

# Metabolomic Data Analysis with MetaboAnalyst 5.0

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## 1 Background

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

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

## 2 MSEA Overview

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

## 3 Data Input

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

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

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

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

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

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

## 4 Data Process

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

	Query	Match
1	HMDB0000123	Glycine
2	HMDB0014691	Acetohydroxamic Acid
3	HMDB0031239	Ethyl nitrite
4	HMDB0161401	NA
5	HMDB0000925	Trimethylamine N-oxide
6	HMDB0142449	NA
7	HMDB0140038	NA
8	HMDB0012136	1-Amino-propan-2-ol
9	HMDB0062143	NA
10	HMDB0031558	Methyloxirane
11	HMDB0031652	Allyl alcohol
12	HMDB0003366	Propanal
13	HMDB0001659	Acetone
14	HMDB0031404	Cyclohexylamine
15	HMDB0032416	2-Methylpiperidine
16	HMDB0031544	3-Methylcyclopentene
17	HMDB0062716	NA
18	HMDB0033971	2-Diethylaminoethanol
19	HMDB0000630	Cytosine
20	HMDB0031335	2-Chloro-1-propanol
21	HMDB0011601	3-Methylcytosine
22	HMDB0004339	2-O-Methylcytosine
23	HMDB0002894	5-Methylcytosine
24	HMDB0128943	NA
25	HMDB0132477	NA
26	HMDB0129097	NA
27	HMDB0168839	NA
28	HMDB0128916	NA
29	HMDB0012233	Glutarate semialdehyde
30	HMDB0029172	3-keto-2-Methylbutyrate
31	HMDB0001865	2-Oxovaleric acid
32	HMDB0000310	Methylacetoacetic acid
33	HMDB0031643	Ethyl pyruvate
34	HMDB0000019	Alpha-ketoisovaleric acid
35	HMDB0003771	2-Methylacetoacetic acid
36	HMDB0000720	Levulinic acid
37	HMDB0034466	Acetoxyacetone
38	HMDB0128917	NA
39	HMDB0129096	NA
40	HMDB0129098	NA
41	HMDB0168838	NA
42	HMDB0177210	NA
43	HMDB0169666	NA
44	HMDB0177209	NA
45	HMDB0171727	NA
46	HMDB0032356	N-Lactoyl ethanolamine
47	HMDB0039499	NA
48	HMDB0031658	L-2-Amino-5-hydroxypentanoic acid
49	HMDB0039790	NA
50	HMDB0038974	NA
51	HMDB0039789	NA
52	HMDB0000786	Oxypurinol
53	HMDB0000292	Xanthine
54	HMDB0001182	6,8-Dihydroxypurine
55	HMDB0000744	Malic acid
56	HMDB0031518	D-Malic acid
57	HMDB0000156	L-Malic acid
58	HMDB0032872	Velcorin
59	HMDB0061971	NA

60	HMDB0166738	NA
61	HMDB0164724	NA
62	HMDB0165094	NA
63	HMDB0165096	NA
64	HMDB0165095	NA
65	HMDB0165097	NA
66	HMDB0166737	NA
67	HMDB0031484	2-Heptenoic acid
68	HMDB0038962	NA
69	HMDB0031500	Methyl 2E-hexenoate
70	HMDB0166739	NA
71	HMDB0029314	Isopentenyl acetate
72	HMDB0031477	3,4-Heptanedione
73	HMDB0031476	2,3-Heptanedione
74	HMDB0031504	Methyl (Z)-3-hexenoate
75	HMDB0031603	Ethyl 4-pentenoate
76	HMDB0040214	NA
77	HMDB0031342	Cyclohexanecarboxylic acid
78	HMDB0038271	NA
79	HMDB0031174	4-Methyl-5-hexanolide
80	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone
81	HMDB0033793	4-Heptenoic acid
82	HMDB0031593	5-Methyl-2,3-hexanedione
83	HMDB0039819	NA
84	HMDB0166736	NA
85	HMDB0173760	NA
86	HMDB0173761	NA
87	HMDB0173762	NA
88	HMDB0173763	NA
89	HMDB0180322	NA
90	HMDB0180323	NA
91	HMDB0029165	1,3-Diacetylpropane
92	HMDB0031351	Cyclohexyl formate
93	HMDB0032460	4-Pentenyl acetate
94	HMDB0032391	3-Methyl-3-butenyl acetate
95	HMDB0030330	1-Methoxy-3-methylene-2-pentanone
96	HMDB0059876	NA
97	HMDB0040591	NA
98	HMDB0145113	NA
99	HMDB0145114	NA
100	HMDB0145115	NA
101	HMDB0145125	NA
102	HMDB0145116	NA
103	HMDB0094649	2-Amino-heptanoic acid
104	HMDB0001161	4-Trimethylammonibutanoic acid
105	HMDB0006831	3-Dehydroxycarnitine
106	HMDB0000895	Acetylcholine
107	HMDB0013811	1-Nitroheptane
108	HMDB0041477	NA
109	HMDB0031660	Dibutyl sulfide
110	HMDB0168717	NA
111	HMDB0168715	NA
112	HMDB0168716	NA
113	HMDB0168718	NA
114	HMDB0062061	NA
115	HMDB0030302	2,3,4-Trimethylhexane
116	HMDB0029595	Nonane
117	HMDB0030301	2,2,3,4-Tetramethylpentane
118	HMDB0031556	Isononane
119	HMDB0031416	3,4-Dimethylheptane
120	HMDB0062017	NA
121	HMDB0062013	NA
122	HMDB0240251	NA
123	HMDB0061880	NA
124	HMDB0059659	Trans-3-hydroxy-L-proline
125	HMDB0002113	3-Hydroxy-L-proline
126	HMDB0000783	Propionylglycine
127	HMDB0000766	N-Acetyl-L-alanine
128	HMDB0000725	4-Hydroxyproline
129	HMDB0036576	NA
130	HMDB0001149	5-Aminolevulinic acid
131	HMDB0002104	L-Glutamic gamma-semialdehyde
132	HMDB0006055	4-Hydroxy-L-proline
133	HMDB0060460	cis-4-Hydroxy-D-proline
134	HMDB0006272	5-Amino-2-oxopentanoic acid
135	HMDB0177404	NA
136	HMDB0014389	Mesalazine
137	HMDB0164041	NA
138	HMDB0059749	NA
139	HMDB0001972	3-Aminosalicylic acid
140	HMDB0014378	Aminosalicylic Acid
141	HMDB0001476	3-Hydroxyanthranilic acid
142	HMDB0059811	NA
143	HMDB0012289	Tetrahydrodipicolinate
144	HMDB0001280	2-Aminomuconic acid semialdehyde
145	HMDB0031670	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione
146	HMDB0028696	Alanyl-Serine

147	HMDB0029032	Serylalanine
148	HMDB0145395	NA
149	HMDB0029061	Threoninyl-Glycine
150	HMDB0028851	Glycyl-Threonine
151	HMDB0169117	NA
152	HMDB0125105	NA
153	HMDB0038987	NA
154	HMDB0032029	2-Isopropylphenol
155	HMDB0032149	1-Methoxy-2,4-dimethylbenzene
156	HMDB0032625	4-Propylphenol
157	HMDB0029667	2,3,6-Trimethylphenol
158	HMDB0039782	NA
159	HMDB0038986	NA
160	HMDB0032624	2-Propylphenol
161	HMDB0038988	NA
162	HMDB0032621	(2-Methoxyethyl)benzene
163	HMDB0038985	NA
164	HMDB0031312	Benzyl ethyl ether
165	HMDB0033962	3-Phenyl-1-propanol
166	HMDB0031627	1-Phenyl-1-propanol
167	HMDB0034378	( $\Delta^5$ )-1-(4-Methylphenyl)ethanol
168	HMDB0031628	2-Phenyl-1-propanol
169	HMDB0038984	NA
170	HMDB0032544	2,4,6-Trimethylphenol
171	HMDB0031446	p-Isopropylphenol
172	HMDB0032441	Nona-2,4,6-trienal
173	HMDB0059896	NA
174	HMDB0169118	NA
175	HMDB0163316	NA
176	HMDB0163318	NA
177	HMDB0163317	NA
178	HMDB0163315	NA
179	HMDB0163319	NA
180	HMDB0062166	NA
181	HMDB0032164	Allyl valerate
182	HMDB0037624	NA
183	HMDB0029761	Ethyl ( $\Delta^5$ )-2-methyl-4-pentenoate
184	HMDB0031403	Cyclohexaneacetic acid
185	HMDB0035422	4-Butyl-gamma-butyrolactone
186	HMDB0031352	Cyclohexyl acetate
187	HMDB0031343	Methyl cyclohexanecarboxylate
188	HMDB0036212	NA
189	HMDB0032533	trans-3-Hexenyl acetate
190	HMDB0240301	NA
191	HMDB0032266	Ethyl (E)-3-hexenoate
192	HMDB0036236	NA
193	HMDB0032268	Ethyl 2E-hexenoate
194	HMDB0000392	2-Octenoic acid
195	HMDB0001568	trans-2-Octenoic acid
196	HMDB0038036	NA
197	HMDB0039793	NA
198	HMDB0037630	NA
199	HMDB0038310	NA
200	HMDB0039872	NA
201	HMDB0037622	NA
202	HMDB0040215	cis-3-Hexenyl acetate
203	HMDB0040212	NA
204	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate
205	HMDB0031293	2,3-Octanedione
206	HMDB0013904	(3E)-2-Propylpent-3-enoic acid
207	HMDB0059908	NA
208	HMDB0013902	2-ene-Valproic acid
209	HMDB0013897	4-ene-Valproic acid
210	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid
211	HMDB0061342	NA
212	HMDB0032267	Ethyl 5-hexenoate
213	HMDB0032207	cis-5-Octenoic acid
214	HMDB0062077	NA
215	HMDB0240571	NA
216	HMDB0000991	DL-2-Aminooctanoic acid
217	HMDB0240732	NA
218	HMDB0014375	Pregabalin
219	HMDB0013305	Propionylcholine
220	HMDB0015654	Methacholine
221	HMDB0000232	Quinolinic acid
222	HMDB0033161	2,6-Pyridinedicarboxylic acid
223	HMDB0185628	NA
224	HMDB0001330	2-Amino-3-carboxymuconic acid semialdehyde
225	HMDB0062578	NA
226	HMDB0060260	NA
227	HMDB0001552	2-Keto-glutaramic acid
228	HMDB0000289	Uric acid
229	HMDB0037881	NA
230	HMDB0037878	NA
231	HMDB0037880	NA
232	HMDB0037872	NA
233	HMDB0037857	NA

234	HMDB0037862	NA
235	HMDB0037882	NA
236	HMDB0037875	NA
237	HMDB0037856	NA
238	HMDB0037879	NA
239	HMDB0037874	NA
240	HMDB0037876	NA
241	HMDB0037873	NA
242	HMDB0034580	psi-Pelletierine
243	HMDB0000904	Citrulline
244	HMDB0003148	Argininic acid
245	HMDB0060303	(2-Naphthyl)methanol
246	HMDB0060322	1-Hydroxymethylnaphthalene
247	HMDB0061285	NA
248	HMDB0032861	2-Methoxynaphthalene
249	HMDB0162075	NA
250	HMDB0162077	NA
251	HMDB0162076	NA
252	HMDB0162073	NA
253	HMDB0012484	(R)-1,2-dimethyl-5,6-dihydroxy-tetrahydroisoquinoline
254	HMDB0012469	(-)-Salsoline
255	HMDB0035072	2-Methylpropyl 2-aminobenzoate
256	HMDB0037698	NA
257	HMDB0036906	NA
258	HMDB0031797	2-Isopropylphenyl methylcarbamate
259	HMDB0003892	(S)-N-Methylsalsolinol
260	HMDB0003626	(R)-N-Methylsalsolinol
261	HMDB0000462	Allantoin
262	HMDB0170210	NA
263	HMDB0170209	NA
264	HMDB0038896	NA
265	HMDB0033556	2,5-Dimethyl-1,4-dithiane-2,5-diol
266	HMDB0013858	3-Dechloroethylfosfamide
267	HMDB0060881	NA
268	HMDB0013859	2-Dechloroethylfosfamide
269	HMDB0037786	NA
270	HMDB0014480	Nitrofurazone
271	HMDB0029416	L-Targinine
272	HMDB0000670	Homo-L-arginine
273	HMDB0015454	Rasagiline
274	HMDB0032926	Polycartine B
275	HMDB0005973	Dimethyltryptamine
276	HMDB0033961	2-(3-Methylbutyl)-1H-pyrrolo[2,3-b]pyridine
277	HMDB0169421	NA
278	HMDB0163468	NA
279	HMDB0163469	NA
280	HMDB0179168	NA
281	HMDB0163465	NA
282	HMDB0163466	NA
283	HMDB0094711	NA
284	HMDB0059936	NA
285	HMDB0062081	NA
286	HMDB0060287	NA
287	HMDB0059937	NA
288	HMDB0036396	NA
289	HMDB0040165	NA
290	HMDB0036188	NA
291	HMDB0036213	NA
292	HMDB0040203	NA
293	HMDB0040202	NA
294	HMDB0163470	NA
295	HMDB0031016	10-Undecen-1-ol
296	HMDB0032371	1-Menthyl methyl ether
297	HMDB0030943	6-Undecanone
298	HMDB0032379	trans- and cis-1-Methoxy-1-decene
299	HMDB0163244	NA
300	HMDB0030941	Undecanal
301	HMDB0031065	(Ás)-(E)-3-Methyl-4-decen-1-ol
302	HMDB0031064	(Z)-3-Methyl-3-decen-1-ol
303	HMDB0033713	2-Undecanone
304	HMDB0034856	2-Undecen-1-ol
305	HMDB0014631	Altretamine
306	HMDB0041615	NA
307	HMDB0035753	(R)-(E)-4,7-Megastigmadien-9-one
308	HMDB0034959	Egulan I
309	HMDB0036818	NA
310	HMDB0036144	NA
311	HMDB0151804	NA
312	HMDB0034979	gamma-Ionone
313	HMDB0029822	2,5-Diisopropyl-3-methylphenol
314	HMDB0029824	2,4-Diisopropyl-3-methylphenol
315	HMDB0032541	4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one
316	HMDB0029821	2,5-Diisopropyl-4-methylphenol
317	HMDB0036565	NA
318	HMDB0033545	(2E,4Z,7Z)-2,4,7-Tridecatrienal
319	HMDB0035682	delta-Damascone
320	HMDB0034671	(E)-5,8-Megastigmadien-4-one

321	HMDB0036027	alpha-Damascone
322	HMDB0037139	NA
323	HMDB0032498	Pseudoionone
324	HMDB0036022	Isospirene
325	HMDB0031733	4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde
326	HMDB0029823	2,4-Diisopropyl-5-methylphenol
327	HMDB0036684	NA
328	HMDB0029825	2,3-Diisopropyl-5-methylphenol
329	HMDB0059883	NA
330	HMDB0029820	2,6-Diisopropyl-3-methylphenol
331	HMDB0014018	4-Hydroxypropofol
332	HMDB0037389	NA
333	HMDB0038292	NA
334	HMDB0040439	NA
335	HMDB0039685	NA
336	HMDB0041497	NA
337	HMDB0031840	(S,Z)-Lyratol acetate
338	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate
339	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate
340	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate
341	HMDB0132986	NA
342	HMDB0034450	Neocnidilide
343	HMDB0032567	Hexylresorcinol
344	HMDB0035126	(Ás)-Myrtenyl acetate
345	HMDB0041610	NA
346	HMDB0038046	NA
347	HMDB0037018	NA
348	HMDB0037231	NA
349	HMDB0035085	Vulgarole
350	HMDB0041572	NA
351	HMDB0029388	Cucurbic acid
352	HMDB0037326	NA
353	HMDB0033601	Dihydrojasmonic acid
354	HMDB0040195	NA
355	HMDB0035723	(1R,2S,3S,4R)-p-Menthane-2,3-diol
356	HMDB0034457	Propyl heptanoate
357	HMDB0061987	NA
358	HMDB0062146	NA
359	HMDB0038038	NA
360	HMDB0036228	2-Methylpropyl hexanoate
361	HMDB0040167	NA
362	HMDB0036136	NA
363	HMDB0187563	NA
364	HMDB0037387	NA
365	HMDB0000511	Capric acid
366	HMDB0031264	Methyl nonanoate
367	HMDB0094654	1-Methylethyl heptanoic acid
368	HMDB0171179	NA
369	HMDB0171178	NA
370	HMDB0171177	NA
371	HMDB0171176	NA
372	HMDB0179213	NA
373	HMDB0179212	NA
374	HMDB0179927	NA
375	HMDB0180500	NA
376	HMDB0180498	NA
377	HMDB0180499	NA
378	HMDB0180497	NA
379	HMDB0180502	NA
380	HMDB0180501	NA
381	HMDB0180503	NA
382	HMDB0180504	NA
383	HMDB0171175	NA
384	HMDB0061805	NA
385	HMDB0180097	NA
386	HMDB0032302	Heptanal propyleneglycol acetal
387	HMDB0032155	Acetaldehyde 1,3-octanediol acetal
388	HMDB0032264	Ethyl 2-ethylhexanoate
389	HMDB0032315	Hexanal butane-2,3-diol acetal
390	HMDB0032045	Pentyl 3-methylbutanoate
391	HMDB0041216	NA
392	HMDB0034849	4-Methylnonanoic acid
393	HMDB0037849	Hexyl 2-methylpropanoate
394	HMDB0040157	NA
395	HMDB0033620	Hexyl butyrate
396	HMDB0035595	trans-p-Menthane-1,8-diol
397	HMDB0029760	1,1-Diethoxy-2-hexene
398	HMDB0032070	Isooctyl acetate
399	HMDB0040211	NA
400	HMDB0040529	NA
401	HMDB0038783	NA
402	HMDB0036145	NA
403	HMDB0039218	NA
404	HMDB0038602	Octyl acetate
405	HMDB0030029	Isopentyl isopentanoate
406	HMDB0031739	7-Hydroxy-3,7-dimethyloctanal
407	HMDB0035360	N-Methyl-1-deoxynojirimycin

