

Metabolomic Data Analysis with MetaboAnalyst 6.0

Name: guest5869009112759895119

August 2, 2024

1 Background

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

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

2 Data Input

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

3 Compound Name Matching

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

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

	Query	Match	HMDB	PubCh
1	HMDB0000042	Acetic acid	HMDB0000042	176
2	HMDB0003344	Glycolaldehyde	HMDB0003344	756
3	HMDB0002165	NA	NA	NA
4	C00033	NA	NA	NA
5	C00266	NA	NA	NA
6	CHEBI:15366	NA	NA	NA
7	CHEBI:17071	NA	NA	NA
8	CHEBI:77699	NA	NA	NA
9	HMDB0000119	Glyoxylic acid	HMDB0000119	760

10	C00048	NA	NA	NA
11	CHEBI:16891	NA	NA	NA
12	CHEBI:36657	NA	NA	NA
13	HMDB0000123	Glycine	HMDB0000123	750
14	HMDB0014691	Acetohydroxamic Acid	HMDB0014691	1990
15	HMDB0031239	Ethyl nitrite	HMDB0031239	8026
16	C00037	NA	NA	NA
17	C01837	NA	NA	NA
18	C06808	NA	NA	NA
19	C19445	NA	NA	NA
20	CHEBI:15428	NA	NA	NA
21	CHEBI:16268	NA	NA	NA
22	CHEBI:27777	NA	NA	NA
23	CHEBI:30321	NA	NA	NA
24	CHEBI:45379	NA	NA	NA
25	CHEBI:49029	NA	NA	NA
26	CHEBI:57305	NA	NA	NA
27	CHEBI:76606	NA	NA	NA
28	CHEBI:77894	NA	NA	NA
29	HMDB0000115	Glycolic acid	HMDB0000115	757
30	HMDB0031608	Peracetic acid	HMDB0031608	6585
31	HMDB0003035	NA	NA	NA
32	C00160	NA	NA	NA
33	CHEBI:17497	NA	NA	NA
34	HMDB0013749	2-Methylfuran	HMDB0013749	10797
35	HMDB0031597	2,4-Pentadienal	HMDB0031597	535669
36	CHEBI:35592	NA	NA	NA
37	CHEBI:35593	NA	NA	NA
38	CHEBI:969439	NA	NA	NA
39	HMDB0002039	2-Pyrrolidinone	HMDB0002039	12025
40	HMDB0060427	NA	NA	NA
41	C02659	NA	NA	NA
42	C11118	NA	NA	NA
43	CHEBI:15348	NA	NA	NA
44	CHEBI:36592	NA	NA	NA
45	CHEBI:40599	NA	NA	NA
46	CHEBI:51457	NA	NA	NA
47	CHEBI:51759	NA	NA	NA
48	CHEBI:53614	NA	NA	NA
49	HMDB0000056	beta-Alanine	HMDB0000056	239
50	HMDB0000161	L-Alanine	HMDB0000161	5950
51	HMDB0000271	Sarcosine	HMDB0000271	1088
52	HMDB0001310	D-Alanine	HMDB0001310	71080
53	HMDB0031219	Ethyl carbamate	HMDB0031219	5641
54	HMDB0062251	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform A (protein)	HMDB0062251	602
55	C00041	NA	NA	NA
56	C00099	NA	NA	NA
57	C00133	NA	NA	NA
58	C00213	NA	NA	NA
59	C01401	NA	NA	NA
60	C01537	NA	NA	NA
61	C02116	NA	NA	NA
62	C11488	NA	NA	NA
63	CHEBI:15570	NA	NA	NA
64	CHEBI:15611	NA	NA	NA
65	CHEBI:16037	NA	NA	NA
66	CHEBI:16449	NA	NA	NA
67	CHEBI:16958	NA	NA	NA
68	CHEBI:16977	NA	NA	NA
69	CHEBI:17967	NA	NA	NA
70	CHEBI:38544	NA	NA	NA
71	CHEBI:57416	NA	NA	NA
72	CHEBI:57433	NA	NA	NA
73	CHEBI:57966	NA	NA	NA
74	CHEBI:57972	NA	NA	NA
75	CHEBI:64738	NA	NA	NA
76	CHEBI:66916	NA	NA	NA
77	CHEBI:75144	NA	NA	NA
78	CHEBI:76050	NA	NA	NA
79	CHEBI:76261	NA	NA	NA
80	CHEBI:87375	NA	NA	NA
81	HMDB0000718	Isovaleric acid	HMDB0000718	10430
82	HMDB0000892	Valeric acid	HMDB0000892	7991
83	HMDB0002176	Ethylmethylacetic acid	HMDB0002176	8314
84	HMDB0030058	Ethyl propionate	HMDB0030058	7749
85	HMDB0031175	Tetrahydro-2-furanmethanol	HMDB0031175	7360
86	HMDB0031241	Isopropyl acetate	HMDB0031241	7915
87	HMDB0031247	2-Methylpropyl formate	HMDB0031247	10957
88	HMDB0031249	Methyl isobutyrate	HMDB0031249	11039
89	HMDB0031516	3-Hydroxy-2-pentanone	HMDB0031516	62484
90	HMDB0032230	2,4-Dimethyl-1,3-dioxolane	HMDB0032230	102993
91	HMDB0032263	Ethylene oxide/propylene oxide copolymer	HMDB0032263	228958
92	HMDB0033742	(S)-2-Methylbutanoic acid	HMDB0033742	448893
93	HMDB0033890	Methyl butyrate	HMDB0033890	12180
94	HMDB0034237	Propyl acetate	HMDB0034237	7997
95	HMDB0039799	Tetrahydro-2-methyl-3-furanol	HMDB0039799	34742
96	HMDB0040575	Butyl formate	HMDB0040575	11614

97	HMDB0041992	NA	NA	NA
98	HMDB0059678	1-Hydroxy-2-pentanone	HMDB0059678	522131
99	C00803	NA	NA	NA
100	C08262	NA	NA	NA
101	C18319	NA	NA	NA
102	CHEBI:1132558	NA	NA	NA
103	CHEBI:137944	NA	NA	NA
104	CHEBI:167460	NA	NA	NA
105	CHEBI:17418	NA	NA	NA
106	CHEBI:28484	NA	NA	NA
107	CHEBI:32026	NA	NA	NA
108	CHEBI:37070	NA	NA	NA
109	CHEBI:38655	NA	NA	NA
110	CHEBI:40116	NA	NA	NA
111	CHEBI:41330	NA	NA	NA
112	CHEBI:45133	NA	NA	NA
113	CHEBI:45525	NA	NA	NA
114	CHEBI:73689	NA	NA	NA
115	CHEBI:88514	NA	NA	NA
116	HMDB0000092	Dimethylglycine	HMDB0000092	673
117	HMDB0000112	gamma-Aminobutyric acid	HMDB0000112	119
118	HMDB0000452	L-alpha-Aminobutyric acid	HMDB0000452	80283
119	HMDB0000650	D-alpha-Aminobutyric acid	HMDB0000650	439691
120	HMDB0001906	2-Aminoisobutyric acid	HMDB0001906	6119
121	HMDB0002166	(S)-beta-Aminoisobutyric acid	HMDB0002166	439434
122	HMDB0002299	(R)-beta-Aminoisobutyric acid	HMDB0002299	545982
123	HMDB0003911	3-Aminoisobutanoic acid	HMDB0003911	64956
124	HMDB0031329	Butyl nitrite	HMDB0031329	10996
125	HMDB0031654	3-Aminobutanoic acid	HMDB0031654	10932
126	HMDB0038394	O-Acetyethanolamine	HMDB0038394	112720
127	HMDB0041945	N-Ethylglycine	HMDB0041945	699207
128	HMDB0000485	NA	NA	NA
129	HMDB0000581	NA	NA	NA
130	HMDB0094692	N-Methylalanine	HMDB0094692	528872
131	HMDB0005815	NA	NA	NA
132	C00334	NA	NA	NA
133	C01026	NA	NA	NA
134	C01205	NA	NA	NA
135	C02261	NA	NA	NA
136	C02356	NA	NA	NA
137	C02721	NA	NA	NA
138	C03284	NA	NA	NA
139	C03665	NA	NA	NA
140	C05145	NA	NA	NA
141	C11109	NA	NA	NA
142	C11735	NA	NA	NA
143	C19514	NA	NA	NA
144	CHEBI:15620	NA	NA	NA
145	CHEBI:16320	NA	NA	NA
146	CHEBI:16865	NA	NA	NA
147	CHEBI:17519	NA	NA	NA
148	CHEBI:17724	NA	NA	NA
149	CHEBI:27389	NA	NA	NA
150	CHEBI:27971	NA	NA	NA
151	CHEBI:28797	NA	NA	NA
152	CHEBI:33094	NA	NA	NA
153	CHEBI:35619	NA	NA	NA
154	CHEBI:35621	NA	NA	NA
155	CHEBI:37081	NA	NA	NA
156	CHEBI:46643	NA	NA	NA
157	CHEBI:57440	NA	NA	NA
158	CHEBI:57731	NA	NA	NA
159	CHEBI:58175	NA	NA	NA
160	CHEBI:58251	NA	NA	NA
161	CHEBI:58655	NA	NA	NA
162	CHEBI:59888	NA	NA	NA
163	CHEBI:64739	NA	NA	NA
164	CHEBI:74359	NA	NA	NA
165	CHEBI:74687	NA	NA	NA
166	HMDB0000008	2-Hydroxybutyric acid	HMDB0000008	440864
167	HMDB0000011	3-Hydroxybutyric acid	HMDB0000011	441
168	HMDB0000023	(S)-3-Hydroxyisobutyric acid	HMDB0000023	440873
169	HMDB0000336	(R)-3-Hydroxyisobutyric acid	HMDB0000336	112172
170	HMDB0000357	NA	NA	NA
171	HMDB0000442	(S)-3-Hydroxybutyric acid	HMDB0000442	94318
172	HMDB0000710	4-Hydroxybutyric acid	HMDB0000710	10413
173	HMDB0000729	alpha-Hydroxyisobutyric acid	HMDB0000729	11671
174	HMDB0031212	Ethoxyacetic acid	HMDB0031212	12301
175	HMDB0000435	NA	NA	NA
176	HMDB0059748	NA	NA	NA
177	HMDB0000758	NA	NA	NA
178	HMDB0126088	NA	NA	NA
179	HMDB0011597	NA	NA	NA
180	C00989	NA	NA	NA
181	C01089	NA	NA	NA
182	C01188	NA	NA	NA
183	C01991	NA	NA	NA

