0012328
1985	HMDB0171476	NA	NA
1986	HMDB0000756	L-Hexanoylcarnitine	HMDB0000756
1987	HMDB0000705	Hexanoylcarnitine	HMDB0000705
1988	HMDB0014413	Ropinirole	HMDB0014413
1989	HMDB0015070	Oxymetazoline	HMDB0015070
1990	HMDB0061189	NA	NA
1991	HMDB0062555	hydroxyisovaleroyl carnitine	HMDB0062555
1992	HMDB0240421	NA	NA
1993	HMDB0040904	NA	NA
1994	HMDB0168550	NA	NA
1995	HMDB0168551	NA	NA
1996	HMDB0168552	NA	NA
1997	HMDB0168553	NA	NA
1998	HMDB0168554	NA	NA
1999	HMDB0168549	NA	NA
2000	HMDB0137260	NA	NA
2001	HMDB0137271	NA	NA
2002	HMDB0030974	8-Acetoxy-4-acoren-3-one	HMDB0030974
2003	HMDB0031928	Panaxytriol	HMDB0031928
2004	HMDB0030801	1-(4-Hydroxy-3-methoxyphenyl)-3-decanone	HMDB0030801
2005	HMDB0039251	NA	NA
2006	HMDB0134775	NA	NA
2007	HMDB0038798	NA	NA
2008	HMDB0035075	Tanacetol B	HMDB0035075
2009	HMDB0060952	NA	NA
2010	HMDB0014521	Palonosetron	HMDB0014521
2011	HMDB0030283	Hydrocinchonine	HMDB0030283
2012	HMDB0175409	NA	NA
2013	HMDB0175412	NA	NA
2014	HMDB0175413	NA	NA
2015	HMDB0175414	NA	NA
2016	HMDB0175415	NA	NA
2017	HMDB0175408	NA	NA
2018	HMDB0175410	NA	NA
2019	HMDB0175411	NA	NA
2020	HMDB0160594	NA	NA
2021	HMDB0173892	NA	NA
2022	HMDB0175402	NA	NA
2023	HMDB0175403	NA	NA
2024	HMDB0175404	NA	NA
2025	HMDB0175405	NA	NA
2026	HMDB0175406	NA	NA
2027	HMDB0175407	NA	NA
2028	HMDB0030964	Linolenelaidic acid	HMDB0030964
2029	HMDB0001388	Alpha-Linolenic acid	HMDB0001388
2030	HMDB0003073	Gamma-Linolenic acid	HMDB0003073
2031	HMDB0030962	Calendic acid	HMDB0030962
2032	HMDB0030963	Punicic acid	HMDB0030963
2033	HMDB0160589	NA	NA
2034	HMDB0160588	NA	NA
2035	HMDB0112194	NA	NA
2036	HMDB0062652	NA	NA
2037	HMDB0173890	NA	NA
2038	HMDB0160590	NA	NA
2039	HMDB0160592	NA	NA
2040	HMDB0160591	NA	NA
2041	HMDB0160593	NA	NA
2042	HMDB0160595	NA	NA
2043	HMDB0173886	NA	NA
2044	HMDB0173885	NA	NA
2045	HMDB0173887	NA	NA
2046	HMDB0173889	NA	NA
2047	HMDB0173891	NA	NA
2048	HMDB0173888	NA	NA
2049	HMDB0173893	NA	NA
2050	HMDB0004667	13S-hydroxyoctadecadienoic acid	HMDB0004667
2051	HMDB0061708	NA	NA
2052	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	HMDB0029796
2053	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid	HMDB0029998
2054	HMDB0029978	Avenoleic acid	HMDB0029978
2055	HMDB0010223	9-HODE	HMDB0010223
2056	HMDB0004701	9,10-Epoxyoctadecenoic acid	HMDB0004701
2057	HMDB0004702	12,13-EpOME	HMDB0004702
2058	HMDB0004670	Alpha-dimorphecolic acid	HMDB0004670
2059	HMDB0000220	Palmitic acid	HMDB0000220
2060	HMDB0060083	NA	NA

2061	HMDB0061373	NA	NA
2062	HMDB0032324	Hexyl decanoate	HMDB0032324
2063	HMDB0032249	Dodecyl butyrate	HMDB0032249
2064	HMDB0033166	Octyl octanoate	HMDB0033166
2065	HMDB0032065	Butyl dodecanoate	HMDB0032065
2066	HMDB0036210	NA	NA
2067	HMDB0034153	Ethyl tetradecanoate	HMDB0034153
2068	HMDB0031068	Isopalmitic acid	HMDB0031068
2069	HMDB0002396	Trimethyltridecanoic acid	HMDB0002396
2070	HMDB0003950	7-Methylinosine	HMDB0003950
2071	HMDB0002721	1-Methylinosine	HMDB0002721
2072	HMDB0033060	Piperolactam A	HMDB0033060
2073	HMDB0034319	Furofoline	HMDB0034319
2074	HMDB0038882	NA	NA
2075	HMDB0038880	NA	NA
2076	HMDB0029918	Arabinofuranobiose	HMDB0029918
2077	HMDB0029894	Xylobiose	HMDB0029894
2078	HMDB0038855	NA	NA
2079	HMDB0029619	Arabinopyranobiose	HMDB0029619
2080	HMDB0038881	NA	NA
2081	HMDB0179982	NA	NA
2082	HMDB0179983	NA	NA
2083	HMDB0179984	NA	NA
2084	HMDB0028745	Asparaginyln-Gamma-glutamate	HMDB0028745
2085	HMDB0028792	Glutaminylasparagine	HMDB0028792
2086	HMDB0028729	Asparaginyln-Glutamine	HMDB0028729
2087	HMDB0126535	NA	NA
2088	HMDB0126543	NA	NA
2089	HMDB0126529	NA	NA
2090	HMDB0126544	NA	NA
2091	HMDB0126525	NA	NA
2092	HMDB0126540	NA	NA
2093	HMDB0126536	NA	NA
2094	HMDB0126532	NA	NA
2095	HMDB0126531	NA	NA
2096	HMDB0126528	NA	NA
2097	HMDB0126526	NA	NA
2098	HMDB0171819	NA	NA
2099	HMDB0240268	NA	NA
2100	HMDB0035910	Cedryl acetate	HMDB0035910
2101	HMDB0037273	NA	NA
2102	HMDB0039630	NA	NA
2103	HMDB0037218	NA	NA
2104	HMDB0036153	NA	NA
2105	HMDB0037224	NA	NA
2106	HMDB0155179	NA	NA
2107	HMDB0186458	NA	NA
2108	HMDB0062415	NA	NA
2109	HMDB0240353	NA	NA
2110	HMDB0038957	NA	NA
2111	HMDB0000053	Androstenedione	HMDB0000053
2112	HMDB0155184	NA	NA
2113	HMDB0137366	NA	NA
2114	HMDB0137379	NA	NA
2115	HMDB0154824	NA	NA
2116	HMDB0154823	NA	NA
2117	HMDB0155183	NA	NA
2118	HMDB0154825	NA	NA
2119	HMDB0155181	NA	NA
2120	HMDB0154992	NA	NA
2121	HMDB0154837	NA	NA
2122	HMDB0154836	NA	NA
2123	HMDB0154826	NA	NA
2124	HMDB0155182	NA	NA
2125	HMDB0155187	NA	NA
2126	HMDB0174401	NA	NA
2127	HMDB0174398	NA	NA
2128	HMDB0174399	NA	NA
2129	HMDB0186115	NA	NA
2130	HMDB0000324	3a,16a-Dihydroxyandrosthenone	HMDB0000324
2131	HMDB0000309	3a,16b-Dihydroxyandrosthenone	HMDB0000309
2132	HMDB0174400	NA	NA
2133	HMDB0174397	NA	NA
2134	HMDB0169093	NA	NA
2135	HMDB0155186	NA	NA
2136	HMDB0155185	NA	NA
2137	HMDB0155188	NA	NA
2138	HMDB0155961	NA	NA
2139	HMDB0155960	NA	NA
2140	HMDB0155963	NA	NA
2141	HMDB0155962	NA	NA
2142	HMDB0155965	NA	NA
2143	HMDB0155966	NA	NA
2144	HMDB0156602	NA	NA
2145	HMDB0156968	NA	NA
2146	HMDB0159843	NA	NA
2147	HMDB0060339	11-Hydroxytestosterone	HMDB0060339

2148	HMDB0000322	16-Oxoandrostenediol	HMDB0000322
2149	HMDB0000352	16a-Hydroxydehydroisoandrosterone	HMDB0000352
2150	HMDB0000388	3a,16-Dihydroxyandrostenone	HMDB0000388
2151	HMDB0003956	7a-Hydroxytestosterone	HMDB0003956
2152	HMDB0004611	7a-Hydroxydehydroepiandrosterone	HMDB0004611
2153	HMDB0004624	7b-Hydroxydehydroepiandrosterone	HMDB0004624
2154	HMDB0006031	11-Ketoetiocholanolone	HMDB0006031
2155	HMDB0006259	6beta-Hydroxytestosterone	HMDB0006259
2156	HMDB0006769	19-Hydroxytestosterone	HMDB0006769
2157	HMDB0039589	NA	NA
2158	HMDB0039735	NA	NA
2159	HMDB0031464	cis-[8]-Shogaol	HMDB0031464
2160	HMDB0012533	11beta-Hydroxytestosterone	HMDB0012533
2161	HMDB0012654	2beta-Hydroxytestosterone	HMDB0012654
2162	HMDB0060089	NA	NA
2163	HMDB0028901	Isoleucyl-Arginine	HMDB0028901
2164	HMDB0028923	Leucyl-Arginine	HMDB0028923
2165	HMDB0028712	Arginyl-Isoleucine	HMDB0028712
2166	HMDB0028713	Arginyl-Leucine	HMDB0028713
2167	HMDB0002227	Capsaicin	HMDB0002227
2168	HMDB0041142	NA	NA
2169	HMDB0032673	15-Octadecene-9,11,13-triynoic acid	HMDB0032673
2170	HMDB0000145	Estrone	HMDB0000145
2171	HMDB0039096	NA	NA
2172	HMDB0173636	NA	NA
2173	HMDB0041314	NA	NA
2174	HMDB0130350	NA	NA
2175	HMDB0130347	NA	NA
2176	HMDB0175079	NA	NA
2177	HMDB0178312	NA	NA
2178	HMDB0141160	NA	NA
2179	HMDB0141105	NA	NA
2180	HMDB0141099	NA	NA
2181	HMDB0141080	NA	NA
2182	HMDB0141122	NA	NA
2183	HMDB0141079	NA	NA
2184	HMDB0141126	NA	NA
2185	HMDB0141149	NA	NA
2186	HMDB0141119	NA	NA
2187	HMDB0040889	NA	NA
2188	HMDB0129039	NA	NA
2189	HMDB0138953	NA	NA
2190	HMDB0141045	NA	NA
2191	HMDB0138954	NA	NA
2192	HMDB0138952	NA	NA
2193	HMDB0138951	NA	NA
2194	HMDB0138956	NA	NA
2195	HMDB0140994	NA	NA
2196	HMDB0138959	NA	NA
2197	HMDB0138955	NA	NA
2198	HMDB0138957	NA	NA
2199	HMDB0138958	NA	NA
2200	HMDB0141056	NA	NA
2201	HMDB0141150	NA	NA
2202	HMDB0141152	NA	NA
2203	HMDB0141153	NA	NA
2204	HMDB0141164	NA	NA
2205	HMDB0146848	NA	NA
2206	HMDB0146849	NA	NA
2207	HMDB0141181	NA	NA
2208	HMDB0141151	NA	NA
2209	HMDB0141180	NA	NA
2210	HMDB0141162	NA	NA
2211	HMDB0141161	NA	NA
2212	HMDB0141169	NA	NA
2213	HMDB0141163	NA	NA
2214	HMDB0141145	NA	NA
2215	HMDB0141146	NA	NA
2216	HMDB0141057	NA	NA
2217	HMDB0141101	NA	NA
2218	HMDB0141102	NA	NA
2219	HMDB0141100	NA	NA
2220	HMDB0141103	NA	NA
2221	HMDB0141106	NA	NA
2222	HMDB0141107	NA	NA
2223	HMDB0141120	NA	NA
2224	HMDB0141121	NA	NA
2225	HMDB0141130	NA	NA
2226	HMDB0141129	NA	NA
2227	HMDB0141128	NA	NA
2228	HMDB0141127	NA	NA
2229	HMDB0141139	NA	NA
2230	HMDB0141140	NA	NA
2231	HMDB0141170	NA	NA
2232	HMDB0036635	NA	NA
2233	HMDB0041298	NA	NA
2234	HMDB0033310	Moracin C	HMDB0033310

2235	HMDB0031744	Artocarbene	HMDB0031744
2236	HMDB0141044	NA	NA
2237	HMDB0138682	NA	NA
2238	HMDB0011741	gamma-Glutamyltyrosine	HMDB0011741
2239	HMDB0029161	NA	NA
2240	HMDB0029104	Tyrosyl-Glutamate	HMDB0029104
2241	HMDB0028831	Glutamyltyrosine	HMDB0028831
2242	HMDB0062553	NA	NA
2243	HMDB0041309	NA	NA
2244	HMDB0000839	Pentaporphyrin I	HMDB0000839
2245	HMDB0029428	Hypoglycin B	HMDB0029428
2246	HMDB0061318	NA	NA
2247	HMDB0015102	Desloratadine	HMDB0015102
2248	HMDB0170226	NA	NA
2249	HMDB0170229	NA	NA
2250	HMDB0170227	NA	NA
2251	HMDB0170230	NA	NA
2252	HMDB0170228	NA	NA
2253	HMDB0004704	9,10-DHOME	HMDB0004704
2254	HMDB0061650	9,10-Epoxystearic acid	HMDB0061650
2255	HMDB0004705	12,13-DHOME	HMDB0004705
2256	HMDB0041220	NA	NA
2257	HMDB0031679	(9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid	HMDB0031679
2258	HMDB0000782	Octadecanedioic acid	HMDB0000782
2259	HMDB0015401	Nelarabine	HMDB0015401
2260	HMDB0005862	2-Methylguanosine	HMDB0005862
2261	HMDB0006038	3'-O-Methylguanosine	HMDB0006038
2262	HMDB0001563	1-Methylguanosine	HMDB0001563
2263	HMDB0001107	7-Methylguanosine	HMDB0001107
2264	HMDB0029076	Tryptophyl-Alanine	HMDB0029076
2265	HMDB0028698	Alanyl-Tryptophan	HMDB0028698
2266	HMDB0142223	NA	NA
2267	HMDB0013209	Alanyltryptophan	HMDB0013209
2268	HMDB0165476	NA	NA
2269	HMDB0165475	NA	NA
2270	HMDB0165471	NA	NA
2271	HMDB0165472	NA	NA
2272	HMDB0126113	NA	NA
2273	HMDB0130135	NA	NA
2274	HMDB0130132	NA	NA
2275	HMDB0130129	NA	NA
2276	HMDB0145822	NA	NA
2277	HMDB0130130	NA	NA
2278	HMDB0164665	NA	NA
2279	HMDB0130133	NA	NA
2280	HMDB0130019	NA	NA
2281	HMDB0126116	NA	NA
2282	HMDB0126115	NA	NA
2283	HMDB0130136	NA	NA
2284	HMDB0126114	NA	NA
2285	HMDB0178290	NA	NA
2286	HMDB0178289	NA	NA
2287	HMDB0181208	NA	NA
2288	HMDB0183795	NA	NA
2289	HMDB0183794	NA	NA
2290	HMDB0183797	NA	NA
2291	HMDB0183799	NA	NA
2292	HMDB0183798	NA	NA
2293	HMDB0183796	NA	NA
2294	HMDB0183800	NA	NA
2295	HMDB0183802	NA	NA
2296	HMDB0183801	NA	NA
2297	HMDB0186752	NA	NA
2298	HMDB0186756	NA	NA
2299	HMDB0186754	NA	NA
2300	HMDB0183792	NA	NA
2301	HMDB0183793	NA	NA
2302	HMDB0137406	NA	NA
2303	HMDB0157378	NA	NA
2304	HMDB0183791	NA	NA
2305	HMDB0183790	NA	NA
2306	HMDB0186755	NA	NA
2307	HMDB0186753	NA	NA
2308	HMDB0186758	NA	NA
2309	HMDB0186759	NA	NA
2310	HMDB0186757	NA	NA
2311	HMDB0062411	NA	NA
2312	HMDB0062412	NA	NA
2313	HMDB0039484	Gibberellin A12 7-aldehyde	HMDB0039484
2314	HMDB0179080	NA	NA
2315	HMDB0041057	NA	NA
2316	HMDB0034630	(4Z,9a)-9-(3-Methyl-2-butenoyloxy)-4,10(14)-oplopadien-3-one	HMDB0034630
2317	HMDB0036725	NA	NA
2318	HMDB0036747	NA	NA
2319	HMDB0038885	NA	NA
2320	HMDB0036812	NA	NA
2321	HMDB0012452	all-trans-18-Hydroxyretinoic acid	HMDB0012452

