

Metabolomic Data Analysis with MetaboAnalyst 5.0

Name: guest16073378008230990507

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.^{1, 2}

2 MSEA Overview

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

3 Data Input

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

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

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

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

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

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

4 Data Process

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

	Query	Match	HMDB
1	HMDB0000123	Glycine	HMDB0000123
2	HMDB0014691	Acetohydroxamic Acid	HMDB0014691
3	HMDB0031239	Ethyl nitrite	HMDB0031239
4	HMDB0161401	NA	NA
5	HMDB0001858	p-Cresol	HMDB0001858
6	HMDB0033895	Anisole	HMDB0033895
7	HMDB0003119	Benzyl alcohol	HMDB0003119
8	HMDB0002055	o-Cresol	HMDB0002055
9	HMDB0002048	m-Cresol	HMDB0002048
10	HMDB0004983	Dimethyl sulfone	HMDB0004983
11	HMDB0144632	NA	NA
12	HMDB0062140	NA	NA
13	HMDB0034203	N-(2-Methylpropyl)acetamide	HMDB0034203
14	HMDB0031651	N-(3-Methylbutyl)acetamide	HMDB0031651
15	HMDB0062041	NA	NA
16	HMDB0012296	Trimethylaminoacetone	HMDB0012296
17	HMDB0031404	Cyclohexylamine	HMDB0031404
18	HMDB0032416	2-Methylpiperidine	HMDB0032416
19	HMDB0031544	3-Methylcyclopentene	HMDB0031544
20	HMDB0062716	NA	NA
21	HMDB0033971	2-Diethylaminoethanol	HMDB0033971
22	HMDB0167366	NA	NA
23	HMDB0094692	NA	NA
24	HMDB0041945	NA	NA
25	HMDB0167367	NA	NA
26	HMDB0167365	NA	NA
27	HMDB0240305	NA	NA
28	HMDB0031654	3-Aminobutanoic acid	HMDB0031654
29	HMDB0094693	NA	NA
30	HMDB0002166	(S)-b-aminoisobutyric acid	HMDB0002166
31	HMDB0000452	L-Alpha-aminobutyric acid	HMDB0000452
32	HMDB0002299	(R)-b-aminoisobutyric acid	HMDB0002299
33	HMDB0001906	2-Aminoisobutyric acid	HMDB0001906
34	HMDB0003911	3-Aminoisobutanoic acid	HMDB0003911
35	HMDB0000112	Gamma-Aminobutyric acid	HMDB0000112
36	HMDB0038394	NA	NA
37	HMDB0031329	Butyl nitrite	HMDB0031329
38	HMDB0000092	Dimethylglycine	HMDB0000092
39	HMDB0000650	D-Alpha-aminobutyric acid	HMDB0000650
40	HMDB0061050	NA	NA
41	HMDB0167139	NA	NA
42	HMDB0167138	NA	NA
43	HMDB0000549	Gamma-Butyrolactone	HMDB0000549
44	HMDB0002523	Oxolan-3-one	HMDB0002523
45	HMDB0003407	Diacetyl	HMDB0003407
46	HMDB0031209	Ethenyl acetate	HMDB0031209
47	HMDB0034439	Isocrotonic acid	HMDB0034439
48	HMDB0033977	Methyl acrylate	HMDB0033977
49	HMDB0174868	NA	NA
50	HMDB0010720	But-2-enoic acid	HMDB0010720
51	HMDB0240288	NA	NA
52	HMDB0161316	NA	NA
53	HMDB0002994	Erythritol	HMDB0002994
54	HMDB0004136	D-Threitol	HMDB0004136
55	HMDB0094689	NA	NA
56	HMDB0165469	NA	NA
57	HMDB0165470	NA	NA
58	HMDB0062640	NA	NA
59	HMDB0126088	NA	NA

60	HMDB0000710	4-Hydroxybutyric acid	HMDB0000710
61	HMDB0000442	(S)-3-Hydroxybutyric acid	HMDB0000442
62	HMDB0000357	3-Hydroxybutyric acid	HMDB0000357
63	HMDB0000336	(R)-3-Hydroxyisobutyric acid	HMDB0000336
64	HMDB0000011	(R)-3-Hydroxybutyric acid	HMDB0000011
65	HMDB0000023	(S)-3-Hydroxyisobutyric acid	HMDB0000023
66	HMDB0000729	Alpha-Hydroxyisobutyric acid	HMDB0000729
67	HMDB0031212	Ethoxyacetic acid	HMDB0031212
68	HMDB0059748	NA	NA
69	HMDB0000008	2-Hydroxybutyric acid	HMDB0000008
70	HMDB0015507	Gamma Hydroxybutyric Acid	HMDB0015507
71	HMDB0000630	Cytosine	HMDB0000630
72	HMDB0031335	2-Chloro-1-propanol	HMDB0031335
73	HMDB0163354	NA	NA
74	HMDB0163353	NA	NA
75	HMDB0163351	NA	NA
76	HMDB0163350	NA	NA
77	HMDB0163352	NA	NA
78	HMDB0163702	NA	NA
79	HMDB0179351	NA	NA
80	HMDB0179346	NA	NA
81	HMDB0179345	NA	NA
82	HMDB0179344	NA	NA
83	HMDB0179343	NA	NA
84	HMDB0179342	NA	NA
85	HMDB0179341	NA	NA
86	HMDB0169695	NA	NA
87	HMDB0169664	NA	NA
88	HMDB0165583	NA	NA
89	HMDB0165582	NA	NA
90	HMDB0165581	NA	NA
91	HMDB0165584	NA	NA
92	HMDB0163703	NA	NA
93	HMDB0000453	Delta-Hexanolactone	HMDB0000453
94	HMDB0060476	epsilon-Caprolactone	HMDB0060476
95	HMDB0032490	Prenyl formate	HMDB0032490
96	HMDB0039581	NA	NA
97	HMDB0031158	2-Methyl-4-pentenoic acid	HMDB0031158
98	HMDB0031562	2-Methyl-3-pentenoic acid	HMDB0031562
99	HMDB0031559	4-Methyl-2,3-pentanedione	HMDB0031559
100	HMDB0031491	2,3-Hexanedione	HMDB0031491
101	HMDB0031560	2-Methyl-2-pentenoic acid	HMDB0031560
102	HMDB0031501	3-Hexenoic acid	HMDB0031501
103	HMDB0029487	Allyl propionate	HMDB0029487
104	HMDB0033568	5-Oxohexanal	HMDB0033568
105	HMDB0040328	NA	NA
106	HMDB0031492	3,4-Hexanedione	HMDB0031492
107	HMDB0031561	4-Methyl-2-pentenoic acid	HMDB0031561
108	HMDB0010719	trans-Hex-2-enoic acid	HMDB0010719
109	HMDB0003843	Gamma-Caprolactone	HMDB0003843
110	HMDB0240384	NA	NA
111	HMDB0061929	NA	NA
112	HMDB0061965	NA	NA
113	HMDB0062135	NA	NA
114	HMDB0161115	NA	NA
115	HMDB0161116	NA	NA
116	HMDB0163679	NA	NA
117	HMDB0061652	3-hydroxyhexanoic acid	HMDB0061652
118	HMDB0171222	NA	NA
119	HMDB0165042	NA	NA
120	HMDB0165043	NA	NA
121	HMDB0165041	NA	NA
122	HMDB0163682	NA	NA
123	HMDB0163680	NA	NA
124	HMDB0163681	NA	NA
125	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	HMDB0000317
126	HMDB0000409	(5R)-5-Hydroxyhexanoic acid	HMDB0000409
127	HMDB0032158	(+/-)-1-Acetoxy-1-ethoxyethane	HMDB0032158
128	HMDB0000624	D-Leucic acid	HMDB0000624
129	HMDB0000665	Leucinic acid	HMDB0000665
130	HMDB0000746	Hydroxyisocaproic acid	HMDB0000746
131	HMDB0000525	5-Hydroxyhexanoic acid	HMDB0000525
132	HMDB0001624	2-Hydroxycaproic acid	HMDB0001624
133	HMDB0001975	2-Ethyl-2-Hydroxybutyric acid	HMDB0001975
134	HMDB0010718	(R)-3-Hydroxyhexanoic acid	HMDB0010718
135	HMDB0012843	6-Hydroxyhexanoic acid	HMDB0012843
136	HMDB0033851	4,4-Dimethoxy-2-butanone	HMDB0033851
137	HMDB0032456	Paraldehyde	HMDB0032456
138	HMDB0040409	NA	NA
139	HMDB0165040	NA	NA
140	HMDB0059770	NA	NA
141	HMDB0041844	NA	NA
142	HMDB0029166	2-Methyl-3-hydroxyvaleric acid	HMDB0029166
143	HMDB0061950	NA	NA
144	HMDB0000532	Acetyl glycine	HMDB0000532
145	HMDB0006454	L-2-Amino-3-oxobutanoic acid	HMDB0006454
146	HMDB0012249	L-Aspartate-semialdehyde	HMDB0012249

147	HMDB0161181	NA	NA
148	HMDB0187639	NA	NA
149	HMDB0032523	Succinic anhydride	HMDB0032523
150	HMDB0029389	(+)-threo-2-Amino-3,4-dihydroxybutanoic acid	HMDB0029389
151	HMDB0000034	Adenine	HMDB0000034
152	HMDB0002024	Imidazoleacetic acid	HMDB0002024
153	HMDB0060261	NA	NA
154	HMDB0000262	Thymine	HMDB0000262
155	HMDB0029736	1H-Imidazole-1-acetic acid	HMDB0029736
156	HMDB0002006	2,3-Diaminopropionic acid	HMDB0002006
157	HMDB0041946	NA	NA
158	HMDB0128943	NA	NA
159	HMDB0132477	NA	NA
160	HMDB0129097	NA	NA
161	HMDB0168839	NA	NA
162	HMDB0128916	NA	NA
163	HMDB0012233	Glutarate semialdehyde	HMDB0012233
164	HMDB0029172	3-keto-2-Methylbutyrate	HMDB0029172
165	HMDB0001865	2-Oxovaleric acid	HMDB0001865
166	HMDB0000310	Methylacetoacetic acid	HMDB0000310
167	HMDB0031643	Ethyl pyruvate	HMDB0031643
168	HMDB0000019	Alpha-ketoisovaleric acid	HMDB0000019
169	HMDB0003771	2-Methylacetoacetic acid	HMDB0003771
170	HMDB0000720	Levulinic acid	HMDB0000720
171	HMDB0034466	Acetoxyacetone	HMDB0034466
172	HMDB0128917	NA	NA
173	HMDB0129096	NA	NA
174	HMDB0129098	NA	NA
175	HMDB0168838	NA	NA
176	HMDB0177210	NA	NA
177	HMDB0169666	NA	NA
178	HMDB0177209	NA	NA
179	HMDB0171727	NA	NA
180	HMDB0032356	N-Lactoyl ethanolamine	HMDB0032356
181	HMDB0039499	NA	NA
182	HMDB0031658	L-2-Amino-5-hydroxypentanoic acid	HMDB0031658
183	HMDB0039790	NA	NA
184	HMDB0038974	NA	NA
185	HMDB0039789	NA	NA
186	HMDB0000786	Oxypurinol	HMDB0000786
187	HMDB0000292	Xanthine	HMDB0000292
188	HMDB0001182	6,8-Dihydroxypurine	HMDB0001182
189	HMDB0000744	Malic acid	HMDB0000744
190	HMDB0031518	D-Malic acid	HMDB0031518
191	HMDB0000156	L-Malic acid	HMDB0000156
192	HMDB0032872	Velcorin	HMDB0032872
193	HMDB0061971	NA	NA
194	HMDB0124942	NA	NA
195	HMDB0167829	NA	NA
196	HMDB0062810	NA	NA
197	HMDB0125535	NA	NA
198	HMDB0183895	NA	NA
199	HMDB0126385	NA	NA
200	HMDB0031459	3-Methoxybenzaldehyde	HMDB0031459
201	HMDB0002340	2-Methylbenzoic acid	HMDB0002340
202	HMDB0041485	NA	NA
203	HMDB0033968	Methyl benzoate	HMDB0033968
204	HMDB0032400	3-(5-Methyl-2-furyl)prop-2-enal	HMDB0032400
205	HMDB0032603	2-Hydroxy-4-methylbenzaldehyde	HMDB0032603
206	HMDB0029686	4-Methoxybenzaldehyde	HMDB0029686
207	HMDB0040733	Phenyl acetate	HMDB0040733
208	HMDB0032568	2'-Hydroxyacetophenone	HMDB0032568
209	HMDB0167830	NA	NA
210	HMDB0038176	NA	NA
211	HMDB0040638	NA	NA
212	HMDB0029635	4-Methylbenzoic acid	HMDB0029635
213	HMDB0033128	4-(2-Furanyl)-3-buten-2-one	HMDB0033128
214	HMDB0003767	4-Hydroxyphenylacetaldehyde	HMDB0003767
215	HMDB0033766	2-Methoxybenzaldehyde	HMDB0033766
216	HMDB0000209	Phenylacetic acid	HMDB0000209
217	HMDB0126617	NA	NA
218	HMDB0169080	NA	NA
219	HMDB0059966	NA	NA
220	HMDB0131479	NA	NA
221	HMDB0135785	NA	NA
222	HMDB0146894	NA	NA
223	HMDB0146874	NA	NA
224	HMDB0131231	NA	NA
225	HMDB0131232	NA	NA
226	HMDB0125534	NA	NA
227	HMDB0037724	NA	NA
228	HMDB0005784	Hydroxytyrosol	HMDB0005784
229	HMDB0030570	Sylvopinol	HMDB0030570
230	HMDB0032012	4-Hydroxy-3-methoxybenzenemethanol	HMDB0032012
231	HMDB0037728	NA	NA
232	HMDB0034158	2,6-Dimethoxyphenol	HMDB0034158
233	HMDB0041477	NA	NA

234	HMDB0031660	Dibutyl sulfide	HMDB0031660
235	HMDB0240251	NA	NA
236	HMDB0061880	NA	NA
237	HMDB0059659	Trans-3-hydroxy-L-proline	HMDB0059659
238	HMDB0002113	3-Hydroxy-L-proline	HMDB0002113
239	HMDB0000783	Propionylglycine	HMDB0000783
240	HMDB0000766	N-Acetyl-L-alanine	HMDB0000766
241	HMDB0000725	4-Hydroxyproline	HMDB0000725
242	HMDB0036576	NA	NA
243	HMDB0001149	5-Aminolevulinic acid	HMDB0001149
244	HMDB0002104	L-Glutamic gamma-semialdehyde	HMDB0002104
245	HMDB0006055	4-Hydroxy-L-proline	HMDB0006055
246	HMDB0060460	cis-4-Hydroxy-D-proline	HMDB0060460
247	HMDB0006272	5-Amino-2-oxopentanoic acid	HMDB0006272
248	HMDB0177404	NA	NA
249	HMDB0014389	Mesalazine	HMDB0014389
250	HMDB0164041	NA	NA
251	HMDB0059749	NA	NA
252	HMDB0001972	3-Aminosalicylic acid	HMDB0001972
253	HMDB0014378	Aminosalicylic Acid	HMDB0014378
254	HMDB0001476	3-Hydroxyanthranilic acid	HMDB0001476
255	HMDB0059811	NA	NA
256	HMDB0012289	Tetrahydroadipic acid	HMDB0012289
257	HMDB0014447	Tranexamic Acid	HMDB0014447
258	HMDB0033433	(S)-Homotachydrine	HMDB0033433
259	HMDB0039651	NA	NA
260	HMDB0039680	NA	NA
261	HMDB0036176	NA	NA
262	HMDB0037625	NA	NA
263	HMDB0040526	NA	NA
264	HMDB0037196	NA	NA
265	HMDB0037167	NA	NA
266	HMDB0039652	NA	NA
267	HMDB0060682	NA	NA
268	HMDB0032311	2,4-Hexadienyl acetate	HMDB0032311
269	HMDB0039673	NA	NA
270	HMDB0040463	NA	NA
271	HMDB0039681	NA	NA
272	HMDB0033054	Ethyl isopropyl disulfide	HMDB0033054
273	HMDB0033053	Ethyl propyl disulfide	HMDB0033053
274	HMDB0031160	1-Pentanesulfenothioic acid	HMDB0031160
275	HMDB0000157	Hypoxanthine	HMDB0000157
276	HMDB0014581	Allopurinol	HMDB0014581
277	HMDB0000943	Threonic acid	HMDB0000943
278	HMDB0062620	NA	NA
279	HMDB0000613	Erythronic acid	HMDB0000613
280	HMDB0137818	NA	NA
281	HMDB0183470	NA	NA
282	HMDB0060348	Maleylacetic acid	HMDB0060348
283	HMDB0031210	Zymonic acid	HMDB0031210
284	HMDB0037759	NA	NA
285	HMDB0014273	NA	NA
286	HMDB0000044	Ascorbic acid	HMDB0000044
287	HMDB0031193	1,2,3-Propanetricarboxylic acid	HMDB0031193
288	HMDB0006355	D-Glucurono-6,3-lactone	HMDB0006355
289	HMDB0160667	NA	NA
290	HMDB0160666	NA	NA
291	HMDB0160406	NA	NA
292	HMDB0160407	NA	NA
293	HMDB0000694	L-2-Hydroxyglutaric acid	HMDB0000694
294	HMDB0000428	3-Hydroxyglutaric acid	HMDB0000428
295	HMDB0000426	Citramalic acid	HMDB0000426
296	HMDB0000606	D-2-Hydroxyglutaric acid	HMDB0000606
297	HMDB0059655	2-Hydroxyglutarate	HMDB0059655
298	HMDB0001900	Ribonolactone	HMDB0001900
299	HMDB0161319	NA	NA
300	HMDB0011676	D-Xylono-1,5-lactone	HMDB0011676
301	HMDB0061190	NA	NA
302	HMDB0062739	NA	NA
303	HMDB0160668	NA	NA
304	HMDB0041392	NA	NA
305	HMDB0033912	2-Propenyl propyl disulfide	HMDB0033912
306	HMDB0038890	NA	NA
307	HMDB0001566	3-Methylguanine	HMDB0001566
308	HMDB0000897	7-Methylguanine	HMDB0000897
309	HMDB0006040	N2-Methylguanine	HMDB0006040
310	HMDB0003282	1-Methylguanine	HMDB0003282
311	HMDB0011657	2,6-Diamino-4-hydroxy-5-N-methylformamidopyrimidine	HMDB0011657
312	HMDB0000232	Quinolinic acid	HMDB0000232
313	HMDB0033161	2,6-Pyridinedicarboxylic acid	HMDB0033161
314	HMDB0185628	NA	NA
315	HMDB0001330	2-Amino-3-carboxymuconic acid semialdehyde	HMDB0001330
316	HMDB0062578	NA	NA
317	HMDB0060260	NA	NA
318	HMDB0001552	2-Keto-glutaramic acid	HMDB0001552
319	HMDB0166108	NA	NA
320	HMDB0171094	NA	NA