408	HMDB0029741	2-Isopropyl-3,5-dimethoxy-6-methylpyrazine
409	HMDB0040551	NA
410	HMDB0240493	NA
411	HMDB0029224	N-methylphenylalanine
412	HMDB0029223	alpha-Methylphenylalanine
413	HMDB0005199	(R)-Salsolinol
414	HMDB0031811	3,5-Dimethylphenyl methylcarbamate
415	HMDB0039655	NA
416	HMDB0030372	Maltosazine
417	HMDB0040021	NA
418	HMDB0033763	Ethyl N-methylanthranilate
419	HMDB0042012	NA
420	HMDB0001189	2(N)-Methyl-norsalsolinol
421	HMDB0041931	NA
422	HMDB0029135	Valyl-Proline
423	HMDB0003581	Dethiobiotin
424	HMDB0029030	Prolyl-Valine
425	HMDB0036683	NA
426	HMDB0059826	NA
427	HMDB0059696	NA
428	HMDB0061824	NA
429	HMDB0013287	Ne,Ne dimethyllysine
430	HMDB0003269	Nicotinuric acid
431	HMDB0164043	NA
432	HMDB0176142	NA
433	HMDB0041912	NA
434	HMDB0059766	NA
435	HMDB0032055	N-Acetylhistidine
436	HMDB0059663	5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate
437	HMDB0062721	NA
438	HMDB0168420	NA
439	HMDB0062551	4-ethylphenylsulfate
440	HMDB0035593	Rishitin
441	HMDB0037605	NA
442	HMDB0036790	NA
443	HMDB0036791	NA
444	HMDB0037820	NA
445	HMDB0040178	NA
446	HMDB0160293	NA
447	HMDB0160295	NA
448	HMDB0160291	NA
449	HMDB0160290	NA
450	HMDB0160289	NA
451	HMDB0160292	NA
452	HMDB0160296	NA
453	HMDB0160294	NA
454	HMDB0160298	NA
455	HMDB0160297	NA
456	HMDB0032369	L-Menthyl acetoacetate
457	HMDB0033619	Hexyl hexanoate
458	HMDB0059868	NA
459	HMDB0032440	Nonanal propyleneglycol acetal
460	HMDB0061988	NA
461	HMDB0035410	(R)-Dihydrocitronellol acetate
462	HMDB0000638	Dodecanoic acid
463	HMDB0040166	NA
464	HMDB0030998	Ethyl decanoate
465	HMDB0034137	Octyl 2-methylpropanoate
466	HMDB0036225	NA
467	HMDB0034136	Octyl butanoate
468	HMDB0034128	Isopropyl nonanoate
469	HMDB0032310	2-Heptyl butyrate
470	HMDB0168119	NA
471	HMDB0168120	NA
472	HMDB0168121	NA
473	HMDB0015050	Phenformin
474	HMDB0004231	Pantothenol
475	HMDB0061683	NA
476	HMDB0031813	N-Carbamoyl-2-amino-2-(4-hydroxyphenyl)acetic acid
477	HMDB0000014	Deoxycytidine
478	HMDB0028732	Asparaginy-Hydroxyproline
479	HMDB0028858	Hydroxyprolyl-Asparagine
480	HMDB0040046	NA
481	HMDB0161863	NA
482	HMDB0161860	NA
483	HMDB0041444	NA
484	HMDB0033452	Koenoline
485	HMDB0161862	NA
486	HMDB0161861	NA
487	HMDB0161859	NA
488	HMDB0161858	NA
489	HMDB0161857	NA
490	HMDB0094651	PyroGlu-Val
491	HMDB0029018	Prolyl-Hydroxyproline
492	HMDB0028871	Hydroxyprolyl-Proline
493	HMDB0006695	Prolylhydroxyproline
494	HMDB0040573	NA

495	HMDB0060747	NA
496	HMDB0011754	Methyldopa
497	HMDB0001434	3-Methoxytyrosine
498	HMDB0011172	gamma-Glutamylvaline
499	HMDB0029162	NA
500	HMDB0028756	Aspartyl-Isoleucine
501	HMDB0028903	Isoleucyl-Aspartate
502	HMDB0028925	Leucyl-Aspartate
503	HMDB0028832	Glutamylvaline
504	HMDB0059717	NA
505	HMDB0029126	Valyl-Glutamate
506	HMDB0028757	Aspartyl-Leucine
507	HMDB0011166	L-beta-aspartyl-L-leucine
508	HMDB0151781	NA
509	HMDB0151783	NA
510	HMDB0151788	NA
511	HMDB0151787	NA
512	HMDB0151784	NA
513	HMDB0035016	2-Phenylethyl pentanoate
514	HMDB0132932	NA
515	HMDB0132940	NA
516	HMDB0151780	NA
517	HMDB0001925	Ibuprofen
518	HMDB0034472	3-Phenylpropyl 2-methylpropanoate
519	HMDB0034470	2-Phenylpropyl isobutyrate
520	HMDB0038605	NA
521	HMDB0040431	NA
522	HMDB0036391	NA
523	HMDB0036025	2,4,6-Trimethyl-4-phenyl-1,3-dioxane
524	HMDB0037194	NA
525	HMDB0034469	2-Phenylpropyl butyrate
526	HMDB0037623	NA
527	HMDB0036240	NA
528	HMDB0035017	2-Phenylethyl 3-methylbutanoate
529	HMDB0037720	NA
530	HMDB0035008	3-Methylbutyl phenylacetate
531	HMDB0036386	NA
532	HMDB0033196	(E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one
533	HMDB0037604	NA
534	HMDB0029669	Eremopetasinorone A
535	HMDB0035181	xi-8,9-Dehydrotheaspirone
536	HMDB0039101	NA
537	HMDB0034556	3-Acetoxy-3-methyl-1-phenylbutane
538	HMDB0032176	Benzyl hexanoate
539	HMDB0163212	NA
540	HMDB0151805	NA
541	HMDB0151793	NA
542	HMDB0151794	NA
543	HMDB0151789	NA
544	HMDB0151790	NA
545	HMDB0151791	NA
546	HMDB0151785	NA
547	HMDB0151786	NA
548	HMDB0151792	NA
549	HMDB0014604	Nabumetone
550	HMDB0176774	NA
551	HMDB0176773	NA
552	HMDB0176775	NA
553	HMDB0061836	NA
554	HMDB0032133	Bisphenol A
555	HMDB0033878	(S)-Curzeone
556	HMDB0135597	NA
557	HMDB0170855	NA
558	HMDB0179330	NA
559	HMDB0179331	NA
560	HMDB0038202	NA
561	HMDB0036767	NA
562	HMDB0036455	NA
563	HMDB0035902	Enokipodin B
564	HMDB0040903	NA
565	HMDB0038188	NA
566	HMDB0031916	5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran
567	HMDB0037558	NA
568	HMDB0036473	NA
569	HMDB0037801	NA
570	HMDB0030911	2-Oxo-5,11(13)-eudesmadien-12,8-olide
571	HMDB0031900	Methyl (2E,4Z,6E,8E,10E)-4,8-dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoate
572	HMDB0036488	NA
573	HMDB0038547	NA
574	HMDB0041920	NA
575	HMDB0179332	NA
576	HMDB0059946	NA
577	HMDB0041618	NA
578	HMDB0176325	NA
579	HMDB0059947	NA
580	HMDB0176328	NA
581	HMDB0000872	Tetradecanedioic acid



582	HMDB0176327	NA
583	HMDB0040429	NA
584	HMDB0176326	NA
585	HMDB0040219	NA
586	HMDB0060002	NA
587	HMDB0240658	NA
588	HMDB0240657	NA
589	HMDB0006512	3-Mercaptolactate-cysteine disulfide
590	HMDB0169467	NA
591	HMDB0169468	NA
592	HMDB0169469	NA
593	HMDB0172924	NA
594	HMDB0172927	NA
595	HMDB0029397	L-Nicotianine
596	HMDB0000732	Hydroxykynurenine
597	HMDB0012819	5-Hydroxykynurenine
598	HMDB0014787	Stavudine
599	HMDB0011631	L-3-Hydroxykynurenine
600	HMDB0060750	NA
601	HMDB0002224	5-Methyldeoxycytidine
602	HMDB0028861	Hydroxypropyl-Glutamine
603	HMDB0038516	NA
604	HMDB0028798	Glutaminyhydroxyproline
605	HMDB0028877	Hydroxypropyl-Gamma-glutamate
606	HMDB0178266	NA
607	HMDB0037694	NA
608	HMDB0040006	NA
609	HMDB0037695	NA
610	HMDB0042008	NA
611	HMDB0033430	Tanakine
612	HMDB0033429	Tanakamine
613	HMDB0142966	NA
614	HMDB0029448	DL-Ornithino-L-alanine
615	HMDB0041858	NA
616	HMDB0135607	NA
617	HMDB0141386	NA
618	HMDB0135600	NA
619	HMDB0135404	NA
620	HMDB0135599	NA
621	HMDB0141385	NA
622	HMDB0141387	NA
623	HMDB0135604	NA
624	HMDB0135603	NA
625	HMDB0135602	NA
626	HMDB0032584	4-Hydroxychalcone
627	HMDB0037696	NA
628	HMDB0014922	Mefenamic acid
629	HMDB0040380	NA
630	HMDB0029366	N-[2-(4-Hydroxyphenyl)ethyl]benzamide
631	HMDB0147191	NA
632	HMDB0131062	NA
633	HMDB0131065	NA
634	HMDB0036050	NA
635	HMDB0033771	Cyperine
636	HMDB0030690	(E)-Suberenol
637	HMDB0039592	NA
638	HMDB0030788	Citrusal
639	HMDB0135759	NA
640	HMDB0135760	NA
641	HMDB0135761	NA
642	HMDB0141827	NA
643	HMDB0151855	NA
644	HMDB0153660	NA
645	HMDB0135757	NA
646	HMDB0135758	NA
647	HMDB0129916	NA
648	HMDB0129917	NA
649	HMDB0129919	NA
650	HMDB0129920	NA
651	HMDB0129922	NA
652	HMDB0131064	NA
653	HMDB0131066	NA
654	HMDB0131067	NA
655	HMDB0132269	NA
656	HMDB0129918	NA
657	HMDB0030854	(S)-Auraptenol
658	HMDB0030110	Celerin
659	HMDB0030948	Dihydrowyerone
660	HMDB0039142	NA
661	HMDB0041192	NA
662	HMDB0034133	3-(1,1-Dimethylallyl)scopoletin
663	HMDB0030853	(R)-Meranzin
664	HMDB0033015	5,6-Dihydroyangonin
665	HMDB0035254	7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone
666	HMDB0033016	7,8-Dihydroyangonin
667	HMDB0030578	Apigravin
668	HMDB0032953	7-Methoxy-5-prenyloxycoumarin

669	HMDB0061290	NA
670	HMDB0061303	NA
671	HMDB0039146	NA
672	HMDB0037679	NA
673	HMDB0035019	Phenethyl salicylate
674	HMDB0029302	1-Phenyl-6,7-dihydroxy-isochroman
675	HMDB0036347	NA
676	HMDB0002209	Equol
677	HMDB0130495	NA
678	HMDB0014713	Fenoprofen
679	HMDB0135409	NA
680	HMDB0135406	NA
681	HMDB0135408	NA
682	HMDB0135407	NA
683	HMDB0135593	NA
684	HMDB0135594	NA
685	HMDB0135405	NA
686	HMDB0130496	NA
687	HMDB0135355	NA
688	HMDB0135397	NA
689	HMDB0135595	NA
690	HMDB0151857	NA
691	HMDB0130497	NA
692	HMDB0168444	NA
693	HMDB0135601	NA
694	HMDB0168447	NA
695	HMDB0148520	NA
696	HMDB0168443	NA
697	HMDB0182848	NA
698	HMDB0168445	NA
699	HMDB0168442	NA
700	HMDB0135596	NA
701	HMDB0168446	NA
702	HMDB0029953	D-erythro-D-galacto-octitol
703	HMDB0151802	NA
704	HMDB0151796	NA
705	HMDB0151800	NA
706	HMDB0151798	NA
707	HMDB0151801	NA
708	HMDB0151797	NA
709	HMDB0151799	NA
710	HMDB0037492	NA
711	HMDB0032589	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone
712	HMDB0061823	NA
713	HMDB0061942	NA
714	HMDB0040424	NA
715	HMDB0132933	NA
716	HMDB0132935	NA
717	HMDB0132936	NA
718	HMDB0132937	NA
719	HMDB0132939	NA
720	HMDB0132948	NA
721	HMDB0060478	gamma-Glutamyl-beta-cyanoalanine
722	HMDB0000089	Cytidine
723	HMDB0015122	Cytarabine
724	HMDB0155273	NA
725	HMDB0001904	3-Nitrotyrosine
726	HMDB0028751	Aspartyl-Glutamine
727	HMDB0028793	Glutaminylaspartic acid
728	HMDB0029144	gamma-Glutamylasparagine
729	HMDB0028814	Glutamylasparagine
730	HMDB0028730	Asparaginyl-Glutamate
731	HMDB0028767	Aspartyl-Gamma-glutamate
732	HMDB0033701	Hydrocotarnine
733	HMDB0031770	Carbofuran
734	HMDB0014798	Metaxalone
735	HMDB0139892	NA
736	HMDB0138550	NA
737	HMDB0033925	Oroselone
738	HMDB0032998	2-Methoxyxanthone
739	HMDB0161779	NA
740	HMDB0161778	NA
741	HMDB0161783	NA
742	HMDB0161782	NA
743	HMDB0161780	NA
744	HMDB0162111	NA
745	HMDB0162103	NA
746	HMDB0162104	NA
747	HMDB0162105	NA
748	HMDB0162108	NA
749	HMDB0162109	NA
750	HMDB0162106	NA
751	HMDB0162107	NA
752	HMDB0162110	NA
753	HMDB0162112	NA
754	HMDB0161832	NA
755	HMDB0161833	NA

756	HMDB0161834	NA
757	HMDB0149051	NA
758	HMDB0149050	NA
759	HMDB0149006	NA
760	HMDB0148541	NA
761	HMDB0148540	NA
762	HMDB0148786	NA
763	HMDB0148785	NA
764	HMDB0148998	NA
765	HMDB0149048	NA
766	HMDB0147226	NA
767	HMDB0148542	NA
768	HMDB0128505	NA
769	HMDB0148539	NA
770	HMDB0145646	NA
771	HMDB0145647	NA
772	HMDB0145645	NA
773	HMDB0135172	NA
774	HMDB0149007	NA
775	HMDB0128506	NA
776	HMDB0128503	NA
777	HMDB0128504	NA
778	HMDB0040876	NA
779	HMDB0030946	(2E,11Z)-Wyerone acid
780	HMDB0041016	NA
781	HMDB0030595	Suberenone
782	HMDB0033735	Graveolone
783	HMDB0039430	NA
784	HMDB0004215	3,3',4'5-Tetrahydroxystilbene
785	HMDB0170845	NA
786	HMDB0164057	NA
787	HMDB0135900	NA
788	HMDB0135902	NA
789	HMDB0135904	NA
790	HMDB0164055	NA
791	HMDB0164056	NA
792	HMDB0164058	NA
793	HMDB0170846	NA
794	HMDB0170974	NA
795	HMDB0170976	NA
796	HMDB0170979	NA
797	HMDB0170978	NA
798	HMDB0131284	NA
799	HMDB0131285	NA
800	HMDB0127824	NA
801	HMDB0131281	NA
802	HMDB0131283	NA
803	HMDB0170977	NA
804	HMDB0031668	Dihydrodeoxy-8-epiaustdiol
805	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid
806	HMDB0037681	NA
807	HMDB0029470	Isodillapiole
808	HMDB0041379	NA
809	HMDB0135906	NA
810	HMDB0038563	NA
811	HMDB0037130	NA
812	HMDB0094660	Diethyl phthalic acid
813	HMDB0033776	Apiole
814	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone
815	HMDB0135689	NA
816	HMDB0013247	Monobutylphthalate
817	HMDB0030725	Dillapiol
818	HMDB0002056	Monoisobutyl phthalic acid
819	HMDB0147179	NA
820	HMDB0140340	NA
821	HMDB0173973	NA
822	HMDB0173971	NA
823	HMDB0173972	NA
824	HMDB0173975	NA
825	HMDB0173976	NA
826	HMDB0177472	NA
827	HMDB0177470	NA
828	HMDB0173974	NA
829	HMDB0128944	NA
830	HMDB0131630	NA
831	HMDB0128958	NA
832	HMDB0039027	NA
833	HMDB0128963	NA
834	HMDB0138052	NA
835	HMDB0128962	NA
836	HMDB0030882	(S)-Rutaretin
837	HMDB0128960	NA
838	HMDB0128961	NA
839	HMDB0032838	Dorsteniol
840	HMDB0131653	NA
841	HMDB0147178	NA
842	HMDB0131691	NA