2322	HMDB0061095	NA	NA
2323	HMDB0012451	all-trans-5,6-Epoxyretinoic acid	HMDB0012451
2324	HMDB0060093	NA	NA
2325	HMDB0006254	4-Hydroxyretinoic acid	HMDB0006254
2326	HMDB0005832	6b-Hydroxymethandienone	HMDB0005832
2327	HMDB0005079	15-Deoxy-d-12,14-PGJ2	HMDB0005079
2328	HMDB0000344	2-Methoxyestradiol-3-methylether	HMDB0000344
2329	HMDB0156417	NA	NA
2330	HMDB0031773	Phytocassane E	HMDB0031773
2331	HMDB0039442	NA	NA
2332	HMDB0034691	Yucalexin B9	HMDB0034691
2333	HMDB0034631	(4Z,9a)-9-Angeloyloxy-4,10(14)-oplopadien-3-one	HMDB0034631
2334	HMDB0037233	NA	NA
2335	HMDB0036147	NA	NA
2336	HMDB0036750	NA	NA
2337	HMDB0035710	Cafestol	HMDB0035710
2338	HMDB0036762	NA	NA
2339	HMDB0041056	NA	NA
2340	HMDB0014855	Norethindrone	HMDB0014855
2341	HMDB0012794	4-Oxoretinal	HMDB0012794
2342	HMDB0060092	NA	NA
2343	HMDB0138135	NA	NA
2344	HMDB0040644	NA	NA
2345	HMDB0060994	NA	NA
2346	HMDB0183805	NA	NA
2347	HMDB0156418	NA	NA
2348	HMDB0156413	NA	NA
2349	HMDB0156410	NA	NA
2350	HMDB0156411	NA	NA
2351	HMDB0156408	NA	NA
2352	HMDB0156409	NA	NA
2353	HMDB0156404	NA	NA
2354	HMDB0156405	NA	NA
2355	HMDB0061925	NA	NA
2356	HMDB0156406	NA	NA
2357	HMDB0156407	NA	NA
2358	HMDB0156401	NA	NA
2359	HMDB0156403	NA	NA
2360	HMDB0156402	NA	NA
2361	HMDB0001852	All-trans-retinoic acid	HMDB0001852
2362	HMDB0156412	NA	NA
2363	HMDB0179600	NA	NA
2364	HMDB0012874	9,13-cis-Retinoate	HMDB0012874
2365	HMDB0012788	4-OH-Retinal	HMDB0012788
2366	HMDB0036710	NA	NA
2367	HMDB0036564	NA	NA
2368	HMDB0036697	NA	NA
2369	HMDB0036711	NA	NA
2370	HMDB0038702	NA	NA
2371	HMDB0012329	4-Oxoretinol	HMDB0012329
2372	HMDB0006219	13-cis-Retinoic acid	HMDB0006219
2373	HMDB0041925	NA	NA
2374	HMDB0002369	9-cis-Retinoic acid	HMDB0002369
2375	HMDB0179597	NA	NA
2376	HMDB0179596	NA	NA
2377	HMDB0179598	NA	NA
2378	HMDB0183803	NA	NA
2379	HMDB0183804	NA	NA
2380	HMDB0183807	NA	NA
2381	HMDB0183806	NA	NA
2382	HMDB0183808	NA	NA
2383	HMDB0183810	NA	NA
2384	HMDB0183811	NA	NA
2385	HMDB0183813	NA	NA
2386	HMDB0179593	NA	NA
2387	HMDB0179594	NA	NA
2388	HMDB0183809	NA	NA
2389	HMDB0062222	NA	NA
2390	HMDB0062293	NA	NA
2391	HMDB0062296	NA	NA
2392	HMDB0062408	NA	NA
2393	HMDB0137419	NA	NA
2394	HMDB0137428	NA	NA
2395	HMDB0183812	NA	NA
2396	HMDB0183814	NA	NA
2397	HMDB0183815	NA	NA
2398	HMDB0183816	NA	NA
2399	HMDB0001337	Leukotriene A4	HMDB0001337
2400	HMDB0036776	NA	NA
2401	HMDB0036839	NA	NA
2402	HMDB0030101	Methyl [8]-Shogaol	HMDB0030101
2403	HMDB0036930	NA	NA
2404	HMDB0036724	NA	NA
2405	HMDB0035311	Galanal A	HMDB0035311
2406	HMDB0039012	NA	NA
2407	HMDB0036698	NA	NA
2408	HMDB0036706	NA	NA

2409	HMDB0037523	NA	NA
2410	HMDB0036806	NA	NA
2411	HMDB0035116	(ent-7alpha)-7-Hydroxy-8(14),15-pimaradien-19-oic acid	HMDB0035116
2412	HMDB0039716	NA	NA
2413	HMDB0005081	5-HEPE	HMDB0005081
2414	HMDB0006027	Oxymesterone	HMDB0006027
2415	HMDB0010202	12-HEPE	HMDB0010202
2416	HMDB0010205	14,15-EpETE	HMDB0010205
2417	HMDB0010210	15-KETE	HMDB0010210
2418	HMDB0010209	15-HEPE	HMDB0010209
2419	HMDB0010212	17,18-EpETE	HMDB0010212
2420	HMDB0010217	5-KETE	HMDB0010217
2421	HMDB0041058	NA	NA
2422	HMDB0036712	NA	NA
2423	HMDB0038521	NA	NA
2424	HMDB0036752	NA	NA
2425	HMDB0036713	NA	NA
2426	HMDB0012534	11R-HEPE	HMDB0012534
2427	HMDB0012611	18R-HEPE	HMDB0012611
2428	HMDB0013633	12-KETE	HMDB0013633
2429	HMDB0060053	NA	NA
2430	HMDB0061114	NA	NA
2431	HMDB0179595	NA	NA
2432	HMDB0005764	Melanostatin	HMDB0005764
2433	HMDB0036329	NA	NA
2434	HMDB0060578	NA	NA
2435	HMDB0061098	NA	NA
2436	HMDB0161587	NA	NA
2437	HMDB0138221	NA	NA
2438	HMDB0030432	Linalyl cinnamate	HMDB0030432
2439	HMDB0038050	NA	NA
2440	HMDB0003422	Boldione	HMDB0003422
2441	HMDB0029913	Gynocardin	HMDB0029913
2442	HMDB0240490	NA	NA
2443	HMDB0059998	NA	NA
2444	HMDB0041272	NA	NA
2445	HMDB0124997	NA	NA
2446	HMDB0029498	3'-Methoxyfukiic acid	HMDB0029498
2447	HMDB0135181	NA	NA
2448	HMDB0125471	NA	NA
2449	HMDB0004326	2'-O-Methyladenosine	HMDB0004326
2450	HMDB0004044	N6-Methyladenosine	HMDB0004044
2451	HMDB0006023	3'-O-Methyladenosine	HMDB0006023
2452	HMDB0003331	1-Methyladenosine	HMDB0003331
2453	HMDB0006832	S-Glutaryldihydroipoamide	HMDB0006832
2454	HMDB0037843	NA	NA
2455	HMDB0030266	Berberrubine	HMDB0030266
2456	HMDB0187656	NA	NA
2457	HMDB0030391	Cepharadione B	HMDB0030391
2458	HMDB0061366	NA	NA
2459	HMDB0029395	L-L-Homoglutathione	HMDB0029395
2460	HMDB0135641	NA	NA
2461	HMDB0179385	NA	NA
2462	HMDB0179388	NA	NA
2463	HMDB0179383	NA	NA
2464	HMDB0179382	NA	NA
2465	HMDB0163720	NA	NA
2466	HMDB0173550	NA	NA
2467	HMDB0135574	NA	NA
2468	HMDB0135576	NA	NA
2469	HMDB0135572	NA	NA
2470	HMDB0135564	NA	NA
2471	HMDB0135568	NA	NA
2472	HMDB0134573	NA	NA
2473	HMDB0134571	NA	NA
2474	HMDB0135570	NA	NA
2475	HMDB0158752	NA	NA
2476	HMDB0158753	NA	NA
2477	HMDB0155927	NA	NA
2478	HMDB0155928	NA	NA
2479	HMDB0161130	NA	NA
2480	HMDB0041096	NA	NA
2481	HMDB0158750	NA	NA
2482	HMDB0158751	NA	NA
2483	HMDB0159487	NA	NA
2484	HMDB0159488	NA	NA
2485	HMDB0159490	NA	NA
2486	HMDB0159830	NA	NA
2487	HMDB0161128	NA	NA
2488	HMDB0161127	NA	NA
2489	HMDB0161129	NA	NA
2490	HMDB0161132	NA	NA
2491	HMDB0161133	NA	NA
2492	HMDB0166865	NA	NA
2493	HMDB0159483	NA	NA
2494	HMDB0159484	NA	NA
2495	HMDB0159482	NA	NA

2496	HMDB0158755	NA	NA
2497	HMDB0158759	NA	NA
2498	HMDB0158758	NA	NA
2499	HMDB0159491	NA	NA
2500	HMDB0158756	NA	NA
2501	HMDB0158876	NA	NA
2502	HMDB0158877	NA	NA
2503	HMDB0159485	NA	NA
2504	HMDB0061135	NA	NA
2505	HMDB0015176	Melphalan	HMDB0015176
2506	HMDB0127928	NA	NA
2507	HMDB0037110	NA	NA
2508	HMDB0145098	NA	NA
2509	HMDB0175072	NA	NA
2510	HMDB0041450	NA	NA
2511	HMDB0038322	NA	NA
2512	HMDB0032909	2-(4-Methoxyphenyl)naphthalic anhydride	HMDB0032909
2513	HMDB0175074	NA	NA
2514	HMDB0175080	NA	NA
2515	HMDB0175081	NA	NA
2516	HMDB0175083	NA	NA
2517	HMDB0175073	NA	NA
2518	HMDB0175082	NA	NA
2519	HMDB0163581	NA	NA
2520	HMDB0163582	NA	NA
2521	HMDB0163584	NA	NA
2522	HMDB0038580	NA	NA
2523	HMDB0033631	Lactapiperanol D	HMDB0033631
2524	HMDB0180021	NA	NA
2525	HMDB0180098	NA	NA
2526	HMDB0180100	NA	NA
2527	HMDB0180099	NA	NA
2528	HMDB0180102	NA	NA
2529	HMDB0034780	Capsiate	HMDB0034780
2530	HMDB0180103	NA	NA
2531	HMDB0184951	NA	NA
2532	HMDB0184949	NA	NA
2533	HMDB0184953	NA	NA
2534	HMDB0012799	5'-Carboxy-gamma-chromanol	HMDB0012799
2535	HMDB0184954	NA	NA
2536	HMDB0184950	NA	NA
2537	HMDB0061677	NA	NA
2538	HMDB0000552	3-Methylglutaryl carnitine	HMDB0000552
2539	HMDB0015334	Nadolol	HMDB0015334
2540	HMDB0015345	Metipranolol	HMDB0015345
2541	HMDB0137251	NA	NA
2542	HMDB0137254	NA	NA
2543	HMDB0137256	NA	NA
2544	HMDB0137255	NA	NA
2545	HMDB0137252	NA	NA
2546	HMDB0137257	NA	NA
2547	HMDB0137259	NA	NA
2548	HMDB0137261	NA	NA
2549	HMDB0137264	NA	NA
2550	HMDB0137263	NA	NA
2551	HMDB0137265	NA	NA
2552	HMDB0137266	NA	NA
2553	HMDB0137267	NA	NA
2554	HMDB0137268	NA	NA
2555	HMDB0137270	NA	NA
2556	HMDB0179994	NA	NA
2557	HMDB0180049	NA	NA
2558	HMDB0041249	NA	NA
2559	HMDB0036693	NA	NA
2560	HMDB0034930	(3beta,6beta)-Furanoeremophilane-3,6-diol 6-acetate	HMDB0034930
2561	HMDB0034738	Isotrichodermin	HMDB0034738
2562	HMDB0035687	Acetylvalerenolic acid	HMDB0035687
2563	HMDB0039275	NA	NA
2564	HMDB0034658	9-Acetoxyfukinanolide	HMDB0034658
2565	HMDB0000791	L-Octanoylcarnitine	HMDB0000791
2566	HMDB0039044	NA	NA
2567	HMDB0131544	NA	NA
2568	HMDB0153683	NA	NA
2569	HMDB0134716	NA	NA
2570	HMDB0131577	NA	NA
2571	HMDB0140842	NA	NA
2572	HMDB0039858	NA	NA
2573	HMDB0150310	NA	NA
2574	HMDB0150311	NA	NA
2575	HMDB0030019	4'-Methoxymucidin	HMDB0030019
2576	HMDB0125543	NA	NA
2577	HMDB0125544	NA	NA
2578	HMDB0125545	NA	NA
2579	HMDB0125547	NA	NA
2580	HMDB0125546	NA	NA
2581	HMDB0125548	NA	NA
2582	HMDB0129031	NA	NA

2583	HMDB0129032	NA	NA
2584	HMDB0141104	NA	NA
2585	HMDB0141131	NA	NA
2586	HMDB0141141	NA	NA
2587	HMDB0141165	NA	NA
2588	HMDB0141171	NA	NA
2589	HMDB0129034	NA	NA
2590	HMDB0149106	NA	NA
2591	HMDB0140204	NA	NA
2592	HMDB0140116	NA	NA
2593	HMDB0129033	NA	NA
2594	HMDB0129035	NA	NA
2595	HMDB0129037	NA	NA
2596	HMDB0129036	NA	NA
2597	HMDB0129038	NA	NA
2598	HMDB0140114	NA	NA
2599	HMDB0140118	NA	NA
2600	HMDB0140117	NA	NA
2601	HMDB0140115	NA	NA
2602	HMDB0146850	NA	NA
2603	HMDB0040670	NA	NA
2604	HMDB0176556	NA	NA
2605	HMDB0013854	N4-Acetylsulfamethoxazole	HMDB0013854
2606	HMDB0167783	NA	NA
2607	HMDB0167780	NA	NA
2608	HMDB0034058	Quinacridone	HMDB0034058
2609	HMDB0178297	NA	NA
2610	HMDB0178295	NA	NA
2611	HMDB0128029	NA	NA
2612	HMDB0171101	NA	NA
2613	HMDB0151544	NA	NA
2614	HMDB0151545	NA	NA
2615	HMDB0131260	NA	NA
2616	HMDB0240531	NA	NA
2617	HMDB0240529	NA	NA
2618	HMDB0131259	NA	NA
2619	HMDB0131258	NA	NA
2620	HMDB0128028	NA	NA
2621	HMDB0040621	NA	NA
2622	HMDB0180003	NA	NA
2623	HMDB0126429	NA	NA
2624	HMDB0124977	NA	NA
2625	HMDB0124976	NA	NA
2626	HMDB0126430	NA	NA
2627	HMDB0183406	NA	NA
2628	HMDB0167831	NA	NA
2629	HMDB0167833	NA	NA
2630	HMDB0140804	NA	NA
2631	HMDB0128031	NA	NA
2632	HMDB0012267	N-Succinyl-L,L-2,6-diaminopimelate	HMDB0012267
2633	HMDB0062575	NA	NA
2634	HMDB0001235	5-Aminoimidazole ribonucleotide	HMDB0001235
2635	HMDB0029391	N-Jasmonoylisoleucine	HMDB0029391
2636	HMDB0006320	2,6 Dimethylheptanoyl carnitine	HMDB0006320
2637	HMDB0013288	Nonanoylcarnitine	HMDB0013288
2638	HMDB0038944	NA	NA
2639	HMDB0029283	Avenanthramide 1f	HMDB0029283
2640	HMDB0125856	NA	NA
2641	HMDB0146475	NA	NA
2642	HMDB0146474	NA	NA
2643	HMDB0014683	Amoxapine	HMDB0014683
2644	HMDB0178275	NA	NA
2645	HMDB0162434	NA	NA
2646	HMDB0162437	NA	NA
2647	HMDB0162435	NA	NA
2648	HMDB0162438	NA	NA
2649	HMDB0035173	2-Carboxy-1-[5-(2-carboxy-1-pyrrolidinyl)-2-hydroxy-2,4-pentadienylidene]pyrrolidinium	HMDB0035173
2650	HMDB0181175	NA	NA
2651	HMDB0181176	NA	NA
2652	HMDB0181179	NA	NA
2653	HMDB0181180	NA	NA
2654	HMDB0181177	NA	NA
2655	HMDB0181178	NA	NA
2656	HMDB0178438	NA	NA
2657	HMDB0178443	NA	NA
2658	HMDB0032766	N2-(2-Carboxymethyl-2-hydroxysuccinoyl)arginine	HMDB0032766
2659	HMDB0134938	NA	NA
2660	HMDB0013189	3-Indole carboxylic acid glucuronide	HMDB0013189
2661	HMDB0011658	2,8-Dihydroxyquinoline-beta-D-glucuronide	HMDB0011658
2662	HMDB0131931	NA	NA
2663	HMDB0131929	NA	NA
2664	HMDB0137816	NA	NA
2665	HMDB0137819	NA	NA
2666	HMDB0137821	NA	NA
2667	HMDB0140538	NA	NA
2668	HMDB0126563	NA	NA
2669	HMDB0125037	NA	NA