184	C03197	NA	NA	NA
185	C05984	NA	NA	NA
186	C06001	NA	NA	NA
187	C14601	NA	NA	NA
188	CHEBI:1148	NA	NA	NA
189	CHEBI:17066	NA	NA	NA
190	CHEBI:17290	NA	NA	NA
191	CHEBI:18064	NA	NA	NA
192	CHEBI:20067	NA	NA	NA
193	CHEBI:30830	NA	NA	NA
194	CHEBI:37373	NA	NA	NA
195	CHEBI:37551	NA	NA	NA
196	CHEBI:50129	NA	NA	NA
197	CHEBI:50612	NA	NA	NA
198	CHEBI:50613	NA	NA	NA
199	CHEBI:741468	NA	NA	NA
200	CHEBI:74611	NA	NA	NA
201	CHEBI:83221	NA	NA	NA
202	CHEBI:83222	NA	NA	NA
203	HMDB0000187	Serine	HMDB0000187	5951
204	HMDB0003406	D-Serine	HMDB0003406	71077
205	HMDB0000589	NA	NA	NA
206	HMDB0062263	NA	NA	NA
207	C00065	NA	NA	NA
208	C00716	NA	NA	NA
209	C00740	NA	NA	NA
210	CHEBI:16523	NA	NA	NA
211	CHEBI:17115	NA	NA	NA
212	CHEBI:17822	NA	NA	NA
213	CHEBI:33384	NA	NA	NA
214	CHEBI:35243	NA	NA	NA
215	CHEBI:35247	NA	NA	NA
216	CHEBI:49042	NA	NA	NA
217	HMDB0000139	Glyceric acid	HMDB0000139	439194
218	HMDB0006372	L-Glyceric acid	HMDB0006372	632677
219	HMDB0031818	NA	NA	NA
220	C00258	NA	NA	NA
221	CHEBI:32398	NA	NA	NA
222	CHEBI:33508	NA	NA	NA
223	CHEBI:74324	NA	NA	NA
224	HMDB0029734	3-Ethylpyridine	HMDB0029734	10823
225	HMDB0032244	2,4-Dimethylpyridine	HMDB0032244	7936
226	HMDB0032972	2,6-Dimethylpyridine	HMDB0032972	7937
227	HMDB0033871	Benzylamine	HMDB0033871	7504
228	HMDB0041965	O-Toluidine	HMDB0041965	7242
229	C14403	NA	NA	NA
230	C15562	NA	NA	NA
231	CHEBI:127904	NA	NA	NA
232	CHEBI:32548	NA	NA	NA
233	CHEBI:40538	NA	NA	NA
234	CHEBI:66892	NA	NA	NA
235	HMDB0004230	Pyrrole-2-carboxylic acid	HMDB0004230	12473
236	HMDB0038175	2-Acetylloxazole	HMDB0038175	197827
237	HMDB0003094	NA	NA	NA
238	C01059	NA	NA	NA
239	C02932	NA	NA	NA
240	C03056	NA	NA	NA
241	C03927	NA	NA	NA
242	C05942	NA	NA	NA
243	CHEBI:131454	NA	NA	NA
244	CHEBI:16364	NA	NA	NA
245	CHEBI:17681	NA	NA	NA
246	CHEBI:28630	NA	NA	NA
247	CHEBI:29053	NA	NA	NA
248	CHEBI:36751	NA	NA	NA
249	CHEBI:68076	NA	NA	NA
250	HMDB0000870	Histamine	HMDB0000870	774
251	HMDB0014417	Betazole	HMDB0014417	7741
252	HMDB0060263	NA	NA	NA
253	C00388	NA	NA	NA
254	CHEBI:18295	NA	NA	NA
255	CHEBI:59170	NA	NA	NA
256	HMDB0029717	2-Thiophenecarboxaldehyde	HMDB0029717	7364
257	CHEBI:246417	NA	NA	NA
258	CHEBI:87301	NA	NA	NA
259	CHEBI:87611	NA	NA	NA
260	HMDB0001301	1-Pyrroline-5-carboxylic acid	HMDB0001301	440162
261	HMDB0006875	1-Pyrroline-2-carboxylic acid	HMDB0006875	440046
262	HMDB0002240	NA	NA	NA
263	C03564	NA	NA	NA
264	C03912	NA	NA	NA
265	C04322	NA	NA	NA
266	C07275	NA	NA	NA
267	CHEBI:1372	NA	NA	NA
268	CHEBI:24322	NA	NA	NA
269	CHEBI:32475	NA	NA	NA
270	CHEBI:32481	NA	NA	NA