843	HMDB0131700	NA
844	HMDB0167944	NA
845	HMDB0163475	NA
846	HMDB0171044	NA
847	HMDB0167134	NA
848	HMDB0028752	Aspartyl-Glutamate
849	HMDB0029145	NA
850	HMDB0030419	gamma-Glutamylaspartic acid
851	HMDB0062501	NA
852	HMDB0028815	Glutamylaspartic acid
853	HMDB0030413	NA
854	HMDB0011164	L-beta-aspartyl-L-glutamic acid
855	HMDB0000767	Pseudouridine
856	HMDB0000296	Uridine
857	HMDB0156330	NA
858	HMDB0126635	NA
859	HMDB0130466	NA
860	HMDB0130477	NA
861	HMDB0006794	5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate
862	HMDB0157260	NA
863	HMDB0157259	NA
864	HMDB0125157	NA
865	HMDB0166885	NA
866	HMDB0155302	NA
867	HMDB0180914	NA
868	HMDB0177249	NA
869	HMDB0163614	NA
870	HMDB0028930	Leucyl-Hydroxyproline
871	HMDB0028867	Hydroxypropyl-Leucine
872	HMDB0028908	Isoleucyl-Hydroxyproline
873	HMDB0028866	Hydroxypropyl-Isoleucine
874	HMDB0032928	2-Amino-3,4,8-trimethyl-3H-imidazo[4,5-f]quinoxaline
875	HMDB0040300	NA
876	HMDB0134717	NA
877	HMDB0133034	NA
878	HMDB0133061	NA
879	HMDB0137262	NA
880	HMDB0137253	NA
881	HMDB0028833	Glutamyl-Gamma-glutamate
882	HMDB0028796	Glutaminyglutamic acid
883	HMDB0029147	N-gamma-Glutamylglutamine
884	HMDB0028817	Glutamylglutamine
885	HMDB0011738	N2-gamma-Glutamylglutamine
886	HMDB0005766	Norophthalmic acid
887	HMDB0240577	NA
888	HMDB0000982	5-Methylcytidine
889	HMDB0039229	Pyro-L-glutamyl-L-glutamine
890	HMDB0032559	(Á)-2-(1-Methylpropyl)-4,6-dinitrophenol
891	HMDB0033610	Pandamarilactam 3x
892	HMDB0139906	NA
893	HMDB0164387	NA
894	HMDB0000086	Glycerophosphocholine
895	HMDB0142996	NA
896	HMDB0143005	NA
897	HMDB0151865	NA
898	HMDB0137520	NA
899	HMDB0130494	NA
900	HMDB0135588	NA
901	HMDB0135591	NA
902	HMDB0135592	NA
903	HMDB0137534	NA
904	HMDB0135587	NA
905	HMDB0135590	NA
906	HMDB0151856	NA
907	HMDB0032130	3',4'-Dihydroxychalcone
908	HMDB0135586	NA
909	HMDB0153774	NA
910	HMDB0036738	NA
911	HMDB0039612	NA
912	HMDB0032129	2',5'-Dihydroxychalcone
913	HMDB0014643	Tolmetin
914	HMDB0033345	(Á)-Ribaline
915	HMDB0041329	NA
916	HMDB0032924	3-Furanmethanol glucoside
917	HMDB0130798	NA
918	HMDB0130839	NA
919	HMDB0126546	NA
920	HMDB0167013	NA
921	HMDB0175219	NA
922	HMDB0167016	NA
923	HMDB0002091	Isovalerylglucuronide
924	HMDB0167014	NA
925	HMDB0175223	NA
926	HMDB0143217	NA
927	HMDB0175224	NA
928	HMDB0175227	NA
929	HMDB0175220	NA

930	HMDB0033065	(x)-1,2-Propanediol 1-O-b-D-glucopyranoside
931	HMDB0060917	NA
932	HMDB0144816	NA
933	HMDB0184077	NA
934	HMDB0029155	NA
935	HMDB0034367	gamma-Glutamylmethionine
936	HMDB0028972	Methionyl-Glutamate
937	HMDB0028825	Glutamylmethionine
938	HMDB0062160	NA
939	HMDB0002117	Oleamide
940	HMDB0060663	NA
941	HMDB0177722	NA
942	HMDB0175189	NA
943	HMDB0175187	NA
944	HMDB0175188	NA
945	HMDB0162484	NA
946	HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione
947	HMDB0036047	NA
948	HMDB0059661	NA
949	HMDB0015088	Rizatriptan
950	HMDB0014873	Naftifine
951	HMDB0014578	Cyproheptadine
952	HMDB0011687	Phenylbutyrylglutamine
953	HMDB0033514	Fusarochromanone
954	HMDB0181167	NA
955	HMDB0034885	Imazamethabenz
956	HMDB0139531	NA
957	HMDB0139533	NA
958	HMDB0139532	NA
959	HMDB0139535	NA
960	HMDB0139993	NA
961	HMDB0014451	Talbutal
962	HMDB0139534	NA
963	HMDB0059959	NA
964	HMDB0028811	Glutaminy-Gamma-glutamate
965	HMDB0029163	Gamma-glutamyl-Gamma-glutamate
966	HMDB0032764	N2-Succinoylarginine
967	HMDB0028795	Glutaminyglutamine
968	HMDB0186509	NA
969	HMDB0184957	NA
970	HMDB0184936	NA
971	HMDB0062677	NA
972	HMDB0004590	19-Nor-5-androstenediol
973	HMDB0032464	Phenethyl decanoate
974	HMDB0002697	19-Norandrosterone
975	HMDB0032672	4,8,12,15-Octadecatetraenoic acid
976	HMDB0005886	19-Noretiocholanolone
977	HMDB0034382	(E,E)-11,13-Octadecadien-9-ynoic acid
978	HMDB0006547	Stearidonic acid
979	HMDB0186501	NA
980	HMDB0186507	NA
981	HMDB0186508	NA
982	HMDB0062288	NA
983	HMDB0186510	NA
984	HMDB0186500	NA
985	HMDB0186506	NA
986	HMDB0186505	NA
987	HMDB0186504	NA
988	HMDB0186502	NA
989	HMDB0186497	NA
990	HMDB0186499	NA
991	HMDB0186498	NA
992	HMDB0112093	NA
993	HMDB0112099	NA
994	HMDB0112102	NA
995	HMDB0112103	NA
996	HMDB0186503	NA
997	HMDB0034586	(9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid
998	HMDB0031088	12,13-Epoxy-9,15-octadecadienoic acid
999	HMDB0029969	Squamostanal A
1000	HMDB0031103	2-Hydroxylinolenic acid
1001	HMDB0036832	NA
1002	HMDB0030950	15,16-Epoxy-9,12-octadecadienoic acid
1003	HMDB0029786	10-Oxo-11-octadecen-13-olide
1004	HMDB0011108	17-Hydroxylinolenic acid
1005	HMDB0010224	9-HOTE
1006	HMDB0010220	9(10)-EpODE
1007	HMDB0010206	15(16)-EpODE
1008	HMDB0010200	A-12(13)-EpODE
1009	HMDB0010203	13-HOTE
1010	HMDB0004669	9-OxoODE
1011	HMDB0004668	13-OxoODE
1012	HMDB0031934	(9S,10E,12Z,15Z)-9-Hydroxy-10,12,15-octadecatrienoic acid
1013	HMDB0030995	(2'E,4'Z,8E)-Colneleic acid
1014	HMDB0061644	NA
1015	HMDB0039603	NA
1016	HMDB0061979	NA

1017	HMDB0033791	(E)-3-Hexadecenoic acid
1018	HMDB0038958	NA
1019	HMDB0031711	15-Hexadecanolide
1020	HMDB0003229	Palmitoleic acid
1021	HMDB0010735	Trans-Hexa-dec-2-enoic acid
1022	HMDB0037647	NA
1023	HMDB0041422	NA
1024	HMDB0032638	(Z)-5-Hexadecenoic acid
1025	HMDB0031053	(E)-6-Hexadecenoic acid
1026	HMDB0035877	(Z)-13-Hexadecenoic acid
1027	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone
1028	HMDB0002186	Hypogeic acid
1029	HMDB0171478	NA
1030	HMDB0171479	NA
1031	HMDB0171477	NA
1032	HMDB0012328	Palmitelaidic acid
1033	HMDB0171476	NA
1034	HMDB0000756	L-Hexanoylcarnitine
1035	HMDB0000705	Hexanoylcarnitine
1036	HMDB0014413	Ropinirole
1037	HMDB0015070	Oxymetazoline
1038	HMDB0011176	L-phenylalanyl-L-hydroxyproline
1039	HMDB0029113	Tyrosyl-Proline
1040	HMDB0029029	Prolyl-Tyrosine
1041	HMDB0011112	N1-(alpha-D-ribosyl)-5,6-dimethyl-benzimidazole
1042	HMDB0028996	Phenylalanyl-Hydroxyproline
1043	HMDB0139701	NA
1044	HMDB0139704	NA
1045	HMDB0139705	NA
1046	HMDB0139706	NA
1047	HMDB0139702	NA
1048	HMDB0033680	Falcarindione
1049	HMDB0015038	Methdilazine
1050	HMDB0003426	Pantetheine
1051	HMDB0141088	NA
1052	HMDB0133909	NA
1053	HMDB0133903	NA
1054	HMDB0133905	NA
1055	HMDB0133906	NA
1056	HMDB0133907	NA
1057	HMDB0133908	NA
1058	HMDB0133910	NA
1059	HMDB0141089	NA
1060	HMDB0133904	NA
1061	HMDB0060472	Didemethylcitalopram
1062	HMDB0138210	NA
1063	HMDB0138209	NA
1064	HMDB0138206	NA
1065	HMDB0138203	NA
1066	HMDB0138207	NA
1067	HMDB0147305	NA
1068	HMDB0147303	NA
1069	HMDB0147304	NA
1070	HMDB0144709	NA
1071	HMDB0141175	NA
1072	HMDB0141176	NA
1073	HMDB0141177	NA
1074	HMDB0141178	NA
1075	HMDB0141090	NA
1076	HMDB0138208	NA
1077	HMDB0144700	NA
1078	HMDB0138205	NA
1079	HMDB0033950	Parakmerin A
1080	HMDB0030599	5-[(4-Hydroxyphenyl)ethenyl]-2-(3-methyl-1-butenyl)-1,3-benzenediol
1081	HMDB0039071	NA
1082	HMDB0038784	NA
1083	HMDB0035220	Cryptotanshinone
1084	HMDB0138202	NA
1085	HMDB0147319	NA
1086	HMDB0138204	NA
1087	HMDB0061189	NA
1088	HMDB0062555	hydroxyisovaleroyl carnitine
1089	HMDB0240421	NA
1090	HMDB0040904	NA
1091	HMDB0168550	NA
1092	HMDB0168551	NA
1093	HMDB0168552	NA
1094	HMDB0168553	NA
1095	HMDB0168554	NA
1096	HMDB0168549	NA
1097	HMDB0137260	NA
1098	HMDB0137271	NA
1099	HMDB0030974	8-Acetoxy-4-acoren-3-one
1100	HMDB0031928	Panaxxytriol
1101	HMDB0030801	1-(4-Hydroxy-3-methoxyphenyl)-3-decanone
1102	HMDB0039251	NA
1103	HMDB0134775	NA

1104	HMDB0038798	NA
1105	HMDB0035075	Tanacetol B
1106	HMDB0060952	NA
1107	HMDB0014521	Palonosetron
1108	HMDB0030283	Hydrocinchonine
1109	HMDB0175409	NA
1110	HMDB0175412	NA
1111	HMDB0175413	NA
1112	HMDB0175414	NA
1113	HMDB0175415	NA
1114	HMDB0175408	NA
1115	HMDB0175410	NA
1116	HMDB0175411	NA
1117	HMDB0160594	NA
1118	HMDB0173892	NA
1119	HMDB0175402	NA
1120	HMDB0175403	NA
1121	HMDB0175404	NA
1122	HMDB0175405	NA
1123	HMDB0175406	NA
1124	HMDB0175407	NA
1125	HMDB0030964	Linolenelaidic acid
1126	HMDB0001388	Alpha-Linolenic acid
1127	HMDB0003073	Gamma-Linolenic acid
1128	HMDB0030962	Calendic acid
1129	HMDB0030963	Punicic acid
1130	HMDB0160589	NA
1131	HMDB0160588	NA
1132	HMDB0112194	NA
1133	HMDB0062652	NA
1134	HMDB0173890	NA
1135	HMDB0160590	NA
1136	HMDB0160592	NA
1137	HMDB0160591	NA
1138	HMDB0160593	NA
1139	HMDB0160595	NA
1140	HMDB0173886	NA
1141	HMDB0173885	NA
1142	HMDB0173887	NA
1143	HMDB0173889	NA
1144	HMDB0173891	NA
1145	HMDB0173888	NA
1146	HMDB0173893	NA
1147	HMDB0004667	13S-hydroxyoctadecadienoic acid
1148	HMDB0061708	NA
1149	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid
1150	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid
1151	HMDB0029978	Avenoleic acid
1152	HMDB0010223	9-HODE
1153	HMDB0004701	9,10-Epoxyoctadecenoic acid
1154	HMDB0004702	12,13-EpOME
1155	HMDB0004670	Alpha-dimorphecolic acid
1156	HMDB0000220	Palmitic acid
1157	HMDB0060083	NA
1158	HMDB0061373	NA
1159	HMDB0032324	Hexyl decanoate
1160	HMDB0032249	Dodecyl butyrate
1161	HMDB0033166	Octyl octanoate
1162	HMDB0032065	Butyl dodecanoate
1163	HMDB0036210	NA
1164	HMDB0034153	Ethyl tetradecanoate
1165	HMDB0031068	Isopalmitic acid
1166	HMDB0002396	Trimethyltridecanoic acid
1167	HMDB0240660	NA
1168	HMDB0166396	NA
1169	HMDB0155323	NA
1170	HMDB0125616	NA
1171	HMDB0157443	NA
1172	HMDB0125615	NA
1173	HMDB0155324	NA
1174	HMDB0155326	NA
1175	HMDB0155327	NA
1176	HMDB0157445	NA
1177	HMDB0157442	NA
1178	HMDB0166395	NA
1179	HMDB0156225	NA
1180	HMDB0156223	NA
1181	HMDB0156224	NA
1182	HMDB0156222	NA
1183	HMDB0155825	NA
1184	HMDB0166394	NA
1185	HMDB0125614	NA
1186	HMDB0125613	NA
1187	HMDB0157444	NA
1188	HMDB0155325	NA
1189	HMDB0164008	NA
1190	HMDB0062577	NA

1191	HMDB0003950	7-Methylinosine
1192	HMDB0002721	1-Methylinosine
1193	HMDB0003060	Piperolactam A
1194	HMDB00034319	Furofoline
1195	HMDB00038882	NA
1196	HMDB00038880	NA
1197	HMDB0029918	Arabinofuranobiose
1198	HMDB0029894	Xylobiose
1199	HMDB00038855	NA
1200	HMDB0029619	Arabinopyranobiose
1201	HMDB00038881	NA
1202	HMDB0179982	NA
1203	HMDB0179983	NA
1204	HMDB0179984	NA
1205	HMDB0028745	Asparaginylnl-Gamma-glutamate
1206	HMDB0028792	Glutaminylnlasparagine
1207	HMDB0028729	Asparaginylnl-Glutamine
1208	HMDB0126535	NA
1209	HMDB0126543	NA
1210	HMDB0126529	NA
1211	HMDB0126544	NA
1212	HMDB0126525	NA
1213	HMDB0126540	NA
1214	HMDB0126536	NA
1215	HMDB0126532	NA
1216	HMDB0126531	NA
1217	HMDB0126528	NA
1218	HMDB0126526	NA
1219	HMDB0140895	NA
1220	HMDB0140584	NA
1221	HMDB0140434	NA
1222	HMDB0240404	NA
1223	HMDB0132291	NA
1224	HMDB0140896	NA
1225	HMDB0140901	NA
1226	HMDB0140900	NA
1227	HMDB0172131	NA
1228	HMDB0171705	NA
1229	HMDB0168714	NA
1230	HMDB0168707	NA
1231	HMDB0159585	NA
1232	HMDB0157245	NA
1233	HMDB0152783	NA
1234	HMDB0145741	NA
1235	HMDB0145740	NA
1236	HMDB0172133	NA
1237	HMDB0134099	NA
1238	HMDB0159586	NA
1239	HMDB0132292	NA
1240	HMDB0041648	NA
1241	HMDB0041721	NA
1242	HMDB0059967	NA
1243	HMDB0061117	NA
1244	HMDB0011719	Homovanillic acid sulfate
1245	HMDB0002899	Ellagic acid
1246	HMDB0015039	Ethacrynic acid
1247	HMDB0060626	NA
1248	HMDB0039096	NA
1249	HMDB0173636	NA
1250	HMDB0041314	NA
1251	HMDB0130350	NA
1252	HMDB0130347	NA
1253	HMDB0175079	NA
1254	HMDB0178312	NA
1255	HMDB0141160	NA
1256	HMDB0141105	NA
1257	HMDB0141099	NA
1258	HMDB0141080	NA
1259	HMDB0141122	NA
1260	HMDB0141079	NA
1261	HMDB0141126	NA
1262	HMDB0141149	NA
1263	HMDB0141119	NA
1264	HMDB0040889	NA
1265	HMDB0129039	NA
1266	HMDB0138953	NA
1267	HMDB0141045	NA
1268	HMDB0138954	NA
1269	HMDB0138952	NA
1270	HMDB0138951	NA
1271	HMDB0138956	NA
1272	HMDB0140994	NA
1273	HMDB0138959	NA
1274	HMDB0138955	NA
1275	HMDB0138957	NA
1276	HMDB0138958	NA
1277	HMDB0141056	NA