2670	HMDB0126566	NA	NA
2671	HMDB0131932	NA	NA
2672	HMDB0126564	NA	NA
2673	HMDB0126567	NA	NA
2674	HMDB0126570	NA	NA
2675	HMDB0125219	NA	NA
2676	HMDB0125216	NA	NA
2677	HMDB0125207	NA	NA
2678	HMDB0125079	NA	NA
2679	HMDB0125067	NA	NA
2680	HMDB0125052	NA	NA
2681	HMDB0126569	NA	NA
2682	HMDB0128213	NA	NA
2683	HMDB0131759	NA	NA
2684	HMDB0131760	NA	NA
2685	HMDB0131925	NA	NA
2686	HMDB0131928	NA	NA
2687	HMDB0140542	NA	NA
2688	HMDB0140556	NA	NA
2689	HMDB0167579	NA	NA
2690	HMDB0152484	NA	NA
2691	HMDB0167582	NA	NA
2692	HMDB0167580	NA	NA
2693	HMDB0167581	NA	NA
2694	HMDB0030835	trans-3,3',4',5,5',7-Hexahydroxyflavanone	HMDB0030835
2695	HMDB0152029	NA	NA
2696	HMDB0152031	NA	NA
2697	HMDB0152038	NA	NA
2698	HMDB0152035	NA	NA
2699	HMDB0152036	NA	NA
2700	HMDB0152037	NA	NA
2701	HMDB0152402	NA	NA
2702	HMDB0152479	NA	NA
2703	HMDB0039815	NA	NA
2704	HMDB0127839	NA	NA
2705	HMDB0128709	NA	NA
2706	HMDB0125826	NA	NA
2707	HMDB0125820	NA	NA
2708	HMDB0127778	NA	NA
2709	HMDB0127840	NA	NA
2710	HMDB0127779	NA	NA
2711	HMDB0125825	NA	NA
2712	HMDB0172923	NA	NA
2713	HMDB0172926	NA	NA
2714	HMDB0141622	NA	NA
2715	HMDB0034767	(1R*,3R*,3'S*)-1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-beta-carboline-3-carboxylic acid	HMDB0034767
2716	HMDB0142252	NA	NA
2717	HMDB0172514	NA	NA
2718	HMDB0172522	NA	NA
2719	HMDB0158878	NA	NA
2720	HMDB0166871	NA	NA
2721	HMDB0166874	NA	NA
2722	HMDB0166876	NA	NA
2723	HMDB0166877	NA	NA
2724	HMDB0158883	NA	NA
2725	HMDB0158879	NA	NA
2726	HMDB0166873	NA	NA
2727	HMDB0158880	NA	NA
2728	HMDB0158886	NA	NA
2729	HMDB0158885	NA	NA
2730	HMDB0160786	NA	NA
2731	HMDB0160787	NA	NA
2732	HMDB0166859	NA	NA
2733	HMDB0166870	NA	NA
2734	HMDB0158882	NA	NA
2735	HMDB0158881	NA	NA
2736	HMDB0158887	NA	NA
2737	HMDB0157435	NA	NA
2738	HMDB0157434	NA	NA
2739	HMDB0156934	NA	NA
2740	HMDB0156933	NA	NA
2741	HMDB0157433	NA	NA
2742	HMDB0156932	NA	NA
2743	HMDB0152126	NA	NA
2744	HMDB0152125	NA	NA
2745	HMDB0160788	NA	NA
2746	HMDB0039724	NA	NA
2747	HMDB0039726	NA	NA
2748	HMDB0029938	Acaciabiuronic acid	HMDB0029938
2749	HMDB0039722	NA	NA
2750	HMDB0155824	NA	NA
2751	HMDB0156218	NA	NA
2752	HMDB0157438	NA	NA
2753	HMDB0157437	NA	NA
2754	HMDB0157439	NA	NA
2755	HMDB0157441	NA	NA
2756	HMDB0157440	NA	NA

2757	HMDB0166391	NA	NA
2758	HMDB0166390	NA	NA
2759	HMDB0166392	NA	NA
2760	HMDB0156220	NA	NA
2761	HMDB0156219	NA	NA
2762	HMDB0155322	NA	NA
2763	HMDB0125610	NA	NA
2764	HMDB0125611	NA	NA
2765	HMDB0125612	NA	NA
2766	HMDB0125609	NA	NA
2767	HMDB0156221	NA	NA
2768	HMDB0155320	NA	NA
2769	HMDB0155318	NA	NA
2770	HMDB0155319	NA	NA
2771	HMDB0155321	NA	NA
2772	HMDB0166393	NA	NA
2773	HMDB0005011	Clopidogrel	HMDB0005011
2774	HMDB0175192	NA	NA
2775	HMDB0128893	NA	NA
2776	HMDB0062467	NA	NA
2777	HMDB0128890	NA	NA
2778	HMDB0128891	NA	NA
2779	HMDB0149084	NA	NA
2780	HMDB0164007	NA	NA
2781	HMDB0149086	NA	NA
2782	HMDB0033659	Dihydrohydroxy-O-methylsterigmatocystin	HMDB0033659
2783	HMDB0030589	O-Methylsterigmatocystin	HMDB0030589
2784	HMDB0148696	NA	NA
2785	HMDB0148232	NA	NA
2786	HMDB0030619	Ovalitenone	HMDB0030619
2787	HMDB0163589	NA	NA
2788	HMDB0014743	Sulindac	HMDB0014743
2789	HMDB0147815	NA	NA
2790	HMDB0147744	NA	NA
2791	HMDB0147742	NA	NA
2792	HMDB0147651	NA	NA
2793	HMDB0150253	NA	NA
2794	HMDB0147649	NA	NA
2795	HMDB0150255	NA	NA
2796	HMDB0147648	NA	NA
2797	HMDB0033298	3-(3,4-Dihydroxybenzyl)-7-hydroxy-5-methoxy-4-chromanone	HMDB0033298
2798	HMDB0148509	NA	NA
2799	HMDB0148510	NA	NA
2800	HMDB0148508	NA	NA
2801	HMDB0148507	NA	NA
2802	HMDB0148512	NA	NA
2803	HMDB0147889	NA	NA
2804	HMDB0148511	NA	NA
2805	HMDB0147535	NA	NA
2806	HMDB0147529	NA	NA
2807	HMDB0138112	NA	NA
2808	HMDB0137444	NA	NA
2809	HMDB0137443	NA	NA
2810	HMDB0137442	NA	NA
2811	HMDB0135788	NA	NA
2812	HMDB0133961	NA	NA
2813	HMDB0133962	NA	NA
2814	HMDB0133959	NA	NA
2815	HMDB0133957	NA	NA
2816	HMDB0133958	NA	NA
2817	HMDB0133295	NA	NA
2818	HMDB0138110	NA	NA
2819	HMDB0138111	NA	NA
2820	HMDB0146399	NA	NA
2821	HMDB0146753	NA	NA
2822	HMDB0146751	NA	NA
2823	HMDB0146573	NA	NA
2824	HMDB0146572	NA	NA
2825	HMDB0146426	NA	NA
2826	HMDB0146422	NA	NA
2827	HMDB0146412	NA	NA
2828	HMDB0140872	NA	NA
2829	HMDB0138632	NA	NA
2830	HMDB0133294	NA	NA
2831	HMDB0151836	NA	NA
2832	HMDB0037749	NA	NA
2833	HMDB0033797	Olivin	HMDB0033797
2834	HMDB0033924	Cajanol	HMDB0033924
2835	HMDB0030111	Homoferreirin	HMDB0030111
2836	HMDB0041790	NA	NA
2837	HMDB0037481	NA	NA
2838	HMDB0033692	Melilotocarpan D	HMDB0033692
2839	HMDB0037477	NA	NA
2840	HMDB0152003	NA	NA
2841	HMDB0152002	NA	NA
2842	HMDB0033683	Melilotocarpan E	HMDB0033683
2843	HMDB0151832	NA	NA

2844	HMDB0151833	NA	NA
2845	HMDB0151834	NA	NA
2846	HMDB0151632	NA	NA
2847	HMDB0151630	NA	NA
2848	HMDB0151631	NA	NA
2849	HMDB0152601	NA	NA
2850	HMDB0153237	NA	NA
2851	HMDB0037251	NA	NA
2852	HMDB0154307	NA	NA
2853	HMDB0153788	NA	NA
2854	HMDB0041234	NA	NA
2855	HMDB0153512	NA	NA
2856	HMDB0153415	NA	NA
2857	HMDB0151417	NA	NA
2858	HMDB0146221	NA	NA
2859	HMDB0146754	NA	NA
2860	HMDB0147650	NA	NA
2861	HMDB0138109	NA	NA
2862	HMDB0147743	NA	NA
2863	HMDB0132897	NA	NA
2864	HMDB0128591	NA	NA
2865	HMDB0128590	NA	NA
2866	HMDB0128197	NA	NA
2867	HMDB0126060	NA	NA
2868	HMDB0124872	NA	NA
2869	HMDB0130367	NA	NA
2870	HMDB0132894	NA	NA
2871	HMDB0132895	NA	NA
2872	HMDB0132890	NA	NA
2873	HMDB0132891	NA	NA
2874	HMDB0132883	NA	NA
2875	HMDB0132866	NA	NA
2876	HMDB0131742	NA	NA
2877	HMDB0131738	NA	NA
2878	HMDB0130897	NA	NA
2879	HMDB0130669	NA	NA
2880	HMDB0130668	NA	NA
2881	HMDB0130395	NA	NA
2882	HMDB0130391	NA	NA
2883	HMDB0146752	NA	NA
2884	HMDB0154672	NA	NA
2885	HMDB0154674	NA	NA
2886	HMDB0154675	NA	NA
2887	HMDB0154673	NA	NA
2888	HMDB0154671	NA	NA
2889	HMDB0154670	NA	NA
2890	HMDB0029566	Isopulegone caffeate	HMDB0029566
2891	HMDB0154668	NA	NA
2892	HMDB0134704	NA	NA
2893	HMDB0147915	NA	NA
2894	HMDB0154665	NA	NA
2895	HMDB0154669	NA	NA
2896	HMDB0154666	NA	NA
2897	HMDB0154667	NA	NA
2898	HMDB0148183	NA	NA
2899	HMDB0153649	NA	NA
2900	HMDB0125854	NA	NA
2901	HMDB0141256	NA	NA
2902	HMDB0124819	NA	NA
2903	HMDB0125836	NA	NA
2904	HMDB0125842	NA	NA
2905	HMDB0133467	NA	NA
2906	HMDB0041386	NA	NA
2907	HMDB0034412	2'-O-Methylphaseollinisoflavan	HMDB0034412
2908	HMDB0039439	NA	NA
2909	HMDB0033672	4'-O-Methylglabridin	HMDB0033672
2910	HMDB0029514	Licochalcone A	HMDB0029514
2911	HMDB0033782	Bergamottin	HMDB0033782
2912	HMDB0039309	NA	NA
2913	HMDB0030846	Archangelin	HMDB0030846
2914	HMDB0039438	NA	NA
2915	HMDB0033671	2'-O-Methylglabridin	HMDB0033671
2916	HMDB0032665	Licoagrocarpin	HMDB0032665
2917	HMDB0031633	Orientanol B	HMDB0031633
2918	HMDB0001272	Nicotine glucuronide	HMDB0001272
2919	HMDB0032808	Niazirinin	HMDB0032808
2920	HMDB0131864	NA	NA
2921	HMDB0124924	NA	NA
2922	HMDB0131867	NA	NA
2923	HMDB0133539	NA	NA
2924	HMDB0124927	NA	NA
2925	HMDB0125807	NA	NA
2926	HMDB0131075	NA	NA
2927	HMDB0133516	NA	NA
2928	HMDB0133495	NA	NA
2929	HMDB0133485	NA	NA
2930	HMDB0133468	NA	NA

2931	HMDB0131866	NA	NA
2932	HMDB0131865	NA	NA
2933	HMDB0124928	NA	NA
2934	HMDB0124929	NA	NA
2935	HMDB0124838	NA	NA
2936	HMDB0124800	NA	NA
2937	HMDB0124826	NA	NA
2938	HMDB0124829	NA	NA
2939	HMDB0124835	NA	NA
2940	HMDB0124837	NA	NA
2941	HMDB0124922	NA	NA
2942	HMDB0130876	NA	NA
2943	HMDB0138809	NA	NA
2944	HMDB0150217	NA	NA
2945	HMDB0150219	NA	NA
2946	HMDB0124822	NA	NA
2947	HMDB0150216	NA	NA
2948	HMDB0150218	NA	NA
2949	HMDB0150215	NA	NA
2950	HMDB0147761	NA	NA
2951	HMDB0147762	NA	NA
2952	HMDB0147765	NA	NA
2953	HMDB0147767	NA	NA
2954	HMDB0147766	NA	NA
2955	HMDB0147764	NA	NA
2956	HMDB0147768	NA	NA
2957	HMDB0147769	NA	NA
2958	HMDB0149836	NA	NA
2959	HMDB0150181	NA	NA
2960	HMDB0150186	NA	NA
2961	HMDB0150185	NA	NA
2962	HMDB0150182	NA	NA
2963	HMDB0150184	NA	NA
2964	HMDB0150187	NA	NA
2965	HMDB0150214	NA	NA
2966	HMDB0035440	alpha,beta-Dihydroxanthohumol	HMDB0035440
2967	HMDB0030666	Chalepin acetate	HMDB0030666
2968	HMDB0035403	Gingerenone A	HMDB0035403
2969	HMDB0030798	Myricanone	HMDB0030798
2970	HMDB0033880	Mammea B/AC cyclo D	HMDB0033880
2971	HMDB0033879	Mammea B/AD cyclo D	HMDB0033879
2972	HMDB0030333	Fragransol C	HMDB0030333
2973	HMDB0041401	NA	NA
2974	HMDB0138808	NA	NA
2975	HMDB0184970	NA	NA
2976	HMDB0184809	NA	NA
2977	HMDB0030936	5,8,12-Trihydroxy-9-octadecenoic acid	HMDB0030936
2978	HMDB0038555	NA	NA
2979	HMDB0172549	NA	NA
2980	HMDB0004710	9,10,13-TriHOME	HMDB0004710
2981	HMDB0004708	9,12,13-TriHOME	HMDB0004708
2982	HMDB0062299	NA	NA
2983	HMDB0062691	NA	NA
2984	HMDB0186066	NA	NA
2985	HMDB0186064	NA	NA
2986	HMDB0186065	NA	NA
2987	HMDB0186063	NA	NA
2988	HMDB0186062	NA	NA
2989	HMDB0186061	NA	NA
2990	HMDB0186060	NA	NA
2991	HMDB0186059	NA	NA
2992	HMDB0183411	NA	NA
2993	HMDB0164486	NA	NA
2994	HMDB0062798	NA	NA
2995	HMDB0062291	NA	NA
2996	HMDB0005077	8-iso-15-keto-PGF2a	HMDB0005077
2997	HMDB0060042	NA	NA
2998	HMDB0060041	NA	NA
2999	HMDB0012587	15-Epi-lipoxin A4	HMDB0012587
3000	HMDB0012564	13,14-Dihydro-15-oxo-lipoxin A4	HMDB0012564
3001	HMDB0012481	(5Z)-(15S)-11alpha-Hydroxy-9,15-dioxoprostanoate	HMDB0012481
3002	HMDB0002363	Levuglandin E2	HMDB0002363
3003	HMDB0002132	8-iso-PGF3a	HMDB0002132
3004	HMDB0002122	Prostaglandin F3a	HMDB0002122
3005	HMDB0001509	20-Hydroxy-leukotriene B4	HMDB0001509
3006	HMDB0001452	Thromboxane A2	HMDB0001452
3007	HMDB0001381	Prostaglandin H2	HMDB0001381
3008	HMDB0001335	Prostaglandin I2	HMDB0001335
3009	HMDB0001320	(13E)-11a-Hydroxy-9,15-dioxoprost-13-enoic acid	HMDB0001320
3010	HMDB0001403	Prostaglandin D2	HMDB0001403
3011	HMDB0002400	Levuglandin D2	HMDB0002400
3012	HMDB0002776	13,14-Dihydro-15-keto-PGE2	HMDB0002776
3013	HMDB0004240	15-Keto-prostaglandin F2a	HMDB0004240
3014	HMDB0035064	Cinnassiol D4	HMDB0035064
3015	HMDB0034676	Cinnassiol D1	HMDB0034676
3016	HMDB0035338	Sterebin B	HMDB0035338
3017	HMDB0035339	Sterebin C	HMDB0035339

3018	HMDB0036756	NA	NA
3019	HMDB0005844	8-isoprostaglandin E2	HMDB0005844
3020	HMDB0005082	Lipoxin B4	HMDB0005082
3021	HMDB0004385	Lipoxin A4	HMDB0004385
3022	HMDB0001220	Prostaglandin E2	HMDB0001220
3023	HMDB0062746	NA	NA
3024	HMDB0013039	Prostaglandin G1	HMDB0013039
3025	HMDB0012502	10,11-dihydro-20-dihydroxy-LTB4	HMDB0012502
3026	HMDB0004049	20-Hydroxy-PGF2a	HMDB0004049
3027	HMDB0003252	Thromboxane B2	HMDB0003252
3028	HMDB0002886	6-Keto-prostaglandin F1a	HMDB0002886
3029	HMDB0013627	Cervonoyl ethanolamide	HMDB0013627
3030	HMDB0041301	NA	NA
3031	HMDB0014629	Nabilone	HMDB0014629
3032	HMDB0156539	NA	NA
3033	HMDB0159326	NA	NA
3034	HMDB0158258	NA	NA
3035	HMDB0039760	NA	NA
3036	HMDB0185130	NA	NA
3037	HMDB0062725	NA	NA
3038	HMDB0038910	NA	NA
3039	HMDB0035676	1-Hydroxy-1-phenyl-3-hexadecanone	HMDB0035676
3040	HMDB0035677	3-Hydroxy-1-phenyl-1-hexadecanone	HMDB0035677
3041	HMDB0002226	Adrenic acid	HMDB0002226
3042	HMDB0062580	NA	NA
3043	HMDB0184508	NA	NA
3044	HMDB0156540	NA	NA
3045	HMDB0128445	NA	NA
3046	HMDB0128454	NA	NA
3047	HMDB0128439	NA	NA
3048	HMDB0128457	NA	NA
3049	HMDB0128441	NA	NA
3050	HMDB0128456	NA	NA
3051	HMDB0128453	NA	NA
3052	HMDB0128449	NA	NA
3053	HMDB0128450	NA	NA
3054	HMDB0128452	NA	NA
3055	HMDB0128448	NA	NA
3056	HMDB0128446	NA	NA
3057	HMDB0128442	NA	NA
3058	HMDB0128444	NA	NA
3059	HMDB0128438	NA	NA
3060	HMDB0128437	NA	NA
3061	HMDB0128458	NA	NA
3062	HMDB0177036	NA	NA
3063	HMDB0059612	NA	NA
3064	HMDB0177043	NA	NA
3065	HMDB0147189	NA	NA
3066	HMDB0147188	NA	NA
3067	HMDB0148992	NA	NA
3068	HMDB0177490	NA	NA
3069	HMDB0147184	NA	NA
3070	HMDB0140356	NA	NA
3071	HMDB0138063	NA	NA
3072	HMDB0128976	NA	NA
3073	HMDB0128981	NA	NA
3074	HMDB0128983	NA	NA
3075	HMDB0131634	NA	NA
3076	HMDB0131637	NA	NA
3077	HMDB0138062	NA	NA
3078	HMDB0147185	NA	NA
3079	HMDB0041882	NA	NA
3080	HMDB0184507	NA	NA
3081	HMDB0184503	NA	NA
3082	HMDB0157679	NA	NA
3083	HMDB0159749	NA	NA
3084	HMDB0184460	NA	NA
3085	HMDB0184500	NA	NA
3086	HMDB0184502	NA	NA
3087	HMDB0184506	NA	NA
3088	HMDB0184505	NA	NA
3089	HMDB0184504	NA	NA
3090	HMDB0184501	NA	NA
3091	HMDB0240595	NA	NA
3092	HMDB0184271	NA	NA
3093	HMDB0183492	NA	NA
3094	HMDB0156837	NA	NA
3095	HMDB0156831	NA	NA
3096	HMDB0156835	NA	NA
3097	HMDB0156889	NA	NA
3098	HMDB0156836	NA	NA
3099	HMDB0157597	NA	NA
3100	HMDB0157601	NA	NA
3101	HMDB0157602	NA	NA
3102	HMDB0157742	NA	NA
3103	HMDB0157743	NA	NA
3104	HMDB0157738	NA	NA