271	CHEBI:36750	NA	NA	NA
272	CHEBI:36761	NA	NA	NA
273	CHEBI:371	NA	NA	NA
274	CHEBI:39785	NA	NA	NA
275	CHEBI:41433	NA	NA	NA
276	CHEBI:5435	NA	NA	NA
277	CHEBI:61920	NA	NA	NA
278	CHEBI:61965	NA	NA	NA
279	CHEBI:85428	NA	NA	NA
280	CHEBI:90860	NA	NA	NA
281	HMDB0000351	(2S,3R)-3-Hydroxy-2-methylbutanoic acid	HMDB0000351	123133
282	HMDB0000354	2-Methyl-3-hydroxybutyric acid	HMDB0000354	160471
283	HMDB0000396	2-Ethylhydracrylic acid	HMDB0000396	188979
284	HMDB0000407	2-Hydroxy-3-methylbutyric acid	HMDB0000407	99823
285	HMDB0000410	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	HMDB0000410	123133
286	HMDB0000531	3-Hydroxyvaleric acid	HMDB0000531	107802
287	HMDB0000642	Erythronilic acid	HMDB0000642	118158
288	HMDB0000754	3-Hydroxyisovaleric acid	HMDB0000754	69362
289	HMDB0001863	2-Hydroxyvaleric acid	HMDB0001863	98009
290	HMDB0001987	2-Hydroxy-2-methylbutyric acid	HMDB0001987	95433
291	HMDB0002011	4-Hydroxyisovaleric acid	HMDB0002011	131760
292	HMDB0040735	Ethyl lactate	HMDB0040735	7344
293	HMDB0041603	Methyl 3-hydroxybutyrate	HMDB0041603	15146
294	HMDB0000420	NA	NA	NA
295	HMDB0059844	NA	NA	NA
296	HMDB0000605	NA	NA	NA
297	HMDB0061927	5-Hydroxypentanoic acid	HMDB0061927	25945
298	HMDB0062584	NA	NA	NA
299	HMDB0130836	NA	NA	NA
300	HMDB0002187	NA	NA	NA
301	HMDB0002321	NA	NA	NA
302	C02804	NA	NA	NA
303	C20827	NA	NA	NA
304	CHEBI:37051	NA	NA	NA
305	CHEBI:37052	NA	NA	NA
306	CHEBI:37084	NA	NA	NA
307	CHEBI:37552	NA	NA	NA
308	CHEBI:38441.1	NA	NA	NA
309	CHEBI:45564	NA	NA	NA
310	CHEBI:46415	NA	NA	NA
311	CHEBI:60631	NA	NA	NA
312	CHEBI:60645	NA	NA	NA
313	CHEBI:60647	NA	NA	NA
314	CHEBI:68454	NA	NA	NA
315	CHEBI:741550	NA	NA	NA
316	CHEBI:78321	NA	NA	NA
317	CHEBI:78322	NA	NA	NA
318	CHEBI:78323	NA	NA	NA
319	CHEBI:79019	NA	NA	NA
320	CHEBI:82956	NA	NA	NA
321	HMDB0002362	2,4-Diaminobutyric acid	HMDB0002362	470
322	HMDB0006284	L-2,4-diaminobutyric acid	HMDB0006284	134490
323	C03283	NA	NA	NA
324	C08291	NA	NA	NA
325	CHEBI:48950	NA	NA	NA
326	CHEBI:64307	NA	NA	NA
327	CHEBI:73169	NA	NA	NA
328	HMDB0000574	L-Cysteine	HMDB0000574	5862
329	HMDB0003417	D-Cysteine	HMDB0003417	92851
330	C00097	NA	NA	NA
331	C00736	NA	NA	NA
332	C00793	NA	NA	NA
333	CHEBI:15356	NA	NA	NA
334	CHEBI:16375	NA	NA	NA
335	CHEBI:17561	NA	NA	NA
336	CHEBI:35235	NA	NA	NA
337	CHEBI:35236	NA	NA	NA
338	CHEBI:35237	NA	NA	NA
339	HMDB0003903	2-Hydroxyethanesulfonate	HMDB0003903	7866
340	HMDB0031233	Ethyl hydrogen sulfate	HMDB0031233	6004
341	C05123	NA	NA	NA
342	C19177	NA	NA	NA
343	CHEBI:11157	NA	NA	NA
344	CHEBI:59050	NA	NA	NA
345	HMDB0013674	1,2,3-Trihydroxybenzene	HMDB0013674	1057
346	HMDB0013675	1,3,5-Trihydroxybenzene	HMDB0013675	359
347	HMDB0029750	Methyl 2-furoate	HMDB0029750	11902
348	HMDB0030776	Maltol	HMDB0030776	8369
349	HMDB0031256	4-Hydroxy-2H-pyran-3-carboxaldehyde	HMDB0031256	
350	HMDB0032651	(Z)-Tamarindienal	HMDB0032651	134337
351	HMDB0034355	5-Hydroxymethyl-2-furancarboxaldehyde	HMDB0034355	237332
352	HMDB0059735	5-Methylfuran-2-carboxylic acid	HMDB0059735	74710
353	HMDB0124831	NA	NA	NA
354	C01108	NA	NA	NA
355	C02183	NA	NA	NA
356	C02752	NA	NA	NA
357	C02814	NA	NA	NA

358	C11101	NA	NA	NA
359	C11918	NA	NA	NA
360	C20718	NA	NA	NA
361	CHEBI:142577	NA	NA	NA
362	CHEBI:16164	NA	NA	NA
363	CHEBI:16204	NA	NA	NA
364	CHEBI:16458	NA	NA	NA
365	CHEBI:16971	NA	NA	NA
366	CHEBI:30999	NA	NA	NA
367	CHEBI:32577	NA	NA	NA
368	CHEBI:412516	NA	NA	NA
369	CHEBI:76245	NA	NA	NA
370	CHEBI:76246	NA	NA	NA
371	HMDB0000262	Thymine	HMDB0000262	1135
372	HMDB0002024	Imidazoleacetic acid	HMDB0002024	96215
373	HMDB0029736	1H-Imidazole-1-acetic acid	HMDB0029736	656129
374	HMDB0060261	NA	NA	NA
375	C00178	NA	NA	NA
376	C02835	NA	NA	NA
377	CHEBI:16974	NA	NA	NA
378	CHEBI:172070	NA	NA	NA
379	CHEBI:17821	NA	NA	NA
380	CHEBI:43615	NA	NA	NA
381	CHEBI:69445	NA	NA	NA
382	CHEBI:70801	NA	NA	NA
383	CHEBI:70804	NA	NA	NA
384	CHEBI:70806	NA	NA	NA
385	CHEBI:74732	NA	NA	NA
386	CHEBI:74733	NA	NA	NA
387	CHEBI:74737	NA	NA	NA
388	CHEBI:74738	NA	NA	NA
389	CHEBI:74739	NA	NA	NA
390	CHEBI:74740	NA	NA	NA
391	CHEBI:74741	NA	NA	NA
392	CHEBI:74742	NA	NA	NA
393	CHEBI:74743	NA	NA	NA
394	CHEBI:74745	NA	NA	NA
395	CHEBI:74747	NA	NA	NA
396	HMDB0000079	Dihydrothymine	HMDB0000079	676414
397	HMDB0029874	Squamolone	HMDB0029874	326996
398	HMDB0031547	L-Cyclo(alanylglycyl)	HMDB0031547	107297
399	HMDB0062558	Pyroglutamine	HMDB0062558	119841
400	C00906	NA	NA	NA
401	C05715	NA	NA	NA
402	C05717	NA	NA	NA
403	CHEBI:133469	NA	NA	NA
404	CHEBI:27468	NA	NA	NA
405	CHEBI:27578	NA	NA	NA
406	CHEBI:28474	NA	NA	NA
407	CHEBI:30011	NA	NA	NA
408	CHEBI:32677	NA	NA	NA
409	CHEBI:48097	NA	NA	NA
410	CHEBI:50614	NA	NA	NA
411	CHEBI:50615	NA	NA	NA
412	CHEBI:565546	NA	NA	NA
413	CHEBI:61960	NA	NA	NA
414	HMDB0000620	Glutaconic acid	HMDB0000620	528049
415	HMDB0000634	Citraconic acid	HMDB0000634	643798
416	HMDB0000749	Mesaconic acid	HMDB0000749	638129
417	HMDB0002092	Itaconic acid	HMDB0002092	811
418	HMDB0013233	Gamma-delta-Dioxovaleric acid	HMDB0013233	119412
419	HMDB0033809	Methyl hydrogen fumarate	HMDB0033809	535445
420	HMDB0059743	2-Hydroxyglutaric acid lactone	HMDB0059743	251524
421	HMDB0060365	2,5-Dioxopentanoate	HMDB0060365	523
422	HMDB0061185	NA	NA	NA
423	HMDB0001657	NA	NA	NA
424	C00433	NA	NA	NA
425	C00490	NA	NA	NA
426	C01732	NA	NA	NA
427	C02132	NA	NA	NA
428	C02214	NA	NA	NA
429	C02226	NA	NA	NA
430	C02800	NA	NA	NA
431	CHEBI:15670	NA	NA	NA
432	CHEBI:16600	NA	NA	NA
433	CHEBI:17204	NA	NA	NA
434	CHEBI:17415	NA	NA	NA
435	CHEBI:17626	NA	NA	NA
436	CHEBI:2424	NA	NA	NA
437	CHEBI:24309	NA	NA	NA
438	CHEBI:30838	NA	NA	NA
439	CHEBI:30921	NA	NA	NA
440	CHEBI:50429	NA	NA	NA
441	CHEBI:73677	NA	NA	NA
442	CHEBI:74524	NA	NA	NA
443	HMDB0000408	2-Methyl-3-ketovaleric acid	HMDB0000408	189028
444	HMDB0000491	3-Methyl-2-oxovaleric acid	HMDB0000491	439286