321	HMDB0172092	NA	NA
322	HMDB0062005	NA	NA
323	HMDB0124926	NA	NA
324	HMDB0168664	NA	NA
325	HMDB0150437	NA	NA
326	HMDB0125528	NA	NA
327	HMDB0137457	NA	NA
328	HMDB0146870	NA	NA
329	HMDB0146889	NA	NA
330	HMDB0166106	NA	NA
331	HMDB0166109	NA	NA
332	HMDB0182861	NA	NA
333	HMDB0166107	NA	NA
334	HMDB0183905	NA	NA
335	HMDB0183904	NA	NA
336	HMDB0036907	NA	NA
337	HMDB0029660	2',6'-Dihydroxyacetophenone	HMDB0029660
338	HMDB0029657	2,4'-Dihydroxyacetophenone	HMDB0029657
339	HMDB0029659	2',4'-Dihydroxyacetophenone	HMDB0029659
340	HMDB0029658	2',3'-Dihydroxyacetophenone	HMDB0029658
341	HMDB0032594	2-(Hydroxymethyl)benzoic acid	HMDB0032594
342	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	HMDB0033003
343	HMDB0032629	2',5'-Dihydroxyacetophenone	HMDB0032629
344	HMDB0032572	Methylparaben	HMDB0032572
345	HMDB0029662	3',5'-Dihydroxyacetophenone	HMDB0029662
346	HMDB0029661	3',4'-Dihydroxyacetophenone	HMDB0029661
347	HMDB0032604	2-Methoxybenzoic acid	HMDB0032604
348	HMDB0034172	Methyl 2-hydroxybenzoate	HMDB0034172
349	HMDB0032606	3-Methoxybenzoic acid	HMDB0032606
350	HMDB0041283	NA	NA
351	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	HMDB0004815
352	HMDB0012308	Vanillin	HMDB0012308
353	HMDB0032919	Ethyl 2-furanyl diketone	HMDB0032919
354	HMDB0172091	NA	NA
355	HMDB0032399	Methyl furfuracrylate	HMDB0032399
356	HMDB0000703	Mandelic acid	HMDB0000703
357	HMDB0000669	Ortho-Hydroxyphenylacetic acid	HMDB0000669
358	HMDB0060390	NA	NA
359	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	HMDB0003791
360	HMDB0062635	NA	NA
361	HMDB0031609	Phenoxyacetic acid	HMDB0031609
362	HMDB0000440	3-Hydroxyphenylacetic acid	HMDB0000440
363	HMDB0001101	p-Anisic acid	HMDB0001101
364	HMDB0000020	p-Hydroxyphenylacetic acid	HMDB0000020
365	HMDB0002390	3-Cresotinic acid	HMDB0002390
366	HMDB0000216	Norepinephrine	HMDB0000216
367	HMDB0035178	6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	HMDB0035178
368	HMDB0037685	NA	NA
369	HMDB0155164	NA	NA
370	HMDB0001537	6-Hydroxydopamine	HMDB0001537
371	HMDB0000239	Pyridoxine	HMDB0000239
372	HMDB0004817	5-Hydroxydopamine	HMDB0004817
373	HMDB0012150	2-Keto-6-acetamidocaproate	HMDB0012150
374	HMDB0168723	NA	NA
375	HMDB0168724	NA	NA
376	HMDB0142963	NA	NA
377	HMDB0061157	NA	NA
378	HMDB0029449	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	HMDB0029449
379	HMDB0033453	Fagomine	HMDB0033453
380	HMDB0162021	NA	NA
381	HMDB0040972	NA	NA
382	HMDB0038628	NA	NA
383	HMDB0004073	5-Hydroxyindoleacetaldehyde	HMDB0004073
384	HMDB0000197	Indoleacetic acid	HMDB0000197
385	HMDB0166095	NA	NA
386	HMDB0060758	NA	NA
387	HMDB0240317	NA	NA
388	HMDB0162022	NA	NA
389	HMDB0162020	NA	NA
390	HMDB0162023	NA	NA
391	HMDB0013292	p-Methylhippuric acid	HMDB0013292
392	HMDB0000821	Phenylacetylglutamine	HMDB0000821
393	HMDB0000859	Methyl hippurate	HMDB0000859
394	HMDB0011723	2-Methylhippuric acid	HMDB0011723
395	HMDB0060366	3-Carbamoyl-2-phenylpropionaldehyde	HMDB0060366
396	HMDB0060389	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	HMDB0060389
397	HMDB0034250	Betamipron	HMDB0034250
398	HMDB0032388	Methyl n-acetylanthranilate	HMDB0032388
399	HMDB0013245	m-Methylhippuric acid	HMDB0013245
400	HMDB0012309	Vanillylamine	HMDB0012309
401	HMDB0004825	p-Octopamine	HMDB0004825
402	HMDB0156498	NA	NA
403	HMDB0000073	Dopamine	HMDB0000073
404	HMDB0060277	NA	NA
405	HMDB0037786	NA	NA
406	HMDB0172919	NA	NA
407	HMDB0129369	NA	NA

408	HMDB0135530	NA	NA
409	HMDB0135531	NA	NA
410	HMDB0135533	NA	NA
411	HMDB0128615	NA	NA
412	HMDB0135532	NA	NA
413	HMDB0033813	3-(3,4-Methylenedioxyphenyl)propenal	HMDB0033813
414	HMDB0032883	1,4,5-Naphthalenetriol	HMDB0032883
415	HMDB0032990	7-Hydroxy-6-methyl-2H-1-benzopyran-2-one	HMDB0032990
416	HMDB0163660	NA	NA
417	HMDB0029758	Herniarin	HMDB0029758
418	HMDB0059622	NA	NA
419	HMDB0031054	10-Hydroxy-2,8-decadiene-4,6-diyonic acid	HMDB0031054
420	HMDB0060747	NA	NA
421	HMDB0001434	3-Methoxytyrosine	HMDB0001434
422	HMDB0011754	Methyldopa	HMDB0011754
423	HMDB0040003	NA	NA
424	HMDB0172928	NA	NA
425	HMDB0172925	NA	NA
426	HMDB0151309	NA	NA
427	HMDB0037153	NA	NA
428	HMDB0151285	NA	NA
429	HMDB0151284	NA	NA
430	HMDB0062564	NA	NA
431	HMDB0163545	NA	NA
432	HMDB0031437	(-)-Bornesitol	HMDB0031437
433	HMDB0029965	Methyl beta-D-glucopyranoside	HMDB0029965
434	HMDB0031449	Sequoiitol	HMDB0031449
435	HMDB0029915	D-4-O-Methyl-myo-inositol	HMDB0029915
436	HMDB0029916	4-O-Methyl-myo-inositol	HMDB0029916
437	HMDB0033816	Mytilitol	HMDB0033816
438	HMDB0034219	D-Pinitol	HMDB0034219
439	HMDB0034222	L-Pinitol	HMDB0034222
440	HMDB0034221	L-Quebrachitol	HMDB0034221
441	HMDB0033750	D-Glycero-D-galacto-heptitol	HMDB0033750
442	HMDB0037295	NA	NA
443	HMDB0014962	Enprofylline	HMDB0014962
444	HMDB0001847	Caffeine	HMDB0001847
445	HMDB0039467	NA	NA
446	HMDB0031699	S-(3-Methyl-2-butenyl) 2-methylpropanethioate	HMDB0031699
447	HMDB0033843	Polyvidone	HMDB0033843
448	HMDB0028843	Glycyl-Histidine	HMDB0028843
449	HMDB0028885	Histidinyl-Glycine	HMDB0028885
450	HMDB0014814	Benzyl Benzoate	HMDB0014814
451	HMDB0032039	Benzoin	HMDB0032039
452	HMDB0014018	4-Hydroxypropofol	HMDB0014018
453	HMDB0037389	NA	NA
454	HMDB0038292	NA	NA
455	HMDB0040439	NA	NA
456	HMDB0039685	NA	NA
457	HMDB0041497	NA	NA
458	HMDB0031840	(S,Z)-Lyralol acetate	HMDB0031840
459	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	HMDB0035801
460	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate	HMDB0035375
461	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate	HMDB0035376
462	HMDB0132986	NA	NA
463	HMDB0034450	Neocnidilide	HMDB0034450
464	HMDB0032567	Hexylresorcinol	HMDB0032567
465	HMDB0035126	(Áś)-Myrtenyl acetate	HMDB0035126
466	HMDB0041610	NA	NA
467	HMDB0038046	NA	NA
468	HMDB0037018	NA	NA
469	HMDB0037231	NA	NA
470	HMDB0035085	Vulgarole	HMDB0035085
471	HMDB0041572	NA	NA
472	HMDB0029388	Cucurbit acid	HMDB0029388
473	HMDB0037326	NA	NA
474	HMDB0033601	Dihydrojasmonic acid	HMDB0033601
475	HMDB0040195	NA	NA
476	HMDB0035723	(1R,2S,3S,4R)-p-Menthane-2,3-diol	HMDB0035723
477	HMDB0034457	Propyl heptanoate	HMDB0034457
478	HMDB0061987	NA	NA
479	HMDB0062146	NA	NA
480	HMDB0038038	NA	NA
481	HMDB0036228	2-Methylpropyl hexanoate	HMDB0036228
482	HMDB0040167	NA	NA
483	HMDB0036136	NA	NA
484	HMDB0187563	NA	NA
485	HMDB0037387	NA	NA
486	HMDB0000511	Capric acid	HMDB0000511
487	HMDB0031264	Methyl nonanoate	HMDB0031264
488	HMDB0094654	1-Methylethyl heptanoic acid	HMDB0094654
489	HMDB0171179	NA	NA
490	HMDB0171178	NA	NA
491	HMDB0171177	NA	NA
492	HMDB0171176	NA	NA
493	HMDB0179213	NA	NA
494	HMDB0179212	NA	NA

495	HMDB0179927	NA	NA
496	HMDB0180500	NA	NA
497	HMDB0180498	NA	NA
498	HMDB0180499	NA	NA
499	HMDB0180497	NA	NA
500	HMDB0180502	NA	NA
501	HMDB0180501	NA	NA
502	HMDB0180503	NA	NA
503	HMDB0180504	NA	NA
504	HMDB0171175	NA	NA
505	HMDB0061805	NA	NA
506	HMDB0180097	NA	NA
507	HMDB0032302	Heptanal propyleneglycol acetal	HMDB0032302
508	HMDB0032155	Acetaldehyde 1,3-octanediol acetal	HMDB0032155
509	HMDB0032264	Ethyl 2-ethylhexanoate	HMDB0032264
510	HMDB0032315	Hexanal butane-2,3-diol acetal	HMDB0032315
511	HMDB0032045	Pentyl 3-methylbutanoate	HMDB0032045
512	HMDB0041216	NA	NA
513	HMDB0034849	4-Methylnonanoic acid	HMDB0034849
514	HMDB0037849	Hexyl 2-methylpropanoate	HMDB0037849
515	HMDB0040157	NA	NA
516	HMDB0033620	Hexyl butyrate	HMDB0033620
517	HMDB0035595	trans-p-Menthane-1,8-diol	HMDB0035595
518	HMDB0029760	1,1-Diethoxy-2-hexene	HMDB0029760
519	HMDB0032070	Isooctyl acetate	HMDB0032070
520	HMDB0040211	NA	NA
521	HMDB0040529	NA	NA
522	HMDB0038783	NA	NA
523	HMDB0036145	NA	NA
524	HMDB0039218	NA	NA
525	HMDB0038602	Octyl acetate	HMDB0038602
526	HMDB0030029	Isopentyl isopentanoate	HMDB0030029
527	HMDB0031739	7-Hydroxy-3,7-dimethyloctanal	HMDB0031739
528	HMDB0035360	N-Methyl-1-deoxynojirimycin	HMDB0035360
529	HMDB0059660	NA	NA
530	HMDB0000114	Glycerylphosphorylethanolamine	HMDB0000114
531	HMDB0033349	Casimiroin	HMDB0033349
532	HMDB0013859	2-Dechloroethylifosfamide	HMDB0013859
533	HMDB0013858	3-Dechloroethylifosfamide	HMDB0013858
534	HMDB0060881	NA	NA
535	HMDB0028776	Cysteinyl-Hydroxyproline	HMDB0028776
536	HMDB0028860	Hydroxypropyl-Cysteine	HMDB0028860
537	HMDB0032660	(2Z,4'Z)-2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene	HMDB0032660
538	HMDB0004821	Bisnorbiotin	HMDB0004821
539	HMDB0060618	NA	NA
540	HMDB0059798	NA	NA
541	HMDB0059799	NA	NA
542	HMDB0059800	NA	NA
543	HMDB0059797	NA	NA
544	HMDB0059801	NA	NA
545	HMDB0000210	Pantothenic acid	HMDB0000210
546	HMDB0062717	NA	NA
547	HMDB0033092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	HMDB0033092
548	HMDB0032306	4-Heptenal diethyl acetal	HMDB0032306
549	HMDB0062766	4-ethylamino-6-isopropylamino-1,3,5-triazin-2-ol	HMDB0062766
550	HMDB0035175	2-Amino-1,6-dimethylfuro[3,2-e]imidazo[4,5-b]pyridine	HMDB0035175
551	HMDB0012204	Cis-zeatin	HMDB0012204
552	HMDB0040032	NA	NA
553	HMDB0181581	NA	NA
554	HMDB0028797	Glutaminyglycine	HMDB0028797
555	HMDB0028682	Alaninyl-Asparagine	HMDB0028682
556	HMDB0028724	Asparaginylin-Alanine	HMDB0028724
557	HMDB0028855	Glycyl-Gamma-glutamate	HMDB0028855
558	HMDB0028839	Glycyl-Glutamine	HMDB0028839
559	HMDB0033191	2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	HMDB0033191
560	HMDB0150426	NA	NA
561	HMDB0034046	1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene	HMDB0034046
562	HMDB0037492	NA	NA
563	HMDB0040424	NA	NA
564	HMDB0061823	NA	NA
565	HMDB0061942	NA	NA
566	HMDB0032589	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	HMDB0032589
567	HMDB0132937	NA	NA
568	HMDB0132935	NA	NA
569	HMDB0132936	NA	NA
570	HMDB0132939	NA	NA
571	HMDB0132948	NA	NA
572	HMDB0151796	NA	NA
573	HMDB0151797	NA	NA
574	HMDB0151800	NA	NA
575	HMDB0151798	NA	NA
576	HMDB0151799	NA	NA
577	HMDB0151801	NA	NA
578	HMDB0132933	NA	NA
579	HMDB0151802	NA	NA
580	HMDB0035593	Rishitin	HMDB0035593
581	HMDB0037605	NA	NA

582	HMDB0036790	NA	NA
583	HMDB0036791	NA	NA
584	HMDB0037820	NA	NA
585	HMDB0040178	NA	NA
586	HMDB0160293	NA	NA
587	HMDB0160295	NA	NA
588	HMDB0160291	NA	NA
589	HMDB0160290	NA	NA
590	HMDB0160289	NA	NA
591	HMDB0160292	NA	NA
592	HMDB0160296	NA	NA
593	HMDB0160294	NA	NA
594	HMDB0160298	NA	NA
595	HMDB0160297	NA	NA
596	HMDB0032369	L-Menthyl acetoacetate	HMDB0032369
597	HMDB0033619	Hexyl hexanoate	HMDB0033619
598	HMDB0059868	NA	NA
599	HMDB0032440	Nonanal propyleneglycol acetal	HMDB0032440
600	HMDB0061988	NA	NA
601	HMDB0035410	(R)-Dihydrocitronellol acetate	HMDB0035410
602	HMDB0000638	Dodecanoic acid	HMDB0000638
603	HMDB0040166	NA	NA
604	HMDB0030998	Ethyl decanoate	HMDB0030998
605	HMDB0034137	Octyl 2-methylpropanoate	HMDB0034137
606	HMDB0036225	NA	NA
607	HMDB0034136	Octyl butanoate	HMDB0034136
608	HMDB0034128	Isopropyl nonanoate	HMDB0034128
609	HMDB0032310	2-Heptyl butyrate	HMDB0032310
610	HMDB0168119	NA	NA
611	HMDB0168120	NA	NA
612	HMDB0168121	NA	NA
613	HMDB0015050	Phenformin	HMDB0015050
614	HMDB0004231	Pantothenol	HMDB0004231
615	HMDB0094651	PyroGlu-Val	HMDB0094651
616	HMDB0029018	Prolyl-Hydroxyproline	HMDB0029018
617	HMDB0028871	Hydroxyprolyl-Proline	HMDB0028871
618	HMDB0006695	Prolylhydroxyproline	HMDB0006695
619	HMDB0040573	NA	NA
620	HMDB0011172	gamma-Glutamylvaline	HMDB0011172
621	HMDB0029162	NA	NA
622	HMDB0028756	Aspartyl-Isoleucine	HMDB0028756
623	HMDB0028903	Isoleucyl-Aspartate	HMDB0028903
624	HMDB0028925	Leucyl-Aspartate	HMDB0028925
625	HMDB0028832	Glutamylvaline	HMDB0028832
626	HMDB0059717	NA	NA
627	HMDB0029126	Valyl-Glutamate	HMDB0029126
628	HMDB0028757	Aspartyl-Leucine	HMDB0028757
629	HMDB0011166	L-beta-aspartyl-L-leucine	HMDB0011166
630	HMDB0151781	NA	NA
631	HMDB0151783	NA	NA
632	HMDB0151788	NA	NA
633	HMDB0151787	NA	NA
634	HMDB0151784	NA	NA
635	HMDB0035016	2-Phenylethyl pentanoate	HMDB0035016
636	HMDB0132932	NA	NA
637	HMDB0132940	NA	NA
638	HMDB0151780	NA	NA
639	HMDB0001925	Ibuprofen	HMDB0001925
640	HMDB0034472	3-Phenylpropyl 2-methylpropanoate	HMDB0034472
641	HMDB0034470	2-Phenylpropyl isobutyrate	HMDB0034470
642	HMDB0038605	NA	NA
643	HMDB0040431	NA	NA
644	HMDB0036391	NA	NA
645	HMDB0036025	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	HMDB0036025
646	HMDB0037194	NA	NA
647	HMDB0034469	2-Phenylpropyl butyrate	HMDB0034469
648	HMDB0037623	NA	NA
649	HMDB0036240	NA	NA
650	HMDB0035017	2-Phenylethyl 3-methylbutanoate	HMDB0035017
651	HMDB0037720	NA	NA
652	HMDB0035008	3-Methylbutyl phenylacetate	HMDB0035008
653	HMDB0036386	NA	NA
654	HMDB0033196	(E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one	HMDB0033196
655	HMDB0037604	NA	NA
656	HMDB0029669	Eremopetasinorone A	HMDB0029669
657	HMDB0035181	xi-8,9-Dehydrotheaspirone	HMDB0035181
658	HMDB0039101	NA	NA
659	HMDB0034556	3-Acetoxy-3-methyl-1-phenylbutane	HMDB0034556
660	HMDB0032176	Benzyl hexanoate	HMDB0032176
661	HMDB0163212	NA	NA
662	HMDB0151805	NA	NA
663	HMDB0151793	NA	NA
664	HMDB0151794	NA	NA
665	HMDB0151789	NA	NA
666	HMDB0151790	NA	NA
667	HMDB0151791	NA	NA
668	HMDB0151785	NA	NA

669	HMDB0151786	NA	NA
670	HMDB0151792	NA	NA
671	HMDB0014604	Nabumetone	HMDB0014604
672	HMDB0176774	NA	NA
673	HMDB0176773	NA	NA
674	HMDB0176775	NA	NA
675	HMDB0061836	NA	NA
676	HMDB0032133	Bisphenol A	HMDB0032133
677	HMDB0033878	(S)-Curzeone	HMDB0033878
678	HMDB0135597	NA	NA
679	HMDB0170855	NA	NA
680	HMDB0179330	NA	NA
681	HMDB0179331	NA	NA
682	HMDB0038202	NA	NA
683	HMDB0036767	NA	NA
684	HMDB0036455	NA	NA
685	HMDB0035902	Enokipodin B	HMDB0035902
686	HMDB0040903	NA	NA
687	HMDB0038188	NA	NA
688	HMDB0031916	5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran	HMDB0031916
689	HMDB0037558	NA	NA
690	HMDB0036473	NA	NA
691	HMDB0037801	NA	NA
692	HMDB0030911	2-Oxo-5,11(13)-eudesmadien-12,8-olide	HMDB0030911
693	HMDB0031900	Methyl (2E,4Z,6E,8E,10E)-4,8-dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoate	HMDB0031900
694	HMDB0036488	NA	NA
695	HMDB0038547	NA	NA
696	HMDB0041920	NA	NA
697	HMDB0179332	NA	NA
698	HMDB0001319	Pyridoxine 5'-phosphate	HMDB0001319
699	HMDB0039455	NA	NA
700	HMDB0032888	Acetyl vitamin K5	HMDB0032888
701	HMDB0172484	NA	NA
702	HMDB0001389	Melatonin	HMDB0001389
703	HMDB0172486	NA	NA
704	HMDB0172485	NA	NA
705	HMDB0172483	NA	NA
706	HMDB0172489	NA	NA
707	HMDB0172488	NA	NA
708	HMDB0172487	NA	NA
709	HMDB0014501	Aminoglutethimide	HMDB0014501
710	HMDB0015443	Heptabarbital	HMDB0015443
711	HMDB0029876	Paucine	HMDB0029876
712	HMDB0060742	NA	NA
713	HMDB0033462	4-Coumaroyl-2-hydroxyputrescine	HMDB0033462
714	HMDB0139613	NA	NA
715	HMDB0139973	NA	NA
716	HMDB0139529	NA	NA
717	HMDB0139528	NA	NA
718	HMDB0139530	NA	NA
719	HMDB0139526	NA	NA
720	HMDB0139527	NA	NA
721	HMDB0041830	NA	NA
722	HMDB0034276	L,L-Cyclo(leucylprolyl)	HMDB0034276
723	HMDB0181560	NA	NA
724	HMDB0181559	NA	NA
725	HMDB0181561	NA	NA
726	HMDB0039111	NA	NA
727	HMDB0040349	NA	NA
728	HMDB0152315	NA	NA
729	HMDB0142172	NA	NA
730	HMDB0142174	NA	NA
731	HMDB0146404	NA	NA
732	HMDB0146402	NA	NA
733	HMDB0149145	NA	NA
734	HMDB0146405	NA	NA
735	HMDB0146406	NA	NA
736	HMDB0146407	NA	NA
737	HMDB0149144	NA	NA
738	HMDB0149143	NA	NA
739	HMDB0142171	NA	NA
740	HMDB0142170	NA	NA
741	HMDB0128183	NA	NA
742	HMDB0128665	NA	NA
743	HMDB0128667	NA	NA
744	HMDB0128668	NA	NA
745	HMDB0128674	NA	NA
746	HMDB0128673	NA	NA
747	HMDB0137280	NA	NA
748	HMDB0137283	NA	NA
749	HMDB0137284	NA	NA
750	HMDB0137291	NA	NA
751	HMDB0137290	NA	NA
752	HMDB0141325	NA	NA
753	HMDB0142075	NA	NA
754	HMDB0142076	NA	NA
755	HMDB0142169	NA	NA