1278	HMDB0141150	NA
1279	HMDB0141152	NA
1280	HMDB0141153	NA
1281	HMDB0141164	NA
1282	HMDB0146848	NA
1283	HMDB0146849	NA
1284	HMDB0141181	NA
1285	HMDB0141151	NA
1286	HMDB0141180	NA
1287	HMDB0141162	NA
1288	HMDB0141161	NA
1289	HMDB0141169	NA
1290	HMDB0141163	NA
1291	HMDB0141145	NA
1292	HMDB0141146	NA
1293	HMDB0141057	NA
1294	HMDB0141101	NA
1295	HMDB0141102	NA
1296	HMDB0141100	NA
1297	HMDB0141103	NA
1298	HMDB0141106	NA
1299	HMDB0141107	NA
1300	HMDB0141120	NA
1301	HMDB0141121	NA
1302	HMDB0141130	NA
1303	HMDB0141129	NA
1304	HMDB0141128	NA
1305	HMDB0141127	NA
1306	HMDB0141139	NA
1307	HMDB0141140	NA
1308	HMDB0141170	NA
1309	HMDB0036635	NA
1310	HMDB0041298	NA
1311	HMDB0033310	Moracin C
1312	HMDB0031744	Artocarbene
1313	HMDB0141044	NA
1314	HMDB0138682	NA
1315	HMDB0011741	gamma-Glutamyltyrosine
1316	HMDB0029161	NA
1317	HMDB0029104	Tyrosyl-Glutamate
1318	HMDB0028831	Glutamyltyrosine
1319	HMDB0062553	NA
1320	HMDB0041309	NA
1321	HMDB0000839	Pentaporphyrin I
1322	HMDB0029428	Hypoglycin B
1323	HMDB0061318	NA
1324	HMDB0015102	Desloratadine
1325	HMDB0170226	NA
1326	HMDB0170229	NA
1327	HMDB0170227	NA
1328	HMDB0170230	NA
1329	HMDB0170228	NA
1330	HMDB0004704	9,10-DHOME
1331	HMDB0061650	9,10-Epoxystearic acid
1332	HMDB0004705	12,13-DHOME
1333	HMDB0041220	NA
1334	HMDB0031679	(9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid
1335	HMDB0000782	Octadecanedioic acid
1336	HMDB0015401	Nelarabine
1337	HMDB0005862	2-Methylguanosine
1338	HMDB0006038	3'-O-Methylguanosine
1339	HMDB0001563	1-Methylguanosine
1340	HMDB0001107	7-Methylguanosine
1341	HMDB0029076	Tryptophyl-Alanine
1342	HMDB0028698	Alanyl-Tryptophan
1343	HMDB0142223	NA
1344	HMDB0013209	Alanyltryptophan
1345	HMDB0165476	NA
1346	HMDB0165475	NA
1347	HMDB0165471	NA
1348	HMDB0165472	NA
1349	HMDB0126113	NA
1350	HMDB0130135	NA
1351	HMDB0130132	NA
1352	HMDB0130129	NA
1353	HMDB0145822	NA
1354	HMDB0130130	NA
1355	HMDB0164665	NA
1356	HMDB0130133	NA
1357	HMDB0130019	NA
1358	HMDB0126116	NA
1359	HMDB0126115	NA
1360	HMDB0130136	NA
1361	HMDB0126114	NA
1362	HMDB0178290	NA
1363	HMDB0178289	NA
1364	HMDB0181208	NA

1365	HMDB0060994	NA
1366	HMDB0183805	NA
1367	HMDB0156418	NA
1368	HMDB0156413	NA
1369	HMDB0156410	NA
1370	HMDB0156411	NA
1371	HMDB0156408	NA
1372	HMDB0156409	NA
1373	HMDB0156404	NA
1374	HMDB0156405	NA
1375	HMDB0061925	NA
1376	HMDB0156406	NA
1377	HMDB0156407	NA
1378	HMDB0156401	NA
1379	HMDB0156403	NA
1380	HMDB0156402	NA
1381	HMDB0001852	All-trans-retinoic acid
1382	HMDB0156412	NA
1383	HMDB0179600	NA
1384	HMDB0012874	9,13-cis-Retinoate
1385	HMDB0012788	4-OH-Retinal
1386	HMDB0036710	NA
1387	HMDB0036564	NA
1388	HMDB0036697	NA
1389	HMDB0036711	NA
1390	HMDB0038702	NA
1391	HMDB0012329	4-Oxoretinol
1392	HMDB0006219	13-cis-Retinoic acid
1393	HMDB0041925	NA
1394	HMDB0002369	9-cis-Retinoic acid
1395	HMDB0179597	NA
1396	HMDB0179596	NA
1397	HMDB0179598	NA
1398	HMDB0183803	NA
1399	HMDB0183804	NA
1400	HMDB0183807	NA
1401	HMDB0183806	NA
1402	HMDB0183808	NA
1403	HMDB0183810	NA
1404	HMDB0183811	NA
1405	HMDB0183813	NA
1406	HMDB0179593	NA
1407	HMDB0179594	NA
1408	HMDB0183809	NA
1409	HMDB0062222	NA
1410	HMDB0062293	NA
1411	HMDB0062296	NA
1412	HMDB0062408	NA
1413	HMDB0137419	NA
1414	HMDB0137428	NA
1415	HMDB0183812	NA
1416	HMDB0183814	NA
1417	HMDB0183815	NA
1418	HMDB0183816	NA
1419	HMDB0001337	Leukotriene A4
1420	HMDB0036776	NA
1421	HMDB0036839	NA
1422	HMDB0030101	Methyl [8]-Shogaol
1423	HMDB0036930	NA
1424	HMDB0036724	NA
1425	HMDB0035311	Galanal A
1426	HMDB0039012	NA
1427	HMDB0036698	NA
1428	HMDB0036706	NA
1429	HMDB0037523	NA
1430	HMDB0036806	NA
1431	HMDB0035116	(ent-7alpha)-7-Hydroxy-8(14),15-pimaradien-19-oic acid
1432	HMDB0039716	NA
1433	HMDB0005081	5-HEPE
1434	HMDB0006027	Oxymesterone
1435	HMDB0010202	12-HEPE
1436	HMDB0010205	14,15-EpETE
1437	HMDB0010210	15-KETE
1438	HMDB0010209	15-HEPE
1439	HMDB0010212	17,18-EpETE
1440	HMDB0010217	5-KETE
1441	HMDB0041058	NA
1442	HMDB0036712	NA
1443	HMDB0038521	NA
1444	HMDB0036752	NA
1445	HMDB0036713	NA
1446	HMDB0012534	11R-HEPE
1447	HMDB0012611	18R-HEPE
1448	HMDB0013633	12-KETE
1449	HMDB0060053	NA
1450	HMDB0061114	NA
1451	HMDB0179595	NA

1452	HMDB0005764	Melanostatin
1453	HMDB0036329	NA
1454	HMDB0060578	NA
1455	HMDB0061098	NA
1456	HMDB0161587	NA
1457	HMDB0138221	NA
1458	HMDB0030432	Linalyl cinnamate
1459	HMDB0038050	NA
1460	HMDB0003422	Boldione
1461	HMDB0029913	Gynocardin
1462	HMDB0240490	NA
1463	HMDB0059998	NA
1464	HMDB0041272	NA
1465	HMDB0124997	NA
1466	HMDB0029498	3'-Methoxyfukiic acid
1467	HMDB0135181	NA
1468	HMDB0125471	NA
1469	HMDB0004326	2'-O-Methyladenosine
1470	HMDB0004044	N6-Methyladenosine
1471	HMDB0006023	3'-O-Methyladenosine
1472	HMDB0003331	1-Methyladenosine
1473	HMDB0006832	S-Glutaryldihydrolipoamide
1474	HMDB0037843	NA
1475	HMDB0030266	Berberrubine
1476	HMDB0187656	NA
1477	HMDB0030391	Cepharadione B
1478	HMDB0061366	NA
1479	HMDB0029395	L-L-Homoglutathione
1480	HMDB0135641	NA
1481	HMDB0179385	NA
1482	HMDB0179388	NA
1483	HMDB0179383	NA
1484	HMDB0179382	NA
1485	HMDB0163720	NA
1486	HMDB0173550	NA
1487	HMDB0135574	NA
1488	HMDB0135576	NA
1489	HMDB0135572	NA
1490	HMDB0135564	NA
1491	HMDB0135568	NA
1492	HMDB0134573	NA
1493	HMDB0134571	NA
1494	HMDB0135570	NA
1495	HMDB0158752	NA
1496	HMDB0158753	NA
1497	HMDB0155927	NA
1498	HMDB0155928	NA
1499	HMDB0161130	NA
1500	HMDB0041096	NA
1501	HMDB0158750	NA
1502	HMDB0158751	NA
1503	HMDB0159487	NA
1504	HMDB0159488	NA
1505	HMDB0159490	NA
1506	HMDB0159830	NA
1507	HMDB0161128	NA
1508	HMDB0161127	NA
1509	HMDB0161129	NA
1510	HMDB0161132	NA
1511	HMDB0161133	NA
1512	HMDB0166865	NA
1513	HMDB0159483	NA
1514	HMDB0159484	NA
1515	HMDB0159482	NA
1516	HMDB0158755	NA
1517	HMDB0158759	NA
1518	HMDB0158758	NA
1519	HMDB0159491	NA
1520	HMDB0158756	NA
1521	HMDB0158876	NA
1522	HMDB0158877	NA
1523	HMDB0159485	NA
1524	HMDB0061135	NA
1525	HMDB0015176	Melphalan
1526	HMDB0127928	NA
1527	HMDB0037110	NA
1528	HMDB0145098	NA
1529	HMDB0175072	NA
1530	HMDB0041450	NA
1531	HMDB0038322	NA
1532	HMDB0032909	2-(4-Methoxyphenyl)naphthalic anhydride
1533	HMDB0175074	NA
1534	HMDB0175080	NA
1535	HMDB0175081	NA
1536	HMDB0175083	NA
1537	HMDB0175073	NA
1538	HMDB0175082	NA

1539	HMDB0163581	NA
1540	HMDB0163582	NA
1541	HMDB0163584	NA
1542	HMDB0038580	NA
1543	HMDB0033631	Lactapiperanol D
1544	HMDB0180021	NA
1545	HMDB0180098	NA
1546	HMDB0180100	NA
1547	HMDB0180099	NA
1548	HMDB0180102	NA
1549	HMDB0034780	Capsiate
1550	HMDB0180103	NA
1551	HMDB0184951	NA
1552	HMDB0184949	NA
1553	HMDB0184953	NA
1554	HMDB0012799	5'-Carboxy-gamma-chromanol
1555	HMDB0184954	NA
1556	HMDB0184950	NA
1557	HMDB0061677	NA
1558	HMDB0000552	3-Methylglutaryl carnitine
1559	HMDB0015334	Nadolol
1560	HMDB0015345	Metipranolol
1561	HMDB0137251	NA
1562	HMDB0137254	NA
1563	HMDB0137256	NA
1564	HMDB0137255	NA
1565	HMDB0137252	NA
1566	HMDB0137257	NA
1567	HMDB0137259	NA
1568	HMDB0137261	NA
1569	HMDB0137264	NA
1570	HMDB0137263	NA
1571	HMDB0137265	NA
1572	HMDB0137266	NA
1573	HMDB0137267	NA
1574	HMDB0137268	NA
1575	HMDB0137270	NA
1576	HMDB0179994	NA
1577	HMDB0180049	NA
1578	HMDB0041249	NA
1579	HMDB0036693	NA
1580	HMDB0034930	(3beta,6beta)-Furanoeremophilane-3,6-diol 6-acetate
1581	HMDB0034738	Isotrichodermin
1582	HMDB0035687	Acetylvalerenolic acid
1583	HMDB0039275	NA
1584	HMDB0034658	9-Acetoxyfukinanolide
1585	HMDB0000791	L-Octanoyl carnitine
1586	HMDB0039044	NA
1587	HMDB0131544	NA
1588	HMDB0153683	NA
1589	HMDB0134716	NA
1590	HMDB0131577	NA
1591	HMDB0140842	NA
1592	HMDB0039858	NA
1593	HMDB0150310	NA
1594	HMDB0150311	NA
1595	HMDB0030019	4'-Methoxymucidin
1596	HMDB0125543	NA
1597	HMDB0125544	NA
1598	HMDB0125545	NA
1599	HMDB0125547	NA
1600	HMDB0125546	NA
1601	HMDB0125548	NA
1602	HMDB0129031	NA
1603	HMDB0129032	NA
1604	HMDB0141104	NA
1605	HMDB0141131	NA
1606	HMDB0141141	NA
1607	HMDB0141165	NA
1608	HMDB0141171	NA
1609	HMDB0129034	NA
1610	HMDB0149106	NA
1611	HMDB0140204	NA
1612	HMDB0140116	NA
1613	HMDB0129033	NA
1614	HMDB0129035	NA
1615	HMDB0129037	NA
1616	HMDB0129036	NA
1617	HMDB0129038	NA
1618	HMDB0140114	NA
1619	HMDB0140118	NA
1620	HMDB0140117	NA
1621	HMDB0140115	NA
1622	HMDB0146850	NA
1623	HMDB0040670	NA
1624	HMDB0176556	NA
1625	HMDB0000495	Androstanediol

1626	HMDB0159493	NA
1627	HMDB0158029	NA
1628	HMDB0000554	Dihydroandrosterone
1629	HMDB0000551	Etiocholanediol
1630	HMDB0000458	5a-Androstane-3a,17a-diol
1631	HMDB0000383	3a,17a-Dihydroxy-5b-androstane
1632	HMDB0000493	5a-Androstane-3b,17b-diol
1633	HMDB0000369	3b,17b-Dihydroxyetiocholane
1634	HMDB0000412	3b,17a-Dihydroxy-5a-androstane
1635	HMDB0060437	Androstan-3alpha,17beta-diol
1636	HMDB0167160	NA
1637	HMDB0167157	NA
1638	HMDB0156083	NA
1639	HMDB0167154	NA
1640	HMDB0167155	NA
1641	HMDB0167156	NA
1642	HMDB0062521	NA
1643	HMDB0167161	NA
1644	HMDB0167158	NA
1645	HMDB0173640	NA
1646	HMDB0186461	NA
1647	HMDB0167171	NA
1648	HMDB0167170	NA
1649	HMDB0186443	NA
1650	HMDB0167159	NA
1651	HMDB0167165	NA
1652	HMDB0167163	NA
1653	HMDB0167162	NA
1654	HMDB0167164	NA
1655	HMDB0167169	NA
1656	HMDB0167168	NA
1657	HMDB0167167	NA
1658	HMDB0167166	NA
1659	HMDB0014613	Dronabinol
1660	HMDB0038533	NA
1661	HMDB0013121	7-Dehydropregnenolone
1662	HMDB0031924	4-Nerolidylcatechol
1663	HMDB0041865	NA
1664	HMDB0001830	Progesterone
1665	HMDB0156085	NA
1666	HMDB0137415	NA
1667	HMDB0137402	NA
1668	HMDB0156084	NA
1669	HMDB0156089	NA
1670	HMDB0186441	NA
1671	HMDB0186440	NA
1672	HMDB0186438	NA
1673	HMDB0186439	NA
1674	HMDB0186444	NA
1675	HMDB0186457	NA
1676	HMDB0186462	NA
1677	HMDB0186435	NA
1678	HMDB0186437	NA
1679	HMDB0156091	NA
1680	HMDB0156092	NA
1681	HMDB0156093	NA
1682	HMDB0156090	NA
1683	HMDB0156094	NA
1684	HMDB0156095	NA
1685	HMDB0156840	NA
1686	HMDB0158166	NA
1687	HMDB0173643	NA
1688	HMDB0173642	NA
1689	HMDB0173641	NA
1690	HMDB0173645	NA
1691	HMDB0173644	NA
1692	HMDB0173646	NA
1693	HMDB0173647	NA
1694	HMDB0173648	NA
1695	HMDB0186436	NA
1696	HMDB0062609	NA
1697	HMDB0060424	7alpha-Hydroxypregnenolone
1698	HMDB0060407	5alpha-Dihydrodeoxycorticosterone
1699	HMDB0031462	[10]-Shogaol
1700	HMDB0033918	(15alpha,20R)-15,20-Dihydroxypregn-4-en-3-one
1701	HMDB0011653	17-alpha,20-alpha-Dihydroxypregn-4-en-3-one
1702	HMDB0004026	21-Hydroxypregnenolone
1703	HMDB0003851	3a,7a-Dihydroxy-5b-cholestanate
1704	HMDB0000363	17a-Hydroxypregnenolone
1705	HMDB0000315	16-a-Hydroxypregnenolone
1706	HMDB0173549	NA
1707	HMDB0125510	NA
1708	HMDB0125509	NA
1709	HMDB0060017	NA
1710	HMDB0125511	NA
1711	HMDB0125508	NA
1712	HMDB0125512	NA

1713	HMDB0187598	NA
1714	HMDB0015513	Fludiazepam
1715	HMDB0162772	NA
1716	HMDB0162714	NA
1717	HMDB0162760	NA
1718	HMDB0162710	NA
1719	HMDB0162708	NA
1720	HMDB0162758	NA
1721	HMDB0033374	Benzyl glycinate 4-methylbenzenesulfonate salt
1722	HMDB0161228	NA
1723	HMDB0161229	NA
1724	HMDB0159742	NA
1725	HMDB0185385	NA
1726	HMDB0181751	NA
1727	HMDB0181741	NA
1728	HMDB0039733	NA
1729	HMDB0004662	S-(Hydroxymethyl)glutathione
1730	HMDB0014848	Ibandronate
1731	HMDB0029391	N-Jasmonoylisoleucine
1732	HMDB0006320	2,6 Dimethylheptanoyl carnitine
1733	HMDB0013288	Nonanoylcarnitine
1734	HMDB0013189	3-Indole carboxylic acid glucuronide
1735	HMDB0011658	2,8-Dihydroxyquinoline-beta-D-glucuronide
1736	HMDB0134938	NA
1737	HMDB0137819	NA
1738	HMDB0137816	NA
1739	HMDB0137821	NA
1740	HMDB0140538	NA
1741	HMDB0140542	NA
1742	HMDB0140556	NA
1743	HMDB0152029	NA
1744	HMDB0125037	NA
1745	HMDB0126563	NA
1746	HMDB0131929	NA
1747	HMDB0131931	NA
1748	HMDB0126570	NA
1749	HMDB0126567	NA
1750	HMDB0126564	NA
1751	HMDB0126566	NA
1752	HMDB0126569	NA
1753	HMDB0128213	NA
1754	HMDB0131759	NA
1755	HMDB0125219	NA
1756	HMDB0125216	NA
1757	HMDB0125207	NA
1758	HMDB0125079	NA
1759	HMDB0125067	NA
1760	HMDB0125052	NA
1761	HMDB0131760	NA
1762	HMDB0131925	NA
1763	HMDB0131928	NA
1764	HMDB0131932	NA
1765	HMDB0167582	NA
1766	HMDB0152484	NA
1767	HMDB0167580	NA
1768	HMDB0167581	NA
1769	HMDB0030835	trans-3,3',4',5,5',7-Hexahydroxyflavanone
1770	HMDB0152031	NA
1771	HMDB0152038	NA
1772	HMDB0152035	NA
1773	HMDB0152036	NA
1774	HMDB0167579	NA
1775	HMDB0152479	NA
1776	HMDB0152402	NA
1777	HMDB0152037	NA
1778	HMDB0039815	NA
1779	HMDB0127840	NA
1780	HMDB0127779	NA
1781	HMDB0128709	NA
1782	HMDB0125820	NA
1783	HMDB0125826	NA
1784	HMDB0127839	NA
1785	HMDB0127778	NA
1786	HMDB0125825	NA
1787	HMDB0172923	NA
1788	HMDB0172926	NA
1789	HMDB0141622	NA
1790	HMDB0142252	NA
1791	HMDB0034767	(1R*,3R*,3'S*)-1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-beta-carboline-3-carboxylic acid
1792	HMDB0172522	NA
1793	HMDB0172514	NA
1794	HMDB0154672	NA
1795	HMDB0154674	NA
1796	HMDB0154675	NA
1797	HMDB0154673	NA
1798	HMDB0154671	NA
1799	HMDB0154670	NA