445	HMDB0000695	Ketoleucine	HMDB0000695	70
446	HMDB0001864	2-Ketohexanoic acid	HMDB0001864	159664
447	HMDB0006024	Mevalonolactone	HMDB0006024	532592
448	HMDB0010717	3-Oxohexanoic acid	HMDB0010717	439658
449	HMDB0012882	Adipate semialdehyde	HMDB0012882	440918
450	HMDB0031214	5-Ethoxy-4,5-dihydro-2(3H)furanone	HMDB0031214	356063
451	HMDB0031216	Ethyl acetoacetate	HMDB0031216	8868
452	HMDB0031218	NA	NA	NA
453	HMDB0033286	Sherry lactone	HMDB0033286	100900
454	HMDB0033302	(4S,6S)-3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2H-pyran-2-one	HMDB0033302	241025
455	HMDB0033698	Acetoin acetate	HMDB0033698	521246
456	HMDB0041602	Methyl levulinate	HMDB0041602	69354
457	HMDB0059876	NA	NA	NA
458	HMDB0061881	4-Acetylbutyrate	HMDB0061881	18407
459	HMDB0000762	NA	NA	NA
460	HMDB0001962	NA	NA	NA
461	HMDB0002254	NA	NA	NA
462	HMDB0003736	NA	NA	NA
463	HMDB0004750	NA	NA	NA
464	HMDB0011647	NA	NA	NA
465	C00233	NA	NA	NA
466	C00671	NA	NA	NA
467	C00902	NA	NA	NA
468	C01012	NA	NA	NA
469	C02122	NA	NA	NA
470	C02129	NA	NA	NA
471	C03241	NA	NA	NA
472	C03465	NA	NA	NA
473	C03467	NA	NA	NA
474	C03500	NA	NA	NA
475	C06008	NA	NA	NA
476	C06102	NA	NA	NA
477	C12314	NA	NA	NA
478	C14530	NA	NA	NA
479	CHEBI:15614	NA	NA	NA
480	CHEBI:15888	NA	NA	NA
481	CHEBI:16719	NA	NA	NA
482	CHEBI:17075	NA	NA	NA
483	CHEBI:17308	NA	NA	NA
484	CHEBI:2490	NA	NA	NA
485	CHEBI:28379	NA	NA	NA
486	CHEBI:28422	NA	NA	NA
487	CHEBI:29024	NA	NA	NA
488	CHEBI:31046	NA	NA	NA
489	CHEBI:34288	NA	NA	NA
490	CHEBI:35932	NA	NA	NA
491	CHEBI:386429	NA	NA	NA
492	CHEBI:48430	NA	NA	NA
493	CHEBI:49293	NA	NA	NA
494	CHEBI:86365	NA	NA	NA
495	CHEBI:87282	NA	NA	NA
496	CHEBI:87296	NA	NA	NA
497	CHEBI:87307	NA	NA	NA
498	CHEBI:87390	NA	NA	NA
499	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	HMDB0000317	107967
500	HMDB0000409	(5R)-5-Hydroxyhexanoic acid	HMDB0000409	713104
501	HMDB0000525	5-Hydroxyhexanoic acid	HMDB0000525	170748
502	HMDB0000624	D-Leucic acid	HMDB0000624	439960
503	HMDB0000665	Leucinic acid	HMDB0000665	92779
504	HMDB0000746	Hydroxyisocaproic acid	HMDB0000746	83697
505	HMDB0001624	2-Hydroxycaproic acid	HMDB0001624	99824
506	HMDB0001975	2-Ethyl-2-Hydroxybutyric acid	HMDB0001975	77199
507	HMDB0010718	(R)-3-Hydroxyhexanoic acid	HMDB0010718	101977
508	HMDB0012843	6-Hydroxyhexanoic acid	HMDB0012843	14490
509	HMDB0029166	2-Methyl-3-hydroxyvaleric acid	HMDB0029166	152968
510	HMDB0032158	(+/-)-1-Acetoxy-1-ethoxyethane	HMDB0032158	97895
511	HMDB0032456	Paraldehyde	HMDB0032456	31264
512	HMDB0033851	4,4-Dimethoxy-2-butanone	HMDB0033851	228548
513	HMDB0040409	Ethyl (±)-3-hydroxybutyrate	HMDB0040409	62572
514	HMDB0041844	NA	NA	NA
515	HMDB0059770	Threo-3-Hydroxy-2-methylbutyric acid	HMDB0059770	642248
516	HMDB0061652	3-Hydroxyhexanoic acid	HMDB0061652	118294
517	C03264	NA	NA	NA
518	C03499	NA	NA	NA
519	C06103	NA	NA	NA
520	C07834	NA	NA	NA
521	CHEBI:131434	NA	NA	NA
522	CHEBI:17869	NA	NA	NA
523	CHEBI:27909	NA	NA	NA
524	CHEBI:28707	NA	NA	NA
525	CHEBI:30941	NA	NA	NA
526	CHEBI:32400	NA	NA	NA
527	CHEBI:32485	NA	NA	NA
528	CHEBI:37035	NA	NA	NA
529	CHEBI:37049	NA	NA	NA
530	CHEBI:37553	NA	NA	NA
531	CHEBI:44510	NA	NA	NA

532	CHEBI:55434	NA	NA	NA
533	CHEBI:55534	NA	NA	NA
534	CHEBI:55536	NA	NA	NA
535	CHEBI:59783	NA	NA	NA
536	CHEBI:78842	NA	NA	NA
537	CHEBI:86542	NA	NA	NA
538	CHEBI:87685	NA	NA	NA
539	HMDB0000214	Ornithine	HMDB0000214	6262
540	HMDB0003374	D-Ornithine	HMDB0003374	71082
541	HMDB0000818	NA	NA	NA
542	HMDB0004984	NA	NA	NA
543	C00077	NA	NA	NA
544	C00515	NA	NA	NA
545	C01602	NA	NA	NA
546	C03943	NA	NA	NA
547	C11320	NA	NA	NA
548	CHEBI:15729	NA	NA	NA
549	CHEBI:16176	NA	NA	NA
550	CHEBI:18257	NA	NA	NA
551	CHEBI:25234	NA	NA	NA
552	CHEBI:4280	NA	NA	NA
553	CHEBI:74403	NA	NA	NA
554	CHEBI:88163	NA	NA	NA
555	CHEBI:904	NA	NA	NA
556	HMDB0029639	(4-Methylphenyl)acetaldehyde	HMDB0029639	61006
557	HMDB0029697	Cinnamyl alcohol	HMDB0029697	528051
558	HMDB0029698	trans-Cinnamyl alcohol	HMDB0029698	531589
559	HMDB0030839	(Z)-4-(1-Propenyl)phenol	HMDB0030839	579113
560	HMDB0031626	2-Phenylpropanal	HMDB0031626	7146
561	HMDB0032024	4-Ethylbenzaldehyde	HMDB0032024	20861
562	HMDB0032142	2,4-Dimethylbenzaldehyde	HMDB0032142	61814
563	HMDB0032608	4'-Methylacetophenone	HMDB0032608	8500
564	HMDB0032623	1-Phenyl-1-propanone	HMDB0032623	7148
565	HMDB0033716	3-Phenylpropanal	HMDB0033716	7707
566	HMDB0034107	Chavicol	HMDB0034107	68148
567	HMDB0034563	7-Nonene-3,5-dien-1-ol	HMDB0034563	101407
568	HMDB0036441	o-Vinylanisole	HMDB0036441	61153
569	HMDB0059601	Indan-1-ol	HMDB0059601	22819
570	HMDB0059895	m-Methylacetophenone	HMDB0059895	11455
571	C01710	NA	NA	NA
572	C02394	NA	NA	NA
573	C15512	NA	NA	NA
574	C16930	NA	NA	NA
575	C20464	NA	NA	NA
576	CHEBI:16697	NA	NA	NA
577	CHEBI:17177	NA	NA	NA
578	CHEBI:33224	NA	NA	NA
579	CHEBI:33225	NA	NA	NA
580	CHEBI:33226	NA	NA	NA
581	CHEBI:33227	NA	NA	NA
582	CHEBI:39826	NA	NA	NA
583	CHEBI:425902	NA	NA	NA
584	CHEBI:50158	NA	NA	NA
585	CHEBI:52052	NA	NA	NA
586	CHEBI:59311	NA	NA	NA
587	CHEBI:73343	NA	NA	NA
588	HMDB0000306	Tyramine	HMDB0000306	5610
589	HMDB0001065	2-Hydroxyphenethylamine	HMDB0001065	1000
590	HMDB0001466	Dimethylaniline-N-oxide	HMDB0001466	950
591	HMDB0004989	m-Tyramine	HMDB0004989	11492
592	HMDB0029759	2-Acetyl-1-ethylpyrrole	HMDB0029759	61988
593	HMDB0039657	1,2,3,4,5,6-Hexahydro-7H-cyclopenta[b]pyridin-7-one	HMDB0039657	642897
594	HMDB0040059	(±)-2-(2-Furanyl)pyrrolidine	HMDB0040059	367598
595	HMDB0060681	4-Hydroxy-2,6-dimethylaniline	HMDB0060681	76543
596	C00483	NA	NA	NA
597	C01183	NA	NA	NA
598	C02735	NA	NA	NA
599	C03473	NA	NA	NA
600	C16570	NA	NA	NA
601	C18396	NA	NA	NA
602	C19216	NA	NA	NA
603	C19376	NA	NA	NA
604	CHEBI:15760	NA	NA	NA
605	CHEBI:16343	NA	NA	NA
606	CHEBI:17735	NA	NA	NA
607	CHEBI:341165	NA	NA	NA
608	CHEBI:49837	NA	NA	NA
609	CHEBI:55545	NA	NA	NA
610	CHEBI:85505	NA	NA	NA
611	HMDB0032311	2,4-Hexadienyl acetate	HMDB0032311	536349
612	HMDB0036176	3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one	HMDB0036176	528698
613	HMDB0037167	3-Ethyl-5-methyl-1,2-cyclopentanedione	HMDB0037167	158255
614	HMDB0037196	Ethyl 2-methyl-3,4-pentadienoate	HMDB0037196	62166
615	HMDB0037625	Allyl tiglate	HMDB0037625	604848
616	HMDB0039651	3-Propyl-1,2-cyclopentanedione	HMDB0039651	542192
617	HMDB0039652	2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one	HMDB0039652	528707
618	HMDB0039673	4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one	HMDB0039673	528704