756	HMDB0179746	NA	NA
757	HMDB0142173	NA	NA
758	HMDB0041691	NA	NA
759	HMDB0030018	Elenolide	HMDB0030018
760	HMDB0140920	NA	NA
761	HMDB0032616	Sinapic acid	HMDB0032616
762	HMDB0034069	cis-Sinapic acid	HMDB0034069
763	HMDB0127488	NA	NA
764	HMDB0014567	Methocarbamol	HMDB0014567
765	HMDB0013134	Fumarycarnitine	HMDB0013134
766	HMDB0032769	Osmaronin	HMDB0032769
767	HMDB0147191	NA	NA
768	HMDB0131062	NA	NA
769	HMDB0131065	NA	NA
770	HMDB0036050	NA	NA
771	HMDB0033771	Cyperine	HMDB0033771
772	HMDB0030690	(E)-Suberenol	HMDB0030690
773	HMDB0039592	NA	NA
774	HMDB0030788	Citrusal	HMDB0030788
775	HMDB0135759	NA	NA
776	HMDB0135760	NA	NA
777	HMDB0135761	NA	NA
778	HMDB0141827	NA	NA
779	HMDB0151855	NA	NA
780	HMDB0153660	NA	NA
781	HMDB0135757	NA	NA
782	HMDB0135758	NA	NA
783	HMDB0129916	NA	NA
784	HMDB0129917	NA	NA
785	HMDB0129919	NA	NA
786	HMDB0129920	NA	NA
787	HMDB0129922	NA	NA
788	HMDB0131064	NA	NA
789	HMDB0131066	NA	NA
790	HMDB0131067	NA	NA
791	HMDB0132269	NA	NA
792	HMDB0129918	NA	NA
793	HMDB0030854	(S)-Auraptenol	HMDB0030854
794	HMDB0030110	Celerin	HMDB0030110
795	HMDB0030948	Dihydrowyerone	HMDB0030948
796	HMDB0039142	NA	NA
797	HMDB0041192	NA	NA
798	HMDB0034133	3-(1,1-Dimethylallyl)scopoletin	HMDB0034133
799	HMDB0030853	(R)-Meranzin	HMDB0030853
800	HMDB0033015	5,6-Dihydroyangonin	HMDB0033015
801	HMDB0035254	7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone	HMDB0035254
802	HMDB0033016	7,8-Dihydroyangonin	HMDB0033016
803	HMDB0030578	Apigravin	HMDB0030578
804	HMDB0032953	7-Methoxy-5-prenyloxycoumarin	HMDB0032953
805	HMDB0061290	NA	NA
806	HMDB0061303	NA	NA
807	HMDB0039146	NA	NA
808	HMDB0037679	NA	NA
809	HMDB0035019	Phenethyl salicylate	HMDB0035019
810	HMDB0029302	1-Phenyl-6,7-dihydroxy-isochroman	HMDB0029302
811	HMDB0036347	NA	NA
812	HMDB0002209	Equol	HMDB0002209
813	HMDB0130495	NA	NA
814	HMDB0014713	Fenoprofen	HMDB0014713
815	HMDB0135409	NA	NA
816	HMDB0135406	NA	NA
817	HMDB0135408	NA	NA
818	HMDB0135407	NA	NA
819	HMDB0135593	NA	NA
820	HMDB0135594	NA	NA
821	HMDB0135405	NA	NA
822	HMDB0130496	NA	NA
823	HMDB0135355	NA	NA
824	HMDB0135397	NA	NA
825	HMDB0135595	NA	NA
826	HMDB0151857	NA	NA
827	HMDB0130497	NA	NA
828	HMDB0168444	NA	NA
829	HMDB0135601	NA	NA
830	HMDB0168447	NA	NA
831	HMDB0148520	NA	NA
832	HMDB0168443	NA	NA
833	HMDB0182848	NA	NA
834	HMDB0168445	NA	NA
835	HMDB0168442	NA	NA
836	HMDB0135596	NA	NA
837	HMDB0168446	NA	NA
838	HMDB0029953	D-erythro-D-galacto-octitol	HMDB0029953
839	HMDB0060478	gamma-Glutamyl-beta-cyanoalanine	HMDB0060478
840	HMDB0000089	Cytidine	HMDB0000089
841	HMDB0015122	Cytarabine	HMDB0015122
842	HMDB0155273	NA	NA

843	HMDB0001904	3-Nitrotyrosine	HMDB0001904
844	HMDB0028751	Aspartyl-Glutamine	HMDB0028751
845	HMDB0028793	Glutaminylaspartic acid	HMDB0028793
846	HMDB0029144	gamma-Glutamylasparagine	HMDB0029144
847	HMDB0028814	Glutamylasparagine	HMDB0028814
848	HMDB0028730	Asparaginy-Glutamate	HMDB0028730
849	HMDB0028767	Aspartyl-Gamma-glutamate	HMDB0028767
850	HMDB0033701	Hydrocotarnine	HMDB0033701
851	HMDB0031770	Carbofuran	HMDB0031770
852	HMDB0014798	Metaxalone	HMDB0014798
853	HMDB0139892	NA	NA
854	HMDB0138550	NA	NA
855	HMDB0033925	Oroselone	HMDB0033925
856	HMDB0032998	2-Methoxyxanthone	HMDB0032998
857	HMDB0161779	NA	NA
858	HMDB0161778	NA	NA
859	HMDB0161783	NA	NA
860	HMDB0161782	NA	NA
861	HMDB0161780	NA	NA
862	HMDB0162111	NA	NA
863	HMDB0162103	NA	NA
864	HMDB0162104	NA	NA
865	HMDB0162105	NA	NA
866	HMDB0162108	NA	NA
867	HMDB0162109	NA	NA
868	HMDB0162106	NA	NA
869	HMDB0162107	NA	NA
870	HMDB0162110	NA	NA
871	HMDB0162112	NA	NA
872	HMDB0161832	NA	NA
873	HMDB0161833	NA	NA
874	HMDB0161834	NA	NA
875	HMDB0149051	NA	NA
876	HMDB0149050	NA	NA
877	HMDB0149006	NA	NA
878	HMDB0148541	NA	NA
879	HMDB0148540	NA	NA
880	HMDB0148786	NA	NA
881	HMDB0148785	NA	NA
882	HMDB0148998	NA	NA
883	HMDB0149048	NA	NA
884	HMDB0147226	NA	NA
885	HMDB0148542	NA	NA
886	HMDB0128505	NA	NA
887	HMDB0148539	NA	NA
888	HMDB0145646	NA	NA
889	HMDB0145647	NA	NA
890	HMDB0145645	NA	NA
891	HMDB0135172	NA	NA
892	HMDB0149007	NA	NA
893	HMDB0128506	NA	NA
894	HMDB0128503	NA	NA
895	HMDB0128504	NA	NA
896	HMDB0040876	NA	NA
897	HMDB0030946	(2E,11Z)-Wyerone acid	HMDB0030946
898	HMDB0041016	NA	NA
899	HMDB0030595	Suberenone	HMDB0030595
900	HMDB0033735	Graveolone	HMDB0033735
901	HMDB0039430	NA	NA
902	HMDB0004215	3,3',4'5-Tetrahydroxystilbene	HMDB0004215
903	HMDB0170845	NA	NA
904	HMDB0164057	NA	NA
905	HMDB0135900	NA	NA
906	HMDB0135902	NA	NA
907	HMDB0135904	NA	NA
908	HMDB0164055	NA	NA
909	HMDB0164056	NA	NA
910	HMDB0164058	NA	NA
911	HMDB0170846	NA	NA
912	HMDB0170974	NA	NA
913	HMDB0170976	NA	NA
914	HMDB0170979	NA	NA
915	HMDB0170978	NA	NA
916	HMDB0131284	NA	NA
917	HMDB0131285	NA	NA
918	HMDB0127824	NA	NA
919	HMDB0131281	NA	NA
920	HMDB0131283	NA	NA
921	HMDB0170977	NA	NA
922	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	HMDB0031668
923	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	HMDB0034056
924	HMDB0037681	NA	NA
925	HMDB0029470	Isodillapiole	HMDB0029470
926	HMDB0041379	NA	NA
927	HMDB0135906	NA	NA
928	HMDB0038563	NA	NA
929	HMDB0037130	NA	NA

930	HMDB0094660	Diethyl phthalic acid	HMDB0094660
931	HMDB0033776	Apiole	HMDB0033776
932	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	HMDB0029226
933	HMDB0135689	NA	NA
934	HMDB0013247	Monobutylphthalate	HMDB0013247
935	HMDB0030725	Dillapiol	HMDB0030725
936	HMDB0002056	Monoisobutyl phthalic acid	HMDB0002056
937	HMDB0147179	NA	NA
938	HMDB0140340	NA	NA
939	HMDB0173973	NA	NA
940	HMDB0173971	NA	NA
941	HMDB0173972	NA	NA
942	HMDB0173975	NA	NA
943	HMDB0173976	NA	NA
944	HMDB0177472	NA	NA
945	HMDB0177470	NA	NA
946	HMDB0173974	NA	NA
947	HMDB0128944	NA	NA
948	HMDB0131630	NA	NA
949	HMDB0128958	NA	NA
950	HMDB0039027	NA	NA
951	HMDB0128963	NA	NA
952	HMDB0138052	NA	NA
953	HMDB0128962	NA	NA
954	HMDB0030882	(S)-Rutaretin	HMDB0030882
955	HMDB0128960	NA	NA
956	HMDB0128961	NA	NA
957	HMDB0032838	Dorsteniol	HMDB0032838
958	HMDB0131653	NA	NA
959	HMDB0147178	NA	NA
960	HMDB0131691	NA	NA
961	HMDB0131700	NA	NA
962	HMDB0167944	NA	NA
963	HMDB0163475	NA	NA
964	HMDB0171044	NA	NA
965	HMDB0167134	NA	NA
966	HMDB0028752	Aspartyl-Glutamate	HMDB0028752
967	HMDB0029145	NA	NA
968	HMDB0030419	gamma-Glutamylaspartic acid	HMDB0030419
969	HMDB0062501	NA	NA
970	HMDB0028815	Glutamylaspartic acid	HMDB0028815
971	HMDB0030413	NA	NA
972	HMDB0011164	L-beta-aspartyl-L-glutamic acid	HMDB0011164
973	HMDB0000767	Pseudouridine	HMDB0000767
974	HMDB0000296	Uridine	HMDB0000296
975	HMDB0156330	NA	NA
976	HMDB0126635	NA	NA
977	HMDB0130466	NA	NA
978	HMDB0130477	NA	NA
979	HMDB0006794	5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate	HMDB0006794
980	HMDB0157260	NA	NA
981	HMDB0157259	NA	NA
982	HMDB0125157	NA	NA
983	HMDB0166885	NA	NA
984	HMDB0155302	NA	NA
985	HMDB0180914	NA	NA
986	HMDB0177249	NA	NA
987	HMDB0163614	NA	NA
988	HMDB0168264	NA	NA
989	HMDB0029971	Coriandrone E	HMDB0029971
990	HMDB0169152	NA	NA
991	HMDB0137140	NA	NA
992	HMDB0137141	NA	NA
993	HMDB0137143	NA	NA
994	HMDB0137139	NA	NA
995	HMDB0172322	NA	NA
996	HMDB0172318	NA	NA
997	HMDB0170970	NA	NA
998	HMDB0170968	NA	NA
999	HMDB0170967	NA	NA
1000	HMDB0172321	NA	NA
1001	HMDB0141329	NA	NA
1002	HMDB0128670	NA	NA
1003	HMDB0128677	NA	NA
1004	HMDB0133894	NA	NA
1005	HMDB0124956	NA	NA
1006	HMDB0166533	NA	NA
1007	HMDB0169509	NA	NA
1008	HMDB0169510	NA	NA
1009	HMDB0166535	NA	NA
1010	HMDB0166534	NA	NA
1011	HMDB0149147	NA	NA
1012	HMDB0137286	NA	NA
1013	HMDB0137294	NA	NA
1014	HMDB0137727	NA	NA
1015	HMDB0140941	NA	NA
1016	HMDB0141547	NA	NA

1017	HMDB0142081	NA	NA
1018	HMDB0146414	NA	NA
1019	HMDB0146428	NA	NA
1020	HMDB0146425	NA	NA
1021	HMDB0146431	NA	NA
1022	HMDB0149148	NA	NA
1023	HMDB0149146	NA	NA
1024	HMDB0141549	NA	NA
1025	HMDB0060736	NA	NA
1026	HMDB0041679	NA	NA
1027	HMDB0041727	NA	NA
1028	HMDB0035830	Genipin	HMDB0035830
1029	HMDB0031722	3,4,5-Trimethoxyphenyl acetate	HMDB0031722
1030	HMDB0146421	NA	NA
1031	HMDB0041560	NA	NA
1032	HMDB0240455	NA	NA
1033	HMDB0142080	NA	NA
1034	HMDB0182642	NA	NA
1035	HMDB0181717	NA	NA
1036	HMDB0182640	NA	NA
1037	HMDB0182638	NA	NA
1038	HMDB0182636	NA	NA
1039	HMDB0176292	NA	NA
1040	HMDB0163151	NA	NA
1041	HMDB0163154	NA	NA
1042	HMDB0163155	NA	NA
1043	HMDB0163161	NA	NA
1044	HMDB0163165	NA	NA
1045	HMDB0163169	NA	NA
1046	HMDB0181721	NA	NA
1047	HMDB0181643	NA	NA
1048	HMDB0181656	NA	NA
1049	HMDB0181713	NA	NA
1050	HMDB0181710	NA	NA
1051	HMDB0181714	NA	NA
1052	HMDB0181718	NA	NA
1053	HMDB0181653	NA	NA
1054	HMDB0182687	NA	NA
1055	HMDB0136711	NA	NA
1056	HMDB0163137	NA	NA
1057	HMDB0163139	NA	NA
1058	HMDB0163145	NA	NA
1059	HMDB0182803	NA	NA
1060	HMDB0163150	NA	NA
1061	HMDB0163147	NA	NA
1062	HMDB0182809	NA	NA
1063	HMDB0182805	NA	NA
1064	HMDB0182690	NA	NA
1065	HMDB0182693	NA	NA
1066	HMDB0182695	NA	NA
1067	HMDB0182801	NA	NA
1068	HMDB0182807	NA	NA
1069	HMDB0180579	NA	NA
1070	HMDB0163833	NA	NA
1071	HMDB0164904	NA	NA
1072	HMDB0181029	NA	NA
1073	HMDB0180584	NA	NA
1074	HMDB0180576	NA	NA
1075	HMDB0180573	NA	NA
1076	HMDB0180570	NA	NA
1077	HMDB0180567	NA	NA
1078	HMDB0180564	NA	NA
1079	HMDB0180158	NA	NA
1080	HMDB0164973	NA	NA
1081	HMDB0180087	NA	NA
1082	HMDB0180093	NA	NA
1083	HMDB0180096	NA	NA
1084	HMDB0180157	NA	NA
1085	HMDB0028749	Aspartyl-Aspartate	HMDB0028749
1086	HMDB0011163	L-beta-aspartyl-L-aspartic acid	HMDB0011163
1087	HMDB0028833	Glutamyl-Gamma-glutamate	HMDB0028833
1088	HMDB0028796	Glutaminylglutamic acid	HMDB0028796
1089	HMDB0029147	N-gamma-Glutamylglutamine	HMDB0029147
1090	HMDB0028817	Glutamylglutamine	HMDB0028817
1091	HMDB0011738	N2-gamma-Glutamylglutamine	HMDB0011738
1092	HMDB0005766	Norophthalmic acid	HMDB0005766
1093	HMDB0240577	NA	NA
1094	HMDB0000982	5-Methylcytidine	HMDB0000982
1095	HMDB0039229	Pyro-L-glutaminy-L-glutamine	HMDB0039229
1096	HMDB0032559	(Áś)-2-(1-Methylpropyl)-4,6-dinitrophenol	HMDB0032559
1097	HMDB0033610	Pandamarilactam 3x	HMDB0033610
1098	HMDB0139906	NA	NA
1099	HMDB0164387	NA	NA
1100	HMDB0000086	Glycerophosphocholine	HMDB0000086
1101	HMDB0142996	NA	NA
1102	HMDB0143005	NA	NA
1103	HMDB0151865	NA	NA

1104	HMDB0137520	NA	NA
1105	HMDB0130494	NA	NA
1106	HMDB0135588	NA	NA
1107	HMDB0135591	NA	NA
1108	HMDB0135592	NA	NA
1109	HMDB0137534	NA	NA
1110	HMDB0135587	NA	NA
1111	HMDB0135590	NA	NA
1112	HMDB0151856	NA	NA
1113	HMDB0032130	3',4'-Dihydroxychalcone	HMDB0032130
1114	HMDB0135586	NA	NA
1115	HMDB0153774	NA	NA
1116	HMDB0036738	NA	NA
1117	HMDB0039612	NA	NA
1118	HMDB0032129	2',5'-Dihydroxychalcone	HMDB0032129
1119	HMDB0014643	Tolmetin	HMDB0014643
1120	HMDB0033345	(Ás)-Ribaline	HMDB0033345
1121	HMDB0041329	NA	NA
1122	HMDB0032924	3-Furanmethanol glucoside	HMDB0032924
1123	HMDB0130798	NA	NA
1124	HMDB0130839	NA	NA
1125	HMDB0126546	NA	NA
1126	HMDB0167013	NA	NA
1127	HMDB0175219	NA	NA
1128	HMDB0167016	NA	NA
1129	HMDB0002091	Isovalerylglucuronide	HMDB0002091
1130	HMDB0167014	NA	NA
1131	HMDB0175223	NA	NA
1132	HMDB0143217	NA	NA
1133	HMDB0175224	NA	NA
1134	HMDB0175227	NA	NA
1135	HMDB0175220	NA	NA
1136	HMDB0033065	(x)-1,2-Propanediol 1-O-b-D-glucopyranoside	HMDB0033065
1137	HMDB0060917	NA	NA
1138	HMDB0144816	NA	NA
1139	HMDB0184077	NA	NA
1140	HMDB0029155	NA	NA
1141	HMDB0034367	gamma-Glutamylmethionine	HMDB0034367
1142	HMDB0028972	Methionyl-Glutamate	HMDB0028972
1143	HMDB0028825	Glutamylmethionine	HMDB0028825
1144	HMDB0000273	Thymidine	HMDB0000273
1145	HMDB0015394	Telbivudine	HMDB0015394
1146	HMDB0136645	NA	NA
1147	HMDB0128628	NA	NA
1148	HMDB0015017	Emtricitabine	HMDB0015017
1149	HMDB0032560	Dinoseb acetate	HMDB0032560
1150	HMDB0015521	Sulfamerazine	HMDB0015521
1151	HMDB0060663	NA	NA
1152	HMDB0177722	NA	NA
1153	HMDB0040790	NA	NA
1154	HMDB0033351	Methoxybrassinin	HMDB0033351
1155	HMDB0155171	NA	NA
1156	HMDB0002062	Norepinephrine sulfate	HMDB0002062
1157	HMDB0156032	NA	NA
1158	HMDB0155175	NA	NA
1159	HMDB0155133	NA	NA
1160	HMDB0156031	NA	NA
1161	HMDB0155132	NA	NA
1162	HMDB0240695	NA	NA
1163	HMDB0168085	NA	NA
1164	HMDB0167573	NA	NA
1165	HMDB0153240	NA	NA
1166	HMDB0148680	NA	NA
1167	HMDB0130908	NA	NA
1168	HMDB0150257	NA	NA
1169	HMDB0150666	NA	NA
1170	HMDB0150667	NA	NA
1171	HMDB0151413	NA	NA
1172	HMDB0151710	NA	NA
1173	HMDB0151717	NA	NA
1174	HMDB0151989	NA	NA
1175	HMDB0152004	NA	NA
1176	HMDB0152130	NA	NA
1177	HMDB0153396	NA	NA
1178	HMDB0147592	NA	NA
1179	HMDB0128588	NA	NA
1180	HMDB0130320	NA	NA
1181	HMDB0130374	NA	NA
1182	HMDB0130909	NA	NA
1183	HMDB0130905	NA	NA
1184	HMDB0130928	NA	NA
1185	HMDB0130926	NA	NA
1186	HMDB0132873	NA	NA
1187	HMDB0140458	NA	NA
1188	HMDB0140466	NA	NA
1189	HMDB0140465	NA	NA
1190	HMDB0140471	NA	NA