3105	HMDB0157739	NA	NA
3106	HMDB0157603	NA	NA
3107	HMDB0157604	NA	NA
3108	HMDB0157599	NA	NA
3109	HMDB0157600	NA	NA
3110	HMDB0156838	NA	NA
3111	HMDB0156832	NA	NA
3112	HMDB0155046	NA	NA
3113	HMDB0156806	NA	NA
3114	HMDB0156826	NA	NA
3115	HMDB0156827	NA	NA
3116	HMDB0156829	NA	NA
3117	HMDB0156830	NA	NA
3118	HMDB0156828	NA	NA
3119	HMDB0156834	NA	NA
3120	HMDB0156833	NA	NA
3121	HMDB0157740	NA	NA
3122	HMDB0157741	NA	NA
3123	HMDB0158276	NA	NA
3124	HMDB0167960	NA	NA
3125	HMDB0167961	NA	NA
3126	HMDB0167962	NA	NA
3127	HMDB0167964	NA	NA
3128	HMDB0167963	NA	NA
3129	HMDB0167966	NA	NA
3130	HMDB0167965	NA	NA
3131	HMDB0167968	NA	NA
3132	HMDB0167967	NA	NA
3133	HMDB0170452	NA	NA
3134	HMDB0170451	NA	NA
3135	HMDB0186750	NA	NA
3136	HMDB0000903	Tetrahydrocortisone	HMDB0000903
3137	HMDB0003259	Dihydrocortisol	HMDB0003259
3138	HMDB0006753	3a,11b,21-Trihydroxy-20-oxo-5b-pregnan-18-al	HMDB0006753
3139	HMDB0006754	11b,21-Dihydroxy-3,20-oxo-5b-pregnan-18-al	HMDB0006754
3140	HMDB0006760	11b,17a,21-Trihydroxypreg-nenolone	HMDB0006760
3141	HMDB0032553	Vanillin 3-(L-menthoxy)propane-1,2-diol acetal	HMDB0032553
3142	HMDB0013157	18-Hydroxy-11-dehydrotetrahydrocorticosterone	HMDB0013157
3143	HMDB0013164	2-Hydroxy-lauroylcarnitine	HMDB0013164
3144	HMDB0061638	NA	NA
3145	HMDB0159333	NA	NA
3146	HMDB0030730	3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin	HMDB0030730
3147	HMDB0144961	NA	NA
3148	HMDB0144931	NA	NA
3149	HMDB0033084	7-Hydroxydehydroglaucone	HMDB0033084
3150	HMDB0061331	NA	NA
3151	HMDB0036765	NA	NA
3152	HMDB0176548	NA	NA
3153	HMDB0035212	Sonchuionoside C	HMDB0035212
3154	HMDB0182762	NA	NA
3155	HMDB0030370	Citroside A	HMDB0030370
3156	HMDB0182758	NA	NA
3157	HMDB0182757	NA	NA
3158	HMDB0182755	NA	NA
3159	HMDB0182753	NA	NA
3160	HMDB0178171	NA	NA
3161	HMDB0178167	NA	NA
3162	HMDB0178165	NA	NA
3163	HMDB0178164	NA	NA
3164	HMDB0178162	NA	NA
3165	HMDB0178160	NA	NA
3166	HMDB0029772	Corchoionol C 9-glucoside	HMDB0029772
3167	HMDB0182760	NA	NA
3168	HMDB0157683	NA	NA
3169	HMDB0157685	NA	NA
3170	HMDB0157684	NA	NA
3171	HMDB0157680	NA	NA
3172	HMDB0157682	NA	NA
3173	HMDB0157681	NA	NA
3174	HMDB0157452	NA	NA
3175	HMDB0157454	NA	NA
3176	HMDB0157451	NA	NA
3177	HMDB0157453	NA	NA
3178	HMDB0157449	NA	NA
3179	HMDB0157450	NA	NA
3180	HMDB0157448	NA	NA
3181	HMDB0157447	NA	NA
3182	HMDB0000865	Muricholic acid	HMDB0000865
3183	HMDB0000760	Hyochoolic acid	HMDB0000760
3184	HMDB0000527	6a,12a-Dihydroxylithocholic acid	HMDB0000527
3185	HMDB0000432	3a,7b,12a-Trihydroxy-5a-Cholanoic acid	HMDB0000432
3186	HMDB0000427	3b,7b,12a-Trihydroxy-5a-Cholanoic acid	HMDB0000427
3187	HMDB0000419	3b,7a,12a-Trihydroxy-5b-cholanoic acid	HMDB0000419
3188	HMDB0000415	3a,6b,7b-Trihydroxy-5b-cholanoic acid	HMDB0000415
3189	HMDB0000414	1b,3a,7a-Trihydroxy-5b-cholanoic acid	HMDB0000414
3190	HMDB0000404	2b,3a,7a-Trihydroxy-5b-cholanoic acid	HMDB0000404
3191	HMDB0000395	3b,7b,12a-Trihydroxy-5b-cholanoic acid	HMDB0000395

3192	HMDB0000390	3a,7b,12b-Trihydroxy-5b-cholanoic acid	HMDB0000390
3193	HMDB0000917	Ursocholic acid	HMDB0000917
3194	HMDB0000376	3b,7a,12a-Trihydroxy-5a-Cholanoic acid	HMDB0000376
3195	HMDB0158259	NA	NA
3196	HMDB0184509	NA	NA
3197	HMDB0184414	NA	NA
3198	HMDB0184360	NA	NA
3199	HMDB0184356	NA	NA
3200	HMDB0184355	NA	NA
3201	HMDB0184316	NA	NA
3202	HMDB0184317	NA	NA
3203	HMDB0184318	NA	NA
3204	HMDB0184314	NA	NA
3205	HMDB0184313	NA	NA
3206	HMDB0184315	NA	NA
3207	HMDB0161001	NA	NA
3208	HMDB0161003	NA	NA
3209	HMDB0184510	NA	NA
3210	HMDB0184511	NA	NA
3211	HMDB0184514	NA	NA
3212	HMDB0000506	Alpha-Muricholic acid	HMDB0000506
3213	HMDB0000505	Allocholic acid	HMDB0000505
3214	HMDB0184519	NA	NA
3215	HMDB0184520	NA	NA
3216	HMDB0184517	NA	NA
3217	HMDB0184516	NA	NA
3218	HMDB0184515	NA	NA
3219	HMDB0184518	NA	NA
3220	HMDB0184513	NA	NA
3221	HMDB0184512	NA	NA
3222	HMDB0161002	NA	NA
3223	HMDB0161000	NA	NA
3224	HMDB0159761	NA	NA
3225	HMDB0158766	NA	NA
3226	HMDB0158272	NA	NA
3227	HMDB0158270	NA	NA
3228	HMDB0158269	NA	NA
3229	HMDB0158271	NA	NA
3230	HMDB0158268	NA	NA
3231	HMDB0158265	NA	NA
3232	HMDB0158264	NA	NA
3233	HMDB0158266	NA	NA
3234	HMDB0158267	NA	NA
3235	HMDB0158262	NA	NA
3236	HMDB0158261	NA	NA
3237	HMDB0158260	NA	NA
3238	HMDB0158764	NA	NA
3239	HMDB0158765	NA	NA
3240	HMDB0158767	NA	NA
3241	HMDB0159758	NA	NA
3242	HMDB0159757	NA	NA
3243	HMDB0159754	NA	NA
3244	HMDB0159755	NA	NA
3245	HMDB0159753	NA	NA
3246	HMDB0159756	NA	NA
3247	HMDB0159751	NA	NA
3248	HMDB0159750	NA	NA
3249	HMDB0159752	NA	NA
3250	HMDB0158771	NA	NA
3251	HMDB0158769	NA	NA
3252	HMDB0158770	NA	NA
3253	HMDB0158768	NA	NA
3254	HMDB0158263	NA	NA
3255	HMDB0000371	1,3,12-Trihydroxy-24-oic acid	HMDB0000371
3256	HMDB0000364	3a,6a,7b-Trihydroxy-5b-cholanoic acid	HMDB0000364
3257	HMDB0000330	3a,4b,12a-Trihydroxy-5b-cholanoic acid	HMDB0000330
3258	HMDB0000326	1b,3a,12a-Trihydroxy-5b-cholanoic acid	HMDB0000326
3259	HMDB0000320	3a,4b,7a-Trihydroxy-5b-cholanoic acid	HMDB0000320
3260	HMDB0000312	3a,7a,12b-Trihydroxy-5b-cholanoic acid	HMDB0000312
3261	HMDB0000619	Cholic acid	HMDB0000619
3262	HMDB0184357	NA	NA
3263	HMDB0000467	Nutriacholic acid	HMDB0000467
3264	HMDB0000460	7-Hydroxy-3-oxocholanoic acid	HMDB0000460
3265	HMDB0000328	12-Ketodeoxycholic acid	HMDB0000328
3266	HMDB0041454	NA	NA
3267	HMDB0012866	9'-Carboxy-alpha-chromanol	HMDB0012866
3268	HMDB0159167	NA	NA
3269	HMDB0157686	NA	NA
3270	HMDB0157455	NA	NA
3271	HMDB0157446	NA	NA
3272	HMDB0156548	NA	NA
3273	HMDB0184495	NA	NA
3274	HMDB0156546	NA	NA
3275	HMDB0156545	NA	NA
3276	HMDB0156543	NA	NA
3277	HMDB0156544	NA	NA
3278	HMDB0156542	NA	NA

3279	HMDB0156541	NA	NA
3280	HMDB0062742	NA	NA
3281	HMDB0184497	NA	NA
3282	HMDB0158251	NA	NA
3283	HMDB0158250	NA	NA
3284	HMDB0158772	NA	NA
3285	HMDB0159748	NA	NA
3286	HMDB0158273	NA	NA
3287	HMDB0158257	NA	NA
3288	HMDB0158256	NA	NA
3289	HMDB0159759	NA	NA
3290	HMDB0159760	NA	NA
3291	HMDB0158253	NA	NA
3292	HMDB0160999	NA	NA
3293	HMDB0158254	NA	NA
3294	HMDB0184494	NA	NA
3295	HMDB0158255	NA	NA
3296	HMDB0156547	NA	NA
3297	HMDB0062796	NA	NA
3298	HMDB0000503	7a-Hydroxy-3-oxo-5b-cholanoic acid	HMDB0000503
3299	HMDB0158252	NA	NA
3300	HMDB0184496	NA	NA
3301	HMDB0184498	NA	NA
3302	HMDB0184499	NA	NA
3303	HMDB0038073	NA	NA
3304	HMDB0013327	Dodecanedioylcarnitine	HMDB0013327
3305	HMDB0061030	NA	NA
3306	HMDB0030198	(-)-Folicanthine	HMDB0030198
3307	HMDB0000222	L-Palmitoylcarnitine	HMDB0000222
3308	HMDB0011574	MG(20:2(11Z,14Z)/0:0/0:0)	HMDB0011574
3309	HMDB0011544	MG(0:0/20:2(11Z,14Z)/0:0)	HMDB0011544
3310	HMDB0036865	NA	NA
3311	HMDB0035959	Persenone B	HMDB0035959
3312	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol	HMDB0011644
3313	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al	HMDB0006894
3314	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one	HMDB0006887
3315	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one	HMDB0006886
3316	HMDB0006764	17a,20a-Dihydroxycholesterol	HMDB0006764
3317	HMDB0006763	20a,22b-Dihydroxycholesterol	HMDB0006763
3318	HMDB0006281	7-a,27-Dihydroxycholesterol	HMDB0006281
3319	HMDB0060136	7alpha,24S-Dihydroxycholesterol	HMDB0060136
3320	HMDB0006280	7-a,25-Dihydroxycholesterol	HMDB0006280
3321	HMDB0159657	NA	NA
3322	HMDB0172272	NA	NA
3323	HMDB0172271	NA	NA
3324	HMDB0172269	NA	NA
3325	HMDB0172270	NA	NA
3326	HMDB0172267	NA	NA
3327	HMDB0172265	NA	NA
3328	HMDB0172268	NA	NA
3329	HMDB0172266	NA	NA
3330	HMDB0185566	NA	NA
3331	HMDB0185568	NA	NA
3332	HMDB0185575	NA	NA
3333	HMDB0185573	NA	NA
3334	HMDB0185574	NA	NA
3335	HMDB0185571	NA	NA
3336	HMDB0185572	NA	NA
3337	HMDB0185569	NA	NA
3338	HMDB0185567	NA	NA
3339	HMDB0185570	NA	NA
3340	HMDB0172262	NA	NA
3341	HMDB0172264	NA	NA
3342	HMDB0062675	NA	NA
3343	HMDB0062664	NA	NA
3344	HMDB0062607	NA	NA
3345	HMDB0062420	NA	NA
3346	HMDB0062419	NA	NA
3347	HMDB0159652	NA	NA
3348	HMDB0159656	NA	NA
3349	HMDB0172263	NA	NA
3350	HMDB0159658	NA	NA
3351	HMDB0159655	NA	NA
3352	HMDB0159654	NA	NA
3353	HMDB0159653	NA	NA
3354	HMDB0159651	NA	NA
3355	HMDB0184845	NA	NA
3356	HMDB0184846	NA	NA
3357	HMDB0155084	NA	NA
3358	HMDB0184842	NA	NA
3359	HMDB0184843	NA	NA
3360	HMDB0184841	NA	NA
3361	HMDB0184844	NA	NA
3362	HMDB0184848	NA	NA
3363	HMDB0184847	NA	NA
3364	HMDB0184849	NA	NA
3365	HMDB0184851	NA	NA



3366	HMDB0184850	NA	NA
3367	HMDB0185576	NA	NA
3368	HMDB0185577	NA	NA
3369	HMDB0185578	NA	NA
3370	HMDB0184168	NA	NA
3371	HMDB0003550	Calcidiol	HMDB0003550
3372	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	HMDB0036012
3373	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	HMDB0034328
3374	HMDB0035585	1-Phenyl-1,3-heneicosanedione	HMDB0035585
3375	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	HMDB0006721
3376	HMDB0006722	25-Hydroxytachysterol3	HMDB0006722
3377	HMDB0001993	7a-Hydroxy-cholestene-3-one	HMDB0001993
3378	HMDB0000501	7-Ketocholesterol	HMDB0000501
3379	HMDB0015504	Alfalcidol	HMDB0015504
3380	HMDB0039871	NA	NA
3381	HMDB0060132	NA	NA
3382	HMDB0060131	NA	NA
3383	HMDB0184149	NA	NA
3384	HMDB0174260	NA	NA
3385	HMDB0174261	NA	NA
3386	HMDB0172274	NA	NA
3387	HMDB0172275	NA	NA
3388	HMDB0172273	NA	NA
3389	HMDB0155085	NA	NA
3390	HMDB0155087	NA	NA
3391	HMDB0155086	NA	NA
3392	HMDB0155081	NA	NA
3393	HMDB0155082	NA	NA
3394	HMDB0174265	NA	NA
3395	HMDB0174262	NA	NA
3396	HMDB0174263	NA	NA
3397	HMDB0184150	NA	NA
3398	HMDB0184148	NA	NA
3399	HMDB0184147	NA	NA
3400	HMDB0184145	NA	NA
3401	HMDB0184146	NA	NA
3402	HMDB0184144	NA	NA
3403	HMDB0174268	NA	NA
3404	HMDB0174267	NA	NA
3405	HMDB0174266	NA	NA
3406	HMDB0174264	NA	NA
3407	HMDB0155083	NA	NA
3408	HMDB0155080	NA	NA
3409	HMDB0184143	NA	NA
3410	HMDB0154867	NA	NA
3411	HMDB0154866	NA	NA
3412	HMDB0035951	Erucoylacetone	HMDB0035951
3413	HMDB0164879	NA	NA
3414	HMDB0037260	NA	NA
3415	HMDB0158333	NA	NA
3416	HMDB0150478	NA	NA
3417	HMDB0150475	NA	NA
3418	HMDB0162509	NA	NA
3419	HMDB0150477	NA	NA
3420	HMDB0038347	NA	NA
3421	HMDB0150474	NA	NA
3422	HMDB0150463	NA	NA
3423	HMDB0150458	NA	NA
3424	HMDB0150468	NA	NA
3425	HMDB0150470	NA	NA
3426	HMDB0150457	NA	NA
3427	HMDB0150453	NA	NA
3428	HMDB0150469	NA	NA
3429	HMDB0150452	NA	NA
3430	HMDB0149868	NA	NA
3431	HMDB0150462	NA	NA
3432	HMDB0140070	NA	NA
3433	HMDB0153459	NA	NA
3434	HMDB0153444	NA	NA
3435	HMDB0153474	NA	NA
3436	HMDB0153627	NA	NA
3437	HMDB0153466	NA	NA
3438	HMDB0139521	NA	NA
3439	HMDB0139520	NA	NA
3440	HMDB0139517	NA	NA
3441	HMDB0139504	NA	NA
3442	HMDB0139507	NA	NA
3443	HMDB0139514	NA	NA
3444	HMDB0149502	NA	NA
3445	HMDB0153458	NA	NA
3446	HMDB0153451	NA	NA
3447	HMDB0153443	NA	NA
3448	HMDB0139516	NA	NA
3449	HMDB0139508	NA	NA
3450	HMDB0139513	NA	NA
3451	HMDB0164958	NA	NA
3452	HMDB0035876	Mesuagin	HMDB0035876