619	HMDB0039680	3,5,5-Trimethyl-1,2-cyclopentanedione	HMDB0039680	696988
620	HMDB0039681	3-Isopropyl-1,2-cyclopentanedione	HMDB0039681	129144
621	HMDB0040463	Ethyl sorbate	HMDB0040463	155047
622	HMDB0040526	3,4,4-Trimethyl-1,2-cyclopentanedione	HMDB0040526	642878
623	HMDB0060682	2-Propyl-2,4-pentadienoic acid	HMDB0060682	644180
624	C06727	NA	NA	NA
625	C16656	NA	NA	NA
626	C18011	NA	NA	NA
627	C19311	NA	NA	NA
628	CHEBI:16843	NA	NA	NA
629	CHEBI:51922	NA	NA	NA
630	CHEBI:53533	NA	NA	NA
631	CHEBI:59001	NA	NA	NA
632	CHEBI:60295	NA	NA	NA
633	CHEBI:72819	NA	NA	NA
634	CHEBI:80642	NA	NA	NA
635	HMDB0000392	2-Octenoic acid	HMDB0000392	528271
636	HMDB0001568	trans-2-Octenoic acid	HMDB0001568	528271
637	HMDB0013897	4-ene-Valproic acid	HMDB0013897	104896
638	HMDB0013902	2-ene-Valproic acid	HMDB0013902	643706
639	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid	HMDB0013903	248928
640	HMDB0013904	(3E)-2-Propylpent-3-enoic acid	HMDB0013904	643974
641	HMDB0029761	Ethyl (±)-2-methyl-4-pentenoate	HMDB0029761	62024
642	HMDB0031293	2,3-Octanedione	HMDB0031293	11449
643	HMDB0031343	Methyl cyclohexanecarboxylate	HMDB0031343	20748
644	HMDB0031352	Cyclohexyl acetate	HMDB0031352	12146
645	HMDB0031403	Cyclohexanecetic acid	HMDB0031403	21363
646	HMDB0032164	Allyl valerate	HMDB0032164	80606
647	HMDB0032207	cis-5-Octenoic acid	HMDB0032207	528271
648	HMDB0032266	Ethyl (E)-3-hexenoate	HMDB0032266	536262
649	HMDB0032267	Ethyl 5-hexenoate	HMDB0032267	642025
650	HMDB0032268	Ethyl 2E-hexenoate	HMDB0032268	536477
651	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate	HMDB0032278	643631
652	HMDB0032533	trans-3-Hexenyl acetate	HMDB0032533	535255
653	HMDB0035422	4-Butyl-gamma-butyrolactone	HMDB0035422	7704
654	HMDB0036212	2-Methylpropyl (2E)-butenoate	HMDB0036212	643582
655	HMDB0036236	2-Methylallyl butyrate	HMDB0036236	251530
656	HMDB0037622	Ethyl 2-methyl-3-pentenoate	HMDB0037622	144233
657	HMDB0037624	Isopropyl tiglate	HMDB0037624	643290
658	HMDB0037630	xi-Tetrahydro-3-propyl-2H-pyran-2-one	HMDB0037630	90840
659	HMDB0038036	2-Propenyl 3-methylbutanoate	HMDB0038036	17816
660	HMDB0038310	xi-Tetrahydro-6-propyl-2H-pyran-2-one	HMDB0038310	12777
661	HMDB0039793	(E)-4-Octenoic acid	HMDB0039793	643371
662	HMDB0039872	Methyl 2-heptenoate	HMDB0039872	536808
663	HMDB0040212	2-Hexenyl acetate	HMDB0040212	273329
664	HMDB0040215	cis-3-Hexenyl acetate	HMDB0040215	536338
665	HMDB0059908	Ethyl-3-hexanoate	HMDB0059908	61312
666	HMDB0010723	NA	NA	NA
667	C12104	NA	NA	NA
668	C12297	NA	NA	NA
669	C16648	NA	NA	NA
670	C16653	NA	NA	NA
671	C16654	NA	NA	NA
672	C19318	NA	NA	NA
673	C19757	NA	NA	NA
674	CHEBI:23705	NA	NA	NA
675	CHEBI:288752	NA	NA	NA
676	CHEBI:37277	NA	NA	NA
677	CHEBI:37316	NA	NA	NA
678	CHEBI:39355	NA	NA	NA
679	CHEBI:410867	NA	NA	NA
680	CHEBI:50899	NA	NA	NA
681	CHEBI:61316	NA	NA	NA
682	CHEBI:86544	NA	NA	NA
683	CHEBI:87275	NA	NA	NA
684	CHEBI:87299	NA	NA	NA
685	CHEBI:87416	NA	NA	NA
686	CHEBI:87514	NA	NA	NA
687	CHEBI:87560	NA	NA	NA
688	HMDB0013821	2-Methyl-4-heptanone	HMDB0013821	7958
689	HMDB0029557	Dihydroisophorol	HMDB0029557	8298
690	HMDB0030959	(Z)-3-Nonen-1-ol	HMDB0030959	536463
691	HMDB0031266	2-Nonanone	HMDB0031266	13187
692	HMDB0031267	3-Nonanone	HMDB0031267	61235
693	HMDB0031268	Amyl propyl ketone	HMDB0031268	78236
694	HMDB0031417	2,6-Dimethyl-4-heptanone	HMDB0031417	7958
695	HMDB0031684	2-Methyl octanal	HMDB0031684	24583
696	HMDB0031730	3,5,5-Trimethylhexanal	HMDB0031730	21574
697	HMDB0034152	1-Nonen-3-ol	HMDB0034152	89560
698	HMDB0037304	(±)-2,6-Dimethyl-6-hepten-1-ol	HMDB0037304	169818
699	HMDB0040581	(Z)-6-Nonen-1-ol	HMDB0040581	536279
700	HMDB0041498	2-Nonen-1-ol	HMDB0041498	536494
701	HMDB0041499	(Z)-2-Nonen-1-ol	HMDB0041499	536502
702	HMDB0041601	(E)-3-Nonen-1-ol	HMDB0041601	535280
703	HMDB0059835	Nonanal	HMDB0059835	31289
704	HMDB0059887	(E)-6-Nonenol	HMDB0059887	536281
705	HMDB0013822	NA	NA	NA