1191	HMDB0140478	NA	NA
1192	HMDB0141217	NA	NA
1193	HMDB0128584	NA	NA
1194	HMDB0146278	NA	NA
1195	HMDB0132455	NA	NA
1196	HMDB0130379	NA	NA
1197	HMDB0036629	NA	NA
1198	HMDB0029522	5,7-Dihydroxy-3-methoxyflavone	HMDB0029522
1199	HMDB0133330	NA	NA
1200	HMDB0132457	NA	NA
1201	HMDB0031428	Farnisin	HMDB0031428
1202	HMDB0039166	NA	NA
1203	HMDB0039578	NA	NA
1204	HMDB0005781	Glycitein	HMDB0005781
1205	HMDB0002338	Biochanin A	HMDB0002338
1206	HMDB0034127	Prunetin	HMDB0034127
1207	HMDB0180733	NA	NA
1208	HMDB0147591	NA	NA
1209	HMDB0041758	NA	NA
1210	HMDB0041776	NA	NA
1211	HMDB0031720	Xenognosin B	HMDB0031720
1212	HMDB0030768	2-(6-Hydroxy-2-methoxy-3,4-methylenedioxyphenyl)benzofuran	HMDB0030768
1213	HMDB0141945	NA	NA
1214	HMDB0132850	NA	NA
1215	HMDB0147530	NA	NA
1216	HMDB0150245	NA	NA
1217	HMDB0132886	NA	NA
1218	HMDB0130929	NA	NA
1219	HMDB0134889	NA	NA
1220	HMDB0137557	NA	NA
1221	HMDB0125118	NA	NA
1222	HMDB0145984	NA	NA
1223	HMDB0060791	NA	NA
1224	HMDB0061269	NA	NA
1225	HMDB0175189	NA	NA
1226	HMDB0175187	NA	NA
1227	HMDB0175188	NA	NA
1228	HMDB0162484	NA	NA
1229	HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	HMDB0033197
1230	HMDB0036047	NA	NA
1231	HMDB0059661	NA	NA
1232	HMDB0015088	Rizatriptan	HMDB0015088
1233	HMDB0014873	Naftifine	HMDB0014873
1234	HMDB0014578	Cyproheptadine	HMDB0014578
1235	HMDB0006023	3'-O-Methyladenosine	HMDB0006023
1236	HMDB0004326	2'-O-Methyladenosine	HMDB0004326
1237	HMDB0003331	1-Methyladenosine	HMDB0003331
1238	HMDB0004044	N6-Methyladenosine	HMDB0004044
1239	HMDB0060966	NA	NA
1240	HMDB0037843	NA	NA
1241	HMDB0126095	NA	NA
1242	HMDB0034681	3-Hydroxy-4-butanolide	HMDB0034681
1243	HMDB0167145	NA	NA
1244	HMDB0130127	NA	NA
1245	HMDB0159320	NA	NA
1246	HMDB0159322	NA	NA
1247	HMDB0167143	NA	NA
1248	HMDB0172032	NA	NA
1249	HMDB0159324	NA	NA
1250	HMDB0172030	NA	NA
1251	HMDB0154807	NA	NA
1252	HMDB0030327	Perlolyrine	HMDB0030327
1253	HMDB0240660	NA	NA
1254	HMDB0166396	NA	NA
1255	HMDB0155323	NA	NA
1256	HMDB0125616	NA	NA
1257	HMDB0157443	NA	NA
1258	HMDB0125615	NA	NA
1259	HMDB0155324	NA	NA
1260	HMDB0155326	NA	NA
1261	HMDB0155327	NA	NA
1262	HMDB0157445	NA	NA
1263	HMDB0157442	NA	NA
1264	HMDB0166395	NA	NA
1265	HMDB0156225	NA	NA
1266	HMDB0156223	NA	NA
1267	HMDB0156224	NA	NA
1268	HMDB0156222	NA	NA
1269	HMDB0155825	NA	NA
1270	HMDB0166394	NA	NA
1271	HMDB0125614	NA	NA
1272	HMDB0125613	NA	NA
1273	HMDB0157444	NA	NA
1274	HMDB0155325	NA	NA
1275	HMDB0164008	NA	NA
1276	HMDB0062577	NA	NA
1277	HMDB0003950	7-Methylinosine	HMDB0003950

1278	HMDB0002721	1-Methylinosine	HMDB0002721
1279	HMDB0033060	Piperolactam A	HMDB0033060
1280	HMDB0034319	Furofoline	HMDB0034319
1281	HMDB0038882	NA	NA
1282	HMDB0038880	NA	NA
1283	HMDB0029918	Arabinofuranobiose	HMDB0029918
1284	HMDB0029894	Xylobiose	HMDB0029894
1285	HMDB0038855	NA	NA
1286	HMDB0029619	Arabinopyranobiose	HMDB0029619
1287	HMDB0038881	NA	NA
1288	HMDB0179982	NA	NA
1289	HMDB0179983	NA	NA
1290	HMDB0179984	NA	NA
1291	HMDB0028745	Asparaginylnl-Gamma-glutamate	HMDB0028745
1292	HMDB0028792	Glutaminylasparagine	HMDB0028792
1293	HMDB0028729	Asparaginylnl-Glutamine	HMDB0028729
1294	HMDB0126535	NA	NA
1295	HMDB0126543	NA	NA
1296	HMDB0126529	NA	NA
1297	HMDB0126544	NA	NA
1298	HMDB0126525	NA	NA
1299	HMDB0126540	NA	NA
1300	HMDB0126536	NA	NA
1301	HMDB0126532	NA	NA
1302	HMDB0126531	NA	NA
1303	HMDB0126528	NA	NA
1304	HMDB0126526	NA	NA
1305	HMDB0130026	NA	NA
1306	HMDB0157544	NA	NA
1307	HMDB0157677	NA	NA
1308	HMDB0157676	NA	NA
1309	HMDB0157545	NA	NA
1310	HMDB0160744	NA	NA
1311	HMDB0187647	NA	NA
1312	HMDB0187648	NA	NA
1313	HMDB0130027	NA	NA
1314	HMDB0160630	NA	NA
1315	HMDB0160631	NA	NA
1316	HMDB0160633	NA	NA
1317	HMDB0160632	NA	NA
1318	HMDB0061311	NA	NA
1319	HMDB0155720	NA	NA
1320	HMDB0135202	NA	NA
1321	HMDB0037131	NA	NA
1322	HMDB0171351	NA	NA
1323	HMDB0171346	NA	NA
1324	HMDB0132963	NA	NA
1325	HMDB0171349	NA	NA
1326	HMDB0132998	NA	NA
1327	HMDB0171344	NA	NA
1328	HMDB0154060	NA	NA
1329	HMDB0170885	NA	NA
1330	HMDB0170883	NA	NA
1331	HMDB0170882	NA	NA
1332	HMDB0170888	NA	NA
1333	HMDB0170889	NA	NA
1334	HMDB0041097	NA	NA
1335	HMDB0037101	NA	NA
1336	HMDB0033915	Aloe emodin w-acetate	HMDB0033915
1337	HMDB0030563	3',4,4'-Trihydroxypulvinone	HMDB0030563
1338	HMDB0033658	De-O-methylhydrosterigmatocystin	HMDB0033658
1339	HMDB0033993	Wairol	HMDB0033993
1340	HMDB0030561	3-Hydroxy-8,9-dimethoxycoumestan	HMDB0030561
1341	HMDB0006552	Aflatoxin B1	HMDB0006552
1342	HMDB0154061	NA	NA
1343	HMDB0170884	NA	NA
1344	HMDB0112194	NA	NA
1345	HMDB0160588	NA	NA
1346	HMDB0160590	NA	NA
1347	HMDB0160589	NA	NA
1348	HMDB0160593	NA	NA
1349	HMDB0160591	NA	NA
1350	HMDB0160592	NA	NA
1351	HMDB0160595	NA	NA
1352	HMDB0062652	NA	NA
1353	HMDB0173890	NA	NA
1354	HMDB0173885	NA	NA
1355	HMDB0173886	NA	NA
1356	HMDB0173888	NA	NA
1357	HMDB0173887	NA	NA
1358	HMDB0173891	NA	NA
1359	HMDB0173889	NA	NA
1360	HMDB0173893	NA	NA
1361	HMDB0004701	9,10-Epoxyoctadecenoic acid	HMDB0004701
1362	HMDB0004702	12,13-EpOME	HMDB0004702
1363	HMDB0004670	Alpha-dimorphecolic acid	HMDB0004670
1364	HMDB0010223	9-HODE	HMDB0010223

1365	HMDB0029978	Avenoleic acid	HMDB0029978
1366	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	HMDB0029796
1367	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid	HMDB0029998
1368	HMDB0004667	13S-hydroxyoctadecadienoic acid	HMDB0004667
1369	HMDB0061708	NA	NA
1370	HMDB0170226	NA	NA
1371	HMDB0170229	NA	NA
1372	HMDB0170227	NA	NA
1373	HMDB0170230	NA	NA
1374	HMDB0170228	NA	NA
1375	HMDB0004704	9,10-DHOME	HMDB0004704
1376	HMDB0061650	9,10-Epoxystearic acid	HMDB0061650
1377	HMDB0004705	12,13-DHOME	HMDB0004705
1378	HMDB0041220	NA	NA
1379	HMDB0031679	(9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid	HMDB0031679
1380	HMDB0000782	Octadecanedioic acid	HMDB0000782
1381	HMDB0015401	Nelarabine	HMDB0015401
1382	HMDB0005862	2-Methylguanosine	HMDB0005862
1383	HMDB0006038	3'-O-Methylguanosine	HMDB0006038
1384	HMDB0001563	1-Methylguanosine	HMDB0001563
1385	HMDB0001107	7-Methylguanosine	HMDB0001107
1386	HMDB0029076	Tryptophyl-Alanine	HMDB0029076
1387	HMDB0028698	Alanyl-Tryptophan	HMDB0028698
1388	HMDB0142223	NA	NA
1389	HMDB0013209	Alanyltryptophan	HMDB0013209
1390	HMDB0165476	NA	NA
1391	HMDB0165475	NA	NA
1392	HMDB0165471	NA	NA
1393	HMDB0165472	NA	NA
1394	HMDB0126113	NA	NA
1395	HMDB0130135	NA	NA
1396	HMDB0130132	NA	NA
1397	HMDB0130129	NA	NA
1398	HMDB0145822	NA	NA
1399	HMDB0130130	NA	NA
1400	HMDB0164665	NA	NA
1401	HMDB0130133	NA	NA
1402	HMDB0130019	NA	NA
1403	HMDB0126116	NA	NA
1404	HMDB0126115	NA	NA
1405	HMDB0130136	NA	NA
1406	HMDB0126114	NA	NA
1407	HMDB0178290	NA	NA
1408	HMDB0178289	NA	NA
1409	HMDB0181208	NA	NA
1410	HMDB0015469	Magnesium salicylate	HMDB0015469
1411	HMDB0037270	NA	NA
1412	HMDB0185229	NA	NA
1413	HMDB0179599	NA	NA
1414	HMDB0036728	ent-16-Kauren-19-al	HMDB0036728
1415	HMDB0034735	Abietinal	HMDB0034735
1416	HMDB0156414	NA	NA
1417	HMDB0000305	Vitamin A	HMDB0000305
1418	HMDB0006216	11-cis-Retinol	HMDB0006216
1419	HMDB0006217	9-cis-Retinol	HMDB0006217
1420	HMDB0006221	13-cis Retinol	HMDB0006221
1421	HMDB0030403	(x)-p-Menth-1-en-4-yl 5-isopropyl-2-methylphenyl ether	HMDB0030403
1422	HMDB0036841	NA	NA
1423	HMDB0038709	NA	NA
1424	HMDB0013624	Alpha-Linolenoyl ethanolamide	HMDB0013624
1425	HMDB0060628	NA	NA
1426	HMDB0002117	Oleamide	HMDB0002117
1427	HMDB0135641	NA	NA
1428	HMDB0179385	NA	NA
1429	HMDB0179388	NA	NA
1430	HMDB0179383	NA	NA
1431	HMDB0179382	NA	NA
1432	HMDB0163720	NA	NA
1433	HMDB0173550	NA	NA
1434	HMDB0135574	NA	NA
1435	HMDB0135576	NA	NA
1436	HMDB0135572	NA	NA
1437	HMDB0135564	NA	NA
1438	HMDB0135568	NA	NA
1439	HMDB0134573	NA	NA
1440	HMDB0134571	NA	NA
1441	HMDB0135570	NA	NA
1442	HMDB0158752	NA	NA
1443	HMDB0158753	NA	NA
1444	HMDB0155927	NA	NA
1445	HMDB0155928	NA	NA
1446	HMDB0161130	NA	NA
1447	HMDB0041096	NA	NA
1448	HMDB0158750	NA	NA
1449	HMDB0158751	NA	NA
1450	HMDB0159487	NA	NA
1451	HMDB0159488	NA	NA

1452	HMDB0159490	NA	NA
1453	HMDB0159830	NA	NA
1454	HMDB0161128	NA	NA
1455	HMDB0161127	NA	NA
1456	HMDB0161129	NA	NA
1457	HMDB0161132	NA	NA
1458	HMDB0161133	NA	NA
1459	HMDB0166865	NA	NA
1460	HMDB0159483	NA	NA
1461	HMDB0159484	NA	NA
1462	HMDB0159482	NA	NA
1463	HMDB0158755	NA	NA
1464	HMDB0158759	NA	NA
1465	HMDB0158758	NA	NA
1466	HMDB0159491	NA	NA
1467	HMDB0158756	NA	NA
1468	HMDB0158876	NA	NA
1469	HMDB0158877	NA	NA
1470	HMDB0159485	NA	NA
1471	HMDB0061135	NA	NA
1472	HMDB0015176	Melphalan	HMDB0015176
1473	HMDB0127928	NA	NA
1474	HMDB0037110	NA	NA
1475	HMDB0145098	NA	NA
1476	HMDB0175072	NA	NA
1477	HMDB0041450	NA	NA
1478	HMDB0038322	NA	NA
1479	HMDB0032909	2-(4-Methoxyphenyl)naphthalic anhydride	HMDB0032909
1480	HMDB0175074	NA	NA
1481	HMDB0175080	NA	NA
1482	HMDB0175081	NA	NA
1483	HMDB0175083	NA	NA
1484	HMDB0175073	NA	NA
1485	HMDB0175082	NA	NA
1486	HMDB0163581	NA	NA
1487	HMDB0163582	NA	NA
1488	HMDB0163584	NA	NA
1489	HMDB0042049	Trichloroethanol glucuronide	HMDB0042049
1490	HMDB0038580	NA	NA
1491	HMDB0033631	Lactapiperanol D	HMDB0033631
1492	HMDB0180021	NA	NA
1493	HMDB0180098	NA	NA
1494	HMDB0180100	NA	NA
1495	HMDB0180099	NA	NA
1496	HMDB0180102	NA	NA
1497	HMDB0034780	Capsiate	HMDB0034780
1498	HMDB0180103	NA	NA
1499	HMDB0184951	NA	NA
1500	HMDB0184949	NA	NA
1501	HMDB0184953	NA	NA
1502	HMDB0012799	5'-Carboxy-gamma-chromanol	HMDB0012799
1503	HMDB0184954	NA	NA
1504	HMDB0184950	NA	NA
1505	HMDB0061677	NA	NA
1506	HMDB0000552	3-Methylglutaryl carnitine	HMDB0000552
1507	HMDB0141924	NA	NA
1508	HMDB0005923	N4-Acetylcytidine	HMDB0005923
1509	HMDB0240452	NA	NA
1510	HMDB0135701	NA	NA
1511	HMDB0125823	NA	NA
1512	HMDB0127756	NA	NA
1513	HMDB0127760	NA	NA
1514	HMDB0132282	NA	NA
1515	HMDB0132579	NA	NA
1516	HMDB0182829	NA	NA
1517	HMDB0182831	NA	NA
1518	HMDB0171701	NA	NA
1519	HMDB0162417	NA	NA
1520	HMDB0135715	NA	NA
1521	HMDB0135714	NA	NA
1522	HMDB0135712	NA	NA
1523	HMDB0135711	NA	NA
1524	HMDB0135708	NA	NA
1525	HMDB0135702	NA	NA
1526	HMDB0132598	NA	NA
1527	HMDB0240447	NA	NA
1528	HMDB0171698	NA	NA
1529	HMDB0059976	NA	NA
1530	HMDB0059975	NA	NA
1531	HMDB0062192	NA	NA
1532	HMDB0061242	NA	NA
1533	HMDB0059997	NA	NA
1534	HMDB0178044	NA	NA
1535	HMDB0038641	NA	NA
1536	HMDB0000495	Androstenediol	HMDB0000495
1537	HMDB0159493	NA	NA
1538	HMDB0158029	NA	NA

1539	HMDB0000554	Dihydroandrosterone	HMDB0000554
1540	HMDB0000551	Etiocholenediol	HMDB0000551
1541	HMDB0000458	5a-Androstane-3a,17a-diol	HMDB0000458
1542	HMDB0000383	3a,17a-Dihydroxy-5b-androstane	HMDB0000383
1543	HMDB0000493	5a-Androstane-3b,17b-diol	HMDB0000493
1544	HMDB0000369	3b,17b-Dihydroxyetiocholane	HMDB0000369
1545	HMDB0000412	3b,17a-Dihydroxy-5a-androstane	HMDB0000412
1546	HMDB0060437	Androstan-3alpha,17beta-diol	HMDB0060437
1547	HMDB0167160	NA	NA
1548	HMDB0167157	NA	NA
1549	HMDB0156083	NA	NA
1550	HMDB0167154	NA	NA
1551	HMDB0167155	NA	NA
1552	HMDB0167156	NA	NA
1553	HMDB0062521	NA	NA
1554	HMDB0167161	NA	NA
1555	HMDB0167158	NA	NA
1556	HMDB0173640	NA	NA
1557	HMDB0186461	NA	NA
1558	HMDB0167171	NA	NA
1559	HMDB0167170	NA	NA
1560	HMDB0186443	NA	NA
1561	HMDB0167159	NA	NA
1562	HMDB0167165	NA	NA
1563	HMDB0167163	NA	NA
1564	HMDB0167162	NA	NA
1565	HMDB0167164	NA	NA
1566	HMDB0167169	NA	NA
1567	HMDB0167168	NA	NA
1568	HMDB0167167	NA	NA
1569	HMDB0167166	NA	NA
1570	HMDB0014613	Dronabinol	HMDB0014613
1571	HMDB0038533	NA	NA
1572	HMDB0013121	7-Dehydropregnenolone	HMDB0013121
1573	HMDB0031924	4-Nerolidylcatechol	HMDB0031924
1574	HMDB0041865	NA	NA
1575	HMDB0001830	Progesterone	HMDB0001830
1576	HMDB0156085	NA	NA
1577	HMDB0137415	NA	NA
1578	HMDB0137402	NA	NA
1579	HMDB0156084	NA	NA
1580	HMDB0156089	NA	NA
1581	HMDB0186441	NA	NA
1582	HMDB0186440	NA	NA
1583	HMDB0186438	NA	NA
1584	HMDB0186439	NA	NA
1585	HMDB0186444	NA	NA
1586	HMDB0186457	NA	NA
1587	HMDB0186462	NA	NA
1588	HMDB0186435	NA	NA
1589	HMDB0186437	NA	NA
1590	HMDB0156091	NA	NA
1591	HMDB0156092	NA	NA
1592	HMDB0156093	NA	NA
1593	HMDB0156090	NA	NA
1594	HMDB0156094	NA	NA
1595	HMDB0156095	NA	NA
1596	HMDB0156840	NA	NA
1597	HMDB0158166	NA	NA
1598	HMDB0173643	NA	NA
1599	HMDB0173642	NA	NA
1600	HMDB0173641	NA	NA
1601	HMDB0173645	NA	NA
1602	HMDB0173644	NA	NA
1603	HMDB0173646	NA	NA
1604	HMDB0173647	NA	NA
1605	HMDB0173648	NA	NA
1606	HMDB0186436	NA	NA
1607	HMDB0062609	NA	NA
1608	HMDB0060424	7alpha-Hydroxypregnenolone	HMDB0060424
1609	HMDB0060407	5alpha-Dihydrodeoxycorticosterone	HMDB0060407
1610	HMDB0031462	[10]-Shogaol	HMDB0031462
1611	HMDB0033918	(15alpha,20R)-15,20-Dihydroxypregn-4-en-3-one	HMDB0033918
1612	HMDB0011653	17-alpha,20-alpha-Dihydroxypregn-4-en-3-one	HMDB0011653
1613	HMDB0004026	21-Hydroxypregnenolone	HMDB0004026
1614	HMDB0003851	3a,7a-Dihydroxy-5b-cholestanate	HMDB0003851
1615	HMDB0000363	17a-Hydroxypregnenolone	HMDB0000363
1616	HMDB0000315	16-a-Hydroxypregnenolone	HMDB0000315
1617	HMDB0173549	NA	NA
1618	HMDB0125510	NA	NA
1619	HMDB0125509	NA	NA
1620	HMDB0060017	NA	NA
1621	HMDB0125511	NA	NA
1622	HMDB0125508	NA	NA
1623	HMDB0125512	NA	NA
1624	HMDB0187598	NA	NA
1625	HMDB0015513	Fludiazepam	HMDB0015513