1800	HMDB0029566	Isopulegone caffeate
1801	HMDB0154668	NA
1802	HMDB0134704	NA
1803	HMDB0147915	NA
1804	HMDB0154665	NA
1805	HMDB0154669	NA
1806	HMDB0154666	NA
1807	HMDB0154667	NA
1808	HMDB0148183	NA
1809	HMDB0153649	NA
1810	HMDB0125854	NA
1811	HMDB0141256	NA
1812	HMDB0124819	NA
1813	HMDB0125836	NA
1814	HMDB0125842	NA
1815	HMDB0133467	NA
1816	HMDB0041386	NA
1817	HMDB0034412	2'-O-Methylphaseollinisoflavan
1818	HMDB0039439	NA
1819	HMDB0033672	4'-O-Methylglabridin
1820	HMDB0029514	Licochalcone A
1821	HMDB0033782	Bergamottin
1822	HMDB0039309	NA
1823	HMDB0030846	Archangelin
1824	HMDB0039438	NA
1825	HMDB0033671	2'-O-Methylglabridin
1826	HMDB0032665	Licoagrocarpin
1827	HMDB0031633	Orientanol B
1828	HMDB0001272	Nicotine glucuronide
1829	HMDB0032808	Niazirinin
1830	HMDB0131864	NA
1831	HMDB0124924	NA
1832	HMDB0131867	NA
1833	HMDB0133539	NA
1834	HMDB0124927	NA
1835	HMDB0125807	NA
1836	HMDB0131075	NA
1837	HMDB0133516	NA
1838	HMDB0133495	NA
1839	HMDB0133485	NA
1840	HMDB0133468	NA
1841	HMDB0131866	NA
1842	HMDB0131865	NA
1843	HMDB0124928	NA
1844	HMDB0124929	NA
1845	HMDB0124838	NA
1846	HMDB0124800	NA
1847	HMDB0124826	NA
1848	HMDB0124829	NA
1849	HMDB0124835	NA
1850	HMDB0124837	NA
1851	HMDB0124922	NA
1852	HMDB0130876	NA
1853	HMDB0138809	NA
1854	HMDB0150217	NA
1855	HMDB0150219	NA
1856	HMDB0124822	NA
1857	HMDB0150216	NA
1858	HMDB0150218	NA
1859	HMDB0150215	NA
1860	HMDB0147761	NA
1861	HMDB0147762	NA
1862	HMDB0147765	NA
1863	HMDB0147767	NA
1864	HMDB0147766	NA
1865	HMDB0147764	NA
1866	HMDB0147768	NA
1867	HMDB0147769	NA
1868	HMDB0149836	NA
1869	HMDB0150181	NA
1870	HMDB0150186	NA
1871	HMDB0150185	NA
1872	HMDB0150182	NA
1873	HMDB0150184	NA
1874	HMDB0150187	NA
1875	HMDB0150214	NA
1876	HMDB0035440	alpha,beta-Dihydroxanthohumol
1877	HMDB0030666	Chalepin acetate
1878	HMDB0035403	Gingerenone A
1879	HMDB0030798	Myricanone
1880	HMDB0033880	Mammea B/AC cyclo D
1881	HMDB0033879	Mammea B/AD cyclo D
1882	HMDB0030333	Fragransol C
1883	HMDB0041401	NA
1884	HMDB0138808	NA
1885	HMDB0184970	NA
1886	HMDB0184809	NA

1887	HMDB0005026	Rabeprazole
1888	HMDB0129572	NA
1889	HMDB0149073	NA
1890	HMDB0150818	NA
1891	HMDB0154339	NA
1892	HMDB0168985	NA
1893	HMDB0168989	NA
1894	HMDB0168988	NA
1895	HMDB0168990	NA
1896	HMDB0172299	NA
1897	HMDB0149076	NA
1898	HMDB0149075	NA
1899	HMDB0168986	NA
1900	HMDB0137123	NA
1901	HMDB0146792	NA
1902	HMDB0149074	NA
1903	HMDB0059746	NA
1904	HMDB0030575	4',5,6,7-Tetramethoxyflavone
1905	HMDB0031289	1,4,6-Trihydroxy-5-methoxy-7-prenylxanthone
1906	HMDB0032736	Dulxanthone D
1907	HMDB0031992	Dulxanthone A
1908	HMDB0029461	Zapotin
1909	HMDB0034182	1,5,8-Trihydroxy-3-methyl-2-prenylxanthone
1910	HMDB0146780	NA
1911	HMDB0136442	NA
1912	HMDB0136453	NA
1913	HMDB0014739	Linezolid
1914	HMDB0181080	NA
1915	HMDB0181070	NA
1916	HMDB0181085	NA
1917	HMDB0181076	NA
1918	HMDB0033108	Semilepidinoside B
1919	HMDB0240296	NA
1920	HMDB0166033	NA
1921	HMDB0012492	1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylate
1922	HMDB0029992	Tetrahydropentoxylene
1923	HMDB0166038	NA
1924	HMDB0166035	NA
1925	HMDB0166036	NA
1926	HMDB0014720	Voriconazole
1927	HMDB0014258	R-138727
1928	HMDB0131015	NA
1929	HMDB0131014	NA
1930	HMDB0131011	NA
1931	HMDB0131013	NA
1932	HMDB0136701	NA
1933	HMDB0140161	NA
1934	HMDB0171360	NA
1935	HMDB0171359	NA
1936	HMDB0171362	NA
1937	HMDB0171358	NA
1938	HMDB0171355	NA
1939	HMDB0171354	NA
1940	HMDB0032955	5-(6-Hydroxy-3,7-dimethyl-2,7-octadienyloxy)-7-methoxycoumarin
1941	HMDB0038690	NA
1942	HMDB0171361	NA
1943	HMDB0034179	Malabaricano
1944	HMDB0031889	(1(10)E,4E,6a,8b)-8-Angeloyloxy-14-oxo-1(10),4,11(13)-germacatrien-12,6-olide
1945	HMDB0031753	2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol
1946	HMDB0038219	NA
1947	HMDB0040388	NA
1948	HMDB0040421	NA
1949	HMDB0036691	NA
1950	HMDB0039610	NA
1951	HMDB0125864	NA
1952	HMDB0172929	NA
1953	HMDB0148194	NA
1954	HMDB0040834	NA
1955	HMDB0040809	NA
1956	HMDB0041100	NA
1957	HMDB0041417	NA
1958	HMDB0035427	Glicoisoflavanone
1959	HMDB0014559	Ampicillin
1960	HMDB0015428	Cefradine
1961	HMDB0062731	Dodecamethylpentasiloxane
1962	HMDB0004239	13,14-Dihydro PGF2a
1963	HMDB0002689	13,14-Dihydro PGE1
1964	HMDB0002685	Prostaglandin F1a
1965	HMDB0165171	NA
1966	HMDB0035508	Annoglabasin F
1967	HMDB0014701	Doxapram
1968	HMDB0175496	NA
1969	HMDB0175499	NA
1970	HMDB0175502	NA
1971	HMDB0175506	NA
1972	HMDB0175509	NA
1973	HMDB0175505	NA



1974	HMDB0175517	NA
1975	HMDB0175521	NA
1976	HMDB0175520	NA
1977	HMDB0175516	NA
1978	HMDB0175513	NA
1979	HMDB0175512	NA
1980	HMDB0012280	Phytosphingosine-1-P
1981	HMDB0062531	NA
1982	HMDB0000277	Sphingosine 1-phosphate
1983	HMDB0059630	NA
1984	HMDB0094648	Leu-Leu-Leu
1985	HMDB0005076	13,14-Dihydro PGF-1a
1986	HMDB0164534	NA
1987	HMDB0002082	Bisnorcholic acid
1988	HMDB0040698	NA
1989	HMDB0184271	NA
1990	HMDB0183492	NA
1991	HMDB0156837	NA
1992	HMDB0156831	NA
1993	HMDB0156835	NA
1994	HMDB0156889	NA
1995	HMDB0156836	NA
1996	HMDB0157597	NA
1997	HMDB0157601	NA
1998	HMDB0157602	NA
1999	HMDB0157742	NA
2000	HMDB0157743	NA
2001	HMDB0157738	NA
2002	HMDB0157739	NA
2003	HMDB0157603	NA
2004	HMDB0157604	NA
2005	HMDB0157599	NA
2006	HMDB0157600	NA
2007	HMDB0156838	NA
2008	HMDB0156832	NA
2009	HMDB0155046	NA
2010	HMDB0156806	NA
2011	HMDB0156826	NA
2012	HMDB0156827	NA
2013	HMDB0156829	NA
2014	HMDB0156830	NA
2015	HMDB0156828	NA
2016	HMDB0156834	NA
2017	HMDB0156833	NA
2018	HMDB0157740	NA
2019	HMDB0157741	NA
2020	HMDB0158276	NA
2021	HMDB0167960	NA
2022	HMDB0167961	NA
2023	HMDB0167962	NA
2024	HMDB0167964	NA
2025	HMDB0167963	NA
2026	HMDB0167966	NA
2027	HMDB0167965	NA
2028	HMDB0167968	NA
2029	HMDB0167967	NA
2030	HMDB0170452	NA
2031	HMDB0170451	NA
2032	HMDB0186750	NA
2033	HMDB0000903	Tetrahydrocortisone
2034	HMDB0003259	Dihydrocortisol
2035	HMDB0006753	3a,11b,21-Trihydroxy-20-oxo-5b-pregnan-18-al
2036	HMDB0006754	11b,21-Dihydroxy-3,20-oxo-5b-pregnan-18-al
2037	HMDB0006760	11b,17a,21-Trihydroxypreg-nenolone
2038	HMDB0032553	Vanillin 3-(L-menthoxy)propane-1,2-diol acetal
2039	HMDB0013157	18-Hydroxy-11-dehydrotetrahydrocorticosterone
2040	HMDB0013164	2-Hydroxy-lauroylcarnitine
2041	HMDB0061638	NA
2042	HMDB0185679	NA
2043	HMDB0185658	NA
2044	HMDB0185694	NA
2045	HMDB0185682	NA
2046	HMDB0185676	NA
2047	HMDB0185661	NA
2048	HMDB0185673	NA
2049	HMDB0185698	NA
2050	HMDB0185670	NA
2051	HMDB0185667	NA
2052	HMDB0185664	NA
2053	HMDB0179611	NA
2054	HMDB0179614	NA
2055	HMDB0179608	NA
2056	HMDB0179615	NA
2057	HMDB0179605	NA
2058	HMDB0179606	NA
2059	HMDB0179618	NA
2060	HMDB0179619	NA

2061	HMDB0179623	NA
2062	HMDB0179626	NA
2063	HMDB0182175	NA
2064	HMDB0179627	NA
2065	HMDB0182176	NA
2066	HMDB0014334	Bortezomib
2067	HMDB0061005	NA
2068	HMDB0060583	NA
2069	HMDB0030868	Citreoviridin A
2070	HMDB0030523	Citreoviridin C
2071	HMDB0036462	NA
2072	HMDB0035027	Melleolide F
2073	HMDB0035774	Armillyl orsellinate
2074	HMDB0015459	Cortisone acetate
2075	HMDB0038917	NA
2076	HMDB0031380	(6beta,7alpha,12beta,13beta)-7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide
2077	HMDB0179899	NA
2078	HMDB0179900	NA
2079	HMDB0179898	NA
2080	HMDB0179897	NA
2081	HMDB0179895	NA
2082	HMDB0179894	NA
2083	HMDB0179893	NA
2084	HMDB0179896	NA
2085	HMDB0060833	NA
2086	HMDB0185381	NA
2087	HMDB0002873	Deacetyldiltiazem
2088	HMDB0124912	NA
2089	HMDB0124915	NA
2090	HMDB0124828	NA
2091	HMDB0124911	NA
2092	HMDB0124914	NA
2093	HMDB0124913	NA
2094	HMDB0125800	NA
2095	HMDB0131078	NA
2096	HMDB0131080	NA
2097	HMDB0131077	NA
2098	HMDB0130292	NA
2099	HMDB0130291	NA
2100	HMDB0130288	NA
2101	HMDB0130290	NA
2102	HMDB0130289	NA
2103	HMDB0130100	NA
2104	HMDB0130099	NA
2105	HMDB0124817	NA
2106	HMDB0124816	NA
2107	HMDB0124815	NA
2108	HMDB0124810	NA
2109	HMDB0124811	NA
2110	HMDB0124813	NA
2111	HMDB0124812	NA
2112	HMDB0133480	NA
2113	HMDB0149865	NA
2114	HMDB0149860	NA
2115	HMDB0149855	NA
2116	HMDB0149846	NA
2117	HMDB0149841	NA
2118	HMDB0149835	NA
2119	HMDB0149834	NA
2120	HMDB0146994	NA
2121	HMDB0146992	NA
2122	HMDB0146993	NA
2123	HMDB0146989	NA
2124	HMDB0133520	NA
2125	HMDB0133514	NA
2126	HMDB0133513	NA
2127	HMDB0133493	NA
2128	HMDB0133492	NA
2129	HMDB0133481	NA
2130	HMDB0146939	NA
2131	HMDB0131836	NA
2132	HMDB0131837	NA
2133	HMDB0131838	NA
2134	HMDB0133527	NA
2135	HMDB0133537	NA
2136	HMDB0137511	NA
2137	HMDB0146987	NA
2138	HMDB0146988	NA
2139	HMDB0146986	NA
2140	HMDB0146947	NA
2141	HMDB0146945	NA
2142	HMDB0146944	NA
2143	HMDB0146941	NA
2144	HMDB0146940	NA
2145	HMDB0146938	NA
2146	HMDB0138813	NA
2147	HMDB0131079	NA

2148	HMDB0039066	NA
2149	HMDB0041416	NA
2150	HMDB0030826	2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-methylenedioxyphenyl)-1-propanol
2151	HMDB0035182	Licoriphenone
2152	HMDB0032733	(8R,8'R,9S)-9-Hydroxy-3,4-dimethoxy-3',4'-methylenoxy-9,9'-epoxylignan
2153	HMDB0005789	Tetrahydrocurcumin
2154	HMDB0030087	(-)-Arctigenin
2155	HMDB0032734	9-Hydroxy-3',4'-dimethoxy-3,4-methylenedioxy-9,9'-epoxylignan
2156	HMDB0164958	NA
2157	HMDB0029510	Garcinone B
2158	HMDB0034436	Rotenone
2159	HMDB0036984	NA
2160	HMDB0148796	NA
2161	HMDB0146129	NA
2162	HMDB0173953	NA
2163	HMDB0184813	NA
2164	HMDB0184985	NA
2165	HMDB0184812	NA
2166	HMDB0184811	NA
2167	HMDB0184810	NA
2168	HMDB0173968	NA
2169	HMDB0173965	NA
2170	HMDB0173956	NA
2171	HMDB0000222	L-Palmitoylcarnitine
2172	HMDB0011574	MG(20:2(11Z,14Z)/0:0/0:0)
2173	HMDB0011544	MG(0:0/20:2(11Z,14Z)/0:0)
2174	HMDB0036865	NA
2175	HMDB0035959	Persenone B
2176	HMDB0172273	NA
2177	HMDB0172275	NA
2178	HMDB0172274	NA
2179	HMDB0174261	NA
2180	HMDB0174260	NA
2181	HMDB0174265	NA
2182	HMDB0174262	NA
2183	HMDB0174263	NA
2184	HMDB0174264	NA
2185	HMDB0174266	NA
2186	HMDB0155085	NA
2187	HMDB0155087	NA
2188	HMDB0154867	NA
2189	HMDB0154866	NA
2190	HMDB0155080	NA
2191	HMDB0155083	NA
2192	HMDB0155082	NA
2193	HMDB0155081	NA
2194	HMDB0155084	NA
2195	HMDB0155086	NA
2196	HMDB0174267	NA
2197	HMDB0174268	NA
2198	HMDB0184842	NA
2199	HMDB0184845	NA
2200	HMDB0184846	NA
2201	HMDB0184848	NA
2202	HMDB0184847	NA
2203	HMDB0184849	NA
2204	HMDB0184851	NA
2205	HMDB0184850	NA
2206	HMDB0185576	NA
2207	HMDB0185577	NA
2208	HMDB0184843	NA
2209	HMDB0184841	NA
2210	HMDB0184144	NA
2211	HMDB0184143	NA
2212	HMDB0184146	NA
2213	HMDB0184145	NA
2214	HMDB0184147	NA
2215	HMDB0184148	NA
2216	HMDB0184150	NA
2217	HMDB0184149	NA
2218	HMDB0184168	NA
2219	HMDB0184844	NA
2220	HMDB0185578	NA
2221	HMDB0003550	Calcidiol
2222	HMDB0060132	NA
2223	HMDB0060131	NA
2224	HMDB0015504	Alfacalcidol
2225	HMDB0000501	7-Ketocholesterol
2226	HMDB0001993	7a-Hydroxy-cholestene-3-one
2227	HMDB0006722	25-Hydroxytachysterol3
2228	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3
2229	HMDB0035585	1-Phenyl-1,3-heneicosanedione
2230	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol
2231	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone
2232	HMDB0039871	NA
2233	HMDB0159655	NA
2234	HMDB0159658	NA