706	CHEBI:59065	NA	NA	NA
707	CHEBI:77927	NA	NA	NA
708	CHEBI:84268	NA	NA	NA
709	CHEBI:87594	NA	NA	NA
710	HMDB0000894	Vinylacetylglycine	HMDB0000894	534777
711	HMDB0014491	Trimethadione	HMDB0014491	5576
712	HMDB0032161	NA	NA	NA
713	HMDB0061082	5-ethyl-5-methyl-2,4-oxazolidinedione	HMDB0061082	232592
714	HMDB0061705	6-Oxopiperidine-2-carboxylic acid	HMDB0061705	301423
715	HMDB0006723	NA	NA	NA
716	HMDB0006724	NA	NA	NA
717	C17357	NA	NA	NA
718	CHEBI:131804	NA	NA	NA
719	CHEBI:415036	NA	NA	NA
720	CHEBI:74435	NA	NA	NA
721	CHEBI:82795	NA	NA	NA
722	CHEBI:87998	NA	NA	NA
723	HMDB0004827	Proline betaine	HMDB0004827	115244
724	HMDB0030410	L-2-Amino-3-methylenehexanoic acid	HMDB0030410	762235
725	HMDB0038949	3beta,6beta-Dihydroxynortropane	HMDB0038949	222975
726	C04114	NA	NA	NA
727	C10172	NA	NA	NA
728	CHEBI:11946	NA	NA	NA
729	CHEBI:17237	NA	NA	NA
730	CHEBI:35280	NA	NA	NA
731	CHEBI:86534	NA	NA	NA
732	HMDB0032429	3-(Methylthio)methylthiophene	HMDB0032429	201580
733	HMDB0034901	2-Vinyl-4H-1,3-dithiine	HMDB0034901	133337
734	HMDB0040259	2-Methyl-5-(methylthio)thiophene	HMDB0040259	142508
735	HMDB0000482	Caprylic acid	HMDB0000482	379
736	HMDB0001877	Valproic acid	HMDB0001877	3121
737	HMDB0029980	Hexyl acetate	HMDB0029980	8908
738	HMDB0030368	(3R,5Z)-5-Octene-1,3-diol	HMDB0030368	211594
739	HMDB0031230	2-Ethylhexanoic acid	HMDB0031230	8697
740	HMDB0031290	1-Hydroxy-3-octanone	HMDB0031290	138647
741	HMDB0031478	Methyl heptanoate	HMDB0031478	7826
742	HMDB0031579	Ethyl (±)-2-methylpentanoate	HMDB0031579	62902
743	HMDB0031587	2-Methylheptanoic acid	HMDB0031587	14475
744	HMDB0031588	6-Methylheptanoic acid	HMDB0031588	90716
745	HMDB0031596	Methyl 5-methylhexanoate	HMDB0031596	519894
746	HMDB0031638	Pentyl propanoate	HMDB0031638	12217
747	HMDB0031703	2-Ethylbutyl acetate	HMDB0031703	61448
748	HMDB0032046	Isopropyl 3-methylbutanoate	HMDB0032046	61914
749	HMDB0032047	Propyl 3-methylbutanoate	HMDB0032047	11176
750	HMDB0032203	cis- and trans-2-Isobutyl-4-methyl-1,3-dioxolane	HMDB0032203	86733
751	HMDB0032225	1,1-Dimethoxy-trans-2-hexene	HMDB0032225	643648
752	HMDB0032272	Ethyl 4-methylpentanoate	HMDB0032272	117477
753	HMDB0032335	3-Hydroxy-2-octanone	HMDB0032335	642854
754	HMDB0032551	Valeraldehyde propyleneglycol acetal	HMDB0032551	156273
755	HMDB0034161	2-Methylpropyl butanoate	HMDB0034161	10885
756	HMDB0034164	3-Methylbutyl propanoate	HMDB0034164	7772
757	HMDB0034234	Ethyl (±)-3-methylpentanoate	HMDB0034234	560255
758	HMDB0034459	Heptyl formate	HMDB0034459	8169
759	HMDB0035457	(±)-5-Hydroxy-4-octanone	HMDB0035457	219794
760	HMDB0036165	3-(Hydroxymethyl)-2-heptanone	HMDB0036165	536256
761	HMDB0039217	Isopropyl 2-methylbutanoate	HMDB0039217	522214
762	HMDB0039620	Butyl butyrate	HMDB0039620	7983
763	HMDB0040209	Ethyl hexanoate	HMDB0040209	31265
764	HMDB0040251	Butyl isobutyrate	HMDB0040251	7353
765	HMDB0040252	Isobutyl isobutyrate	HMDB0040252	7351
766	HMDB0040296	Propyl pentanoate	HMDB0040296	67328
767	HMDB0040298	Ethyl 2-ethylbutanoate	HMDB0040298	76326
768	HMDB0061931	Tetrahydro-2,5-dimethyl-2H-pyranmethanol	HMDB0061931	98034
769	C06423	NA	NA	NA
770	C07185	NA	NA	NA
771	CHEBI:28837	NA	NA	NA
772	CHEBI:39867	NA	NA	NA
773	CHEBI:744024	NA	NA	NA
774	CHEBI:86055	NA	NA	NA
775	CHEBI:87318	NA	NA	NA
776	CHEBI:87373	NA	NA	NA
777	CHEBI:87419	NA	NA	NA
778	CHEBI:87429	NA	NA	NA
779	CHEBI:87510	NA	NA	NA
780	CHEBI:87683	NA	NA	NA
781	CHEBI:88826	NA	NA	NA
782	HMDB0001552	2-Keto-glutaramic acid	HMDB0001552	48
783	C00940	NA	NA	NA
784	C05572	NA	NA	NA
785	CHEBI:16378	NA	NA	NA
786	CHEBI:29987	NA	NA	NA
787	CHEBI:29988	NA	NA	NA
788	CHEBI:29989	NA	NA	NA
789	CHEBI:30882	NA	NA	NA
790	CHEBI:30883	NA	NA	NA
791	HMDB0000641	Glutamine	HMDB0000641	5961
792	HMDB0002031	Ureidoisobutyric acid	HMDB0002031	885587

793	HMDB0003423	D-Glutamine	HMDB0003423	145815
794	HMDB0006899	Alanylglycine	HMDB0006899	699802
795	HMDB0028687	NA	NA	NA
796	C00064	NA	NA	NA
797	C00303	NA	NA	NA
798	C00819	NA	NA	NA
799	C05100	NA	NA	NA
800	C16673	NA	NA	NA
801	CHEBI:1670	NA	NA	NA
802	CHEBI:17061	NA	NA	NA
803	CHEBI:18050	NA	NA	NA
804	CHEBI:185249	NA	NA	NA
805	CHEBI:28300	NA	NA	NA
806	CHEBI:44079	NA	NA	NA
807	CHEBI:58000	NA	NA	NA
808	CHEBI:58359	NA	NA	NA
809	CHEBI:73757	NA	NA	NA
810	CHEBI:73786	NA	NA	NA
811	CHEBI:73834	NA	NA	NA
812	CHEBI:73836	NA	NA	NA
813	CHEBI:73855	NA	NA	NA
814	CHEBI:73891	NA	NA	NA
815	HMDB0000182	Lysine	HMDB0000182	5962
816	HMDB0003405	D-Lysine	HMDB0003405	57449
817	HMDB0012114	(3S)-3,6-Diaminohexanoate	HMDB0012114	439417
818	HMDB0012115	(3S,5S)-3,5-Diaminohexanoate	HMDB0012115	439430
819	HMDB0142894	NA	NA	NA
820	C00047	NA	NA	NA
821	C00739	NA	NA	NA
822	C01142	NA	NA	NA
823	C01186	NA	NA	NA
824	C05161	NA	NA	NA
825	C16440	NA	NA	NA
826	C20277	NA	NA	NA
827	CHEBI:131843	NA	NA	NA
828	CHEBI:15613	NA	NA	NA
829	CHEBI:15616	NA	NA	NA
830	CHEBI:16855	NA	NA	NA
831	CHEBI:16926	NA	NA	NA
832	CHEBI:18019	NA	NA	NA
833	CHEBI:25094	NA	NA	NA
834	CHEBI:32573	NA	NA	NA
835	CHEBI:64693	NA	NA	NA
836	CHEBI:72340	NA	NA	NA
837	CHEBI:85040	NA	NA	NA
838	HMDB0029449	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	HMDB0029449	354197
839	HMDB0033453	Fagomine	HMDB0033453	72259
840	HMDB0061157	N-(2-Hydroxyethyl)-morpholine N-oxide	HMDB0061157	130392
841	HMDB0142963	NA	NA	NA
842	C10144	NA	NA	NA
843	C20310	NA	NA	NA
844	C20802	NA	NA	NA
845	CHEBI:32537	NA	NA	NA
846	CHEBI:32539	NA	NA	NA
847	CHEBI:435538	NA	NA	NA
848	CHEBI:4969	NA	NA	NA
849	CHEBI:61129	NA	NA	NA
850	CHEBI:78247	NA	NA	NA
851	CHEBI:79079	NA	NA	NA
852	HMDB0002214	Cuminaldehyde	HMDB0002214	326
853	HMDB0030837	Anethole	HMDB0030837	154904
854	HMDB0031616	4-Phenyl-3-buten-2-ol	HMDB0031616	114691
855	HMDB0032014	2,3,6-Trimethylbenzaldehyde	HMDB0032014	102360
856	HMDB0032015	Duryl aldehyde	HMDB0032015	22013
857	HMDB0032016	2,4,6-Trimethylbenzaldehyde	HMDB0032016	10254
858	HMDB0032017	3,4,5-Trimethylbenzaldehyde	HMDB0032017	122871
859	HMDB0032140	2',4'-Dimethylacetophenone	HMDB0032140	6985
860	HMDB0033382	2-(4-Methylphenyl)propanal	HMDB0033382	60990
861	HMDB0034121	1-Methoxy-4-(2-propenyl)benzene	HMDB0034121	8815
862	HMDB0059845	p-Ethylacetophenone	HMDB0059845	13642
863	HMDB0133593	NA	NA	NA
864	HMDB0133746	NA	NA	NA
865	C06577	NA	NA	NA
866	C10428	NA	NA	NA
867	C10452	NA	NA	NA
868	C14309	NA	NA	NA
869	C17965	NA	NA	NA
870	CHEBI:2716	NA	NA	NA
871	CHEBI:28671	NA	NA	NA
872	CHEBI:34448	NA	NA	NA
873	CHEBI:35616	NA	NA	NA
874	CHEBI:366706	NA	NA	NA
875	CHEBI:38475	NA	NA	NA
876	CHEBI:45900	NA	NA	NA
877	CHEBI:59335	NA	NA	NA
878	CHEBI:78412	NA	NA	NA
879	CHEBI:992716	NA	NA	NA