1626	HMDB0162772	NA	NA
1627	HMDB0162714	NA	NA
1628	HMDB0162760	NA	NA
1629	HMDB0162710	NA	NA
1630	HMDB0162708	NA	NA
1631	HMDB0162758	NA	NA
1632	HMDB0033374	Benzyl glycinate 4-methylbenzenesulfonate salt	HMDB0033374
1633	HMDB0161228	NA	NA
1634	HMDB0161229	NA	NA
1635	HMDB0159742	NA	NA
1636	HMDB0185385	NA	NA
1637	HMDB0181751	NA	NA
1638	HMDB0181741	NA	NA
1639	HMDB0039733	NA	NA
1640	HMDB0004662	S-(Hydroxymethyl)glutathione	HMDB0004662
1641	HMDB0014848	Ibandronate	HMDB0014848
1642	HMDB0038582	NA	NA
1643	HMDB0154970	NA	NA
1644	HMDB0156936	NA	NA
1645	HMDB0158197	NA	NA
1646	HMDB0158606	NA	NA
1647	HMDB0012782	4-Methoxy-17beta-estradiol	HMDB0012782
1648	HMDB0155194	NA	NA
1649	HMDB0155195	NA	NA
1650	HMDB0137388	NA	NA
1651	HMDB0137399	NA	NA
1652	HMDB0154971	NA	NA
1653	HMDB0154972	NA	NA
1654	HMDB0154973	NA	NA
1655	HMDB0154976	NA	NA
1656	HMDB0154995	NA	NA
1657	HMDB0155190	NA	NA
1658	HMDB0155192	NA	NA
1659	HMDB0155191	NA	NA
1660	HMDB0155189	NA	NA
1661	HMDB0155193	NA	NA
1662	HMDB0006773	11b-Hydroxyandrost-4-ene-3,17-dione	HMDB0006773
1663	HMDB0039568	NA	NA
1664	HMDB0034167	Falcarindiol 3-acetate	HMDB0034167
1665	HMDB0040927	NA	NA
1666	HMDB0033125	[8]-Dehydroshogaol	HMDB0033125
1667	HMDB0006771	7a-Hydroxyandrost-4-ene-3,17-dione	HMDB0006771
1668	HMDB0006774	16a-Hydroxyandrost-4-ene-3,17-dione	HMDB0006774
1669	HMDB0003959	19-Oxotestosterone	HMDB0003959
1670	HMDB0003955	19-Hydroxyandrost-4-ene-3,17-dione	HMDB0003955
1671	HMDB0000405	2-Methoxyestradiol	HMDB0000405
1672	HMDB0000380	2-Hydroxyestradiol-3-methyl ether	HMDB0000380
1673	HMDB0034028	2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone	HMDB0034028
1674	HMDB0154977	NA	NA
1675	HMDB0041204	NA	NA
1676	HMDB0031038	(2Z,8S,9Z)-2,9-Heptadecadiene-8-hydroxy-4,6-diyne-1-yl acetate	HMDB0031038
1677	HMDB0036696	NA	NA
1678	HMDB0060359	2,3-Epoxymenaquinone	HMDB0060359
1679	HMDB0184900	NA	NA
1680	HMDB0184898	NA	NA
1681	HMDB0184895	NA	NA
1682	HMDB0184897	NA	NA
1683	HMDB0184899	NA	NA
1684	HMDB0184896	NA	NA
1685	HMDB0184903	NA	NA
1686	HMDB0184902	NA	NA
1687	HMDB0184904	NA	NA
1688	HMDB0184908	NA	NA
1689	HMDB0184905	NA	NA
1690	HMDB0184901	NA	NA
1691	HMDB0005038	Citalopram	HMDB0005038
1692	HMDB0005028	Escitalopram	HMDB0005028
1693	HMDB0186295	NA	NA
1694	HMDB0186306	NA	NA
1695	HMDB0186305	NA	NA
1696	HMDB0186302	NA	NA
1697	HMDB0186303	NA	NA
1698	HMDB0186304	NA	NA
1699	HMDB0186299	NA	NA
1700	HMDB0186301	NA	NA
1701	HMDB0186297	NA	NA
1702	HMDB0186300	NA	NA
1703	HMDB0186296	NA	NA
1704	HMDB0029525	7-(4-Hydroxy-3-methoxyphenyl)-5-methoxy-1-phenyl-3-heptanone	HMDB0029525
1705	HMDB0131863	NA	NA
1706	HMDB0032549	N-Undecylbenzenesulfonic acid	HMDB0032549
1707	HMDB0171053	NA	NA
1708	HMDB0171052	NA	NA
1709	HMDB0180006	NA	NA
1710	HMDB0179178	NA	NA
1711	HMDB0179822	NA	NA
1712	HMDB0179824	NA	NA

1713	HMDB0163506	NA	NA
1714	HMDB0179826	NA	NA
1715	HMDB0179828	NA	NA
1716	HMDB0171049	NA	NA
1717	HMDB0171046	NA	NA
1718	HMDB0040461	NA	NA
1719	HMDB0163490	NA	NA
1720	HMDB0163491	NA	NA
1721	HMDB0163494	NA	NA
1722	HMDB0163498	NA	NA
1723	HMDB0163499	NA	NA
1724	HMDB0163495	NA	NA
1725	HMDB0170942	NA	NA
1726	HMDB0163526	NA	NA
1727	HMDB0163505	NA	NA
1728	HMDB0163502	NA	NA
1729	HMDB0171045	NA	NA
1730	HMDB0029084	Tryptophyl-Hydroxyproline	HMDB0029084
1731	HMDB0181182	NA	NA
1732	HMDB0028874	Hydroxyprolyl-Tryptophan	HMDB0028874
1733	HMDB0138126	NA	NA
1734	HMDB0138125	NA	NA
1735	HMDB0138129	NA	NA
1736	HMDB0138130	NA	NA
1737	HMDB0138127	NA	NA
1738	HMDB0179081	NA	NA
1739	HMDB0138131	NA	NA
1740	HMDB0138132	NA	NA
1741	HMDB0138128	NA	NA
1742	HMDB0138133	NA	NA
1743	HMDB0138134	NA	NA
1744	HMDB0138276	NA	NA
1745	HMDB0171363	NA	NA
1746	HMDB0186298	NA	NA
1747	HMDB0031976	Methyl (9Z)-10'-oxo-6,10'-diapo-6-carotenoate	HMDB0031976
1748	HMDB0033294	5-Methoxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	HMDB0033294
1749	HMDB0040761	NA	NA
1750	HMDB0061027	NA	NA
1751	HMDB0015191	Praziquantel	HMDB0015191
1752	HMDB0033108	Semilepidinoside B	HMDB0033108
1753	HMDB0240296	NA	NA
1754	HMDB0166033	NA	NA
1755	HMDB0012492	1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylate	HMDB0012492
1756	HMDB0029992	Tetrahydropentoxylone	HMDB0029992
1757	HMDB0166038	NA	NA
1758	HMDB0166035	NA	NA
1759	HMDB0166036	NA	NA
1760	HMDB0014720	Voriconazole	HMDB0014720
1761	HMDB0014258	R-138727	HMDB0014258
1762	HMDB0131015	NA	NA
1763	HMDB0131014	NA	NA
1764	HMDB0131011	NA	NA
1765	HMDB0131013	NA	NA
1766	HMDB0136701	NA	NA
1767	HMDB0140161	NA	NA
1768	HMDB0171360	NA	NA
1769	HMDB0171359	NA	NA
1770	HMDB0171362	NA	NA
1771	HMDB0171358	NA	NA
1772	HMDB0171355	NA	NA
1773	HMDB0171354	NA	NA
1774	HMDB0032955	5-(6-Hydroxy-3,7-dimethyl-2,7-octadienyloxy)-7-methoxycoumarin	HMDB0032955
1775	HMDB0038690	NA	NA
1776	HMDB0171361	NA	NA
1777	HMDB0034179	Malabaricano	HMDB0034179
1778	HMDB0031889	(1(10)E,4E,6a,8b)-8-Angeloyloxy-14-oxo-1(10),4,11(13)-germacatrien-12,6-olide	HMDB0031889
1779	HMDB0031753	2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol	HMDB0031753
1780	HMDB0038219	NA	NA
1781	HMDB0040388	NA	NA
1782	HMDB0040421	NA	NA
1783	HMDB0036691	NA	NA
1784	HMDB0039610	NA	NA
1785	HMDB0125864	NA	NA
1786	HMDB0172929	NA	NA
1787	HMDB0148194	NA	NA
1788	HMDB0040834	NA	NA
1789	HMDB0040809	NA	NA
1790	HMDB0041100	NA	NA
1791	HMDB0041417	NA	NA
1792	HMDB0035427	Glicoisoflavanone	HMDB0035427
1793	HMDB0014559	Ampicillin	HMDB0014559
1794	HMDB0015428	Cefradine	HMDB0015428
1795	HMDB0062731	Dodecamethylpentasiloxane	HMDB0062731
1796	HMDB0012983	Kinetensin 1-3	HMDB0012983
1797	HMDB0011568	MG(18:2(9Z,12Z)/0:0/0:0)	HMDB0011568
1798	HMDB0011538	MG(0:0/18:2(9Z,12Z)/0:0)	HMDB0011538
1799	HMDB0012868	9'-Carboxy-gamma-chromanol	HMDB0012868

1800	HMDB0167759	NA	NA
1801	HMDB0039278	NA	NA
1802	HMDB0011550	MG(0:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	HMDB0011550
1803	HMDB0011580	MG(20:5(5Z,8Z,11Z,14Z,17Z)/0:0/0:0)	HMDB0011580
1804	HMDB0013651	2-(14,15-Epoxyeicosatrienoyl) Glycerol	HMDB0013651
1805	HMDB0012530	11-Hydroxyeicosatetraenoate glyceryl ester	HMDB0012530
1806	HMDB0004239	13,14-Dihydro PGF2a	HMDB0004239
1807	HMDB0002689	13,14-Dihydro PGE1	HMDB0002689
1808	HMDB0002685	Prostaglandin F1a	HMDB0002685
1809	HMDB0165171	NA	NA
1810	HMDB0035508	Annoglabasin F	HMDB0035508
1811	HMDB0014701	Doxapram	HMDB0014701
1812	HMDB0175496	NA	NA
1813	HMDB0175499	NA	NA
1814	HMDB0175502	NA	NA
1815	HMDB0175506	NA	NA
1816	HMDB0175509	NA	NA
1817	HMDB0175505	NA	NA
1818	HMDB0175517	NA	NA
1819	HMDB0175521	NA	NA
1820	HMDB0175520	NA	NA
1821	HMDB0175516	NA	NA
1822	HMDB0175513	NA	NA
1823	HMDB0175512	NA	NA
1824	HMDB0011131	MG(18:0/0:0/0:0)	HMDB0011131
1825	HMDB0031075	Glycerol 1-octadecanoate	HMDB0031075
1826	HMDB0072842	NA	NA
1827	HMDB0011535	MG(0:0/18:0/0:0)	HMDB0011535
1828	HMDB0072877	NA	NA
1829	HMDB0032735	Isopersin	HMDB0032735
1830	HMDB0039403	NA	NA
1831	HMDB0011577	MG(20:3(8Z,11Z,14Z)/0:0/0:0)	HMDB0011577
1832	HMDB0011576	MG(20:3(5Z,8Z,11Z)/0:0/0:0)	HMDB0011576
1833	HMDB0011575	MG(20:3(11Z,14Z,17Z)/0:0/0:0)	HMDB0011575
1834	HMDB0011547	MG(0:0/20:3(8Z,11Z,14Z)/0:0)	HMDB0011547
1835	HMDB0011545	MG(0:0/20:3(11Z,14Z,17Z)/0:0)	HMDB0011545
1836	HMDB0011546	MG(0:0/20:3(5Z,8Z,11Z)/0:0)	HMDB0011546
1837	HMDB0041103	NA	NA
1838	HMDB0185679	NA	NA
1839	HMDB0185658	NA	NA
1840	HMDB0185694	NA	NA
1841	HMDB0185682	NA	NA
1842	HMDB0185676	NA	NA
1843	HMDB0185661	NA	NA
1844	HMDB0185673	NA	NA
1845	HMDB0185698	NA	NA
1846	HMDB0185670	NA	NA
1847	HMDB0185667	NA	NA
1848	HMDB0185664	NA	NA
1849	HMDB0179611	NA	NA
1850	HMDB0179614	NA	NA
1851	HMDB0179608	NA	NA
1852	HMDB0179615	NA	NA
1853	HMDB0179605	NA	NA
1854	HMDB0179606	NA	NA
1855	HMDB0179618	NA	NA
1856	HMDB0179619	NA	NA
1857	HMDB0179623	NA	NA
1858	HMDB0179626	NA	NA
1859	HMDB0182175	NA	NA
1860	HMDB0179627	NA	NA
1861	HMDB0182176	NA	NA
1862	HMDB0014334	Bortezomib	HMDB0014334
1863	HMDB0061005	NA	NA
1864	HMDB0060583	NA	NA
1865	HMDB0030868	Citreoviridin A	HMDB0030868
1866	HMDB0030523	Citreoviridin C	HMDB0030523
1867	HMDB0036462	NA	NA
1868	HMDB0035027	Melleolide F	HMDB0035027
1869	HMDB0035774	Armillyl orsellinate	HMDB0035774
1870	HMDB0015459	Cortisone acetate	HMDB0015459
1871	HMDB0038917	NA	NA
1872	HMDB0031380	(6beta,7alpha,12beta,13beta)-7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide	HMDB0031380
1873	HMDB0179899	NA	NA
1874	HMDB0179900	NA	NA
1875	HMDB0179898	NA	NA
1876	HMDB0179897	NA	NA
1877	HMDB0179895	NA	NA
1878	HMDB0179894	NA	NA
1879	HMDB0179893	NA	NA
1880	HMDB0179896	NA	NA
1881	HMDB0161492	NA	NA
1882	HMDB0161493	NA	NA
1883	HMDB0161490	NA	NA
1884	HMDB0029360	Isorheagenine	HMDB0029360
1885	HMDB0029401	Ochratoxin B	HMDB0029401
1886	HMDB0015068	Mesoridazine	HMDB0015068

1887	HMDB0030785	Mammeigin	HMDB0030785
1888	HMDB0015248	Trimethaphan	HMDB0015248
1889	HMDB0180131	NA	NA
1890	HMDB0180133	NA	NA
1891	HMDB0180134	NA	NA
1892	HMDB0180137	NA	NA
1893	HMDB0180138	NA	NA
1894	HMDB0180139	NA	NA
1895	HMDB0180595	NA	NA
1896	HMDB0180596	NA	NA
1897	HMDB0180594	NA	NA
1898	HMDB0180593	NA	NA
1899	HMDB0180599	NA	NA
1900	HMDB0180598	NA	NA
1901	HMDB0180601	NA	NA
1902	HMDB0180602	NA	NA
1903	HMDB0180604	NA	NA
1904	HMDB0180605	NA	NA
1905	HMDB0179947	NA	NA
1906	HMDB0180130	NA	NA
1907	HMDB0180128	NA	NA
1908	HMDB0180129	NA	NA
1909	HMDB0179950	NA	NA
1910	HMDB0179946	NA	NA
1911	HMDB0179945	NA	NA
1912	HMDB0179942	NA	NA
1913	HMDB0179943	NA	NA
1914	HMDB0179941	NA	NA
1915	HMDB0164899	NA	NA
1916	HMDB0164897	NA	NA
1917	HMDB0164898	NA	NA
1918	HMDB0163827	NA	NA
1919	HMDB0163828	NA	NA
1920	HMDB0179951	NA	NA
1921	HMDB0179955	NA	NA
1922	HMDB0163826	NA	NA
1923	HMDB0179962	NA	NA
1924	HMDB0179960	NA	NA
1925	HMDB0179961	NA	NA
1926	HMDB0179957	NA	NA
1927	HMDB0179956	NA	NA
1928	HMDB0180124	NA	NA
1929	HMDB0180118	NA	NA
1930	HMDB0180115	NA	NA
1931	HMDB0180117	NA	NA
1932	HMDB0180112	NA	NA
1933	HMDB0180114	NA	NA
1934	HMDB0012240	Isopentenyladenine-9-N-glucoside	HMDB0012240
1935	HMDB0014828	Flurazepam	HMDB0014828
1936	HMDB0126243	NA	NA
1937	HMDB0133257	NA	NA
1938	HMDB0133256	NA	NA
1939	HMDB0133260	NA	NA
1940	HMDB0133258	NA	NA
1941	HMDB0133261	NA	NA
1942	HMDB0133254	NA	NA
1943	HMDB0133265	NA	NA
1944	HMDB0133262	NA	NA
1945	HMDB0133264	NA	NA
1946	HMDB0132557	NA	NA
1947	HMDB0135675	NA	NA
1948	HMDB0133252	NA	NA
1949	HMDB0126244	NA	NA
1950	HMDB0126245	NA	NA
1951	HMDB0126247	NA	NA
1952	HMDB0126372	NA	NA
1953	HMDB0132287	NA	NA
1954	HMDB0132286	NA	NA
1955	HMDB0132293	NA	NA
1956	HMDB0132294	NA	NA
1957	HMDB0126241	NA	NA
1958	HMDB0132556	NA	NA
1959	HMDB0133251	NA	NA
1960	HMDB0135697	NA	NA
1961	HMDB0151258	NA	NA
1962	HMDB0163653	NA	NA
1963	HMDB0163655	NA	NA
1964	HMDB0163657	NA	NA
1965	HMDB0163654	NA	NA
1966	HMDB0163658	NA	NA
1967	HMDB0164136	NA	NA
1968	HMDB0164140	NA	NA
1969	HMDB0164138	NA	NA
1970	HMDB0166270	NA	NA
1971	HMDB0166272	NA	NA
1972	HMDB0182840	NA	NA
1973	HMDB0163651	NA	NA