3453	HMDB0180147	NA	NA
3454	HMDB0013842	O-Deethylated candesartan	HMDB0013842
3455	HMDB0144444	NA	NA
3456	HMDB0144965	NA	NA
3457	HMDB0144871	NA	NA
3458	HMDB0142647	NA	NA
3459	HMDB0144859	NA	NA
3460	HMDB0144408	NA	NA
3461	HMDB0144379	NA	NA
3462	HMDB0142761	NA	NA
3463	HMDB0142694	NA	NA
3464	HMDB0144418	NA	NA
3465	HMDB0144964	NA	NA
3466	HMDB0142682	NA	NA
3467	HMDB0144733	NA	NA
3468	HMDB0038793	NA	NA
3469	HMDB0038787	NA	NA
3470	HMDB0175541	NA	NA
3471	HMDB0175538	NA	NA
3472	HMDB0175530	NA	NA
3473	HMDB0175535	NA	NA
3474	HMDB0147021	NA	NA
3475	HMDB0147024	NA	NA
3476	HMDB0147025	NA	NA
3477	HMDB0147019	NA	NA
3478	HMDB0147020	NA	NA
3479	HMDB0148764	NA	NA
3480	HMDB0147022	NA	NA
3481	HMDB0147023	NA	NA
3482	HMDB0148762	NA	NA
3483	HMDB0168741	NA	NA
3484	HMDB0148763	NA	NA
3485	HMDB0148761	NA	NA
3486	HMDB0148760	NA	NA
3487	HMDB0148765	NA	NA
3488	HMDB0148759	NA	NA
3489	HMDB0147026	NA	NA
3490	HMDB0147018	NA	NA
3491	HMDB0168749	NA	NA
3492	HMDB0168747	NA	NA
3493	HMDB0168748	NA	NA
3494	HMDB0168750	NA	NA
3495	HMDB0168746	NA	NA
3496	HMDB0168744	NA	NA
3497	HMDB0168740	NA	NA
3498	HMDB0168742	NA	NA
3499	HMDB0168743	NA	NA
3500	HMDB0168739	NA	NA
3501	HMDB0168745	NA	NA
3502	HMDB0041407	NA	NA
3503	HMDB0014838	Eplerenone	HMDB0014838
3504	HMDB0037039	NA	NA
3505	HMDB0030404	Armillaripin	HMDB0030404
3506	HMDB0039380	NA	NA
3507	HMDB0173691	NA	NA
3508	HMDB0173689	NA	NA
3509	HMDB0173685	NA	NA
3510	HMDB0173687	NA	NA
3511	HMDB0173683	NA	NA
3512	HMDB0062274	NA	NA
3513	HMDB0062282	NA	NA
3514	HMDB0062292	NA	NA
3515	HMDB0034662	Dihydrofukinolide	HMDB0034662
3516	HMDB0164538	NA	NA
3517	HMDB0164537	NA	NA
3518	HMDB0164536	NA	NA
3519	HMDB0240233	NA	NA
3520	HMDB0139759	NA	NA
3521	HMDB0139773	NA	NA
3522	HMDB0139772	NA	NA
3523	HMDB0139774	NA	NA
3524	HMDB0139775	NA	NA
3525	HMDB0139761	NA	NA
3526	HMDB0139764	NA	NA
3527	HMDB0139762	NA	NA
3528	HMDB0139760	NA	NA
3529	HMDB0139763	NA	NA
3530	HMDB0139766	NA	NA
3531	HMDB0139767	NA	NA
3532	HMDB0139765	NA	NA
3533	HMDB0139768	NA	NA
3534	HMDB0139769	NA	NA
3535	HMDB0139771	NA	NA
3536	HMDB0139770	NA	NA
3537	HMDB0139778	NA	NA
3538	HMDB0139776	NA	NA
3539	HMDB0139777	NA	NA

3540	HMDB0038618	NA	NA
3541	HMDB0183867	NA	NA
3542	HMDB0183864	NA	NA
3543	HMDB0183876	NA	NA
3544	HMDB0183860	NA	NA
3545	HMDB0183873	NA	NA
3546	HMDB0183891	NA	NA
3547	HMDB0183870	NA	NA
3548	HMDB0183894	NA	NA
3549	HMDB0036548	NA	NA
3550	HMDB0006226	24R,25-Dihydroxyvitamin D3	HMDB0006226
3551	HMDB0062401	NA	NA
3552	HMDB0062610	NA	NA
3553	HMDB0062736	NA	NA
3554	HMDB0159642	NA	NA
3555	HMDB0159643	NA	NA
3556	HMDB0159645	NA	NA
3557	HMDB0159644	NA	NA
3558	HMDB0174275	NA	NA
3559	HMDB0174276	NA	NA
3560	HMDB0174277	NA	NA
3561	HMDB0174278	NA	NA
3562	HMDB0174280	NA	NA
3563	HMDB0174279	NA	NA
3564	HMDB0174281	NA	NA
3565	HMDB0174282	NA	NA
3566	HMDB0174283	NA	NA
3567	HMDB0174274	NA	NA
3568	HMDB0174272	NA	NA
3569	HMDB0159649	NA	NA
3570	HMDB0159646	NA	NA
3571	HMDB0159647	NA	NA
3572	HMDB0159648	NA	NA
3573	HMDB0159650	NA	NA
3574	HMDB0172935	NA	NA
3575	HMDB0172936	NA	NA
3576	HMDB0174269	NA	NA
3577	HMDB0174271	NA	NA
3578	HMDB0174270	NA	NA
3579	HMDB0174273	NA	NA
3580	HMDB0012453	3 beta-Hydroxy-5-cholestenoate	HMDB0012453
3581	HMDB0001903	Calcitriol	HMDB0001903
3582	HMDB0030024	Sarsasapogenin	HMDB0030024
3583	HMDB0060133	NA	NA
3584	HMDB0060425	7alpha,25-Dihydroxy-4-cholesten-3-one	HMDB0060425
3585	HMDB0060508	NA	NA
3586	HMDB0030048	Smilagenin	HMDB0030048
3587	HMDB0030047	Neotigogenin	HMDB0030047
3588	HMDB0015046	Paricalcitol	HMDB0015046
3589	HMDB0000430	24,25-Dihydroxyvitamin D	HMDB0000430
3590	HMDB0001420	25,26-dihydroxyvitamin D	HMDB0001420
3591	HMDB0002197	7a,12a-Dihydroxy-cholestene-3-one	HMDB0002197
3592	HMDB0006720	23S,25-dihydroxyvitamin D3	HMDB0006720
3593	HMDB0012459	7 alpha,26-Dihydroxy-4-cholesten-3-one	HMDB0012459
3594	HMDB0012457	7 alpha,24-Dihydroxy-4-cholesten-3-one	HMDB0012457
3595	HMDB0035300	Octadecyl cis-p-coumarate	HMDB0035300
3596	HMDB0162231	NA	NA
3597	HMDB0159898	NA	NA
3598	HMDB0159886	NA	NA
3599	HMDB0159887	NA	NA
3600	HMDB0159775	NA	NA
3601	HMDB0159762	NA	NA
3602	HMDB0159763	NA	NA
3603	HMDB0062208	NA	NA
3604	HMDB0000359	3a,7a-Dihydroxycoprostanic acid	HMDB0000359
3605	HMDB0003533	3a,7a,12a-Trihydroxy-5b-cholestan-26-al	HMDB0003533
3606	HMDB0172392	NA	NA
3607	HMDB0172390	NA	NA
3608	HMDB0167571	NA	NA
3609	HMDB0167569	NA	NA
3610	HMDB0167567	NA	NA
3611	HMDB0167565	NA	NA
3612	HMDB0167563	NA	NA
3613	HMDB0159764	NA	NA
3614	HMDB0159888	NA	NA
3615	HMDB0005814	Testosterone enanthate	HMDB0005814
3616	HMDB0040994	NA	NA
3617	HMDB0040993	NA	NA
3618	HMDB0041990	NA	NA
3619	HMDB0041212	NA	NA
3620	HMDB0033806	2'-O-Methylcajanone	HMDB0033806
3621	HMDB0030849	Artocarpin	HMDB0030849
3622	HMDB0140394	NA	NA
3623	HMDB0129645	NA	NA
3624	HMDB0134743	NA	NA
3625	HMDB0162013	NA	NA
3626	HMDB0162016	NA	NA

3627	HMDB0162004	NA	NA
3628	HMDB0142798	NA	NA
3629	HMDB0142979	NA	NA
3630	HMDB0142983	NA	NA
3631	HMDB0142989	NA	NA
3632	HMDB0142992	NA	NA
3633	HMDB0142993	NA	NA
3634	HMDB0143013	NA	NA
3635	HMDB0143016	NA	NA
3636	HMDB0142982	NA	NA
3637	HMDB0142838	NA	NA
3638	HMDB0142799	NA	NA
3639	HMDB0142805	NA	NA
3640	HMDB0142795	NA	NA
3641	HMDB0142808	NA	NA
3642	HMDB0142824	NA	NA
3643	HMDB0142822	NA	NA
3644	HMDB0142828	NA	NA
3645	HMDB0142834	NA	NA
3646	HMDB0142809	NA	NA
3647	HMDB0143017	NA	NA
3648	HMDB0143090	NA	NA
3649	HMDB0143094	NA	NA
3650	HMDB0143096	NA	NA
3651	HMDB0143100	NA	NA
3652	HMDB0143110	NA	NA
3653	HMDB0143964	NA	NA
3654	HMDB0143966	NA	NA
3655	HMDB0143091	NA	NA
3656	HMDB0143087	NA	NA
3657	HMDB0143080	NA	NA
3658	HMDB0143023	NA	NA
3659	HMDB0143026	NA	NA
3660	HMDB0143027	NA	NA
3661	HMDB0143067	NA	NA
3662	HMDB0143070	NA	NA
3663	HMDB0143071	NA	NA
3664	HMDB0143106	NA	NA
3665	HMDB0143081	NA	NA
3666	HMDB0142788	NA	NA
3667	HMDB0142729	NA	NA
3668	HMDB0142725	NA	NA
3669	HMDB0142719	NA	NA
3670	HMDB0142718	NA	NA
3671	HMDB0142715	NA	NA
3672	HMDB0142739	NA	NA
3673	HMDB0143077	NA	NA
3674	HMDB0142728	NA	NA
3675	HMDB0142735	NA	NA
3676	HMDB0142738	NA	NA
3677	HMDB0142789	NA	NA
3678	HMDB0142785	NA	NA
3679	HMDB0142758	NA	NA
3680	HMDB0142759	NA	NA
3681	HMDB0142755	NA	NA
3682	HMDB0142748	NA	NA
3683	HMDB0142749	NA	NA
3684	HMDB0142745	NA	NA
3685	HMDB0035858	Obacunone	HMDB0035858
3686	HMDB0035031	Desoxylimonin	HMDB0035031
3687	HMDB0039920	NA	NA
3688	HMDB0039918	NA	NA
3689	HMDB0039919	NA	NA
3690	HMDB0015013	Flupenthixol	HMDB0015013
3691	HMDB0184201	NA	NA
3692	HMDB0183261	NA	NA
3693	HMDB0183260	NA	NA
3694	HMDB0183262	NA	NA
3695	HMDB0183264	NA	NA
3696	HMDB0183267	NA	NA
3697	HMDB0183269	NA	NA
3698	HMDB0184206	NA	NA
3699	HMDB0184207	NA	NA
3700	HMDB0183254	NA	NA
3701	HMDB0183258	NA	NA
3702	HMDB0183250	NA	NA
3703	HMDB0183251	NA	NA
3704	HMDB0039214	NA	NA
3705	HMDB0036631	NA	NA
3706	HMDB0030688	Cyclomulberrin	HMDB0030688
3707	HMDB0040480	NA	NA
3708	HMDB0029506	Kuwanon B	HMDB0029506
3709	HMDB0029505	Kuwanon A	HMDB0029505
3710	HMDB0131612	NA	NA
3711	HMDB0131610	NA	NA
3712	HMDB0131607	NA	NA
3713	HMDB0131606	NA	NA

3714	HMDB0131608	NA	NA
3715	HMDB0131609	NA	NA
3716	HMDB0131611	NA	NA
3717	HMDB0166772	NA	NA
3718	HMDB0166773	NA	NA
3719	HMDB0185408	NA	NA
3720	HMDB0185426	NA	NA
3721	HMDB0160312	NA	NA
3722	HMDB0160311	NA	NA
3723	HMDB0160309	NA	NA
3724	HMDB0160306	NA	NA
3725	HMDB0160305	NA	NA
3726	HMDB0160308	NA	NA
3727	HMDB0160314	NA	NA
3728	HMDB0160317	NA	NA
3729	HMDB0160320	NA	NA
3730	HMDB0036340	NA	NA
3731	HMDB0160333	NA	NA
3732	HMDB0160330	NA	NA
3733	HMDB0160332	NA	NA
3734	HMDB0160329	NA	NA
3735	HMDB0160327	NA	NA
3736	HMDB0160326	NA	NA
3737	HMDB0160324	NA	NA
3738	HMDB0160323	NA	NA
3739	HMDB0160321	NA	NA
3740	HMDB0165007	NA	NA
3741	HMDB0165008	NA	NA
3742	HMDB0175389	NA	NA
3743	HMDB0175386	NA	NA
3744	HMDB0038562	NA	NA
3745	HMDB0014843	Delavirdine	HMDB0014843
3746	HMDB0014565	Spirolactone	HMDB0014565
3747	HMDB0180016	NA	NA
3748	HMDB0180015	NA	NA
3749	HMDB0015164	Topotecan	HMDB0015164
3750	HMDB0145175	NA	NA
3751	HMDB0139832	NA	NA
3752	HMDB0139824	NA	NA
3753	HMDB0139838	NA	NA
3754	HMDB0139829	NA	NA
3755	HMDB0139833	NA	NA
3756	HMDB0139834	NA	NA
3757	HMDB0139836	NA	NA
3758	HMDB0139835	NA	NA
3759	HMDB0139837	NA	NA
3760	HMDB0139830	NA	NA
3761	HMDB0139831	NA	NA
3762	HMDB0139826	NA	NA
3763	HMDB0139825	NA	NA
3764	HMDB0139823	NA	NA
3765	HMDB0042019	NA	NA
3766	HMDB0165600	NA	NA
3767	HMDB0165605	NA	NA
3768	HMDB0163371	NA	NA
3769	HMDB0165603	NA	NA
3770	HMDB0165607	NA	NA
3771	HMDB0179376	NA	NA
3772	HMDB0179375	NA	NA
3773	HMDB0179380	NA	NA
3774	HMDB0179379	NA	NA
3775	HMDB0163370	NA	NA
3776	HMDB0041991	NA	NA
3777	HMDB0014780	Pemetrexed	HMDB0014780
3778	HMDB0181044	NA	NA
3779	HMDB0181045	NA	NA
3780	HMDB0139597	NA	NA
3781	HMDB0139606	NA	NA
3782	HMDB0139601	NA	NA
3783	HMDB0139602	NA	NA
3784	HMDB0029900	Lucuminoside	HMDB0029900
3785	HMDB0164389	NA	NA
3786	HMDB0164395	NA	NA
3787	HMDB0164391	NA	NA
3788	HMDB0036334	NA	NA
3789	HMDB0142846	NA	NA
3790	HMDB0132661	NA	NA
3791	HMDB0155455	NA	NA
3792	HMDB0155391	NA	NA
3793	HMDB0155394	NA	NA
3794	HMDB0155396	NA	NA
3795	HMDB0155406	NA	NA
3796	HMDB0158123	NA	NA
3797	HMDB0155403	NA	NA
3798	HMDB0155401	NA	NA
3799	HMDB0155400	NA	NA
3800	HMDB0155388	NA	NA