880	HMDB0001878	Thymol	HMDB0001878	6989
881	HMDB0003647	Perillyl aldehyde	HMDB0003647	16441
882	HMDB0004487	(S)-Carvone	HMDB0004487	16724
883	HMDB0029652	2-(4-Methylphenyl)-2-propanol	HMDB0029652	14529
884	HMDB0031570	2-Methyl-1-phenyl-2-propanol	HMDB0031570	7531
885	HMDB0031613	4-Phenyl-2-butanol	HMDB0031613	61302
886	HMDB0031817	Cumyl alcohol	HMDB0031817	325
887	HMDB0032063	4-tert-Butylphenol	HMDB0032063	7393
888	HMDB0032213	2-trans-4-trans-7-cis-Decatrienal	HMDB0032213	644264
889	HMDB0032626	1-Methoxy-4-propylbenzene	HMDB0032626	7702
890	HMDB0033544	(2E,4Z,7Z)-2,4,7-Decatrienal	HMDB0033544	644263
891	HMDB0034846	2-(4-Methylphenyl)-1-propanol	HMDB0034846	95376
892	HMDB0034921	Teresantalal	HMDB0034921	858612
893	HMDB0035089	(R)-Carvone	HMDB0035089	439570
894	HMDB0035172	2,6,6-Trimethyl-1,4-cyclohexadiene-1-carboxaldehyde	HMDB0035172	118192
895	HMDB0035250	Myrtenal	HMDB0035250	61130
896	HMDB0035591	3-Carene-5-one	HMDB0035591	135028
897	HMDB0035761	(-)-Pinocarvone	HMDB0035761	121719
898	HMDB0035770	5-Isopropyl-2-methylphenol	HMDB0035770	10364
899	HMDB0035824	Carvone	HMDB0035824	7439
900	HMDB0036061	Safranal	HMDB0036061	61041
901	HMDB0036070	1-Acetyl-4-isopropenylcyclopentene	HMDB0036070	126345
902	HMDB0036089	(R)-Menthofuran	HMDB0036089	329983
903	HMDB0036999	Piperitenone	HMDB0036999	381152
904	HMDB0037561	Linden ether	HMDB0037561	216061
905	HMDB0038913	4,6-Decadien-1-ol	HMDB0038913	247406
906	HMDB0061788	NA	NA	NA
907	HMDB0133616	NA	NA	NA
908	HMDB0006315	NA	NA	NA
909	C01767	NA	NA	NA
910	C01868	NA	NA	NA
911	C01951	NA	NA	NA
912	C02289	NA	NA	NA
913	C02485	NA	NA	NA
914	C02576	NA	NA	NA
915	C06576	NA	NA	NA
916	C09840	NA	NA	NA
917	C09843	NA	NA	NA
918	C09868	NA	NA	NA
919	C09884	NA	NA	NA
920	C09908	NA	NA	NA
921	C09911	NA	NA	NA
922	C09913	NA	NA	NA
923	C11383	NA	NA	NA
924	C11394	NA	NA	NA
925	C11939	NA	NA	NA
926	C14130	NA	NA	NA
927	C14138	NA	NA	NA
928	C14139	NA	NA	NA
929	C14188	NA	NA	NA
930	C14200	NA	NA	NA
931	C14464	NA	NA	NA
932	C14741	NA	NA	NA
933	C16955	NA	NA	NA
934	C17062	NA	NA	NA
935	C18025	NA	NA	NA
936	CHEBI:15399	NA	NA	NA
937	CHEBI:15400	NA	NA	NA
938	CHEBI:15403	NA	NA	NA
939	CHEBI:15408	NA	NA	NA
940	CHEBI:15421	NA	NA	NA
941	CHEBI:17304	NA	NA	NA
942	CHEBI:27607	NA	NA	NA
943	CHEBI:28996	NA	NA	NA
944	CHEBI:34303	NA	NA	NA
945	CHEBI:3440	NA	NA	NA
946	CHEBI:34444	NA	NA	NA
947	CHEBI:37001	NA	NA	NA
948	CHEBI:38265	NA	NA	NA
949	CHEBI:40611	NA	NA	NA
950	CHEBI:50110	NA	NA	NA
951	CHEBI:50542	NA	NA	NA
952	CHEBI:50544	NA	NA	NA
953	CHEBI:53169	NA	NA	NA
954	CHEBI:6041	NA	NA	NA
955	CHEBI:6750	NA	NA	NA
956	CHEBI:74039	NA	NA	NA
957	CHEBI:78315	NA	NA	NA
958	CHEBI:78316	NA	NA	NA
959	CHEBI:84966	NA	NA	NA
960	CHEBI:9955	NA	NA	NA
961	HMDB0000292	Xanthine	HMDB0000292	1188
962	HMDB0000786	Oxy purinol	HMDB0000786	4644
963	HMDB0001182	6,8-Dihydroxypurine	HMDB0001182	83252
964	C00385	NA	NA	NA
965	C07599	NA	NA	NA
966	CHEBI:17712	NA	NA	NA