1974	HMDB0163650	NA	NA
1975	HMDB0151257	NA	NA
1976	HMDB0151255	NA	NA
1977	HMDB0151261	NA	NA
1978	HMDB0151262	NA	NA
1979	HMDB0151267	NA	NA
1980	HMDB0151269	NA	NA
1981	HMDB0152804	NA	NA
1982	HMDB0152821	NA	NA
1983	HMDB0163644	NA	NA
1984	HMDB0163645	NA	NA
1985	HMDB0163647	NA	NA
1986	HMDB0163646	NA	NA
1987	HMDB0163652	NA	NA
1988	HMDB0059980	NA	NA
1989	HMDB0040865	NA	NA
1990	HMDB0041115	NA	NA
1991	HMDB0030380	Brevianamide B	HMDB0030380
1992	HMDB0153959	NA	NA
1993	HMDB0176911	NA	NA
1994	HMDB0165595	NA	NA
1995	HMDB0061060	NA	NA
1996	HMDB0061059	NA	NA
1997	HMDB0031754	Nequinatate	HMDB0031754
1998	HMDB0060833	NA	NA
1999	HMDB0185381	NA	NA
2000	HMDB0002873	Deacetyldiltiazem	HMDB0002873
2001	HMDB0124912	NA	NA
2002	HMDB0124915	NA	NA
2003	HMDB0124828	NA	NA
2004	HMDB0124911	NA	NA
2005	HMDB0124914	NA	NA
2006	HMDB0124913	NA	NA
2007	HMDB0125800	NA	NA
2008	HMDB0131078	NA	NA
2009	HMDB0131080	NA	NA
2010	HMDB0131077	NA	NA
2011	HMDB0130292	NA	NA
2012	HMDB0130291	NA	NA
2013	HMDB0130288	NA	NA
2014	HMDB0130290	NA	NA
2015	HMDB0130289	NA	NA
2016	HMDB0130100	NA	NA
2017	HMDB0130099	NA	NA
2018	HMDB0124817	NA	NA
2019	HMDB0124816	NA	NA
2020	HMDB0124815	NA	NA
2021	HMDB0124810	NA	NA
2022	HMDB0124811	NA	NA
2023	HMDB0124813	NA	NA
2024	HMDB0124812	NA	NA
2025	HMDB0133480	NA	NA
2026	HMDB0149865	NA	NA
2027	HMDB0149860	NA	NA
2028	HMDB0149855	NA	NA
2029	HMDB0149846	NA	NA
2030	HMDB0149841	NA	NA
2031	HMDB0149835	NA	NA
2032	HMDB0149834	NA	NA
2033	HMDB0146994	NA	NA
2034	HMDB0146992	NA	NA
2035	HMDB0146993	NA	NA
2036	HMDB0146989	NA	NA
2037	HMDB0133520	NA	NA
2038	HMDB0133514	NA	NA
2039	HMDB0133513	NA	NA
2040	HMDB0133493	NA	NA
2041	HMDB0133492	NA	NA
2042	HMDB0133481	NA	NA
2043	HMDB0146939	NA	NA
2044	HMDB0131836	NA	NA
2045	HMDB0131837	NA	NA
2046	HMDB0131838	NA	NA
2047	HMDB0133527	NA	NA
2048	HMDB0133537	NA	NA
2049	HMDB0137511	NA	NA
2050	HMDB0146987	NA	NA
2051	HMDB0146988	NA	NA
2052	HMDB0146986	NA	NA
2053	HMDB0146947	NA	NA
2054	HMDB0146945	NA	NA
2055	HMDB0146944	NA	NA
2056	HMDB0146941	NA	NA
2057	HMDB0146940	NA	NA
2058	HMDB0146938	NA	NA
2059	HMDB0138813	NA	NA
2060	HMDB0131079	NA	NA

2061	HMDB0039066	NA	NA
2062	HMDB0041416	NA	NA
2063	HMDB0030826	2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-methylenedioxyphenyl)-1-propanol	HMDB0030826
2064	HMDB0035182	Licoriphenone	HMDB0035182
2065	HMDB0032733	(8R,8'R,9S)-9-Hydroxy-3,4-dimethoxy-3',4'-methylenoxy-9,9'-epoxylignan	HMDB0032733
2066	HMDB0005789	Tetrahydrocurcumin	HMDB0005789
2067	HMDB0030087	(-)-Arctigenin	HMDB0030087
2068	HMDB0032734	9-Hydroxy-3',4'-dimethoxy-3,4-methylenedioxy-9,9'-epoxylignan	HMDB0032734
2069	HMDB0164958	NA	NA
2070	HMDB0029510	Garcinone B	HMDB0029510
2071	HMDB0034436	Rotenone	HMDB0034436
2072	HMDB0036984	NA	NA
2073	HMDB0148796	NA	NA
2074	HMDB0146129	NA	NA
2075	HMDB0173953	NA	NA
2076	HMDB0184813	NA	NA
2077	HMDB0184985	NA	NA
2078	HMDB0184812	NA	NA
2079	HMDB0184811	NA	NA
2080	HMDB0184810	NA	NA
2081	HMDB0173968	NA	NA
2082	HMDB0173965	NA	NA
2083	HMDB0173956	NA	NA
2084	HMDB0183162	NA	NA
2085	HMDB0039867	NA	NA
2086	HMDB0035584	1-Phenyl-1,3-nonadecanedione	HMDB0035584
2087	HMDB0038506	NA	NA
2088	HMDB0174608	NA	NA
2089	HMDB0173235	NA	NA
2090	HMDB0171546	NA	NA
2091	HMDB0036848	NA	NA
2092	HMDB0039022	NA	NA
2093	HMDB0036849	NA	NA
2094	HMDB0040749	NA	NA
2095	HMDB0040765	NA	NA
2096	HMDB0015567	Calcipotriol	HMDB0015567
2097	HMDB0172273	NA	NA
2098	HMDB0172275	NA	NA
2099	HMDB0172274	NA	NA
2100	HMDB0174261	NA	NA
2101	HMDB0174260	NA	NA
2102	HMDB0174265	NA	NA
2103	HMDB0174262	NA	NA
2104	HMDB0174263	NA	NA
2105	HMDB0174264	NA	NA
2106	HMDB0174266	NA	NA
2107	HMDB0155085	NA	NA
2108	HMDB0155087	NA	NA
2109	HMDB0154867	NA	NA
2110	HMDB0154866	NA	NA
2111	HMDB0155080	NA	NA
2112	HMDB0155083	NA	NA
2113	HMDB0155082	NA	NA
2114	HMDB0155081	NA	NA
2115	HMDB0155084	NA	NA
2116	HMDB0155086	NA	NA
2117	HMDB0174267	NA	NA
2118	HMDB0174268	NA	NA
2119	HMDB0184842	NA	NA
2120	HMDB0184845	NA	NA
2121	HMDB0184846	NA	NA
2122	HMDB0184848	NA	NA
2123	HMDB0184847	NA	NA
2124	HMDB0184849	NA	NA
2125	HMDB0184851	NA	NA
2126	HMDB0184850	NA	NA
2127	HMDB0185576	NA	NA
2128	HMDB0185577	NA	NA
2129	HMDB0184843	NA	NA
2130	HMDB0184841	NA	NA
2131	HMDB0184144	NA	NA
2132	HMDB0184143	NA	NA
2133	HMDB0184146	NA	NA
2134	HMDB0184145	NA	NA
2135	HMDB0184147	NA	NA
2136	HMDB0184148	NA	NA
2137	HMDB0184150	NA	NA
2138	HMDB0184149	NA	NA
2139	HMDB0184168	NA	NA
2140	HMDB0184844	NA	NA
2141	HMDB0185578	NA	NA
2142	HMDB0003550	Calcidiol	HMDB0003550
2143	HMDB0060132	NA	NA
2144	HMDB0060131	NA	NA
2145	HMDB0015504	Alfacalcidol	HMDB0015504
2146	HMDB0000501	7-Ketocholesterol	HMDB0000501
2147	HMDB0001993	7a-Hydroxy-cholestene-3-one	HMDB0001993

2148	HMDB0006722	25-Hydroxytachysterol3	HMDB0006722
2149	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	HMDB0006721
2150	HMDB0035585	1-Phenyl-1,3-heneicosanedione	HMDB0035585
2151	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	HMDB0034328
2152	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	HMDB0036012
2153	HMDB0039871	NA	NA
2154	HMDB0159655	NA	NA
2155	HMDB0159658	NA	NA
2156	HMDB0159656	NA	NA
2157	HMDB0159657	NA	NA
2158	HMDB0159654	NA	NA
2159	HMDB0159653	NA	NA
2160	HMDB0159651	NA	NA
2161	HMDB0159652	NA	NA
2162	HMDB0062675	NA	NA
2163	HMDB0062664	NA	NA
2164	HMDB0062419	NA	NA
2165	HMDB0062420	NA	NA
2166	HMDB0062607	NA	NA
2167	HMDB0172263	NA	NA
2168	HMDB0172264	NA	NA
2169	HMDB0185568	NA	NA
2170	HMDB0185570	NA	NA
2171	HMDB0185567	NA	NA
2172	HMDB0185569	NA	NA
2173	HMDB0185572	NA	NA
2174	HMDB0185575	NA	NA
2175	HMDB0185571	NA	NA
2176	HMDB0185574	NA	NA
2177	HMDB0185566	NA	NA
2178	HMDB0172272	NA	NA
2179	HMDB0172262	NA	NA
2180	HMDB0172266	NA	NA
2181	HMDB0172268	NA	NA
2182	HMDB0172265	NA	NA
2183	HMDB0172267	NA	NA
2184	HMDB0172270	NA	NA
2185	HMDB0172269	NA	NA
2186	HMDB0172271	NA	NA
2187	HMDB0185573	NA	NA
2188	HMDB0006280	7-a,25-Dihydroxycholesterol	HMDB0006280
2189	HMDB0060136	7alpha,24S-Dihydroxycholesterol	HMDB0060136
2190	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol	HMDB0011644
2191	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al	HMDB0006894
2192	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one	HMDB0006887
2193	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one	HMDB0006886
2194	HMDB0006764	17a,20a-Dihydroxycholesterol	HMDB0006764
2195	HMDB0006763	20a,22b-Dihydroxycholesterol	HMDB0006763
2196	HMDB0006281	7-a,27-Dihydroxycholesterol	HMDB0006281
2197	HMDB0035951	Erucoylacetone	HMDB0035951
2198	HMDB0165504	NA	NA
2199	HMDB0014902	Mometasone	HMDB0014902
2200	HMDB0149450	NA	NA
2201	HMDB0165831	NA	NA
2202	HMDB0138170	NA	NA
2203	HMDB0138169	NA	NA
2204	HMDB0138189	NA	NA
2205	HMDB0138192	NA	NA
2206	HMDB0138175	NA	NA
2207	HMDB0138176	NA	NA
2208	HMDB0138179	NA	NA
2209	HMDB0138182	NA	NA
2210	HMDB0138183	NA	NA
2211	HMDB0138186	NA	NA
2212	HMDB0138188	NA	NA
2213	HMDB0138191	NA	NA
2214	HMDB0138195	NA	NA
2215	HMDB0138172	NA	NA
2216	HMDB0138173	NA	NA
2217	HMDB0171434	NA	NA
2218	HMDB0171377	NA	NA
2219	HMDB0171432	NA	NA
2220	HMDB0171436	NA	NA
2221	HMDB0180057	NA	NA
2222	HMDB0180127	NA	NA
2223	HMDB0183179	NA	NA
2224	HMDB0183180	NA	NA
2225	HMDB0167778	NA	NA
2226	HMDB0172090	NA	NA
2227	HMDB0144261	NA	NA
2228	HMDB0136130	NA	NA
2229	HMDB0136128	NA	NA
2230	HMDB0130041	NA	NA
2231	HMDB0130042	NA	NA
2232	HMDB0130038	NA	NA
2233	HMDB0130035	NA	NA
2234	HMDB0130037	NA	NA

2235	HMDB0136134	NA	NA
2236	HMDB0141975	NA	NA
2237	HMDB0154071	NA	NA
2238	HMDB0154072	NA	NA
2239	HMDB0148956	NA	NA
2240	HMDB0145713	NA	NA
2241	HMDB0144028	NA	NA
2242	HMDB0141974	NA	NA
2243	HMDB0138050	NA	NA
2244	HMDB0138003	NA	NA
2245	HMDB0137957	NA	NA
2246	HMDB0136144	NA	NA
2247	HMDB0136137	NA	NA
2248	HMDB0145714	NA	NA
2249	HMDB0136139	NA	NA
2250	HMDB0038066	NA	NA
2251	HMDB0180987	NA	NA
2252	HMDB0164391	NA	NA
2253	HMDB0164389	NA	NA
2254	HMDB0164395	NA	NA
2255	HMDB0036334	NA	NA
2256	HMDB0029900	Lucuminoside	HMDB0029900
2257	HMDB0014780	Pemetrexed	HMDB0014780
2258	HMDB0037260	NA	NA
2259	HMDB0158333	NA	NA
2260	HMDB0150478	NA	NA
2261	HMDB0150475	NA	NA
2262	HMDB0162509	NA	NA
2263	HMDB0150477	NA	NA
2264	HMDB0038347	NA	NA
2265	HMDB0150474	NA	NA
2266	HMDB0150463	NA	NA
2267	HMDB0150458	NA	NA
2268	HMDB0150468	NA	NA
2269	HMDB0150470	NA	NA
2270	HMDB0150457	NA	NA
2271	HMDB0150453	NA	NA
2272	HMDB0150469	NA	NA
2273	HMDB0150452	NA	NA
2274	HMDB0149868	NA	NA
2275	HMDB0150462	NA	NA
2276	HMDB0140070	NA	NA
2277	HMDB0153459	NA	NA
2278	HMDB0153444	NA	NA
2279	HMDB0153474	NA	NA
2280	HMDB0153627	NA	NA
2281	HMDB0153466	NA	NA
2282	HMDB0139521	NA	NA
2283	HMDB0139520	NA	NA
2284	HMDB0139517	NA	NA
2285	HMDB0139504	NA	NA
2286	HMDB0139507	NA	NA
2287	HMDB0139514	NA	NA
2288	HMDB0149502	NA	NA
2289	HMDB0153458	NA	NA
2290	HMDB0153451	NA	NA
2291	HMDB0153443	NA	NA
2292	HMDB0139516	NA	NA
2293	HMDB0139508	NA	NA
2294	HMDB0139513	NA	NA
2295	HMDB0035876	Mesuagin	HMDB0035876
2296	HMDB0180147	NA	NA
2297	HMDB0013842	O-Deethylated candesartan	HMDB0013842
2298	HMDB0144444	NA	NA
2299	HMDB0144965	NA	NA
2300	HMDB0144871	NA	NA
2301	HMDB0142647	NA	NA
2302	HMDB0144859	NA	NA
2303	HMDB0144408	NA	NA
2304	HMDB0144379	NA	NA
2305	HMDB0142761	NA	NA
2306	HMDB0142694	NA	NA
2307	HMDB0144418	NA	NA
2308	HMDB0144964	NA	NA
2309	HMDB0142682	NA	NA
2310	HMDB0144733	NA	NA
2311	HMDB0169644	NA	NA
2312	HMDB0059970	NA	NA
2313	HMDB0147118	NA	NA
2314	HMDB0128714	NA	NA
2315	HMDB0142099	NA	NA
2316	HMDB0142100	NA	NA
2317	HMDB0147119	NA	NA
2318	HMDB0147120	NA	NA
2319	HMDB0128706	NA	NA
2320	HMDB0128702	NA	NA
2321	HMDB0128698	NA	NA

2322	HMDB0142101	NA	NA
2323	HMDB0178475	NA	NA
2324	HMDB0187594	NA	NA
2325	HMDB0138865	NA	NA
2326	HMDB0160312	NA	NA
2327	HMDB0160311	NA	NA
2328	HMDB0160309	NA	NA
2329	HMDB0160306	NA	NA
2330	HMDB0160305	NA	NA
2331	HMDB0160308	NA	NA
2332	HMDB0160314	NA	NA
2333	HMDB0160317	NA	NA
2334	HMDB0160320	NA	NA
2335	HMDB0036340	NA	NA
2336	HMDB0160333	NA	NA
2337	HMDB0160330	NA	NA
2338	HMDB0160332	NA	NA
2339	HMDB0160329	NA	NA
2340	HMDB0160327	NA	NA
2341	HMDB0160326	NA	NA
2342	HMDB0160324	NA	NA
2343	HMDB0160323	NA	NA
2344	HMDB0160321	NA	NA
2345	HMDB0165007	NA	NA
2346	HMDB0165008	NA	NA
2347	HMDB0175389	NA	NA
2348	HMDB0175386	NA	NA
2349	HMDB0038562	NA	NA
2350	HMDB0014843	Delavirdine	HMDB0014843
2351	HMDB0014565	Spirolactone	HMDB0014565
2352	HMDB0180016	NA	NA
2353	HMDB0180015	NA	NA
2354	HMDB0015164	Topotecan	HMDB0015164
2355	HMDB0145175	NA	NA
2356	HMDB0139832	NA	NA
2357	HMDB0139824	NA	NA
2358	HMDB0139838	NA	NA
2359	HMDB0139829	NA	NA
2360	HMDB0139833	NA	NA
2361	HMDB0139834	NA	NA
2362	HMDB0139836	NA	NA
2363	HMDB0139835	NA	NA
2364	HMDB0139837	NA	NA
2365	HMDB0139830	NA	NA
2366	HMDB0139831	NA	NA
2367	HMDB0139826	NA	NA
2368	HMDB0139825	NA	NA
2369	HMDB0139823	NA	NA
2370	HMDB0042019	NA	NA
2371	HMDB0165600	NA	NA
2372	HMDB0165605	NA	NA
2373	HMDB0163371	NA	NA
2374	HMDB0165603	NA	NA
2375	HMDB0165607	NA	NA
2376	HMDB0179376	NA	NA
2377	HMDB0179375	NA	NA
2378	HMDB0179380	NA	NA
2379	HMDB0179379	NA	NA
2380	HMDB0163370	NA	NA
2381	HMDB0041991	NA	NA
2382	HMDB0035973	Lucidenic acid M	HMDB0035973
2383	HMDB0164014	NA	NA
2384	HMDB0171518	NA	NA
2385	HMDB0174361	NA	NA
2386	HMDB0174360	NA	NA
2387	HMDB0174359	NA	NA
2388	HMDB0174715	NA	NA
2389	HMDB0174374	NA	NA
2390	HMDB0174370	NA	NA
2391	HMDB0174371	NA	NA
2392	HMDB0174372	NA	NA
2393	HMDB0174373	NA	NA
2394	HMDB0174367	NA	NA
2395	HMDB0174363	NA	NA
2396	HMDB0174364	NA	NA
2397	HMDB0174362	NA	NA
2398	HMDB0174365	NA	NA
2399	HMDB0174366	NA	NA
2400	HMDB0174369	NA	NA
2401	HMDB0174368	NA	NA
2402	HMDB0183788	NA	NA
2403	HMDB0183785	NA	NA
2404	HMDB0183779	NA	NA
2405	HMDB0183773	NA	NA
2406	HMDB0183776	NA	NA
2407	HMDB0174714	NA	NA
2408	HMDB0174358	NA	NA