3801	HMDB0155385	NA	NA
3802	HMDB0155412	NA	NA
3803	HMDB0154709	NA	NA
3804	HMDB0154708	NA	NA
3805	HMDB0155409	NA	NA
3806	HMDB0155398	NA	NA
3807	HMDB0035864	13-Hydroxy-5'-O-methylmelledonal	HMDB0035864
3808	HMDB0038159	NA	NA
3809	HMDB0035690	6-O-Methylarmillaridin	HMDB0035690
3810	HMDB0157763	NA	NA
3811	HMDB0157761	NA	NA
3812	HMDB0157764	NA	NA
3813	HMDB0157766	NA	NA
3814	HMDB0157765	NA	NA
3815	HMDB0158281	NA	NA
3816	HMDB0170458	NA	NA
3817	HMDB0170461	NA	NA
3818	HMDB0157760	NA	NA
3819	HMDB0157759	NA	NA
3820	HMDB0157609	NA	NA
3821	HMDB0157611	NA	NA
3822	HMDB0157614	NA	NA
3823	HMDB0156809	NA	NA
3824	HMDB0157607	NA	NA
3825	HMDB0157758	NA	NA
3826	HMDB0157613	NA	NA
3827	HMDB0157610	NA	NA
3828	HMDB0157612	NA	NA
3829	HMDB0014818	Moricizine	HMDB0014818
3830	HMDB0172090	NA	NA
3831	HMDB0030452	Blasticidin S	HMDB0030452
3832	HMDB0035973	Lucidenic acid M	HMDB0035973
3833	HMDB0164014	NA	NA
3834	HMDB0171518	NA	NA
3835	HMDB0174361	NA	NA
3836	HMDB0174360	NA	NA
3837	HMDB0174359	NA	NA
3838	HMDB0174715	NA	NA
3839	HMDB0174374	NA	NA
3840	HMDB0174370	NA	NA
3841	HMDB0174371	NA	NA
3842	HMDB0174372	NA	NA
3843	HMDB0174373	NA	NA
3844	HMDB0174367	NA	NA
3845	HMDB0174363	NA	NA
3846	HMDB0174364	NA	NA
3847	HMDB0174362	NA	NA
3848	HMDB0174365	NA	NA
3849	HMDB0174366	NA	NA
3850	HMDB0174369	NA	NA
3851	HMDB0174368	NA	NA
3852	HMDB0183788	NA	NA
3853	HMDB0183785	NA	NA
3854	HMDB0183779	NA	NA
3855	HMDB0183773	NA	NA
3856	HMDB0183776	NA	NA
3857	HMDB0174714	NA	NA
3858	HMDB0174358	NA	NA
3859	HMDB0174356	NA	NA
3860	HMDB0174357	NA	NA
3861	HMDB0174355	NA	NA
3862	HMDB0000969	1,25-Dihydroxyvitamin D3-26,23-lactone	HMDB0000969
3863	HMDB0164012	NA	NA
3864	HMDB0174354	NA	NA
3865	HMDB0174353	NA	NA
3866	HMDB0174352	NA	NA
3867	HMDB0171517	NA	NA
3868	HMDB0015200	Glipizide	HMDB0015200
3869	HMDB0041221	NA	NA
3870	HMDB0177910	NA	NA
3871	HMDB0183673	NA	NA
3872	HMDB0183665	NA	NA
3873	HMDB0183643	NA	NA
3874	HMDB0183669	NA	NA
3875	HMDB0183658	NA	NA
3876	HMDB0183654	NA	NA
3877	HMDB0177913	NA	NA
3878	HMDB0183650	NA	NA
3879	HMDB0060821	NA	NA
3880	HMDB0060820	NA	NA
3881	HMDB0060916	NA	NA
3882	HMDB0061137	NA	NA
3883	HMDB0030246	Narceine	HMDB0030246
3884	HMDB0139781	NA	NA
3885	HMDB0139782	NA	NA
3886	HMDB0139784	NA	NA
3887	HMDB0139783	NA	NA

3888	HMDB0139793	NA	NA
3889	HMDB0139789	NA	NA
3890	HMDB0139791	NA	NA
3891	HMDB0139792	NA	NA
3892	HMDB0139790	NA	NA
3893	HMDB0139787	NA	NA
3894	HMDB0139788	NA	NA
3895	HMDB0139786	NA	NA
3896	HMDB0139785	NA	NA
3897	HMDB0139794	NA	NA
3898	HMDB0144925	NA	NA
3899	HMDB0144855	NA	NA
3900	HMDB0144858	NA	NA
3901	HMDB0144867	NA	NA
3902	HMDB0144870	NA	NA
3903	HMDB0144924	NA	NA
3904	HMDB0144954	NA	NA
3905	HMDB0144955	NA	NA
3906	HMDB0162826	NA	NA
3907	HMDB0162834	NA	NA
3908	HMDB0162874	NA	NA
3909	HMDB0162872	NA	NA
3910	HMDB0162824	NA	NA
3911	HMDB0030329	Neopetasitenine	HMDB0030329
3912	HMDB0162882	NA	NA
3913	HMDB0001846	Tetrahydrofolic acid	HMDB0001846
3914	HMDB0062806	NA	NA
3915	HMDB0012936	Dynorphin B (10-13)	HMDB0012936
3916	HMDB0240599	NA	NA
3917	HMDB0155347	NA	NA
3918	HMDB0155348	NA	NA
3919	HMDB0034064	2-Angeloyl-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one	HMDB0034064
3920	HMDB0035068	Melleolide M	HMDB0035068
3921	HMDB0179387	NA	NA
3922	HMDB0179386	NA	NA
3923	HMDB0179390	NA	NA
3924	HMDB0179389	NA	NA
3925	HMDB0061104	NA	NA
3926	HMDB0139815	NA	NA
3927	HMDB0144973	NA	NA
3928	HMDB0144948	NA	NA
3929	HMDB0144943	NA	NA
3930	HMDB0144938	NA	NA
3931	HMDB0139798	NA	NA
3932	HMDB0139801	NA	NA
3933	HMDB0139799	NA	NA
3934	HMDB0139800	NA	NA
3935	HMDB0139797	NA	NA
3936	HMDB0144978	NA	NA
3937	HMDB0139796	NA	NA
3938	HMDB0139795	NA	NA
3939	HMDB0144983	NA	NA
3940	HMDB0144998	NA	NA
3941	HMDB0144988	NA	NA
3942	HMDB0144933	NA	NA
3943	HMDB0144918	NA	NA
3944	HMDB0139811	NA	NA
3945	HMDB0139813	NA	NA
3946	HMDB0139809	NA	NA
3947	HMDB0139806	NA	NA
3948	HMDB0139807	NA	NA
3949	HMDB0139808	NA	NA
3950	HMDB0139814	NA	NA
3951	HMDB0139816	NA	NA
3952	HMDB0139805	NA	NA
3953	HMDB0139817	NA	NA
3954	HMDB0139812	NA	NA
3955	HMDB0139818	NA	NA
3956	HMDB0139804	NA	NA
3957	HMDB0139820	NA	NA
3958	HMDB0139819	NA	NA
3959	HMDB0139803	NA	NA
3960	HMDB0144913	NA	NA
3961	HMDB0139802	NA	NA
3962	HMDB0145003	NA	NA
3963	HMDB0144993	NA	NA
3964	HMDB0145038	NA	NA
3965	HMDB0145034	NA	NA
3966	HMDB0145032	NA	NA
3967	HMDB0139810	NA	NA
3968	HMDB0145018	NA	NA
3969	HMDB0145013	NA	NA
3970	HMDB0145008	NA	NA
3971	HMDB0032622	Phenethyl rutinoside	HMDB0032622
3972	HMDB0094682	5alpha-Androstan-3alpha,17beta-diol disulfate	HMDB0094682
3973	HMDB0240625	NA	NA
3974	HMDB0172330	NA	NA

3975	HMDB0034065	2,9-Bis(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one	HMDB0034065
3976	HMDB0032601	Muzanzagenin	HMDB0032601
3977	HMDB0014936	Gentamicin	HMDB0014936
3978	HMDB0168556	NA	NA
3979	HMDB0168555	NA	NA
3980	HMDB0015019	Quinapril	HMDB0015019
3981	HMDB0138286	NA	NA
3982	HMDB0175209	NA	NA
3983	HMDB0015560	Thiothixene	HMDB0015560
3984	HMDB0157393	NA	NA
3985	HMDB0158619	NA	NA
3986	HMDB0169094	NA	NA
3987	HMDB0171247	NA	NA
3988	HMDB0006765	2-Methoxy-estradiol-17b 3-glucuronide	HMDB0006765
3989	HMDB0010315	4-Hydroxyandrostenedione glucuronide	HMDB0010315
3990	HMDB0145075	NA	NA
3991	HMDB0145086	NA	NA
3992	HMDB0144922	NA	NA
3993	HMDB0144879	NA	NA
3994	HMDB0144952	NA	NA
3995	HMDB0144894	NA	NA
3996	HMDB0144844	NA	NA
3997	HMDB0144847	NA	NA
3998	HMDB0144882	NA	NA
3999	HMDB0144891	NA	NA
4000	HMDB0031918	Suspensolide F	HMDB0031918
4001	HMDB0061351	NA	NA
4002	HMDB0160543	NA	NA
4003	HMDB0160539	NA	NA
4004	HMDB0160541	NA	NA
4005	HMDB0160540	NA	NA
4006	HMDB0160542	NA	NA
4007	HMDB0160544	NA	NA
4008	HMDB0160545	NA	NA
4009	HMDB0160516	NA	NA
4010	HMDB0160517	NA	NA
4011	HMDB0160518	NA	NA
4012	HMDB0160515	NA	NA
4013	HMDB0160519	NA	NA
4014	HMDB0160522	NA	NA
4015	HMDB0160521	NA	NA
4016	HMDB0160520	NA	NA
4017	HMDB0160523	NA	NA
4018	HMDB0160526	NA	NA
4019	HMDB0160524	NA	NA
4020	HMDB0160525	NA	NA
4021	HMDB0160528	NA	NA
4022	HMDB0160529	NA	NA
4023	HMDB0160527	NA	NA
4024	HMDB0160530	NA	NA
4025	HMDB0172528	NA	NA
4026	HMDB0170464	NA	NA
4027	HMDB0059931	NA	NA
4028	HMDB0040118	NA	NA
4029	HMDB0184359	NA	NA
4030	HMDB0000722	Lithocholytaurine	HMDB0000722
4031	HMDB0184197	NA	NA
4032	HMDB0155893	NA	NA
4033	HMDB0184199	NA	NA
4034	HMDB0184202	NA	NA
4035	HMDB0184203	NA	NA
4036	HMDB0184192	NA	NA
4037	HMDB0184200	NA	NA
4038	HMDB0184193	NA	NA
4039	HMDB0184189	NA	NA
4040	HMDB0184187	NA	NA
4041	HMDB0155900	NA	NA
4042	HMDB0155896	NA	NA
4043	HMDB0155897	NA	NA
4044	HMDB0155894	NA	NA
4045	HMDB0184196	NA	NA
4046	HMDB0184333	NA	NA
4047	HMDB0184190	NA	NA
4048	HMDB0155899	NA	NA
4049	HMDB0060547	NA	NA
4050	HMDB0010380	LysoPC(14:1(9Z))	HMDB0010380
4051	HMDB0184086	NA	NA
4052	HMDB0002385	Celastrol	HMDB0002385
4053	HMDB0015057	Buprenorphine	HMDB0015057
4054	HMDB0062331	NA	NA
4055	HMDB0010379	LysoPC(14:0)	HMDB0010379
4056	HMDB0061691	NA	NA
4057	HMDB0161447	NA	NA
4058	HMDB0179451	NA	NA
4059	HMDB0062337	NA	NA
4060	HMDB0138981	NA	NA
4061	HMDB0138985	NA	NA



4062	HMDB0138983	NA	NA
4063	HMDB0138982	NA	NA
4064	HMDB0138963	NA	NA
4065	HMDB0138657	NA	NA
4066	HMDB0138986	NA	NA
4067	HMDB0138990	NA	NA
4068	HMDB0138994	NA	NA
4069	HMDB0138995	NA	NA
4070	HMDB0138999	NA	NA
4071	HMDB0138976	NA	NA
4072	HMDB0138978	NA	NA
4073	HMDB0138977	NA	NA
4074	HMDB0138656	NA	NA
4075	HMDB0134169	NA	NA
4076	HMDB0134170	NA	NA
4077	HMDB0134168	NA	NA
4078	HMDB0129088	NA	NA
4079	HMDB0129087	NA	NA
4080	HMDB0129086	NA	NA
4081	HMDB0138698	NA	NA
4082	HMDB0138699	NA	NA
4083	HMDB0138964	NA	NA
4084	HMDB0138967	NA	NA
4085	HMDB0138970	NA	NA
4086	HMDB0138969	NA	NA
4087	HMDB0138968	NA	NA
4088	HMDB0138971	NA	NA
4089	HMDB0138972	NA	NA
4090	HMDB0139000	NA	NA
4091	HMDB0141014	NA	NA
4092	HMDB0138697	NA	NA
4093	HMDB0138984	NA	NA
4094	HMDB0138989	NA	NA
4095	HMDB0138973	NA	NA
4096	HMDB0129052	NA	NA
4097	HMDB0125560	NA	NA
4098	HMDB0125552	NA	NA
4099	HMDB0125562	NA	NA
4100	HMDB0125561	NA	NA
4101	HMDB0125558	NA	NA
4102	HMDB0125554	NA	NA
4103	HMDB0125559	NA	NA
4104	HMDB0125553	NA	NA
4105	HMDB0125556	NA	NA
4106	HMDB0125555	NA	NA
4107	HMDB0140120	NA	NA
4108	HMDB0125564	NA	NA
4109	HMDB0125563	NA	NA
4110	HMDB0129075	NA	NA
4111	HMDB0129073	NA	NA
4112	HMDB0129066	NA	NA
4113	HMDB0129068	NA	NA
4114	HMDB0129067	NA	NA
4115	HMDB0129063	NA	NA
4116	HMDB0129064	NA	NA
4117	HMDB0129062	NA	NA
4118	HMDB0129061	NA	NA
4119	HMDB0129074	NA	NA
4120	HMDB0129081	NA	NA
4121	HMDB0140238	NA	NA
4122	HMDB0140127	NA	NA
4123	HMDB0140130	NA	NA
4124	HMDB0140124	NA	NA
4125	HMDB0140122	NA	NA
4126	HMDB0129571	NA	NA
4127	HMDB0129082	NA	NA
4128	HMDB0129080	NA	NA
4129	HMDB0129059	NA	NA
4130	HMDB0129058	NA	NA
4131	HMDB0129054	NA	NA
4132	HMDB0125577	NA	NA
4133	HMDB0125578	NA	NA
4134	HMDB0125576	NA	NA
4135	HMDB0125566	NA	NA
4136	HMDB0125573	NA	NA
4137	HMDB0125569	NA	NA
4138	HMDB0125571	NA	NA
4139	HMDB0125572	NA	NA
4140	HMDB0125568	NA	NA
4141	HMDB0129040	NA	NA
4142	HMDB0129041	NA	NA
4143	HMDB0129057	NA	NA
4144	HMDB0129055	NA	NA
4145	HMDB0129053	NA	NA
4146	HMDB0129048	NA	NA
4147	HMDB0129049	NA	NA
4148	HMDB0129046	NA	NA

4149	HMDB0129047	NA	NA
4150	HMDB0129045	NA	NA
4151	HMDB0129042	NA	NA
4152	HMDB0125567	NA	NA
4153	HMDB0150327	NA	NA
4154	HMDB0150323	NA	NA
4155	HMDB0131587	NA	NA
4156	HMDB0131586	NA	NA
4157	HMDB0131555	NA	NA
4158	HMDB0131554	NA	NA
4159	HMDB0034608	PSF-A	HMDB0034608
4160	HMDB0187185	NA	NA
4161	HMDB0187161	NA	NA
4162	HMDB0187164	NA	NA
4163	HMDB0187169	NA	NA
4164	HMDB0187172	NA	NA
4165	HMDB0187181	NA	NA
4166	HMDB0176585	NA	NA
4167	HMDB0176586	NA	NA
4168	HMDB0176925	NA	NA
4169	HMDB0176921	NA	NA
4170	HMDB0039706	NA	NA
4171	HMDB0034072	Gentianose	HMDB0034072
4172	HMDB0006599	3-Galactosyllactose	HMDB0006599
4173	HMDB0001262	Maltotriose	HMDB0001262
4174	HMDB0033748	Umbelliferose	HMDB0033748
4175	HMDB0040984	NA	NA
4176	HMDB0029930	beta-D-Fructofuranosyl alpha-D-glucopyranosyl-(1->4)-D-glucopyranoside	HMDB0029930
4177	HMDB0040181	NA	NA
4178	HMDB0039708	NA	NA
4179	HMDB0029929	6-O-Glucosylmaltose	HMDB0029929
4180	HMDB0033673	6-Kestose	HMDB0033673
4181	HMDB0038853	NA	NA
4182	HMDB0003213	Raffinose	HMDB0003213
4183	HMDB0039704	NA	NA
4184	HMDB0039707	NA	NA
4185	HMDB0029921	Neokestose	HMDB0029921
4186	HMDB0060468	D-Gal alpha 1->6D-Gal alpha 1->6D-Glucose	HMDB0060468
4187	HMDB0041948	NA	NA
4188	HMDB0003539	Levan	HMDB0003539
4189	HMDB0038852	NA	NA
4190	HMDB0029910	Gentiotriose	HMDB0029910
4191	HMDB0006857	Dextrin	HMDB0006857
4192	HMDB0011729	1-Kestose	HMDB0011729
4193	HMDB0011730	Melezitose	HMDB0011730
4194	HMDB0038851	NA	NA
4195	HMDB0035322	Fagopyritol B2	HMDB0035322
4196	HMDB0029922	Galactotriose	HMDB0029922
4197	HMDB0029937	Panose	HMDB0029937
4198	HMDB0039703	NA	NA
4199	HMDB0142726	NA	NA
4200	HMDB0142746	NA	NA
4201	HMDB0144455	NA	NA
4202	HMDB0142823	NA	NA
4203	HMDB0144467	NA	NA
4204	HMDB0143965	NA	NA
4205	HMDB0144465	NA	NA
4206	HMDB0144463	NA	NA
4207	HMDB0144459	NA	NA
4208	HMDB0144439	NA	NA
4209	HMDB0144435	NA	NA
4210	HMDB0144431	NA	NA
4211	HMDB0142806	NA	NA
4212	HMDB0142827	NA	NA
4213	HMDB0142796	NA	NA
4214	HMDB0144443	NA	NA
4215	HMDB0142736	NA	NA
4216	HMDB0142716	NA	NA
4217	HMDB0142756	NA	NA
4218	HMDB0142786	NA	NA
4219	HMDB0031674	Armillarinin	HMDB0031674
4220	HMDB0041532	NA	NA
4221	HMDB0030901	Eremopetasitenin B2	HMDB0030901
4222	HMDB0039930	NA	NA
4223	HMDB0164234	NA	NA
4224	HMDB0135504	NA	NA
4225	HMDB0135508	NA	NA
4226	HMDB0135506	NA	NA
4227	HMDB0031943	(Z)-N-[(4-hydroxyphenyl)methyl]ethoxycarbothioamide 4'-(tri-acetylRhamnoside)	HMDB0031943
4228	HMDB0133632	NA	NA
4229	HMDB0133629	NA	NA
4230	HMDB0133763	NA	NA
4231	HMDB0133762	NA	NA
4232	HMDB0135654	NA	NA
4233	HMDB0179487	NA	NA
4234	HMDB0179486	NA	NA
4235	HMDB0133631	NA	NA