2235	HMDB0159656	NA
2236	HMDB0159657	NA
2237	HMDB0159654	NA
2238	HMDB0159653	NA
2239	HMDB0159651	NA
2240	HMDB0159652	NA
2241	HMDB0062675	NA
2242	HMDB0062664	NA
2243	HMDB0062419	NA
2244	HMDB0062420	NA
2245	HMDB0062607	NA
2246	HMDB0172263	NA
2247	HMDB0172264	NA
2248	HMDB0185568	NA
2249	HMDB0185570	NA
2250	HMDB0185567	NA
2251	HMDB0185569	NA
2252	HMDB0185572	NA
2253	HMDB0185575	NA
2254	HMDB0185571	NA
2255	HMDB0185574	NA
2256	HMDB0185566	NA
2257	HMDB0172272	NA
2258	HMDB0172262	NA
2259	HMDB0172266	NA
2260	HMDB0172268	NA
2261	HMDB0172265	NA
2262	HMDB0172267	NA
2263	HMDB0172270	NA
2264	HMDB0172269	NA
2265	HMDB0172271	NA
2266	HMDB0185573	NA
2267	HMDB0006280	7-a,25-Dihydroxycholesterol
2268	HMDB0060136	7alpha,24S-Dihydroxycholesterol
2269	HMDB0011644	(24R)-Cholest-5-ene-3-beta,7-alpha,24-triol
2270	HMDB0006894	3a,7a-Dihydroxy-5b-cholestan-26-al
2271	HMDB0006887	7a,12a-Dihydroxy-5b-cholestan-3-one
2272	HMDB0006886	7a,12a-Dihydroxy-5a-cholestan-3-one
2273	HMDB0006764	17a,20a-Dihydroxycholesterol
2274	HMDB0006763	20a,22b-Dihydroxycholesterol
2275	HMDB0006281	7-a,27-Dihydroxycholesterol
2276	HMDB0035951	Erucylacetone
2277	HMDB0164879	NA
2278	HMDB0037260	NA
2279	HMDB0158333	NA
2280	HMDB0150478	NA
2281	HMDB0150475	NA
2282	HMDB0162509	NA
2283	HMDB0150477	NA
2284	HMDB0038347	NA
2285	HMDB0150474	NA
2286	HMDB0150463	NA
2287	HMDB0150458	NA
2288	HMDB0150468	NA
2289	HMDB0150470	NA
2290	HMDB0150457	NA
2291	HMDB0150453	NA
2292	HMDB0150469	NA
2293	HMDB0150452	NA
2294	HMDB0149868	NA
2295	HMDB0150462	NA
2296	HMDB0140070	NA
2297	HMDB0153459	NA
2298	HMDB0153444	NA
2299	HMDB0153474	NA
2300	HMDB0153627	NA
2301	HMDB0153466	NA
2302	HMDB0139521	NA
2303	HMDB0139520	NA
2304	HMDB0139517	NA
2305	HMDB0139504	NA
2306	HMDB0139507	NA
2307	HMDB0139514	NA
2308	HMDB0149502	NA
2309	HMDB0153458	NA
2310	HMDB0153451	NA
2311	HMDB0153443	NA
2312	HMDB0139516	NA
2313	HMDB0139508	NA
2314	HMDB0139513	NA
2315	HMDB0035876	Mesuagin
2316	HMDB0180147	NA
2317	HMDB0013842	O-Deethylated candesartan
2318	HMDB0144444	NA
2319	HMDB0144965	NA
2320	HMDB0144871	NA
2321	HMDB0142647	NA

2322	HMDB0144859	NA
2323	HMDB0144408	NA
2324	HMDB0144379	NA
2325	HMDB0142761	NA
2326	HMDB0142694	NA
2327	HMDB0144418	NA
2328	HMDB0144964	NA
2329	HMDB0142682	NA
2330	HMDB0144733	NA
2331	HMDB0038793	NA
2332	HMDB0038787	NA
2333	HMDB0175541	NA
2334	HMDB0175538	NA
2335	HMDB0175530	NA
2336	HMDB0175535	NA
2337	HMDB0147021	NA
2338	HMDB0147024	NA
2339	HMDB0147025	NA
2340	HMDB0147019	NA
2341	HMDB0147020	NA
2342	HMDB0148764	NA
2343	HMDB0147022	NA
2344	HMDB0147023	NA
2345	HMDB0148762	NA
2346	HMDB0168741	NA
2347	HMDB0148763	NA
2348	HMDB0148761	NA
2349	HMDB0148760	NA
2350	HMDB0148765	NA
2351	HMDB0148759	NA
2352	HMDB0147026	NA
2353	HMDB0147018	NA
2354	HMDB0168749	NA
2355	HMDB0168747	NA
2356	HMDB0168748	NA
2357	HMDB0168750	NA
2358	HMDB0168746	NA
2359	HMDB0168744	NA
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2362	HMDB0168743	NA
2363	HMDB0168739	NA
2364	HMDB0168745	NA
2365	HMDB0041407	NA
2366	HMDB0014838	Eplerenone
2367	HMDB0037039	NA
2368	HMDB0030404	Armillaripin
2369	HMDB0039380	NA
2370	HMDB0173691	NA
2371	HMDB0173689	NA
2372	HMDB0173685	NA
2373	HMDB0173687	NA
2374	HMDB0173683	NA
2375	HMDB0062274	NA
2376	HMDB0062282	NA
2377	HMDB0062292	NA
2378	HMDB0034662	Dihydrofukinolide
2379	HMDB0164538	NA
2380	HMDB0164537	NA
2381	HMDB0164536	NA
2382	HMDB0240233	NA
2383	HMDB0139759	NA
2384	HMDB0139773	NA
2385	HMDB0139772	NA
2386	HMDB0139774	NA
2387	HMDB0139775	NA
2388	HMDB0139761	NA
2389	HMDB0139764	NA
2390	HMDB0139762	NA
2391	HMDB0139760	NA
2392	HMDB0139763	NA
2393	HMDB0139766	NA
2394	HMDB0139767	NA
2395	HMDB0139765	NA
2396	HMDB0139768	NA
2397	HMDB0139769	NA
2398	HMDB0139771	NA
2399	HMDB0139770	NA
2400	HMDB0139778	NA
2401	HMDB0139776	NA
2402	HMDB0139777	NA
2403	HMDB0038618	NA
2404	HMDB0183867	NA
2405	HMDB0183864	NA
2406	HMDB0183876	NA
2407	HMDB0183860	NA
2408	HMDB0183873	NA

2409	HMDB0183891	NA
2410	HMDB0183870	NA
2411	HMDB0183894	NA
2412	HMDB0036548	NA
2413	HMDB0012560	13'-Hydroxy-alpha-tocotrienol
2414	HMDB0035730	Camellectedionol
2415	HMDB0041212	NA
2416	HMDB0033806	2'-O-Methylcajanone
2417	HMDB0030849	Artocarpin
2418	HMDB0140394	NA
2419	HMDB0129645	NA
2420	HMDB0134743	NA
2421	HMDB0162013	NA
2422	HMDB0162016	NA
2423	HMDB0162004	NA
2424	HMDB0142798	NA
2425	HMDB0142979	NA
2426	HMDB0142983	NA
2427	HMDB0142989	NA
2428	HMDB0142992	NA
2429	HMDB0142993	NA
2430	HMDB0143013	NA
2431	HMDB0143016	NA
2432	HMDB0142982	NA
2433	HMDB0142838	NA
2434	HMDB0142799	NA
2435	HMDB0142805	NA
2436	HMDB0142795	NA
2437	HMDB0142808	NA
2438	HMDB0142824	NA
2439	HMDB0142822	NA
2440	HMDB0142828	NA
2441	HMDB0142834	NA
2442	HMDB0142809	NA
2443	HMDB0143017	NA
2444	HMDB0143090	NA
2445	HMDB0143094	NA
2446	HMDB0143096	NA
2447	HMDB0143100	NA
2448	HMDB0143110	NA
2449	HMDB0143964	NA
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2451	HMDB0143091	NA
2452	HMDB0143087	NA
2453	HMDB0143080	NA
2454	HMDB0143023	NA
2455	HMDB0143026	NA
2456	HMDB0143027	NA
2457	HMDB0143067	NA
2458	HMDB0143070	NA
2459	HMDB0143071	NA
2460	HMDB0143106	NA
2461	HMDB0143081	NA
2462	HMDB0142788	NA
2463	HMDB0142729	NA
2464	HMDB0142725	NA
2465	HMDB0142719	NA
2466	HMDB0142718	NA
2467	HMDB0142715	NA
2468	HMDB0142739	NA
2469	HMDB0143077	NA
2470	HMDB0142728	NA
2471	HMDB0142735	NA
2472	HMDB0142738	NA
2473	HMDB0142789	NA
2474	HMDB0142785	NA
2475	HMDB0142758	NA
2476	HMDB0142759	NA
2477	HMDB0142755	NA
2478	HMDB0142748	NA
2479	HMDB0142749	NA
2480	HMDB0142745	NA
2481	HMDB0035858	Obacunone
2482	HMDB0035031	Desoxylimonin
2483	HMDB0039920	NA
2484	HMDB0039918	NA
2485	HMDB0039919	NA
2486	HMDB0015013	Flupenthixol
2487	HMDB0184201	NA
2488	HMDB0183261	NA
2489	HMDB0183260	NA
2490	HMDB0183262	NA
2491	HMDB0183264	NA
2492	HMDB0183267	NA
2493	HMDB0183269	NA
2494	HMDB0184206	NA
2495	HMDB0184207	NA

2496	HMDB0183254	NA
2497	HMDB0183258	NA
2498	HMDB0183250	NA
2499	HMDB0183251	NA
2500	HMDB0039214	NA
2501	HMDB0036631	NA
2502	HMDB0030688	Cyclomulberrin
2503	HMDB0040480	NA
2504	HMDB0029506	Kuwanon B
2505	HMDB0029505	Kuwanon A
2506	HMDB0131612	NA
2507	HMDB0131610	NA
2508	HMDB0131607	NA
2509	HMDB0131606	NA
2510	HMDB0131608	NA
2511	HMDB0131609	NA
2512	HMDB0131611	NA
2513	HMDB0166772	NA
2514	HMDB0166773	NA
2515	HMDB0185408	NA
2516	HMDB0185426	NA
2517	HMDB0160312	NA
2518	HMDB0160311	NA
2519	HMDB0160309	NA
2520	HMDB0160306	NA
2521	HMDB0160305	NA
2522	HMDB0160308	NA
2523	HMDB0160314	NA
2524	HMDB0160317	NA
2525	HMDB0160320	NA
2526	HMDB0036340	NA
2527	HMDB0160333	NA
2528	HMDB0160330	NA
2529	HMDB0160332	NA
2530	HMDB0160329	NA
2531	HMDB0160327	NA
2532	HMDB0160326	NA
2533	HMDB0160324	NA
2534	HMDB0160323	NA
2535	HMDB0160321	NA
2536	HMDB0165007	NA
2537	HMDB0165008	NA
2538	HMDB0175389	NA
2539	HMDB0175386	NA
2540	HMDB0038562	NA
2541	HMDB0014843	Delavirdine
2542	HMDB0014565	Spironolactone
2543	HMDB0180016	NA
2544	HMDB0180015	NA
2545	HMDB0015164	Topotecan
2546	HMDB0145175	NA
2547	HMDB0139832	NA
2548	HMDB0139824	NA
2549	HMDB0139838	NA
2550	HMDB0139829	NA
2551	HMDB0139833	NA
2552	HMDB0139834	NA
2553	HMDB0139836	NA
2554	HMDB0139835	NA
2555	HMDB0139837	NA
2556	HMDB0139830	NA
2557	HMDB0139831	NA
2558	HMDB0139826	NA
2559	HMDB0139825	NA
2560	HMDB0139823	NA
2561	HMDB0042019	NA
2562	HMDB0165600	NA
2563	HMDB0165605	NA
2564	HMDB0163371	NA
2565	HMDB0165603	NA
2566	HMDB0165607	NA
2567	HMDB0179376	NA
2568	HMDB0179375	NA
2569	HMDB0179380	NA
2570	HMDB0179379	NA
2571	HMDB0163370	NA
2572	HMDB0041991	NA
2573	HMDB0035142	(3beta,17alpha,23S)-17,23-Epoxy-3,29-dihydroxy-27-norlanost-8-en-24-one
2574	HMDB0035995	2-(Methoxycarbonyl)-5-methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone
2575	HMDB0164769	NA
2576	HMDB0032669	(3beta,5alpha,9alpha,22E,24R)-3,5,9-Trihydroxy-23-methylergosta-7,22-dien-6-one
2577	HMDB0014780	Pemetrexed
2578	HMDB0181044	NA
2579	HMDB0181045	NA
2580	HMDB0139597	NA
2581	HMDB0139606	NA
2582	HMDB0139601	NA

2583	HMDB0139602	NA
2584	HMDB0029900	Lucuminoside
2585	HMDB0164389	NA
2586	HMDB0164395	NA
2587	HMDB0164391	NA
2588	HMDB0036334	NA
2589	HMDB0142846	NA
2590	HMDB0132661	NA
2591	HMDB0155455	NA
2592	HMDB0155391	NA
2593	HMDB0155394	NA
2594	HMDB0155396	NA
2595	HMDB0155406	NA
2596	HMDB0158123	NA
2597	HMDB0155403	NA
2598	HMDB0155401	NA
2599	HMDB0155400	NA
2600	HMDB0155388	NA
2601	HMDB0155385	NA
2602	HMDB0155412	NA
2603	HMDB0154709	NA
2604	HMDB0154708	NA
2605	HMDB0155409	NA
2606	HMDB0155398	NA
2607	HMDB0035864	13-Hydroxy-5'-O-methylmelledonal
2608	HMDB0038159	NA
2609	HMDB0035690	6-O-Methylarmillaridin
2610	HMDB0157763	NA
2611	HMDB0157761	NA
2612	HMDB0157764	NA
2613	HMDB0157766	NA
2614	HMDB0157765	NA
2615	HMDB0158281	NA
2616	HMDB0170458	NA
2617	HMDB0170461	NA
2618	HMDB0157760	NA
2619	HMDB0157759	NA
2620	HMDB0157609	NA
2621	HMDB0157611	NA
2622	HMDB0157614	NA
2623	HMDB0156809	NA
2624	HMDB0157607	NA
2625	HMDB0157758	NA
2626	HMDB0157613	NA
2627	HMDB0157610	NA
2628	HMDB0157612	NA
2629	HMDB0014818	Moricizine
2630	HMDB0172090	NA
2631	HMDB0030452	Blasticidin S
2632	HMDB0035973	Lucidenic acid M
2633	HMDB0164014	NA
2634	HMDB0171518	NA
2635	HMDB0174361	NA
2636	HMDB0174360	NA
2637	HMDB0174359	NA
2638	HMDB0174715	NA
2639	HMDB0174374	NA
2640	HMDB0174370	NA
2641	HMDB0174371	NA
2642	HMDB0174372	NA
2643	HMDB0174373	NA
2644	HMDB0174367	NA
2645	HMDB0174363	NA
2646	HMDB0174364	NA
2647	HMDB0174362	NA
2648	HMDB0174365	NA
2649	HMDB0174366	NA
2650	HMDB0174369	NA
2651	HMDB0174368	NA
2652	HMDB0183788	NA
2653	HMDB0183785	NA
2654	HMDB0183779	NA
2655	HMDB0183773	NA
2656	HMDB0183776	NA
2657	HMDB0174714	NA
2658	HMDB0174358	NA
2659	HMDB0174356	NA
2660	HMDB0174357	NA
2661	HMDB0174355	NA
2662	HMDB0000969	1,25-Dihydroxyvitamin D3-26,23-lactone
2663	HMDB0164012	NA
2664	HMDB0174354	NA
2665	HMDB0174353	NA
2666	HMDB0174352	NA
2667	HMDB0171517	NA
2668	HMDB0015200	Glipizide
2669	HMDB0041221	NA



2670	HMDB0177910	NA
2671	HMDB0183673	NA
2672	HMDB0183665	NA
2673	HMDB0183643	NA
2674	HMDB0183669	NA
2675	HMDB0183658	NA
2676	HMDB0183654	NA
2677	HMDB0177913	NA
2678	HMDB0183650	NA
2679	HMDB0060821	NA
2680	HMDB0060820	NA
2681	HMDB0060916	NA
2682	HMDB0061137	NA
2683	HMDB0030246	Narceine
2684	HMDB0139781	NA
2685	HMDB0139782	NA
2686	HMDB0139784	NA
2687	HMDB0139783	NA
2688	HMDB0139793	NA
2689	HMDB0139789	NA
2690	HMDB0139791	NA
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2693	HMDB0139787	NA
2694	HMDB0139788	NA
2695	HMDB0139786	NA
2696	HMDB0139785	NA
2697	HMDB0139794	NA
2698	HMDB0144925	NA
2699	HMDB0144855	NA
2700	HMDB0144858	NA
2701	HMDB0144867	NA
2702	HMDB0144870	NA
2703	HMDB0144924	NA
2704	HMDB0144954	NA
2705	HMDB0144955	NA
2706	HMDB0162826	NA
2707	HMDB0162834	NA
2708	HMDB0162874	NA
2709	HMDB0162872	NA
2710	HMDB0162824	NA
2711	HMDB0030329	Neopetasitenine
2712	HMDB0162882	NA
2713	HMDB0001846	Tetrahydrofolic acid
2714	HMDB0062806	NA
2715	HMDB0012936	Dynorphin B (10-13)
2716	HMDB0240599	NA
2717	HMDB0155347	NA
2718	HMDB0155348	NA
2719	HMDB0034064	2-Angeloyl-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one
2720	HMDB0035068	Melleolide M
2721	HMDB0179387	NA
2722	HMDB0179386	NA
2723	HMDB0179390	NA
2724	HMDB0179389	NA
2725	HMDB0061104	NA
2726	HMDB0139815	NA
2727	HMDB0144973	NA
2728	HMDB0144948	NA
2729	HMDB0144943	NA
2730	HMDB0144938	NA
2731	HMDB0139798	NA
2732	HMDB0139801	NA
2733	HMDB0139799	NA
2734	HMDB0139800	NA
2735	HMDB0139797	NA
2736	HMDB0144978	NA
2737	HMDB0139796	NA
2738	HMDB0139795	NA
2739	HMDB0144983	NA
2740	HMDB0144998	NA
2741	HMDB0144988	NA
2742	HMDB0144933	NA
2743	HMDB0144918	NA
2744	HMDB0139811	NA
2745	HMDB0139813	NA
2746	HMDB0139809	NA
2747	HMDB0139806	NA
2748	HMDB0139807	NA
2749	HMDB0139808	NA
2750	HMDB0139814	NA
2751	HMDB0139816	NA
2752	HMDB0139805	NA
2753	HMDB0139817	NA
2754	HMDB0139812	NA
2755	HMDB0139818	NA
2756	HMDB0139804	NA