2409	HMDB0174356	NA	NA
2410	HMDB0174357	NA	NA
2411	HMDB0174355	NA	NA
2412	HMDB0000969	1,25-Dihydroxyvitamin D3-26,23-lactone	HMDB0000969
2413	HMDB0164012	NA	NA
2414	HMDB0174354	NA	NA
2415	HMDB0174353	NA	NA
2416	HMDB0174352	NA	NA
2417	HMDB0171517	NA	NA
2418	HMDB0012936	Dynorphin B (10-13)	HMDB0012936
2419	HMDB0240599	NA	NA
2420	HMDB0155347	NA	NA
2421	HMDB0155348	NA	NA
2422	HMDB0034064	2-Angeloyl-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one	HMDB0034064
2423	HMDB0036571	NA	NA
2424	HMDB0035489	Linalool 3,6-oxide primeveroside	HMDB0035489
2425	HMDB0031367	Linalool oxide D 3-[apiosyl-(1->6)-glucoside]	HMDB0031367
2426	HMDB0182246	NA	NA
2427	HMDB0182247	NA	NA
2428	HMDB0182263	NA	NA
2429	HMDB0015631	Alvimopan	HMDB0015631
2430	HMDB0061149	NA	NA
2431	HMDB0029989	Dulciol B	HMDB0029989
2432	HMDB0033316	Garcinone E	HMDB0033316
2433	HMDB0029990	Dulciol A	HMDB0029990
2434	HMDB0156274	NA	NA
2435	HMDB0162419	NA	NA
2436	HMDB0177052	NA	NA
2437	HMDB0040747	NA	NA
2438	HMDB0148895	NA	NA
2439	HMDB0040607	NA	NA
2440	HMDB0034183	Licoricidin	HMDB0034183
2441	HMDB0014420	Olmesartan	HMDB0014420
2442	HMDB0060584	NA	NA
2443	HMDB0159770	NA	NA
2444	HMDB0159769	NA	NA
2445	HMDB0159767	NA	NA
2446	HMDB0159766	NA	NA
2447	HMDB0159765	NA	NA
2448	HMDB0159768	NA	NA
2449	HMDB0062421	NA	NA
2450	HMDB0062416	NA	NA
2451	HMDB0159772	NA	NA
2452	HMDB0159774	NA	NA
2453	HMDB0159773	NA	NA
2454	HMDB0159897	NA	NA
2455	HMDB0159894	NA	NA
2456	HMDB0159896	NA	NA
2457	HMDB0159893	NA	NA
2458	HMDB0159889	NA	NA
2459	HMDB0159890	NA	NA
2460	HMDB0159892	NA	NA
2461	HMDB0159891	NA	NA
2462	HMDB0000558	5a-Cholestane-3a,7a,12a,23,25-pentol	HMDB0000558
2463	HMDB0002208	Cholestane-3,7,12,24,25-pentol	HMDB0002208
2464	HMDB0000483	5b-Cholestane-3a,7a,12a,23S,25-pentol	HMDB0000483
2465	HMDB0000556	5b-Cholestane-3a,7a,12a,24,25-pentol	HMDB0000556
2466	HMDB0000513	5b-Cholestane-3a,7a,12a,23R,25-pentol	HMDB0000513
2467	HMDB0002180	5b-Cholestane-3a,7a,12a,25,26-pentol	HMDB0002180
2468	HMDB0011187	TG(8:0/8:0/8:0)	HMDB0011187
2469	HMDB0059930	NA	NA
2470	HMDB0011503	LysoPE(16:0/0:0)	HMDB0011503
2471	HMDB0011473	LysoPE(0:0/16:0)	HMDB0011473
2472	HMDB0160383	NA	NA
2473	HMDB0007851	LysoPA(0:0/18:1(9Z))	HMDB0007851
2474	HMDB0007855	LysoPA(18:1(9Z)/0:0)	HMDB0007855
2475	HMDB0187017	NA	NA
2476	HMDB0155795	NA	NA
2477	HMDB0160382	NA	NA
2478	HMDB0011133	DHAP(18:0)	HMDB0011133
2479	HMDB0187016	NA	NA
2480	HMDB0161139	NA	NA
2481	HMDB0041085	NA	NA
2482	HMDB0032798	(R)-1-O-[b-D-Apiofuranosyl-(1->2)-b-D-glucopyranoside]-1,3-octanediol	HMDB0032798
2483	HMDB0062208	NA	NA
2484	HMDB0159763	NA	NA
2485	HMDB0159762	NA	NA
2486	HMDB0159775	NA	NA
2487	HMDB0159887	NA	NA
2488	HMDB0159886	NA	NA
2489	HMDB0003533	3a,7a,12a-Trihydroxy-5b-cholestan-26-al	HMDB0003533
2490	HMDB0000359	3a,7a-Dihydroxycoprostanic acid	HMDB0000359
2491	HMDB0159898	NA	NA
2492	HMDB0170385	NA	NA
2493	HMDB0170384	NA	NA
2494	HMDB0035221	(3beta,17alpha,23S)-17,23-Epoxy-3,28,29-trihydroxy-27-norlanost-8-en-24-one	HMDB0035221
2495	HMDB0035144	(3beta,17alpha,23S,24S)-17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-15-one	HMDB0035144

2496	HMDB0172390	NA	NA
2497	HMDB0167571	NA	NA
2498	HMDB0167569	NA	NA
2499	HMDB0167567	NA	NA
2500	HMDB0167565	NA	NA
2501	HMDB0167563	NA	NA
2502	HMDB0172392	NA	NA
2503	HMDB0168556	NA	NA
2504	HMDB0168555	NA	NA
2505	HMDB0015019	Quinapril	HMDB0015019
2506	HMDB0138286	NA	NA
2507	HMDB0175209	NA	NA
2508	HMDB0015560	Thiothixene	HMDB0015560
2509	HMDB0157393	NA	NA
2510	HMDB0158619	NA	NA
2511	HMDB0169094	NA	NA
2512	HMDB0171247	NA	NA
2513	HMDB0006765	2-Methoxy-estradiol-17b 3-glucuronide	HMDB0006765
2514	HMDB0010315	4-Hydroxyandrostenedione glucuronide	HMDB0010315
2515	HMDB0145075	NA	NA
2516	HMDB0145086	NA	NA
2517	HMDB0144922	NA	NA
2518	HMDB0144879	NA	NA
2519	HMDB0144952	NA	NA
2520	HMDB0144894	NA	NA
2521	HMDB0144844	NA	NA
2522	HMDB0144847	NA	NA
2523	HMDB0144882	NA	NA
2524	HMDB0144891	NA	NA
2525	HMDB0031918	Suspensolide F	HMDB0031918
2526	HMDB0061351	NA	NA
2527	HMDB0160543	NA	NA
2528	HMDB0160539	NA	NA
2529	HMDB0160541	NA	NA
2530	HMDB0160540	NA	NA
2531	HMDB0160542	NA	NA
2532	HMDB0160544	NA	NA
2533	HMDB0160545	NA	NA
2534	HMDB0160516	NA	NA
2535	HMDB0160517	NA	NA
2536	HMDB0160518	NA	NA
2537	HMDB0160515	NA	NA
2538	HMDB0160519	NA	NA
2539	HMDB0160522	NA	NA
2540	HMDB0160521	NA	NA
2541	HMDB0160520	NA	NA
2542	HMDB0160523	NA	NA
2543	HMDB0160526	NA	NA
2544	HMDB0160524	NA	NA
2545	HMDB0160525	NA	NA
2546	HMDB0160528	NA	NA
2547	HMDB0160529	NA	NA
2548	HMDB0160527	NA	NA
2549	HMDB0160530	NA	NA
2550	HMDB0172528	NA	NA
2551	HMDB0170464	NA	NA
2552	HMDB0059931	NA	NA
2553	HMDB0040118	NA	NA
2554	HMDB0240598	NA	NA
2555	HMDB0160534	NA	NA
2556	HMDB0160531	NA	NA
2557	HMDB0160532	NA	NA
2558	HMDB0160533	NA	NA
2559	HMDB0160538	NA	NA
2560	HMDB0160535	NA	NA
2561	HMDB0160536	NA	NA
2562	HMDB0160537	NA	NA
2563	HMDB0039079	NA	NA
2564	HMDB0039024	NA	NA
2565	HMDB0184086	NA	NA
2566	HMDB0002385	Celastrol	HMDB0002385
2567	HMDB0015057	Buprenorphine	HMDB0015057
2568	HMDB0062331	NA	NA
2569	HMDB0010379	LysoPC(14:0)	HMDB0010379
2570	HMDB0061691	NA	NA
2571	HMDB0161447	NA	NA
2572	HMDB0179451	NA	NA
2573	HMDB0062337	NA	NA
2574	HMDB0010407	LysoPC(P-16:0)	HMDB0010407
2575	HMDB0039086	NA	NA
2576	HMDB0183486	NA	NA
2577	HMDB0183482	NA	NA
2578	HMDB0183483	NA	NA
2579	HMDB0010381	LysoPC(15:0)	HMDB0010381
2580	HMDB0011130	LysoPE(18:0/0:0)	HMDB0011130
2581	HMDB0011129	LysoPE(0:0/18:0)	HMDB0011129
2582	HMDB0062305	NA	NA

2583	HMDB0172584	NA	NA
2584	HMDB0172583	NA	NA
2585	HMDB0154880	NA	NA
2586	HMDB0184865	NA	NA
2587	HMDB0172431	NA	NA
2588	HMDB0175550	NA	NA
2589	HMDB0172429	NA	NA
2590	HMDB0175542	NA	NA
2591	HMDB0175548	NA	NA
2592	HMDB0175549	NA	NA
2593	HMDB0034216	Adouetine X	HMDB0034216
2594	HMDB0030199	Frangulanine	HMDB0030199
2595	HMDB0032879	all-trans-Carophyll yellow	HMDB0032879
2596	HMDB0010380	LysoPC(14:1(9Z))	HMDB0010380
2597	HMDB0170639	NA	NA
2598	HMDB0170632	NA	NA
2599	HMDB0170638	NA	NA
2600	HMDB0170641	NA	NA
2601	HMDB0170637	NA	NA
2602	HMDB0170661	NA	NA
2603	HMDB0170640	NA	NA
2604	HMDB0170634	NA	NA
2605	HMDB0170636	NA	NA
2606	HMDB0170633	NA	NA
2607	HMDB0170635	NA	NA
2608	HMDB0170642	NA	NA
2609	HMDB0041532	NA	NA
2610	HMDB0030901	Eremopetasitenin B2	HMDB0030901
2611	HMDB0039930	NA	NA
2612	HMDB0164234	NA	NA
2613	HMDB0135504	NA	NA
2614	HMDB0135508	NA	NA
2615	HMDB0135506	NA	NA
2616	HMDB0031943	(Z)-N-[(4-hydroxyphenyl)methyl]ethoxycarbothioamide 4'-(tri-acetylramnoside)	HMDB0031943
2617	HMDB0133632	NA	NA
2618	HMDB0133629	NA	NA
2619	HMDB0133763	NA	NA
2620	HMDB0133762	NA	NA
2621	HMDB0135654	NA	NA
2622	HMDB0179487	NA	NA
2623	HMDB0179486	NA	NA
2624	HMDB0133631	NA	NA
2625	HMDB0133626	NA	NA
2626	HMDB0133623	NA	NA
2627	HMDB0133634	NA	NA
2628	HMDB0170798	NA	NA
2629	HMDB0170797	NA	NA
2630	HMDB0170793	NA	NA
2631	HMDB0170796	NA	NA
2632	HMDB0170791	NA	NA
2633	HMDB0170792	NA	NA
2634	HMDB0061034	NA	NA
2635	HMDB0033709	Desglucocoroloside	HMDB0033709
2636	HMDB0015110	Dipyridamole	HMDB0015110
2637	HMDB0010408	LysoPC(P-18:1(9Z))	HMDB0010408
2638	HMDB0010384	LysoPC(18:0)	HMDB0010384
2639	HMDB0011128	LysoPC(0:0/18:0)	HMDB0011128
2640	HMDB0062195	NA	NA
2641	HMDB0036884	NA	NA
2642	HMDB0181960	NA	NA
2643	HMDB0181959	NA	NA
2644	HMDB0181963	NA	NA
2645	HMDB0181976	NA	NA
2646	HMDB0181975	NA	NA
2647	HMDB0181971	NA	NA
2648	HMDB0181968	NA	NA
2649	HMDB0181967	NA	NA
2650	HMDB0181964	NA	NA
2651	HMDB0158842	NA	NA
2652	HMDB0173534	NA	NA
2653	HMDB0176106	NA	NA
2654	HMDB0173047	NA	NA
2655	HMDB0173001	NA	NA
2656	HMDB0176107	NA	NA
2657	HMDB0172559	NA	NA
2658	HMDB0172560	NA	NA
2659	HMDB0172557	NA	NA
2660	HMDB0172558	NA	NA
2661	HMDB0175792	NA	NA
2662	HMDB0184222	NA	NA
2663	HMDB0183715	NA	NA
2664	HMDB0034679	Cinn cassiol D2 glucoside	HMDB0034679
2665	HMDB0183713	NA	NA
2666	HMDB0183714	NA	NA
2667	HMDB0184220	NA	NA
2668	HMDB0240600	NA	NA
2669	HMDB0184758	NA	NA

2670	HMDB0184757	NA	NA
2671	HMDB0184774	NA	NA
2672	HMDB0184760	NA	NA
2673	HMDB0184759	NA	NA
2674	HMDB0184764	NA	NA
2675	HMDB0184765	NA	NA
2676	HMDB0184770	NA	NA
2677	HMDB0184789	NA	NA
2678	HMDB0184787	NA	NA
2679	HMDB0184784	NA	NA
2680	HMDB0184790	NA	NA
2681	HMDB0184781	NA	NA
2682	HMDB0184783	NA	NA
2683	HMDB0184777	NA	NA
2684	HMDB0184775	NA	NA
2685	HMDB0184776	NA	NA
2686	HMDB0184769	NA	NA
2687	HMDB0184768	NA	NA
2688	HMDB0184767	NA	NA
2689	HMDB0184788	NA	NA
2690	HMDB0184782	NA	NA
2691	HMDB0139969	NA	NA
2692	HMDB0139968	NA	NA
2693	HMDB0139967	NA	NA
2694	HMDB0139970	NA	NA
2695	HMDB0139971	NA	NA
2696	HMDB0139977	NA	NA
2697	HMDB0139976	NA	NA
2698	HMDB0139979	NA	NA
2699	HMDB0139984	NA	NA
2700	HMDB0139983	NA	NA
2701	HMDB0139985	NA	NA
2702	HMDB0139982	NA	NA
2703	HMDB0139980	NA	NA
2704	HMDB0139978	NA	NA
2705	HMDB0139981	NA	NA
2706	HMDB0143771	NA	NA
2707	HMDB0143774	NA	NA
2708	HMDB0143775	NA	NA
2709	HMDB0143791	NA	NA
2710	HMDB0143794	NA	NA
2711	HMDB0143795	NA	NA
2712	HMDB0164483	NA	NA
2713	HMDB0164482	NA	NA
2714	HMDB0164491	NA	NA
2715	HMDB0164495	NA	NA
2716	HMDB0164502	NA	NA
2717	HMDB0164506	NA	NA
2718	HMDB0164474	NA	NA
2719	HMDB0015101	Telmisartan	HMDB0015101
2720	HMDB0159631	NA	NA
2721	HMDB0159632	NA	NA
2722	HMDB0145353	NA	NA
2723	HMDB0034362	Desglucocheirotoxin	HMDB0034362
2724	HMDB0166971	NA	NA
2725	HMDB0166972	NA	NA
2726	HMDB0166970	NA	NA
2727	HMDB0173681	NA	NA
2728	HMDB0173690	NA	NA
2729	HMDB0173684	NA	NA
2730	HMDB0186464	NA	NA
2731	HMDB0177528	NA	NA
2732	HMDB0173682	NA	NA
2733	HMDB0173688	NA	NA
2734	HMDB0173686	NA	NA
2735	HMDB0240602	NA	NA
2736	HMDB0011490	LysoPE(0:0/22:0)	HMDB0011490
2737	HMDB0011520	LysoPE(22:0/0:0)	HMDB0011520
2738	HMDB0114757	NA	NA
2739	HMDB0165392	NA	NA
2740	HMDB0171540	NA	NA
2741	HMDB0015129	Neomycin	HMDB0015129
2742	HMDB0002160	Harderoporpyrinogen	HMDB0002160
2743	HMDB0039454	NA	NA
2744	HMDB0173693	NA	NA
2745	HMDB0173692	NA	NA
2746	HMDB0173699	NA	NA
2747	HMDB0173698	NA	NA
2748	HMDB0142988	NA	NA
2749	HMDB0142998	NA	NA
2750	HMDB0142997	NA	NA
2751	HMDB0143001	NA	NA
2752	HMDB0142987	NA	NA
2753	HMDB0142978	NA	NA
2754	HMDB0142977	NA	NA
2755	HMDB0142917	NA	NA
2756	HMDB0142918	NA	NA

2757	HMDB0142919	NA	NA
2758	HMDB0142921	NA	NA
2759	HMDB0142920	NA	NA
2760	HMDB0142926	NA	NA
2761	HMDB0142929	NA	NA
2762	HMDB0142928	NA	NA
2763	HMDB0142927	NA	NA
2764	HMDB0143002	NA	NA
2765	HMDB0143007	NA	NA
2766	HMDB0143006	NA	NA
2767	HMDB0143108	NA	NA
2768	HMDB0143104	NA	NA
2769	HMDB0143098	NA	NA
2770	HMDB0143093	NA	NA
2771	HMDB0143086	NA	NA
2772	HMDB0143085	NA	NA
2773	HMDB0143076	NA	NA
2774	HMDB0143075	NA	NA
2775	HMDB0143066	NA	NA
2776	HMDB0143065	NA	NA
2777	HMDB0143061	NA	NA
2778	HMDB0143060	NA	NA
2779	HMDB0143022	NA	NA
2780	HMDB0143012	NA	NA
2781	HMDB0143011	NA	NA
2782	HMDB0143021	NA	NA
2783	HMDB0142916	NA	NA
2784	HMDB0142915	NA	NA
2785	HMDB0142901	NA	NA
2786	HMDB0142899	NA	NA
2787	HMDB0142902	NA	NA
2788	HMDB0142900	NA	NA
2789	HMDB0142905	NA	NA
2790	HMDB0142904	NA	NA
2791	HMDB0142903	NA	NA
2792	HMDB0142908	NA	NA
2793	HMDB0142911	NA	NA
2794	HMDB0142913	NA	NA
2795	HMDB0142914	NA	NA
2796	HMDB0142912	NA	NA
2797	HMDB0142930	NA	NA
2798	HMDB0165936	NA	NA
2799	HMDB0165918	NA	NA
2800	HMDB0173230	NA	NA
2801	HMDB0173229	NA	NA
2802	HMDB0165966	NA	NA
2803	HMDB0164809	NA	NA
2804	HMDB0034433	Riboflavine 2',3',4',5'-tetrabutanoate	HMDB0034433
2805	HMDB0157944	NA	NA
2806	HMDB0157945	NA	NA
2807	HMDB0157949	NA	NA
2808	HMDB0157950	NA	NA
2809	HMDB0157951	NA	NA
2810	HMDB0157955	NA	NA
2811	HMDB0157956	NA	NA
2812	HMDB0157943	NA	NA
2813	HMDB0157938	NA	NA
2814	HMDB0157939	NA	NA
2815	HMDB0157937	NA	NA
2816	HMDB0157933	NA	NA
2817	HMDB0157932	NA	NA
2818	HMDB0157931	NA	NA
2819	HMDB0157898	NA	NA
2820	HMDB0157896	NA	NA
2821	HMDB0157957	NA	NA
2822	HMDB0158932	NA	NA
2823	HMDB0158968	NA	NA
2824	HMDB0158964	NA	NA
2825	HMDB0158963	NA	NA
2826	HMDB0158958	NA	NA
2827	HMDB0158959	NA	NA
2828	HMDB0158953	NA	NA
2829	HMDB0158954	NA	NA
2830	HMDB0158949	NA	NA
2831	HMDB0158948	NA	NA
2832	HMDB0158944	NA	NA
2833	HMDB0158943	NA	NA
2834	HMDB0158937	NA	NA
2835	HMDB0158938	NA	NA
2836	HMDB0158939	NA	NA
2837	HMDB0158933	NA	NA
2838	HMDB0158969	NA	NA
2839	HMDB0157897	NA	NA
2840	HMDB0157050	NA	NA
2841	HMDB0157221	NA	NA
2842	HMDB0157842	NA	NA
2843	HMDB0157841	NA	NA