4236	HMDB0133626	NA	NA
4237	HMDB0133623	NA	NA
4238	HMDB0133634	NA	NA
4239	HMDB0170798	NA	NA
4240	HMDB0170797	NA	NA
4241	HMDB0170793	NA	NA
4242	HMDB0170796	NA	NA
4243	HMDB0170791	NA	NA
4244	HMDB0170792	NA	NA
4245	HMDB0184654	NA	NA
4246	HMDB0184468	NA	NA
4247	HMDB0139941	NA	NA
4248	HMDB0139958	NA	NA
4249	HMDB0035635	Kanokoside A	HMDB0035635
4250	HMDB0004482	2-Methoxyestrone 3-glucuronide	HMDB0004482
4251	HMDB0154676	NA	NA
4252	HMDB0169584	NA	NA
4253	HMDB0146115	NA	NA
4254	HMDB0161563	NA	NA
4255	HMDB0161564	NA	NA
4256	HMDB0161602	NA	NA
4257	HMDB0161603	NA	NA
4258	HMDB0011156	PA(20:4(5Z,8Z,11Z,14Z)e/2:0)	HMDB0011156
4259	HMDB0114752	NA	NA
4260	HMDB0062310	NA	NA
4261	HMDB0011485	LysoPE(0:0/20:3(5Z,8Z,11Z))	HMDB0011485
4262	HMDB0011486	LysoPE(0:0/20:3(8Z,11Z,14Z))	HMDB0011486
4263	HMDB0011484	LysoPE(0:0/20:3(11Z,14Z,17Z))	HMDB0011484
4264	HMDB0011514	LysoPE(20:3(11Z,14Z,17Z)/0:0)	HMDB0011514
4265	HMDB0011516	LysoPE(20:3(8Z,11Z,14Z)/0:0)	HMDB0011516
4266	HMDB0011515	LysoPE(20:3(5Z,8Z,11Z)/0:0)	HMDB0011515
4267	HMDB0010381	LysoPC(15:0)	HMDB0010381
4268	HMDB0011130	LysoPE(18:0/0:0)	HMDB0011130
4269	HMDB0011129	LysoPE(0:0/18:0)	HMDB0011129
4270	HMDB0173895	NA	NA
4271	HMDB0173901	NA	NA
4272	HMDB0173913	NA	NA
4273	HMDB0173911	NA	NA
4274	HMDB0173905	NA	NA
4275	HMDB0173903	NA	NA
4276	HMDB0173899	NA	NA
4277	HMDB0173897	NA	NA
4278	HMDB0010408	LysoPC(P-18:1(9Z))	HMDB0010408
4279	HMDB0010384	LysoPC(18:0)	HMDB0010384
4280	HMDB0011128	LysoPC(0:0/18:0)	HMDB0011128
4281	HMDB0062195	NA	NA
4282	HMDB0036884	NA	NA
4283	HMDB0181960	NA	NA
4284	HMDB0181959	NA	NA
4285	HMDB0181963	NA	NA
4286	HMDB0181976	NA	NA
4287	HMDB0181975	NA	NA
4288	HMDB0181971	NA	NA
4289	HMDB0181968	NA	NA
4290	HMDB0181967	NA	NA
4291	HMDB0181964	NA	NA
4292	HMDB0158842	NA	NA
4293	HMDB0011523	LysoPE(22:4(7Z,10Z,13Z,16Z)/0:0)	HMDB0011523
4294	HMDB0011493	LysoPE(0:0/22:4(7Z,10Z,13Z,16Z))	HMDB0011493
4295	HMDB0041430	NA	NA
4296	HMDB0011482	LysoPE(0:0/20:1(11Z))	HMDB0011482
4297	HMDB0011512	LysoPE(20:1(11Z)/0:0)	HMDB0011512
4298	HMDB0010404	LysoPC(22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0010404
4299	HMDB0030528	Janthitrem B	HMDB0030528
4300	HMDB0010393	LysoPC(20:3(5Z,8Z,11Z))	HMDB0010393
4301	HMDB0010394	LysoPC(20:3(8Z,11Z,14Z))	HMDB0010394
4302	HMDB0184561	NA	NA
4303	HMDB0184408	NA	NA
4304	HMDB0156558	NA	NA
4305	HMDB0175799	NA	NA
4306	HMDB0175694	NA	NA
4307	HMDB0175794	NA	NA
4308	HMDB0184131	NA	NA
4309	HMDB0177847	NA	NA
4310	HMDB0175890	NA	NA
4311	HMDB0175811	NA	NA
4312	HMDB0041547	NA	NA
4313	HMDB0061198	NA	NA
4314	HMDB0035388	(24E)-3alpha,15alpha-Diacetoxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid	HMDB0035388
4315	HMDB0171952	NA	NA
4316	HMDB0171971	NA	NA
4317	HMDB0171957	NA	NA
4318	HMDB0171959	NA	NA
4319	HMDB0171967	NA	NA
4320	HMDB0171969	NA	NA
4321	HMDB0171963	NA	NA
4322	HMDB0171965	NA	NA

4323	HMDB0171961	NA	NA
4324	HMDB0039897	NA	NA
4325	HMDB0172989	NA	NA
4326	HMDB0172985	NA	NA
4327	HMDB0172986	NA	NA
4328	HMDB0172988	NA	NA
4329	HMDB0015129	Neomycin	HMDB0015129
4330	HMDB0002160	Harderoporpyrinogen	HMDB0002160
4331	HMDB0039454	NA	NA
4332	HMDB0173693	NA	NA
4333	HMDB0173692	NA	NA
4334	HMDB0173699	NA	NA
4335	HMDB0173698	NA	NA
4336	HMDB0142988	NA	NA
4337	HMDB0142998	NA	NA
4338	HMDB0142997	NA	NA
4339	HMDB0143001	NA	NA
4340	HMDB0142987	NA	NA
4341	HMDB0142978	NA	NA
4342	HMDB0142977	NA	NA
4343	HMDB0142917	NA	NA
4344	HMDB0142918	NA	NA
4345	HMDB0142919	NA	NA
4346	HMDB0142921	NA	NA
4347	HMDB0142920	NA	NA
4348	HMDB0142926	NA	NA
4349	HMDB0142929	NA	NA
4350	HMDB0142928	NA	NA
4351	HMDB0142927	NA	NA
4352	HMDB0143002	NA	NA
4353	HMDB0143007	NA	NA
4354	HMDB0143006	NA	NA
4355	HMDB0143108	NA	NA
4356	HMDB0143104	NA	NA
4357	HMDB0143098	NA	NA
4358	HMDB0143093	NA	NA
4359	HMDB0143086	NA	NA
4360	HMDB0143085	NA	NA
4361	HMDB0143076	NA	NA
4362	HMDB0143075	NA	NA
4363	HMDB0143066	NA	NA
4364	HMDB0143065	NA	NA
4365	HMDB0143061	NA	NA
4366	HMDB0143060	NA	NA
4367	HMDB0143022	NA	NA
4368	HMDB0143012	NA	NA
4369	HMDB0143011	NA	NA
4370	HMDB0143021	NA	NA
4371	HMDB0142916	NA	NA
4372	HMDB0142915	NA	NA
4373	HMDB0142901	NA	NA
4374	HMDB0142899	NA	NA
4375	HMDB0142902	NA	NA
4376	HMDB0142900	NA	NA
4377	HMDB0142905	NA	NA
4378	HMDB0142904	NA	NA
4379	HMDB0142903	NA	NA
4380	HMDB0142908	NA	NA
4381	HMDB0142911	NA	NA
4382	HMDB0142913	NA	NA
4383	HMDB0142914	NA	NA
4384	HMDB0142912	NA	NA
4385	HMDB0142930	NA	NA
4386	HMDB0165936	NA	NA
4387	HMDB0165918	NA	NA
4388	HMDB0173230	NA	NA
4389	HMDB0173229	NA	NA
4390	HMDB0165966	NA	NA
4391	HMDB0164809	NA	NA
4392	HMDB0034433	Riboflavine 2',3',4',5'-tetrabutanoate	HMDB0034433
4393	HMDB0157944	NA	NA
4394	HMDB0157945	NA	NA
4395	HMDB0157949	NA	NA
4396	HMDB0157950	NA	NA
4397	HMDB0157951	NA	NA
4398	HMDB0157955	NA	NA
4399	HMDB0157956	NA	NA
4400	HMDB0157943	NA	NA
4401	HMDB0157938	NA	NA
4402	HMDB0157939	NA	NA
4403	HMDB0157937	NA	NA
4404	HMDB0157933	NA	NA
4405	HMDB0157932	NA	NA
4406	HMDB0157931	NA	NA
4407	HMDB0157898	NA	NA
4408	HMDB0157896	NA	NA
4409	HMDB0157957	NA	NA

4410	HMDB0158932	NA	NA
4411	HMDB0158968	NA	NA
4412	HMDB0158964	NA	NA
4413	HMDB0158963	NA	NA
4414	HMDB0158958	NA	NA
4415	HMDB0158959	NA	NA
4416	HMDB0158953	NA	NA
4417	HMDB0158954	NA	NA
4418	HMDB0158949	NA	NA
4419	HMDB0158948	NA	NA
4420	HMDB0158944	NA	NA
4421	HMDB0158943	NA	NA
4422	HMDB0158937	NA	NA
4423	HMDB0158938	NA	NA
4424	HMDB0158939	NA	NA
4425	HMDB0158933	NA	NA
4426	HMDB0158969	NA	NA
4427	HMDB0157897	NA	NA
4428	HMDB0157050	NA	NA
4429	HMDB0157221	NA	NA
4430	HMDB0157842	NA	NA
4431	HMDB0157841	NA	NA
4432	HMDB0157843	NA	NA
4433	HMDB0157847	NA	NA
4434	HMDB0157846	NA	NA
4435	HMDB0157851	NA	NA
4436	HMDB0157848	NA	NA
4437	HMDB0157853	NA	NA
4438	HMDB0157215	NA	NA
4439	HMDB0157218	NA	NA
4440	HMDB0157212	NA	NA
4441	HMDB0157051	NA	NA
4442	HMDB0157054	NA	NA
4443	HMDB0157057	NA	NA
4444	HMDB0157060	NA	NA
4445	HMDB0157066	NA	NA
4446	HMDB0157063	NA	NA
4447	HMDB0157206	NA	NA
4448	HMDB0157205	NA	NA
4449	HMDB0157209	NA	NA
4450	HMDB0157852	NA	NA
4451	HMDB0157856	NA	NA
4452	HMDB0157857	NA	NA
4453	HMDB0157876	NA	NA
4454	HMDB0157881	NA	NA
4455	HMDB0157882	NA	NA
4456	HMDB0157883	NA	NA
4457	HMDB0157886	NA	NA
4458	HMDB0157887	NA	NA
4459	HMDB0157888	NA	NA
4460	HMDB0157891	NA	NA
4461	HMDB0157892	NA	NA
4462	HMDB0157893	NA	NA
4463	HMDB0157878	NA	NA
4464	HMDB0157877	NA	NA
4465	HMDB0157858	NA	NA
4466	HMDB0157861	NA	NA
4467	HMDB0157862	NA	NA
4468	HMDB0157863	NA	NA
4469	HMDB0157866	NA	NA
4470	HMDB0157867	NA	NA
4471	HMDB0157868	NA	NA
4472	HMDB0157871	NA	NA
4473	HMDB0157873	NA	NA
4474	HMDB0157872	NA	NA
4475	HMDB0038619	NA	NA
4476	HMDB0010698	CerP(d18:0/16:0)	HMDB0010698
4477	HMDB0165986	NA	NA
4478	HMDB0165987	NA	NA
4479	HMDB0166012	NA	NA
4480	HMDB0166013	NA	NA
4481	HMDB0166011	NA	NA
4482	HMDB0166007	NA	NA
4483	HMDB0170721	NA	NA
4484	HMDB0166009	NA	NA
4485	HMDB0166010	NA	NA
4486	HMDB0166004	NA	NA
4487	HMDB0166005	NA	NA
4488	HMDB0166003	NA	NA
4489	HMDB0166006	NA	NA
4490	HMDB0167988	NA	NA
4491	HMDB0167989	NA	NA
4492	HMDB0168064	NA	NA
4493	HMDB0170719	NA	NA
4494	HMDB0170718	NA	NA
4495	HMDB0168079	NA	NA
4496	HMDB0168080	NA	NA

4497	HMDB0168077	NA	NA
4498	HMDB0168076	NA	NA
4499	HMDB0168068	NA	NA
4500	HMDB0168067	NA	NA
4501	HMDB0168065	NA	NA
4502	HMDB0166001	NA	NA
4503	HMDB0166002	NA	NA
4504	HMDB0170734	NA	NA
4505	HMDB0165975	NA	NA
4506	HMDB0165973	NA	NA
4507	HMDB0165879	NA	NA
4508	HMDB0165880	NA	NA
4509	HMDB0170735	NA	NA
4510	HMDB0170737	NA	NA
4511	HMDB0166008	NA	NA
4512	HMDB0165977	NA	NA
4513	HMDB0165978	NA	NA
4514	HMDB0165999	NA	NA
4515	HMDB0165985	NA	NA
4516	HMDB0165984	NA	NA
4517	HMDB0165976	NA	NA
4518	HMDB0165983	NA	NA
4519	HMDB0165980	NA	NA
4520	HMDB0165981	NA	NA
4521	HMDB0165982	NA	NA
4522	HMDB0165979	NA	NA
4523	HMDB0177535	NA	NA
4524	HMDB0177543	NA	NA
4525	HMDB0177537	NA	NA
4526	HMDB0177545	NA	NA
4527	HMDB0177544	NA	NA
4528	HMDB0177546	NA	NA
4529	HMDB0177536	NA	NA
4530	HMDB0166014	NA	NA
4531	HMDB0165988	NA	NA
4532	HMDB0184229	NA	NA
4533	HMDB0186286	NA	NA
4534	HMDB0033242	Glycylserylprolylmethionylphenylalanylvalinamide	HMDB0033242
4535	HMDB0143644	NA	NA
4536	HMDB0041431	NA	NA
4537	HMDB0175656	NA	NA
4538	HMDB0175651	NA	NA
4539	HMDB0175661	NA	NA
4540	HMDB0175662	NA	NA
4541	HMDB0175652	NA	NA
4542	HMDB0175657	NA	NA
4543	HMDB0168025	NA	NA
4544	HMDB0168023	NA	NA
4545	HMDB0165935	NA	NA
4546	HMDB0168024	NA	NA
4547	HMDB0168022	NA	NA
4548	HMDB0168019	NA	NA
4549	HMDB0168021	NA	NA
4550	HMDB0168018	NA	NA
4551	HMDB0168020	NA	NA
4552	HMDB0168017	NA	NA
4553	HMDB0168016	NA	NA
4554	HMDB0168015	NA	NA
4555	HMDB0168014	NA	NA
4556	HMDB0168012	NA	NA
4557	HMDB0168026	NA	NA
4558	HMDB0168027	NA	NA
4559	HMDB0168033	NA	NA
4560	HMDB0168045	NA	NA
4561	HMDB0168044	NA	NA
4562	HMDB0168042	NA	NA
4563	HMDB0168043	NA	NA
4564	HMDB0168041	NA	NA
4565	HMDB0168040	NA	NA
4566	HMDB0168039	NA	NA
4567	HMDB0168038	NA	NA
4568	HMDB0168037	NA	NA
4569	HMDB0168035	NA	NA
4570	HMDB0168036	NA	NA
4571	HMDB0168034	NA	NA
4572	HMDB0168032	NA	NA
4573	HMDB0168030	NA	NA
4574	HMDB0165933	NA	NA
4575	HMDB0165934	NA	NA
4576	HMDB0165912	NA	NA
4577	HMDB0165911	NA	NA
4578	HMDB0165913	NA	NA
4579	HMDB0165914	NA	NA
4580	HMDB0165910	NA	NA
4581	HMDB0165909	NA	NA
4582	HMDB0165907	NA	NA
4583	HMDB0165904	NA	NA