2757	HMDB0139820	NA
2758	HMDB0139819	NA
2759	HMDB0139803	NA
2760	HMDB0144913	NA
2761	HMDB0139802	NA
2762	HMDB0145003	NA
2763	HMDB0144993	NA
2764	HMDB0145038	NA
2765	HMDB0145034	NA
2766	HMDB0145032	NA
2767	HMDB0139810	NA
2768	HMDB0145018	NA
2769	HMDB0145013	NA
2770	HMDB0145008	NA
2771	HMDB0032622	Phenethyl rutinoid
2772	HMDB0094682	5alpha-Androstan-3alpha,17beta-diol disulfate
2773	HMDB0240625	NA
2774	HMDB0172330	NA
2775	HMDB0159770	NA
2776	HMDB0159769	NA
2777	HMDB0159767	NA
2778	HMDB0159766	NA
2779	HMDB0159765	NA
2780	HMDB0159768	NA
2781	HMDB0062421	NA
2782	HMDB0062416	NA
2783	HMDB0159772	NA
2784	HMDB0159774	NA
2785	HMDB0159773	NA
2786	HMDB0159897	NA
2787	HMDB0159894	NA
2788	HMDB0159896	NA
2789	HMDB0159893	NA
2790	HMDB0159889	NA
2791	HMDB0159890	NA
2792	HMDB0159892	NA
2793	HMDB0159891	NA
2794	HMDB0000558	5a-Cholestane-3a,7a,12a,23,25-pentol
2795	HMDB0002208	Cholestane-3,7,12,24,25-pentol
2796	HMDB0000483	5b-Cholestane-3a,7a,12a,23S,25-pentol
2797	HMDB0000556	5b-Cholestane-3a,7a,12a,24,25-pentol
2798	HMDB0000513	5b-Cholestane-3a,7a,12a,23R,25-pentol
2799	HMDB0002180	5b-Cholestane-3a,7a,12a,25,26-pentol
2800	HMDB0011187	TG(8:0/8:0/8:0)
2801	HMDB0059930	NA
2802	HMDB0035144	(3beta,17alpha,23S,24S)-17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-15-one
2803	HMDB0170385	NA
2804	HMDB0035221	(3beta,17alpha,23S)-17,23-Epoxy-3,28,29-trihydroxy-27-norlanost-8-en-24-one
2805	HMDB0170384	NA
2806	HMDB0167563	NA
2807	HMDB0167569	NA
2808	HMDB0167571	NA
2809	HMDB0167565	NA
2810	HMDB0172392	NA
2811	HMDB0172390	NA
2812	HMDB0167567	NA
2813	HMDB0062208	NA
2814	HMDB0159763	NA
2815	HMDB0159762	NA
2816	HMDB0000359	3a,7a-Dihydroxycoprostanic acid
2817	HMDB0159775	NA
2818	HMDB0159887	NA
2819	HMDB0003533	3a,7a,12a-Trihydroxy-5b-cholestan-26-al
2820	HMDB0159898	NA
2821	HMDB0159886	NA
2822	HMDB0034065	2,9-Bis(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one
2823	HMDB0032601	Muzanzagenin
2824	HMDB0014936	Gentamicin
2825	HMDB0168556	NA
2826	HMDB0168555	NA
2827	HMDB0015019	Quinapril
2828	HMDB0138286	NA
2829	HMDB0175209	NA
2830	HMDB0015560	Thiothixene
2831	HMDB0157393	NA
2832	HMDB0158619	NA
2833	HMDB0169094	NA
2834	HMDB0171247	NA
2835	HMDB00006765	2-Methoxy-estradiol-17b 3-glucuronide
2836	HMDB0010315	4-Hydroxyandrostenedione glucuronide
2837	HMDB0145075	NA
2838	HMDB0145086	NA
2839	HMDB0144922	NA
2840	HMDB0144879	NA
2841	HMDB0144952	NA
2842	HMDB0144894	NA
2843	HMDB0144844	NA

2844	HMDB0144847	NA
2845	HMDB0144882	NA
2846	HMDB0144891	NA
2847	HMDB0031918	Suspensolide F
2848	HMDB0061351	NA
2849	HMDB0160543	NA
2850	HMDB0160539	NA
2851	HMDB0160541	NA
2852	HMDB0160540	NA
2853	HMDB0160542	NA
2854	HMDB0160544	NA
2855	HMDB0160545	NA
2856	HMDB0160516	NA
2857	HMDB0160517	NA
2858	HMDB0160518	NA
2859	HMDB0160515	NA
2860	HMDB0160519	NA
2861	HMDB0160522	NA
2862	HMDB0160521	NA
2863	HMDB0160520	NA
2864	HMDB0160523	NA
2865	HMDB0160526	NA
2866	HMDB0160524	NA
2867	HMDB0160525	NA
2868	HMDB0160528	NA
2869	HMDB0160529	NA
2870	HMDB0160527	NA
2871	HMDB0160530	NA
2872	HMDB0172528	NA
2873	HMDB0170464	NA
2874	HMDB0059931	NA
2875	HMDB0040118	NA
2876	HMDB0184086	NA
2877	HMDB0002385	Celastrol
2878	HMDB0015057	Buprenorphine
2879	HMDB0062331	NA
2880	HMDB0010379	LysoPC(14:0)
2881	HMDB0061691	NA
2882	HMDB0161447	NA
2883	HMDB0179451	NA
2884	HMDB0062337	NA
2885	HMDB0133638	NA
2886	HMDB0133618	NA
2887	HMDB0010407	LysoPC(P-16:0)
2888	HMDB0039086	NA
2889	HMDB0183486	NA
2890	HMDB0183482	NA
2891	HMDB0183483	NA
2892	HMDB0041532	NA
2893	HMDB0030901	Eremopetasitenin B2
2894	HMDB0039930	NA
2895	HMDB0164234	NA
2896	HMDB0135504	NA
2897	HMDB0135508	NA
2898	HMDB0135506	NA
2899	HMDB0031943	(Z)-N-[(4-hydroxyphenyl)methyl]ethoxycarbothioamide 4'-(tri-acetylrrhamnoside)
2900	HMDB0133632	NA
2901	HMDB0133629	NA
2902	HMDB0133763	NA
2903	HMDB0133762	NA
2904	HMDB0135654	NA
2905	HMDB0179487	NA
2906	HMDB0179486	NA
2907	HMDB0133631	NA
2908	HMDB0133626	NA
2909	HMDB0133623	NA
2910	HMDB0133634	NA
2911	HMDB0170798	NA
2912	HMDB0170797	NA
2913	HMDB0170793	NA
2914	HMDB0170796	NA
2915	HMDB0170791	NA
2916	HMDB0170792	NA
2917	HMDB0184654	NA
2918	HMDB0184468	NA
2919	HMDB0139941	NA
2920	HMDB0139958	NA
2921	HMDB0035635	Kanokoside A
2922	HMDB0004482	2-Methoxyestrone 3-glucuronide
2923	HMDB0154676	NA
2924	HMDB0169584	NA
2925	HMDB0146115	NA
2926	HMDB0161563	NA
2927	HMDB0161564	NA
2928	HMDB0161602	NA
2929	HMDB0161603	NA
2930	HMDB0061034	NA

2931	HMDB0033709	Desglucocoroloside
2932	HMDB0015110	Dipyridamole
2933	HMDB0010408	LysoPC(P-18:1(9Z))
2934	HMDB0010384	LysoPC(18:0)
2935	HMDB0011128	LysoPC(0:0/18:0)
2936	HMDB0062195	NA
2937	HMDB0036884	NA
2938	HMDB0181960	NA
2939	HMDB0181959	NA
2940	HMDB0181963	NA
2941	HMDB0181976	NA
2942	HMDB0181975	NA
2943	HMDB0181971	NA
2944	HMDB0181968	NA
2945	HMDB0181967	NA
2946	HMDB0181964	NA
2947	HMDB0158842	NA
2948	HMDB0011481	LysoPE(0:0/20:0)
2949	HMDB0012108	LysoPC(17:0)
2950	HMDB0011511	LysoPE(20:0/0:0)
2951	HMDB0114750	NA
2952	HMDB0062304	NA
2953	HMDB0030291	Daphniphylline
2954	HMDB0183973	NA
2955	HMDB0174607	NA
2956	HMDB0174422	NA
2957	HMDB0171595	NA
2958	HMDB0167550	NA
2959	HMDB0167544	NA
2960	HMDB0167357	NA
2961	HMDB0166718	NA
2962	HMDB0166240	NA
2963	HMDB0162256	NA
2964	HMDB0145366	NA
2965	HMDB0145272	NA
2966	HMDB0145271	NA
2967	HMDB0145352	NA
2968	HMDB0145351	NA
2969	HMDB0029429	Malformin
2970	HMDB0015181	Fluocinonide
2971	HMDB0158654	NA
2972	HMDB0169107	NA
2973	HMDB0169101	NA
2974	HMDB0169097	NA
2975	HMDB0169099	NA
2976	HMDB0169095	NA
2977	HMDB0158636	NA
2978	HMDB0158660	NA
2979	HMDB0158646	NA
2980	HMDB0158642	NA
2981	HMDB0158643	NA
2982	HMDB0158650	NA
2983	HMDB0158656	NA
2984	HMDB0158639	NA
2985	HMDB0169105	NA
2986	HMDB0169110	NA
2987	HMDB0171268	NA
2988	HMDB0171269	NA
2989	HMDB0169108	NA
2990	HMDB0171261	NA
2991	HMDB0033412	Gibberellin A20 13-glucoside
2992	HMDB0171272	NA
2993	HMDB0171264	NA
2994	HMDB0171258	NA
2995	HMDB0171257	NA
2996	HMDB0171253	NA
2997	HMDB0171254	NA
2998	HMDB0169103	NA
2999	HMDB0169111	NA
3000	HMDB0171273	NA
3001	HMDB0158225	NA
3002	HMDB0158226	NA
3003	HMDB0158228	NA
3004	HMDB0158231	NA
3005	HMDB0158234	NA
3006	HMDB0158235	NA
3007	HMDB0158238	NA
3008	HMDB0158621	NA
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3012	HMDB0158633	NA
3013	HMDB0038610	NA
3014	HMDB0037084	NA
3015	HMDB0157580	NA
3016	HMDB0158210	NA
3017	HMDB0158213	NA

3018	HMDB0158219	NA
3019	HMDB0158216	NA
3020	HMDB0158221	NA
3021	HMDB0062314	NA
3022	HMDB0114749	NA
3023	HMDB0114769	NA
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3029	HMDB0167195	NA
3030	HMDB0167174	NA
3031	HMDB0167177	NA
3032	HMDB0167180	NA
3033	HMDB0167183	NA
3034	HMDB0167189	NA
3035	HMDB0167186	NA
3036	HMDB0167192	NA
3037	HMDB0167196	NA
3038	HMDB0167197	NA
3039	HMDB0167227	NA
3040	HMDB0167213	NA
3041	HMDB0167212	NA
3042	HMDB0167216	NA
3043	HMDB0167217	NA
3044	HMDB0167220	NA
3045	HMDB0167223	NA
3046	HMDB0035700	Lucidenic acid J
3047	HMDB0157584	NA
3048	HMDB0157593	NA
3049	HMDB0157590	NA
3050	HMDB0157587	NA
3051	HMDB0174900	NA
3052	HMDB0173534	NA
3053	HMDB0176106	NA
3054	HMDB0173047	NA
3055	HMDB0173001	NA
3056	HMDB0176107	NA
3057	HMDB0172559	NA
3058	HMDB0172560	NA
3059	HMDB0172557	NA
3060	HMDB0172558	NA
3061	HMDB0175792	NA
3062	HMDB0184222	NA
3063	HMDB0183715	NA
3064	HMDB0034679	Cinn cassiol D2 glucoside
3065	HMDB0183713	NA
3066	HMDB0183714	NA
3067	HMDB0184220	NA
3068	HMDB0240600	NA
3069	HMDB0184758	NA
3070	HMDB0184757	NA
3071	HMDB0184774	NA
3072	HMDB0184760	NA
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3081	HMDB0184781	NA
3082	HMDB0184783	NA
3083	HMDB0184777	NA
3084	HMDB0184775	NA
3085	HMDB0184776	NA
3086	HMDB0184769	NA
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3092	HMDB0139968	NA
3093	HMDB0139967	NA
3094	HMDB0139970	NA
3095	HMDB0139971	NA
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3099	HMDB0139984	NA
3100	HMDB0139983	NA
3101	HMDB0139985	NA
3102	HMDB0139982	NA
3103	HMDB0139980	NA
3104	HMDB0139978	NA

3105	HMDB0139981	NA
3106	HMDB0143771	NA
3107	HMDB0143774	NA
3108	HMDB0143775	NA
3109	HMDB0143791	NA
3110	HMDB0143794	NA
3111	HMDB0143795	NA
3112	HMDB0034362	Desglucocheirotoxin
3113	HMDB0166971	NA
3114	HMDB0166972	NA
3115	HMDB0166970	NA
3116	HMDB0173681	NA
3117	HMDB0173690	NA
3118	HMDB0173684	NA
3119	HMDB0186464	NA
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3121	HMDB0173682	NA
3122	HMDB0173688	NA
3123	HMDB0173686	NA
3124	HMDB0240602	NA
3125	HMDB0072546	NA
3126	HMDB0072531	NA
3127	HMDB0072529	NA
3128	HMDB0072338	NA
3129	HMDB0072333	NA
3130	HMDB0072245	NA
3131	HMDB0072206	NA
3132	HMDB0071968	NA
3133	HMDB0071738	NA
3134	HMDB0100886	NA
3135	HMDB0100885	NA
3136	HMDB0100884	NA
3137	HMDB0096650	NA
3138	HMDB0096651	NA
3139	HMDB0096564	NA
3140	HMDB0096562	NA
3141	HMDB0096563	NA
3142	HMDB0071685	NA
3143	HMDB0071676	NA
3144	HMDB0071663	NA
3145	HMDB0096649	NA
3146	HMDB0071443	NA
3147	HMDB0071222	NA
3148	HMDB0071165	NA
3149	HMDB0039897	NA
3150	HMDB0172989	NA
3151	HMDB0172985	NA
3152	HMDB0172986	NA
3153	HMDB0172988	NA
3154	HMDB0015129	Neomycin
3155	HMDB0002160	Harderoporpyrinogen
3156	HMDB0039454	NA
3157	HMDB0173693	NA
3158	HMDB0173692	NA
3159	HMDB0173699	NA
3160	HMDB0173698	NA
3161	HMDB0142988	NA
3162	HMDB0142998	NA
3163	HMDB0142997	NA
3164	HMDB0143001	NA
3165	HMDB0142987	NA
3166	HMDB0142978	NA
3167	HMDB0142977	NA
3168	HMDB0142917	NA
3169	HMDB0142918	NA
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3175	HMDB0142928	NA
3176	HMDB0142927	NA
3177	HMDB0143002	NA
3178	HMDB0143007	NA
3179	HMDB0143006	NA
3180	HMDB0143108	NA
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3186	HMDB0143076	NA
3187	HMDB0143075	NA
3188	HMDB0143066	NA
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3195	HMDB0143021	NA
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3197	HMDB0142915	NA
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3200	HMDB0142902	NA
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3209	HMDB0142912	NA
3210	HMDB0142930	NA
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3212	HMDB0165918	NA
3213	HMDB0173230	NA
3214	HMDB0173229	NA
3215	HMDB0165966	NA
3216	HMDB0164809	NA
3217	HMDB0034433	Riboflavine 2',3',4',5'-tetrabutanoate
3218	HMDB0157944	NA
3219	HMDB0157945	NA
3220	HMDB0157949	NA
3221	HMDB0157950	NA
3222	HMDB0157951	NA
3223	HMDB0157955	NA
3224	HMDB0157956	NA
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3233	HMDB0157896	NA
3234	HMDB0157957	NA
3235	HMDB0158932	NA
3236	HMDB0158968	NA
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3238	HMDB0158963	NA
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3240	HMDB0158959	NA
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3292	HMDB0157862	NA
3293	HMDB0157863	NA
3294	HMDB0157866	NA
3295	HMDB0157867	NA
3296	HMDB0157868	NA
3297	HMDB0157871	NA
3298	HMDB0157873	NA
3299	HMDB0157872	NA
3300	HMDB0038619	NA
3301	HMDB0010698	CerP(d18:0/16:0)
3302	HMDB0007094	DG(15:0/24:1(15Z)/0:0)
3303	HMDB0055994	NA
3304	HMDB0007822	DG(24:1(15Z)/15:0/0:0)
3305	HMDB0165986	NA
3306	HMDB0165987	NA
3307	HMDB0166012	NA
3308	HMDB0166013	NA
3309	HMDB0166011	NA
3310	HMDB0166007	NA
3311	HMDB0170721	NA
3312	HMDB0166009	NA
3313	HMDB0166010	NA
3314	HMDB0166004	NA
3315	HMDB0166005	NA
3316	HMDB0166003	NA
3317	HMDB0166006	NA
3318	HMDB0167988	NA
3319	HMDB0167989	NA
3320	HMDB0168064	NA
3321	HMDB0170719	NA
3322	HMDB0170718	NA
3323	HMDB0168079	NA
3324	HMDB0168080	NA
3325	HMDB0168077	NA
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3328	HMDB0168067	NA
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3330	HMDB0166001	NA
3331	HMDB0166002	NA
3332	HMDB0170734	NA
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3334	HMDB0165973	NA
3335	HMDB0165879	NA
3336	HMDB0165880	NA
3337	HMDB0170735	NA
3338	HMDB0170737	NA
3339	HMDB0166008	NA
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3341	HMDB0165978	NA
3342	HMDB0165999	NA
3343	HMDB0165985	NA
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3345	HMDB0165976	NA
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3347	HMDB0165980	NA
3348	HMDB0165981	NA
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3352	HMDB0177543	NA
3353	HMDB0177537	NA
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3358	HMDB0166014	NA
3359	HMDB0165988	NA
3360	HMDB0184229	NA
3361	HMDB0186286	NA
3362	HMDB0033242	Glycylserylprolylmethionylphenylalanylvalinamide
3363	HMDB0143644	NA
3364	HMDB0041431	NA
3365	HMDB0175656	NA