2844	HMDB0157843	NA	NA
2845	HMDB0157847	NA	NA
2846	HMDB0157846	NA	NA
2847	HMDB0157851	NA	NA
2848	HMDB0157848	NA	NA
2849	HMDB0157853	NA	NA
2850	HMDB0157215	NA	NA
2851	HMDB0157218	NA	NA
2852	HMDB0157212	NA	NA
2853	HMDB0157051	NA	NA
2854	HMDB0157054	NA	NA
2855	HMDB0157057	NA	NA
2856	HMDB0157060	NA	NA
2857	HMDB0157066	NA	NA
2858	HMDB0157063	NA	NA
2859	HMDB0157206	NA	NA
2860	HMDB0157205	NA	NA
2861	HMDB0157209	NA	NA
2862	HMDB0157852	NA	NA
2863	HMDB0157856	NA	NA
2864	HMDB0157857	NA	NA
2865	HMDB0157876	NA	NA
2866	HMDB0157881	NA	NA
2867	HMDB0157882	NA	NA
2868	HMDB0157883	NA	NA
2869	HMDB0157886	NA	NA
2870	HMDB0157887	NA	NA
2871	HMDB0157888	NA	NA
2872	HMDB0157891	NA	NA
2873	HMDB0157892	NA	NA
2874	HMDB0157893	NA	NA
2875	HMDB0157878	NA	NA
2876	HMDB0157877	NA	NA
2877	HMDB0157858	NA	NA
2878	HMDB0157861	NA	NA
2879	HMDB0157862	NA	NA
2880	HMDB0157863	NA	NA
2881	HMDB0157866	NA	NA
2882	HMDB0157867	NA	NA
2883	HMDB0157868	NA	NA
2884	HMDB0157871	NA	NA
2885	HMDB0157873	NA	NA
2886	HMDB0157872	NA	NA
2887	HMDB0038619	NA	NA
2888	HMDB0010698	CerP(d18:0/16:0)	HMDB0010698
2889	HMDB0165986	NA	NA
2890	HMDB0165987	NA	NA
2891	HMDB0166012	NA	NA
2892	HMDB0166013	NA	NA
2893	HMDB0166011	NA	NA
2894	HMDB0166007	NA	NA
2895	HMDB0170721	NA	NA
2896	HMDB0166009	NA	NA
2897	HMDB0166010	NA	NA
2898	HMDB0166004	NA	NA
2899	HMDB0166005	NA	NA
2900	HMDB0166003	NA	NA
2901	HMDB0166006	NA	NA
2902	HMDB0167988	NA	NA
2903	HMDB0167989	NA	NA
2904	HMDB0168064	NA	NA
2905	HMDB0170719	NA	NA
2906	HMDB0170718	NA	NA
2907	HMDB0168079	NA	NA
2908	HMDB0168080	NA	NA
2909	HMDB0168077	NA	NA
2910	HMDB0168076	NA	NA
2911	HMDB0168068	NA	NA
2912	HMDB0168067	NA	NA
2913	HMDB0168065	NA	NA
2914	HMDB0166001	NA	NA
2915	HMDB0166002	NA	NA
2916	HMDB0170734	NA	NA
2917	HMDB0165975	NA	NA
2918	HMDB0165973	NA	NA
2919	HMDB0165879	NA	NA
2920	HMDB0165880	NA	NA
2921	HMDB0170735	NA	NA
2922	HMDB0170737	NA	NA
2923	HMDB0166008	NA	NA
2924	HMDB0165977	NA	NA
2925	HMDB0165978	NA	NA
2926	HMDB0165999	NA	NA
2927	HMDB0165985	NA	NA
2928	HMDB0165984	NA	NA
2929	HMDB0165976	NA	NA
2930	HMDB0165983	NA	NA

2931	HMDB0165980	NA	NA
2932	HMDB0165981	NA	NA
2933	HMDB0165982	NA	NA
2934	HMDB0165979	NA	NA
2935	HMDB0177535	NA	NA
2936	HMDB0177543	NA	NA
2937	HMDB0177537	NA	NA
2938	HMDB0177545	NA	NA
2939	HMDB0177544	NA	NA
2940	HMDB0177546	NA	NA
2941	HMDB0177536	NA	NA
2942	HMDB0166014	NA	NA
2943	HMDB0165988	NA	NA
2944	HMDB0184229	NA	NA
2945	HMDB0186286	NA	NA
2946	HMDB0033242	Glycylserylprolylmethionylphenylalanylvalinamide	HMDB0033242
2947	HMDB0143644	NA	NA
2948	HMDB0041431	NA	NA
2949	HMDB0175661	NA	NA
2950	HMDB0175651	NA	NA
2951	HMDB0175656	NA	NA
2952	HMDB0175652	NA	NA
2953	HMDB0175662	NA	NA
2954	HMDB0175657	NA	NA
2955	HMDB0186380	NA	NA
2956	HMDB0186379	NA	NA
2957	HMDB0186374	NA	NA
2958	HMDB0186377	NA	NA
2959	HMDB0186373	NA	NA
2960	HMDB0186376	NA	NA
2961	HMDB0164570	NA	NA
2962	HMDB0168018	NA	NA
2963	HMDB0168019	NA	NA
2964	HMDB0168020	NA	NA
2965	HMDB0168021	NA	NA
2966	HMDB0168022	NA	NA
2967	HMDB0165927	NA	NA
2968	HMDB0168015	NA	NA
2969	HMDB0165929	NA	NA
2970	HMDB0165932	NA	NA
2971	HMDB0165933	NA	NA
2972	HMDB0165931	NA	NA
2973	HMDB0165934	NA	NA
2974	HMDB0165935	NA	NA
2975	HMDB0168012	NA	NA
2976	HMDB0168014	NA	NA
2977	HMDB0168016	NA	NA
2978	HMDB0168017	NA	NA
2979	HMDB0168025	NA	NA
2980	HMDB0168023	NA	NA
2981	HMDB0168044	NA	NA
2982	HMDB0168045	NA	NA
2983	HMDB0168042	NA	NA
2984	HMDB0168041	NA	NA
2985	HMDB0168039	NA	NA
2986	HMDB0168038	NA	NA
2987	HMDB0168040	NA	NA
2988	HMDB0168036	NA	NA
2989	HMDB0168034	NA	NA
2990	HMDB0168035	NA	NA
2991	HMDB0168037	NA	NA
2992	HMDB0168032	NA	NA
2993	HMDB0168030	NA	NA
2994	HMDB0168027	NA	NA
2995	HMDB0168026	NA	NA
2996	HMDB0168024	NA	NA
2997	HMDB0168033	NA	NA
2998	HMDB0165928	NA	NA
2999	HMDB0165913	NA	NA
3000	HMDB0165911	NA	NA
3001	HMDB0165908	NA	NA
3002	HMDB0165909	NA	NA
3003	HMDB0165910	NA	NA
3004	HMDB0165907	NA	NA
3005	HMDB0165906	NA	NA
3006	HMDB0165904	NA	NA
3007	HMDB0165914	NA	NA
3008	HMDB0165912	NA	NA
3009	HMDB0165930	NA	NA
3010	HMDB0165925	NA	NA
3011	HMDB0165926	NA	NA
3012	HMDB0165924	NA	NA
3013	HMDB0165922	NA	NA
3014	HMDB0165917	NA	NA
3015	HMDB0165915	NA	NA
3016	HMDB0165916	NA	NA
3017	HMDB0168043	NA	NA

3018	HMDB0187178	NA	NA
3019	HMDB0187175	NA	NA
3020	HMDB0187177	NA	NA
3021	HMDB0187174	NA	NA
3022	HMDB0178542	NA	NA
3023	HMDB0178548	NA	NA
3024	HMDB0178550	NA	NA
3025	HMDB0178541	NA	NA
3026	HMDB0178540	NA	NA
3027	HMDB0178549	NA	NA
3028	HMDB0036529	NA	NA
3029	HMDB0036528	NA	NA
3030	HMDB0112956	NA	NA
3031	HMDB0112955	NA	NA
3032	HMDB0112957	NA	NA
3033	HMDB0113920	NA	NA
3034	HMDB0113309	NA	NA
3035	HMDB0114067	NA	NA
3036	HMDB0112984	NA	NA
3037	HMDB0113337	NA	NA
3038	HMDB0113167	NA	NA
3039	HMDB0113141	NA	NA
3040	HMDB0113114	NA	NA
3041	HMDB0113042	NA	NA
3042	HMDB0008901	PE(15:0/20:2(11Z,14Z))	HMDB0008901
3043	HMDB0009285	PE(20:2(11Z,14Z)/15:0)	HMDB0009285
3044	HMDB0008130	PC(18:2(9Z,12Z)/14:0)	HMDB0008130
3045	HMDB0007874	PC(14:0/18:2(9Z,12Z))	HMDB0007874
3046	HMDB0008098	PC(18:1(9Z)/14:1(9Z))	HMDB0008098
3047	HMDB0008002	PC(16:1(9Z)/16:1(9Z))	HMDB0008002
3048	HMDB0007906	PC(14:1(9Z)/18:1(9Z))	HMDB0007906
3049	HMDB0007905	PC(14:1(9Z)/18:1(11Z))	HMDB0007905
3050	HMDB0008065	PC(18:1(11Z)/14:1(9Z))	HMDB0008065
3051	HMDB0008460	PC(20:4(8Z,11Z,14Z,17Z)/14:1(9Z))	HMDB0008460
3052	HMDB0007885	PC(14:0/20:5(5Z,8Z,11Z,14Z,17Z))	HMDB0007885
3053	HMDB0007917	PC(14:1(9Z)/20:4(8Z,11Z,14Z,17Z))	HMDB0007917
3054	HMDB0007916	PC(14:1(9Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0007916
3055	HMDB0008233	PC(18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	HMDB0008233
3056	HMDB0008427	PC(20:4(5Z,8Z,11Z,14Z)/14:1(9Z))	HMDB0008427
3057	HMDB0008492	PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:0)	HMDB0008492
3058	HMDB0008911	PE(15:0/22:5(4Z,7Z,10Z,13Z,16Z))	HMDB0008911
3059	HMDB0008912	PE(15:0/22:5(7Z,10Z,13Z,16Z,19Z))	HMDB0008912
3060	HMDB0009615	PE(22:5(4Z,7Z,10Z,13Z,16Z)/15:0)	HMDB0009615
3061	HMDB0009648	PE(22:5(7Z,10Z,13Z,16Z,19Z)/15:0)	HMDB0009648
3062	HMDB0008009	PC(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	HMDB0008009
3063	HMDB0113482	NA	NA
3064	HMDB0113173	NA	NA
3065	HMDB0116726	NA	NA
3066	HMDB0113229	NA	NA
3067	HMDB0113256	NA	NA
3068	HMDB0113257	NA	NA
3069	HMDB0113426	NA	NA
3070	HMDB0113454	NA	NA
3071	HMDB0113174	NA	NA
3072	HMDB0113146	NA	NA
3073	HMDB0113119	NA	NA
3074	HMDB0112994	NA	NA
3075	HMDB0112995	NA	NA
3076	HMDB0113012	NA	NA
3077	HMDB0113051	NA	NA
3078	HMDB0113072	NA	NA
3079	HMDB0113073	NA	NA
3080	HMDB0113593	NA	NA
3081	HMDB0113620	NA	NA
3082	HMDB0114383	NA	NA
3083	HMDB0113646	NA	NA
3084	HMDB0113930	NA	NA
3085	HMDB0041467	NA	NA
3086	HMDB0115979	NA	NA
3087	HMDB0006975	CDP-DG(16:0/22:3(10Z,13Z,16Z))	HMDB0006975
3088	HMDB0145559	NA	NA
3089	HMDB0145553	NA	NA
3090	HMDB0145556	NA	NA
3091	HMDB0145554	NA	NA
3092	HMDB0145560	NA	NA
3093	HMDB0145576	NA	NA
3094	HMDB0145569	NA	NA
3095	HMDB0145561	NA	NA
3096	HMDB0145562	NA	NA
3097	HMDB0145563	NA	NA
3098	HMDB0145558	NA	NA
3099	HMDB0145557	NA	NA
3100	HMDB0145555	NA	NA
3101	HMDB0055799	NA	NA
3102	HMDB0010560	TG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0010560

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

5 Selection of Metabolite Set Library

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

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

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

6 Enrichment Analysis

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

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

Enrichment Overview (top 25)

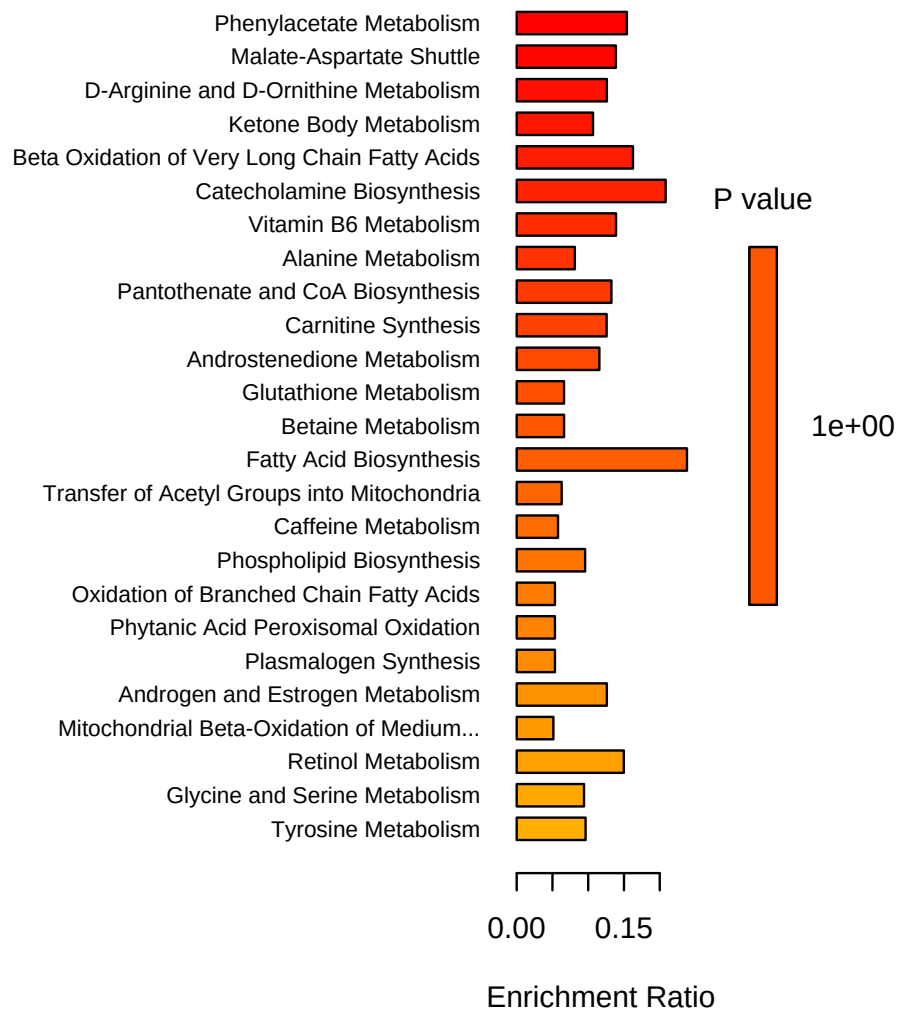


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Phenylacetate Metabolism	9	6.49	1	1.00E+00	1.00E+00	1.00E+00
Malate-Aspartate Shuttle	10	7.21	1	1.00E+00	1.00E+00	1.00E+00
D-Arginine and D-Ornithine Metabolism	11	7.93	1	1.00E+00	1.00E+00	1.00E+00
Ketone Body Metabolism	13	9.37	1	1.00E+00	1.00E+00	1.00E+00
Beta Oxidation of Very Long Chain Fatty Acids	17	12.30	2	1.00E+00	1.00E+00	1.00E+00
Catecholamine Biosynthesis	20	14.40	3	1.00E+00	1.00E+00	1.00E+00
Vitamin B6 Metabolism	20	14.40	2	1.00E+00	1.00E+00	1.00E+00
Alanine Metabolism	17	12.30	1	1.00E+00	1.00E+00	1.00E+00
Pantothenate and CoA Biosynthesis	21	15.10	2	1.00E+00	1.00E+00	1.00E+00
Carnitine Synthesis	22	15.90	2	1.00E+00	1.00E+00	1.00E+00
Androstenedione Metabolism	24	17.30	2	1.00E+00	1.00E+00	1.00E+00
Glutathione Metabolism	21	15.10	1	1.00E+00	1.00E+00	1.00E+00
Betaine Metabolism	21	15.10	1	1.00E+00	1.00E+00	1.00E+00
Fatty Acid Biosynthesis	35	25.20	6	1.00E+00	1.00E+00	1.00E+00
Transfer of Acetyl Groups into Mitochondria	22	15.90	1	1.00E+00	1.00E+00	1.00E+00
Caffeine Metabolism	24	17.30	1	1.00E+00	1.00E+00	1.00E+00
Phospholipid Biosynthesis	29	20.90	2	1.00E+00	1.00E+00	1.00E+00
Oxidation of Branched Chain Fatty Acids	26	18.70	1	1.00E+00	1.00E+00	1.00E+00
Phytanic Acid Peroxisomal Oxidation	26	18.70	1	1.00E+00	1.00E+00	1.00E+00
Plasmalogen Synthesis	26	18.70	1	1.00E+00	1.00E+00	1.00E+00
Androgen and Estrogen Metabolism	33	23.80	3	1.00E+00	1.00E+00	1.00E+00
Mitochondrial Beta-Oxidation of Medium Chain Saturated Fatty Acids	27	19.50	1	1.00E+00	1.00E+00	1.00E+00
Retinol Metabolism	37	26.70	4	1.00E+00	1.00E+00	1.00E+00
Glycine and Serine Metabolism	59	42.50	4	1.00E+00	1.00E+00	1.00E+00
Tyrosine Metabolism	72	51.90	5	1.00E+00	1.00E+00	1.00E+00
Beta-Alanine Metabolism	34	24.50	1	1.00E+00	1.00E+00	1.00E+00
Ammonia Recycling	32	23.10	1	1.00E+00	1.00E+00	1.00E+00
Propanoate Metabolism	42	30.30	1	1.00E+00	1.00E+00	1.00E+00
Arginine and Proline Metabolism	53	38.20	3	1.00E+00	1.00E+00	1.00E+00
Porphyrin Metabolism	40	28.80	2	1.00E+00	1.00E+00	1.00E+00
Valine, Leucine and Isoleucine Degradation	60	43.20	3	1.00E+00	1.00E+00	1.00E+00
Methionine Metabolism	43	31.00	2	1.00E+00	1.00E+00	1.00E+00
Bile Acid Biosynthesis	65	46.80	9	1.00E+00	1.00E+00	1.00E+00
Histidine Metabolism	43	31.00	1	1.00E+00	1.00E+00	1.00E+00
Pyrimidine Metabolism	59	42.50	5	1.00E+00	1.00E+00	1.00E+00
Nicotinate and Nicotinamide Metabolism	37	26.70	1	1.00E+00	1.00E+00	1.00E+00
Purine Metabolism	74	53.30	4	1.00E+00	1.00E+00	1.00E+00
Fatty Acid Elongation In Mitochondria	35	25.20	1	1.00E+00	1.00E+00	1.00E+00
Citric Acid Cycle	32	23.10	1	1.00E+00	1.00E+00	1.00E+00
Starch and Sucrose Metabolism	31	22.30	1	1.00E+00	1.00E+00	1.00E+00
Pyruvate Metabolism	48	34.60	1	1.00E+00	1.00E+00	1.00E+00
Tryptophan Metabolism	60	43.20	6	1.00E+00	1.00E+00	1.00E+00
Glutamate Metabolism	49	35.30	2	1.00E+00	1.00E+00	1.00E+00
Arachidonic Acid Metabolism	69	49.70	1	1.00E+00	1.00E+00	1.00E+00
Gluconeogenesis	35	25.20	1	1.00E+00	1.00E+00	1.00E+00
Steroidogenesis	43	31.00	5	1.00E+00	1.00E+00	1.00E+00
Warburg Effect	58	41.80	1	1.00E+00	1.00E+00	1.00E+00

7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "compd.vec<-c(\"HMDB0000123\", \"HMDB0014691\", \"HMDB0031239\", \"HMDB0161401\", \"HMDB0001858\", \"HMDB0001858\")"
```

```
[3] "mSet<-Setup.MapData(mSet, compd.vec);"
[4] "mSet<-CrossReferencing(mSet, \"hmdb\");"
[5] "mSet<-CreateMappingResultTable(mSet)"
[6] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[7] "mSet<-SetMetabolomeFilter(mSet, F);"
[8] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[9] "mSet<-PlotPathSummary(mSet, F, \"path_view_0\", \"png\", 72, width=NA)"
[10] "mSet<-PlotKEGGPath(mSet, \"Linoleic acid metabolism\", 528, 480, \"png\", NULL)"
[11] "mSet<-RenderMetPAGraph(mSet, \"zoom1621883876437.png\", 528.0, 480.0, 100.0)"
[12] "mSet<-PlotKEGGPath(mSet, \"Linoleic acid metabolism\", 528, 480, \"png\", NULL)"
[13] "mSet<-SaveTransformedData(mSet)"
[14] "UpdateDataObjects(\"conc\", \"msetora\", FALSE)"
[15] "mSet<-SetMetabolomeFilter(mSet, F);"
[16] "mSet<-SetCurrentMsetLib(mSet, \"smpdb_pathway\", 2);"
[17] "mSet<-CalculateHyperScore(mSet)"
[18] "mSet<-PlotORA(mSet, \"ora_0\", \"net\", \"png\", 72, width=NA)"
[19] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_0\", \"png\", 72, width=NA)"
[20] "mSet<-CalculateHyperScore(mSet)"
[21] "mSet<-PlotORA(mSet, \"ora_1\", \"net\", \"png\", 72, width=NA)"
[22] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_1\", \"png\", 72, width=NA)"
[23] "mSet<-SaveTransformedData(mSet)"
[24] "mSet<-PreparePDFReport(mSet, \"guest16073378008230990507\")\\n"
```

The report was generated on Mon May 24 15:18:36 2021 with R version 4.0.2 (2020-06-22).