4584	HMDB0165906	NA	NA
4585	HMDB0165908	NA	NA
4586	HMDB0165917	NA	NA
4587	HMDB0165916	NA	NA
4588	HMDB0165915	NA	NA
4589	HMDB0165932	NA	NA
4590	HMDB0165931	NA	NA
4591	HMDB0165928	NA	NA
4592	HMDB0165930	NA	NA
4593	HMDB0165929	NA	NA
4594	HMDB0165927	NA	NA
4595	HMDB0165924	NA	NA
4596	HMDB0165926	NA	NA
4597	HMDB0165925	NA	NA
4598	HMDB0165922	NA	NA
4599	HMDB0181031	NA	NA
4600	HMDB0177742	NA	NA
4601	HMDB0177531	NA	NA
4602	HMDB0177529	NA	NA
4603	HMDB0177530	NA	NA
4604	HMDB0187178	NA	NA
4605	HMDB0187175	NA	NA
4606	HMDB0187177	NA	NA
4607	HMDB0187174	NA	NA
4608	HMDB0178542	NA	NA
4609	HMDB0178548	NA	NA
4610	HMDB0178550	NA	NA
4611	HMDB0178541	NA	NA
4612	HMDB0178540	NA	NA
4613	HMDB0178549	NA	NA
4614	HMDB0036529	NA	NA
4615	HMDB0036528	NA	NA
4616	HMDB0014454	Vindesine	HMDB0014454
4617	HMDB0116519	NA	NA
4618	HMDB0116569	NA	NA
4619	HMDB0116555	NA	NA
4620	HMDB0116549	NA	NA
4621	HMDB0116538	NA	NA
4622	HMDB0116512	NA	NA
4623	HMDB0176104	NA	NA
4624	HMDB0173004	NA	NA
4625	HMDB0176105	NA	NA
4626	HMDB0040745	NA	NA
4627	HMDB0164979	NA	NA
4628	HMDB0164980	NA	NA
4629	HMDB0164978	NA	NA
4630	HMDB0164977	NA	NA
4631	HMDB0061054	NA	NA
4632	HMDB0061057	NA	NA
4633	HMDB0062582	NA	NA
4634	HMDB0009781	PI(16:0/18:0)	HMDB0009781
4635	HMDB0009805	PI(18:0/16:0)	HMDB0009805
4636	HMDB0112518	NA	NA
4637	HMDB0112350	NA	NA
4638	HMDB0112517	NA	NA
4639	HMDB0112364	NA	NA
4640	HMDB0112910	NA	NA
4641	HMDB0112882	NA	NA
4642	HMDB0112739	NA	NA
4643	HMDB0112711	NA	NA
4644	HMDB0112545	NA	NA
4645	HMDB0112375	NA	NA
4646	HMDB0112392	NA	NA
4647	HMDB0112411	NA	NA
4648	HMDB0112319	NA	NA
4649	HMDB0112307	NA	NA
4650	HMDB0010628	PG(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0010628
4651	HMDB0010627	PG(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0010627
4652	HMDB0010642	PG(18:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0010642
4653	HMDB0010643	PG(18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0010643
4654	HMDB0010614	PG(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0010614
4655	HMDB0010656	PG(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	HMDB0010656
4656	HMDB0116586	NA	NA
4657	HMDB0116593	NA	NA
4658	HMDB0116580	NA	NA
4659	HMDB0116630	NA	NA
4660	HMDB0116624	NA	NA
4661	HMDB0116625	NA	NA
4662	HMDB0116617	NA	NA
4663	HMDB0116583	NA	NA
4664	HMDB0116582	NA	NA
4665	HMDB0116579	NA	NA
4666	HMDB0116616	NA	NA
4667	HMDB0112745	NA	NA
4668	HMDB0112746	NA	NA
4669	HMDB0112769	NA	NA
4670	HMDB0112793	NA	NA

4671	HMDB0112580	NA	NA
4672	HMDB0112606	NA	NA
4673	HMDB0112718	NA	NA
4674	HMDB0112665	NA	NA
4675	HMDB0112640	NA	NA
4676	HMDB0112382	NA	NA
4677	HMDB0112461	NA	NA
4678	HMDB0112478	NA	NA
4679	HMDB0112504	NA	NA
4680	HMDB0112529	NA	NA
4681	HMDB0112528	NA	NA
4682	HMDB0112554	NA	NA
4683	HMDB0112555	NA	NA
4684	HMDB0112626	NA	NA
4685	HMDB0112437	NA	NA
4686	HMDB0169205	NA	NA
4687	HMDB0169206	NA	NA
4688	HMDB0009605	PE(22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0009605
4689	HMDB0009702	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:4(7Z,10Z,13Z,16Z))	HMDB0009702
4690	HMDB0114593	NA	NA
4691	HMDB0009671	PE(22:5(7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0009671
4692	HMDB0009670	PE(22:5(7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0009670
4693	HMDB0009638	PE(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0009638
4694	HMDB0116722	NA	NA
4695	HMDB0114567	NA	NA
4696	HMDB0114540	NA	NA
4697	HMDB0114406	NA	NA
4698	HMDB0114405	NA	NA
4699	HMDB0114378	NA	NA
4700	HMDB0114349	NA	NA
4701	HMDB0009637	PE(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0009637
4702	HMDB0061425	NA	NA
4703	HMDB0061422	NA	NA
4704	HMDB0061438	NA	NA
4705	HMDB0061465	NA	NA
4706	HMDB0113821	NA	NA
4707	HMDB0113813	NA	NA
4708	HMDB0113789	NA	NA
4709	HMDB0113774	NA	NA
4710	HMDB0113764	NA	NA
4711	HMDB0113758	NA	NA
4712	HMDB0113827	NA	NA
4713	HMDB0113828	NA	NA
4714	HMDB0113835	NA	NA
4715	HMDB0114666	NA	NA
4716	HMDB0114680	NA	NA
4717	HMDB0114686	NA	NA
4718	HMDB0114714	NA	NA
4719	HMDB0114729	NA	NA
4720	HMDB0114733	NA	NA
4721	HMDB0114739	NA	NA
4722	HMDB0114721	NA	NA
4723	HMDB0113781	NA	NA
4724	HMDB0061511	NA	NA
4725	HMDB0061507	NA	NA
4726	HMDB0061499	NA	NA
4727	HMDB0061475	NA	NA
4728	HMDB0061483	NA	NA
4729	HMDB0061471	NA	NA
4730	HMDB0061522	NA	NA
4731	HMDB0061530	NA	NA
4732	HMDB0061533	NA	NA
4733	HMDB0061549	NA	NA
4734	HMDB0059616	all-trans-Decaprenyl diphosphate	HMDB0059616



The second step is to check concentration values. For SSP analysis, the concentration must be measured in *umol* for blood and CSF samples. The urinary concentrations must be first converted to *umol/mmol\_creatinine* in order to compare with reported concentrations in literature. No missing or negative values are allowed in SSP analysis. The concentration data for QEA analysis is more flexible. Users can upload either the original concentration data or normalized data. Missing or negative values are allowed (coded as *NA*) for QEA.

## 5 Selection of Metabolite Set Library

Before proceeding to enrichment analysis, a metabolite set library has to be chosen. There are seven built-in libraries offered by MSEA:

- Metabolic pathway associated metabolite sets (*currently contains 99 entries*);
- Disease associated metabolite sets (reported in blood) (*currently contains 344 entries*);
- Disease associated metabolite sets (reported in urine) (*currently contains 384 entries*);
- Disease associated metabolite sets (reported in CSF) (*currently contains 166 entries*);
- Metabolite sets associated with SNPs (*currently contains 4598 entries*);
- Predicted metabolite sets based on computational enzyme knockout model (*currently contains 912 entries*);
- Metabolite sets based on locations (*currently contains 73 entries*);
- Drug pathway associated metabolite sets (*currently contains 461 entries*);

In addition, MSEA also allows user-defined metabolite sets to be uploaded to perform enrichment analysis on arbitrary groups of compounds which researchers want to test. The metabolite set library is simply a two-column comma separated text file with the first column for metabolite set names and the second column for its compound names (**must use HMDB compound name**) separated by "; ". Please note, the built-in libraries are mainly from human studies. The functional grouping of metabolites may not be valid. Therefore, for data from subjects other than human being, users are suggested to upload their self-defined metabolite set libraries for enrichment analysis.

## 6 Enrichment Analysis

Over Representation Analysis (ORA) is performed when a list of compound names is provided. The list of compound list can be obtained through conventional feature selection methods, or from a clustering algorithm, or from the compounds with abnormal concentrations detected in SSP, to investigate if some biologically meaningful patterns can be identified.

ORA was implemented using the *hypergeometric test* to evaluate whether a particular metabolite set is represented more than expected by chance within the given compound list. One-tailed p values are provided after adjusting for multiple testing. **Figure 2** below summarizes the result.

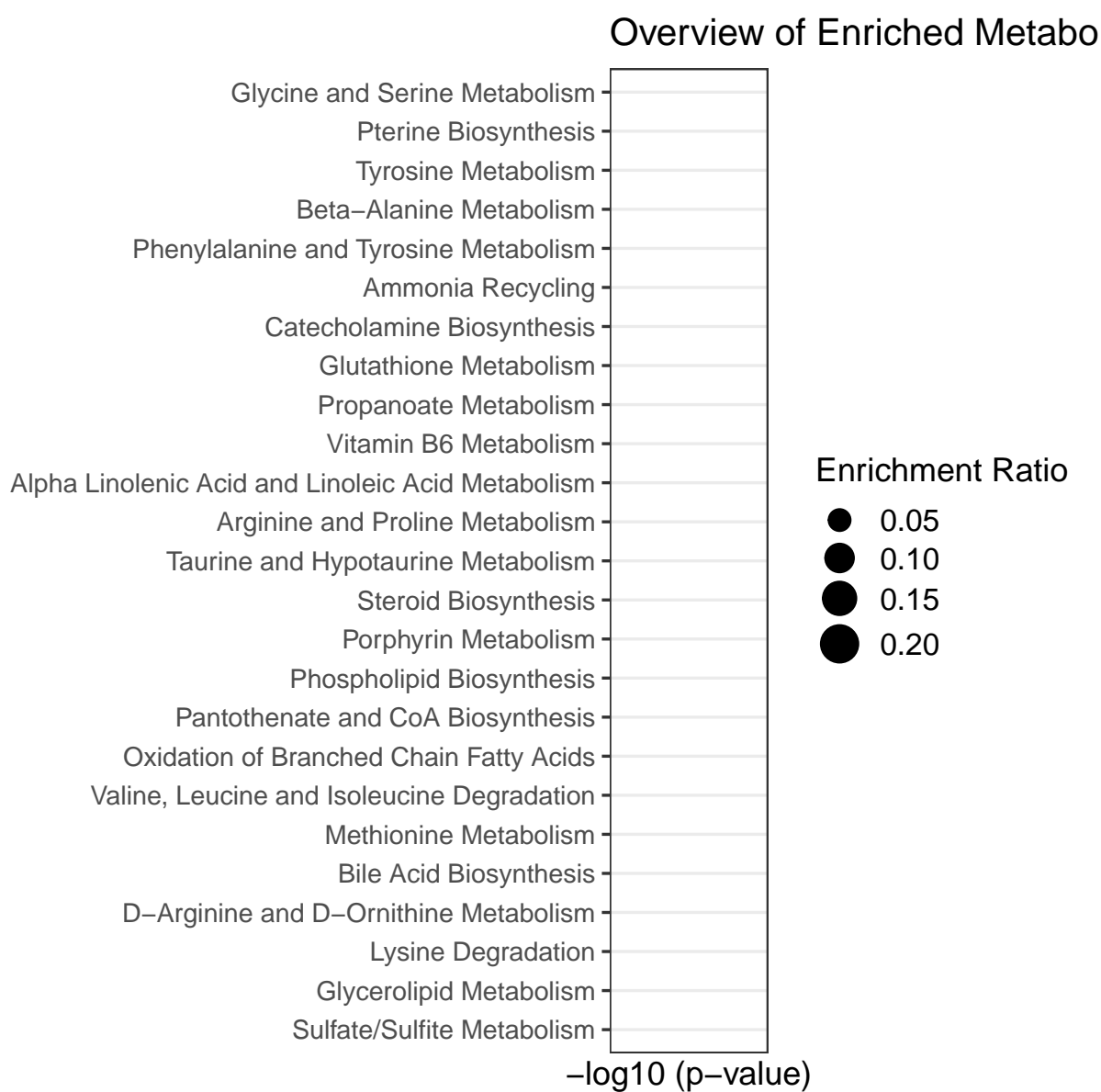


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Glycine and Serine Metabolism	59	71.00	4			
Pterine Biosynthesis	29	34.90	1			
Tyrosine Metabolism	72	86.70	13			
Beta-Alanine Metabolism	34	40.90	1			
Phenylalanine and Tyrosine Metabolism	28	33.70	3			
Ammonia Recycling	32	38.50	3			
Catecholamine Biosynthesis	20	24.10	5			
Glutathione Metabolism	21	25.30	1			
Propanoate Metabolism	42	50.60	1			
Vitamin B6 Metabolism	20	24.10	1			
Alpha Linolenic Acid and Linoleic Acid Metabolism	19	22.90	4			
Arginine and Proline Metabolism	53	63.80	4			
Taurine and Hypotaurine Metabolism	12	14.40	1			
Steroid Biosynthesis	48	57.80	1			
Porphyrin Metabolism	40	48.20	2			
Phospholipid Biosynthesis	29	34.90	2			
Pantothenate and CoA Biosynthesis	21	25.30	2			
Oxidation of Branched Chain Fatty Acids	26	31.30	2			
Valine, Leucine and Isoleucine Degradation	60	72.20	2			
Methionine Metabolism	43	51.80	3			
Bile Acid Biosynthesis	65	78.30	17			
D-Arginine and D-Ornithine Metabolism	11	13.20	1			
Lysine Degradation	30	36.10	2			
Glycerolipid Metabolism	25	30.10	1			
Sulfate/Sulfite Metabolism	22	26.50	1			
Galactose Metabolism	38	45.80	2			
Histidine Metabolism	43	51.80	1			
Pyrimidine Metabolism	59	71.00	3			
Nicotinate and Nicotinamide Metabolism	37	44.60	1			
Purine Metabolism	74	89.10	5			
Fatty acid Metabolism	43	51.80	3			
Beta Oxidation of Very Long Chain Fatty Acids	17	20.50	3			
Folate Metabolism	29	34.90	1			
Fatty Acid Elongation In Mitochondria	35	42.10	2			
Alanine Metabolism	17	20.50	2			
Citric Acid Cycle	32	38.50	1			
Starch and Sucrose Metabolism	31	37.30	1			
Urea Cycle	29	34.90	1			
Pyruvate Metabolism	48	57.80	1			
Tryptophan Metabolism	60	72.20	9			
Fructose and Mannose Degradation	32	38.50	1			
Ubiquinone Biosynthesis	20	24.10	1			
Biotin Metabolism	8	9.63	1			
Aspartate Metabolism	35	42.10	1			
Androgen and Estrogen Metabolism	33	39.70	3			
Ketone Body Metabolism	13	15.70	1			
Glutamate Metabolism	49	59.00	2			
Retinol Metabolism	37	44.60	7			
Arachidonic Acid Metabolism	69	83.10	13			
Betaine Metabolism	21	25.30	2			
Gluconeogenesis	35	42.10	1			
Steroidogenesis	43	51.80	7			
Threonine and 2-Oxobutanoate Degradation	20	24.10	1			
Homocysteine Degradation	9	10.80	1			
Fatty Acid Biosynthesis	35	42.10	6			
Carnitine Synthesis	22	26.50	3			
Transfer of Acetyl Groups into Mitochondria	22	26.50	1			
Mitochondrial Beta-Oxidation of Short Chain Saturated Fatty Acids	27	32.50	2			
Mitochondrial Beta-Oxidation of Medium Chain Saturated Fatty Acids	27	32.50	1			
Mitochondrial Beta-Oxidation of Long Chain Saturated Fatty Acids	28	33.70	1			
Warburg Effect	58	69.80	1			
Thyroid hormone synthesis	13	15.70	1			
Androstenedione Metabolism	24	28.90	2			
Estrone Metabolism	24	28.90	2			

## 7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "compd.vec<-c(\"HMDB0000123\", \"HMDB0014691\", \"HMDB0031239\", \"HMDB0161401\", \"HMDB0000925\", \"HMDB0000925\")"
[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<-SaveTransformedData(mSet)"
[11] "mSet<-PreparePDFReport(mSet, \"guest5553748766599075063\")\n"
[12] "UpdateDataObjects(\"conc\", \"msetora\", FALSE)"
[13] "mSet<-SetMetabolomeFilter(mSet, F);"
[14] "mSet<-SetCurrentMsetLib(mSet, \"smpdb_pathway\", 2);"
[15] "mSet<-CalculateHyperScore(mSet)"
[16] "mSet<-PlotORA(mSet, \"ora_0\", \"net\", \"png\", 72, width=NA)"
[17] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_0\", \"png\", 72, width=NA)"
[18] "mSet<-CalculateHyperScore(mSet)"
[19] "mSet<-PlotORA(mSet, \"ora_1\", \"net\", \"png\", 72, width=NA)"
[20] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_1\", \"png\", 72, width=NA)"
[21] "mSet<-SaveTransformedData(mSet)"
[22] "mSet<-PreparePDFReport(mSet, \"guest5553748766599075063\")\n"
```

The report was generated on Mon May 24 12:56:25 2021 with R version 4.0.2 (2020-06-22).