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3368	HMDB0175662	NA
3369	HMDB0175652	NA
3370	HMDB0175657	NA
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3376	HMDB0186376	NA
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3382	HMDB0168019	NA
3383	HMDB0168021	NA
3384	HMDB0168018	NA
3385	HMDB0168020	NA
3386	HMDB0168017	NA
3387	HMDB0168016	NA
3388	HMDB0168015	NA
3389	HMDB0168014	NA
3390	HMDB0168012	NA
3391	HMDB0168026	NA
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3447	HMDB0166018	NA
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3450	HMDB0161194	NA
3451	HMDB0036400	NA
3452	HMDB0036288	NA

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3457	HMDB0127536	NA
3458	HMDB0127543	NA
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3460	HMDB0127544	NA
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3463	HMDB0174236	NA
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3465	HMDB0174234	NA
3466	HMDB0174235	NA
3467	HMDB0001261	Coproporphyrinogen III
3468	HMDB0002158	Coproporphyrinogen I
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3628	HMDB0187293	NA
3629	HMDB0187126	NA
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3631	HMDB0187130	NA
3632	HMDB0187137	NA
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3671	HMDB0185073	NA
3672	HMDB0185090	NA
3673	HMDB0185085	NA
3674	HMDB0185086	NA
3675	HMDB0185082	NA
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3677	HMDB0185080	NA
3678	HMDB0185076	NA
3679	HMDB0185075	NA
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3681	HMDB0186607	NA
3682	HMDB0185959	NA
3683	HMDB0185958	NA
3684	HMDB0186605	NA
3685	HMDB0185955	NA
3686	HMDB0185954	NA
3687	HMDB0185951	NA
3688	HMDB0185950	NA
3689	HMDB0185947	NA
3690	HMDB0185962	NA
3691	HMDB0185963	NA
3692	HMDB0185966	NA
3693	HMDB0186604	NA
3694	HMDB0186601	NA
3695	HMDB0186600	NA
3696	HMDB0186599	NA
3697	HMDB0186595	NA
3698	HMDB0186593	NA
3699	HMDB0186594	NA
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3701	HMDB0185945	NA
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3708	HMDB0185915	NA
3709	HMDB0185914	NA
3710	HMDB0185909	NA
3711	HMDB0185927	NA
3712	HMDB0185928	NA
3713	HMDB0185931	NA

3714	HMDB0185946	NA
3715	HMDB0185940	NA
3716	HMDB0185941	NA
3717	HMDB0185939	NA
3718	HMDB0185935	NA
3719	HMDB0185936	NA
3720	HMDB0185938	NA
3721	HMDB0185932	NA
3722	HMDB0185910	NA
3723	HMDB0175631	NA
3724	HMDB0034552	Medicagenic acid 3-O-beta-D-glucoside
3725	HMDB0041347	NA
3726	HMDB0169217	NA
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3728	HMDB0169220	NA
3729	HMDB0169219	NA
3730	HMDB0175632	NA
3731	HMDB0175630	NA
3732	HMDB0034636	Phytolaccasaponin G
3733	HMDB0175633	NA
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3741	HMDB0176008	NA
3742	HMDB0176013	NA
3743	HMDB0176014	NA
3744	HMDB0176016	NA
3745	HMDB0176015	NA
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3747	HMDB0176628	NA
3748	HMDB0178344	NA
3749	HMDB0178345	NA
3750	HMDB0178346	NA
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3756	HMDB0175821	NA
3757	HMDB0175820	NA
3758	HMDB0175822	NA
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3762	HMDB0175826	NA
3763	HMDB0175840	NA
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3768	HMDB0175836	NA
3769	HMDB0175837	NA
3770	HMDB0175841	NA
3771	HMDB0178542	NA
3772	HMDB0178541	NA
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3775	HMDB0178548	NA
3776	HMDB0178540	NA
3777	HMDB0036529	NA
3778	HMDB0036528	NA
3779	HMDB0014454	Vindesine
3780	HMDB0116519	NA
3781	HMDB0116569	NA
3782	HMDB0116555	NA
3783	HMDB0116549	NA
3784	HMDB0116538	NA
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3786	HMDB0176104	NA
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3797	HMDB0178529	NA
3798	HMDB0178528	NA
3799	HMDB0178530	NA
3800	HMDB0178531	NA

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3807	HMDB0054629	NA
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3809	HMDB0054889	NA
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3811	HMDB0054844	NA
3812	HMDB0055933	NA
3813	HMDB0055867	NA
3814	HMDB0055077	NA
3815	HMDB0054892	NA
3816	HMDB0060165	NA
3817	HMDB0062518	NA
3818	HMDB0112245	NA
3819	HMDB0100000	NA
3820	HMDB0115979	NA
3821	HMDB0006975	CDP-DG(16:0/22:3(10Z,13Z,16Z))
3822	HMDB0145559	NA
3823	HMDB0145553	NA
3824	HMDB0145556	NA
3825	HMDB0145554	NA
3826	HMDB0145560	NA
3827	HMDB0145576	NA
3828	HMDB0145569	NA
3829	HMDB0145561	NA
3830	HMDB0145562	NA
3831	HMDB0145563	NA
3832	HMDB0145558	NA
3833	HMDB0145557	NA
3834	HMDB0145555	NA
3835	HMDB0055799	NA
3836	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))
3837	HMDB0046646	NA
3838	HMDB0004879	Trihexosylceramide (d18:1/16:0)
3839	HMDB0004889	Ganglioside GA2 (d18:1/9Z-18:1)
3840	HMDB0001543	Diguanosine hexaphosphate
3841	HMDB0006563	Hexaglutamyl folate
3842	HMDB0060217	NA
3843	HMDB0032781	Acetyljuguboside B

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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)

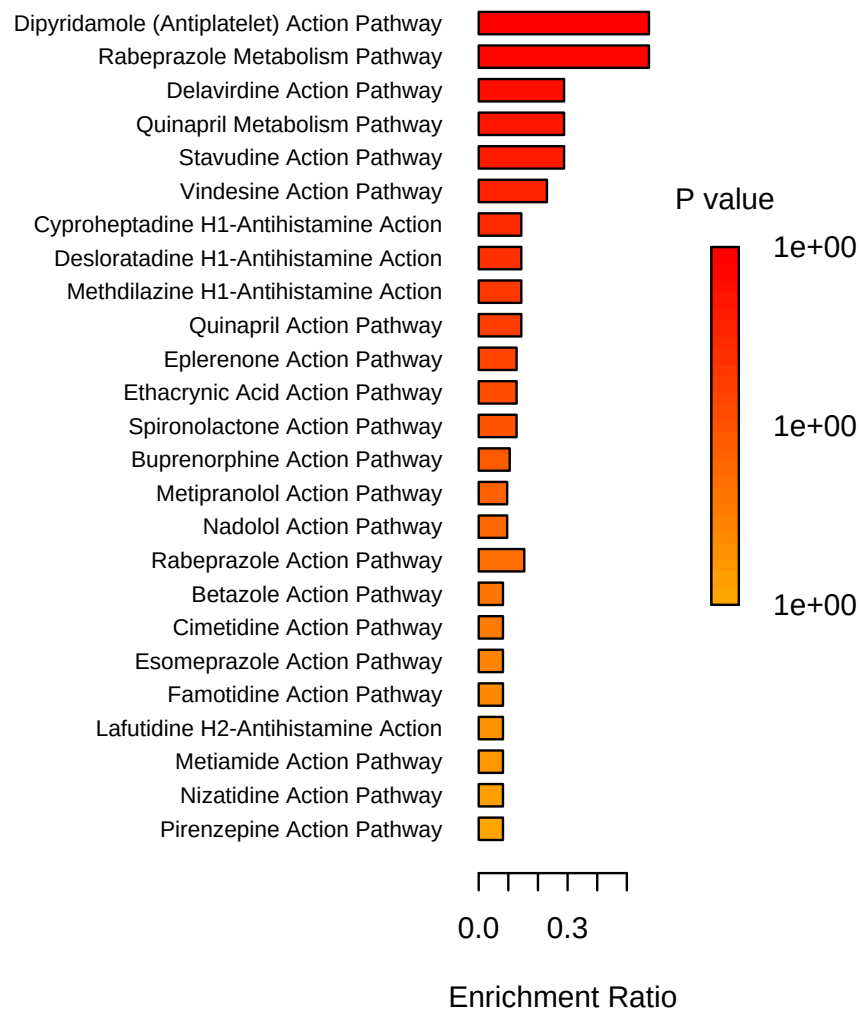


Figure 1: Summary Plot for Over Representation Analysis (ORA)



Table 2: Result from Over Representation Analysis

	total	expected	hits	Raw p	Holm p	FDR
Dipyridamole (Antiplatelet) Action Pathway	2	1.74	1	9.83E-01	1.00E+00	1.00E+00
Rabeprazole Metabolism Pathway	2	1.74	1	9.83E-01	1.00E+00	1.00E+00
Delavirdine Action Pathway	4	3.47	1	1.00E+00	1.00E+00	1.00E+00
Quinapril Metabolism Pathway	4	3.47	1	1.00E+00	1.00E+00	1.00E+00
Stavudine Action Pathway	4	3.47	1	1.00E+00	1.00E+00	1.00E+00
Vindesine Action Pathway	5	4.34	1	1.00E+00	1.00E+00	1.00E+00
Cyproheptadine H1-Antihistamine Action	8	6.95	1	1.00E+00	1.00E+00	1.00E+00
Desloratadine H1-Antihistamine Action	8	6.95	1	1.00E+00	1.00E+00	1.00E+00
Methdilazine H1-Antihistamine Action	8	6.95	1	1.00E+00	1.00E+00	1.00E+00
Quinapril Action Pathway	8	6.95	1	1.00E+00	1.00E+00	1.00E+00
Eplerenone Action Pathway	9	7.82	1	1.00E+00	1.00E+00	1.00E+00
Ethacrynic Acid Action Pathway	9	7.82	1	1.00E+00	1.00E+00	1.00E+00
Spironolactone Action Pathway	9	7.82	1	1.00E+00	1.00E+00	1.00E+00
Buprenorphine Action Pathway	11	9.55	1	1.00E+00	1.00E+00	1.00E+00
Metipranolol Action Pathway	12	10.40	1	1.00E+00	1.00E+00	1.00E+00
Nadolol Action Pathway	12	10.40	1	1.00E+00	1.00E+00	1.00E+00
Rabeprazole Action Pathway	15	13.00	2	1.00E+00	1.00E+00	1.00E+00
Betazole Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Cimetidine Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Esomeprazole Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Famotidine Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Lafutidine H2-Antihistamine Action	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Metiamide Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Nizatidine Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Pirenzepine Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Ranitidine Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Roxatidine acetate Action Pathway	14	12.20	1	1.00E+00	1.00E+00	1.00E+00
Ibuprofen Metabolism Pathway	15	13.00	1	1.00E+00	1.00E+00	1.00E+00
Lansoprazole Action Pathway	15	13.00	1	1.00E+00	1.00E+00	1.00E+00
Pantoprazole Action Pathway	15	13.00	1	1.00E+00	1.00E+00	1.00E+00
Omeprazole Action Pathway	16	13.90	1	1.00E+00	1.00E+00	1.00E+00
Acetaminophen Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Acetylsalicylic Acid Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Alendronate Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Antipyrine Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Antrafenine Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Atorvastatin Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Azathioprine Action Pathway	92	79.90	4	1.00E+00	1.00E+00	1.00E+00
Bromfenac Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Carprofen Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Celecoxib Action Pathway	74	64.30	4	1.00E+00	1.00E+00	1.00E+00
Cerivastatin Action Pathway	47	40.80	1	1.00E+00	1.00E+00	1.00E+00
Citalopram Action Pathway	28	24.30	1	1.00E+00	1.00E+00	1.00E+00
Citalopram Metabolism Pathway	19	16.50	1	1.00E+00	1.00E+00	1.00E+00
Cyclophosphamide Action Pathway	25	21.70	1	1.00E+00	1.00E+00	1.00E+00
Cyclophosphamide Metabolism Pathway	25	21.70	1	1.00E+00	1.00E+00	1.00E+00
Diclofenac Action Pathway	68	59.10	4	1.00E+00	1.00E+00	1.00E+00
Diffunisal Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Etodolac Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Etoricoxib Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Fenoprofen Action Pathway	67	58.20	5	1.00E+00	1.00E+00	1.00E+00
Flurbiprofen Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Fluvastatin Action Pathway	49	42.60	1	1.00E+00	1.00E+00	1.00E+00
Gentamicin Action Pathway	20	17.40	1	1.00E+00	1.00E+00	1.00E+00
Ibandronate Action Pathway	48	41.70	2	1.00E+00	1.00E+00	1.00E+00
Ibuprofen Action Pathway	76	66.00	5	1.00E+00	1.00E+00	1.00E+00
Ifosfamide Action Pathway	23	20.00	2	1.00E+00	1.00E+00	1.00E+00
Ifosfamide Metabolism Pathway	23	20.00	2	1.00E+00	1.00E+00	1.00E+00
Indomethacin Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Ketoprofen Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Ketorolac Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Lornoxicam Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Lovastatin Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Lumiracoxib Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Magnesium salicylate Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Mefenamic Acid Action Pathway	67	58.20	5	1.00E+00	1.00E+00	1.00E+00
Meloxicam Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Mercaptopurine Action Pathway	90	78.20	4	1.00E+00	1.00E+00	1.00E+00
Methotrexate Action Pathway	30	26.10	1	1.00E+00	1.00E+00	1.00E+00
Nabumetone Action Pathway	67	58.20	5	1.00E+00	1.00E+00	1.00E+00
Naproxen Action Pathway	68	59.10	4	1.00E+00	1.00E+00	1.00E+00
Neomycin Action Pathway	20	17.40	1	1.00E+00	1.00E+00	1.00E+00
Nepafenac Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Nicotine Action Pathway	36	31.30	1	1.00E+00	1.00E+00	1.00E+00
Nicotine Metabolism Pathway	26	22.60	1	1.00E+00	1.00E+00	1.00E+00
Oxaprozin Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Pamidronate Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Phenylbutazone Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Piroxicam Action Pathway	68	59.10	4	1.00E+00	1.00E+00	1.00E+00
Pravastatin Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Risedronate Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Rofecoxib Action Pathway	66	57.30	4	1.00E+00	1.00E+00	1.00E+00

Rosuvastatin Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Salicylate-sodium Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Salicylic Acid Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Salsalate Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Simvastatin Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00
Sulindac Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Suprofen Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Tenoxicam Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Thioguanine Action Pathway	91	79.00	4	1.00E+00	1.00E+00	1.00E+00
Tiaprofenic Acid Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Tolmetin Action Pathway	67	58.20	5	1.00E+00	1.00E+00	1.00E+00
Trisalicylate-choline Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Valdecoxib Action Pathway	67	58.20	4	1.00E+00	1.00E+00	1.00E+00
Valproic Acid Metabolism Pathway	37	32.10	3	1.00E+00	1.00E+00	1.00E+00
Zoledronate Action Pathway	48	41.70	1	1.00E+00	1.00E+00	1.00E+00

## 7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "cmpd.vec<-c(\"HMDB0000123\", \"HMDB0014691\", \"HMDB0031239\", \"HMDB0161401\", \"HMDB0000925\", \"I
[3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
[4] "mSet<-CrossReferencing(mSet, \"hmdb\");"
[5] "mSet<-CreateMappingResultTable(mSet)"
[6] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[7] "mSet<-SetMetabolomeFilter(mSet, F);"
[8] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[9] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA)"
[10] "mSet<-SaveTransformedData(mSet)"
[11] "UpdateDataObjects(\"conc\", \"msetora\", FALSE)"
[12] "mSet<-SetMetabolomeFilter(mSet, F);"
[13] "mSet<-SetCurrentMsetLib(mSet, \"smpdb_pathway\", 2);"
[14] "mSet<-CalculateHyperScore(mSet)"
[15] "mSet<-PlotORA(mSet, \"ora_0_\", \"net\", \"png\", 72, width=NA)"
[16] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_0_\", \"png\", 72, width=NA)"
[17] "mSet<-CalculateHyperScore(mSet)"
[18] "mSet<-PlotORA(mSet, \"ora_1_\", \"net\", \"png\", 72, width=NA)"
[19] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_1_\", \"png\", 72, width=NA)"
[20] "mSet<-SaveTransformedData(mSet)"
[21] "UpdateDataObjects(\"conc\", \"pathora\", FALSE)"
[22] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[23] "mSet<-SetMetabolomeFilter(mSet, F);"
[24] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[25] "mSet<-PlotPathSummary(mSet, F, \"path_view_1_\", \"png\", 72, width=NA)"
[26] "mSet<-SaveTransformedData(mSet)"
[27] "UpdateDataObjects(\"conc\", \"msetora\", FALSE)"
[28] "mSet<-SetMetabolomeFilter(mSet, F);"
[29] "mSet<-SetCurrentMsetLib(mSet, \"drug\", 2);"
[30] "mSet<-CalculateHyperScore(mSet)"
[31] "mSet<-PlotORA(mSet, \"ora_2_\", \"net\", \"png\", 72, width=NA)"
[32] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_2_\", \"png\", 72, width=NA)"
[33] "mSet<-CalculateHyperScore(mSet)"
[34] "mSet<-PlotORA(mSet, \"ora_3_\", \"net\", \"png\", 72, width=NA)"
[35] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_3_\", \"png\", 72, width=NA)"
[36] "mSet<-SaveTransformedData(mSet)"
[37] "mSet<-PreparePDFReport(mSet, \"guest16429080455207080108\")\n"
```

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The report was generated on Mon May 24 13:00:17 2021 with R version 4.0.2 (2020-06-22).