967	CHEBI:28315	NA	NA	NA
968	CHEBI:48517	NA	NA	NA
969	CHEBI:72574	NA	NA	NA
970	HMDB0000020	p-Hydroxyphenylacetic acid	HMDB0000020	127
971	HMDB0000440	3-Hydroxyphenylacetic acid	HMDB0000440	12122
972	HMDB0000669	ortho-Hydroxyphenylacetic acid	HMDB0000669	11970
973	HMDB0000703	Mandelic acid	HMDB0000703	439616
974	HMDB0001101	p-Anisic acid	HMDB0001101	7478
975	HMDB0002390	3-Cresotinic acid	HMDB0002390	6738
976	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	HMDB0003791	119219
977	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	HMDB0004815	68138
978	HMDB0012308	Vanillin	HMDB0012308	1183
979	HMDB0029657	2,4'-Dihydroxyacetophenone	HMDB0029657	440082
980	HMDB0029658	2',3'-Dihydroxyacetophenone	HMDB0029658	642911
981	HMDB0029659	2',4'-Dihydroxyacetophenone	HMDB0029659	6990
982	HMDB0029660	2',6'-Dihydroxyacetophenone	HMDB0029660	69687
983	HMDB0029661	3',4'-Dihydroxyacetophenone	HMDB0029661	14530
984	HMDB0029662	3',5'-Dihydroxyacetophenone	HMDB0029662	103993
985	HMDB0031609	Phenoxyacetic acid	HMDB0031609	19188
986	HMDB0032399	Methyl furfuracrylate	HMDB0032399	535541
987	HMDB0032572	Methylparaben	HMDB0032572	7456
988	HMDB0032594	2-(Hydroxymethyl)benzoic acid	HMDB0032594	11920
989	HMDB0032604	2-Methoxybenzoic acid	HMDB0032604	11370
990	HMDB0032606	3-Methoxybenzoic acid	HMDB0032606	11461
991	HMDB0032629	2',5'-Dihydroxyacetophenone	HMDB0032629	10279
992	HMDB0032919	Ethyl 2-furanyl diketone	HMDB0032919	197761
993	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	HMDB0033003	70968
994	HMDB0034172	Methyl 2-hydroxybenzoate	HMDB0034172	4133
995	HMDB0036907	2-Propenyl 2-furancarboxylate	HMDB0036907	61337
996	HMDB0041283	1-(2-Furanyl)-1,3-butanedione	HMDB0041283	12168
997	HMDB0060390	4-Hydroxyphenyl acetate	HMDB0060390	96009
998	HMDB0062635	(R)-mandelic Acid	HMDB0062635	11914
999	HMDB0124926	NA	NA	NA
1000	HMDB0125528	NA	NA	NA
1001	HMDB0137457	NA	NA	NA
1002	HMDB0006256	NA	NA	NA
1003	HMDB0006778	NA	NA	NA
1004	C00642	NA	NA	NA
1005	C00755	NA	NA	NA
1006	C01983	NA	NA	NA
1007	C01984	NA	NA	NA
1008	C02181	NA	NA	NA
1009	C02519	NA	NA	NA
1010	C02639	NA	NA	NA
1011	C02657	NA	NA	NA
1012	C03663	NA	NA	NA
1013	C04043	NA	NA	NA
1014	C05593	NA	NA	NA
1015	C05852	NA	NA	NA
1016	C10675	NA	NA	NA
1017	C10804	NA	NA	NA
1018	C12064	NA	NA	NA
1019	C12305	NA	NA	NA
1020	C13635	NA	NA	NA
1021	C13636	NA	NA	NA
1022	C14088	NA	NA	NA
1023	C14103	NA	NA	NA
1024	C14108	NA	NA	NA
1025	C17900	NA	NA	NA
1026	CHEBI:17445	NA	NA	NA
1027	CHEBI:17637	NA	NA	NA
1028	CHEBI:17656	NA	NA	NA
1029	CHEBI:18101	NA	NA	NA
1030	CHEBI:18346	NA	NA	NA
1031	CHEBI:18414	NA	NA	NA
1032	CHEBI:19868	NA	NA	NA
1033	CHEBI:20141	NA	NA	NA
1034	CHEBI:20414	NA	NA	NA
1035	CHEBI:20450	NA	NA	NA
1036	CHEBI:27978	NA	NA	NA
1037	CHEBI:28478	NA	NA	NA
1038	CHEBI:29672	NA	NA	NA
1039	CHEBI:31128	NA	NA	NA
1040	CHEBI:31832	NA	NA	NA
1041	CHEBI:31835	NA	NA	NA
1042	CHEBI:32800	NA	NA	NA
1043	CHEBI:35164	NA	NA	NA
1044	CHEBI:35825	NA	NA	NA
1045	CHEBI:40813	NA	NA	NA
1046	CHEBI:421840	NA	NA	NA
1047	CHEBI:491876	NA	NA	NA
1048	CHEBI:559127	NA	NA	NA
1049	CHEBI:574890	NA	NA	NA
1050	CHEBI:78339	NA	NA	NA
1051	CHEBI:8075	NA	NA	NA
1052	CHEBI:85239	NA	NA	NA
1053	HMDB0003450	(-)-trans-Carveol	HMDB0003450	94221

1054	HMDB0003634	Perillyl alcohol	HMDB0003634	10819
1055	HMDB0003667	Alpha-Pinene-oxide	HMDB0003667	91508
1056	HMDB0030892	p-Menth-3-en-9-al	HMDB0030892	884256
1057	HMDB0030893	Isocitral	HMDB0030893	642892
1058	HMDB0031854	3-Methyl-5-propyl-2-cyclohexen-1-one	HMDB0031854	378213
1059	HMDB0032120	2,6-Dimethyl-1,7-octadien-3-one	HMDB0032120	158402
1060	HMDB0032242	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	HMDB0032242	62842
1061	HMDB0032536	2-(trans-2-Pentenyl)cyclopentanone	HMDB0032536	643700
1062	HMDB0034715	p-Mentha-1(6),8-dien-3-ol	HMDB0034715	148446
1063	HMDB0034916	cis-2-Thujen-4-ol	HMDB0034916	561870
1064	HMDB0034973	(R)-Campholenic aldehyde	HMDB0034973	98497
1065	HMDB0034974	(R)-Carvotanacetone	HMDB0034974	521267
1066	HMDB0034975	Piperitone	HMDB0034975	6987
1067	HMDB0034985	(+)-Fenchone	HMDB0034985	14525
1068	HMDB0035054	(1S,4R)-p-Mentha-2,8-dien-1-ol	HMDB0035054	111055
1069	HMDB0035077	(1R,4R)-p-Mentha-2,8-dien-1-ol	HMDB0035077	111274
1070	HMDB0035078	Geranial	HMDB0035078	638011
1071	HMDB0035092	cis-Citral	HMDB0035092	643779
1072	HMDB0035100	2-Pinen-10-ol	HMDB0035100	10582
1073	HMDB0035120	Dehydrolinalool	HMDB0035120	854707
1074	HMDB0035125	Darwinol	HMDB0035125	636475
1075	HMDB0035158	1,2-Epoxy-p-menth-8-ene	HMDB0035158	91496
1076	HMDB0035203	(S)-9,10-Cyclo-p-menth-1-en-4-ol	HMDB0035203	738151
1077	HMDB0035241	(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol	HMDB0035241	531972
1078	HMDB0035277	(2S,4R)-p-Mentha-1(7),5-dien-2-ol	HMDB0035277	531936
1079	HMDB0035280	Teresantalol	HMDB0035280	578221
1080	HMDB0035600	(S)-Phellandral	HMDB0035600	89488
1081	HMDB0035604	Pulegone	HMDB0035604	442495
1082	HMDB0035622	(+)-cis-Carveol	HMDB0035622	443177
1083	HMDB0035656	3-Pinanone	HMDB0035656	11038
1084	HMDB0035706	alpha-Cyclocitral	HMDB0035706	94143
1085	HMDB0035737	(R)-Piperitone	HMDB0035737	107561
1086	HMDB0035738	NA	NA	NA
1087	HMDB0035741	(-)-trans-Isopulegone	HMDB0035741	34645
1088	HMDB0035743	Pinocarveol	HMDB0035743	102667
1089	HMDB0035744	(-)-Isopinocampnone	HMDB0035744	84532
1090	HMDB0036044	Marmelo oxide A	HMDB0036044	131751
1091	HMDB0036079	Dihydrocarvone	HMDB0036079	24473
1092	HMDB0036080	(1S,4S)-Dihydrocarvone	HMDB0036080	443180
1093	HMDB0036082	(-)-cis-Carveol	HMDB0036082	330573
1094	HMDB0036083	Carveol	HMDB0036083	7438
1095	HMDB0036085	Dehydro-1,8-cineole	HMDB0036085	523035
1096	HMDB0036087	(R)-p-Mentha-1,8-dien-7-ol	HMDB0036087	117883
1097	HMDB0036088	NA	NA	NA
1098	HMDB0036113	(+)-3-Thujone	HMDB0036113	91456
1099	HMDB0036114	(-)-3-Thujone	HMDB0036114	655387
1100	HMDB0036115	(-)-3-Isotujone	HMDB0036115	261491
1101	HMDB0036127	(-)-Pinocampnone	HMDB0036127	642710
1102	HMDB0036128	(-)-trans-Pinocarveol	HMDB0036128	120153
1103	HMDB0036129	Verbenol	HMDB0036129	61126
1104	HMDB0036598	(E,E)-2,4-Decadienal	HMDB0036598	642708
1105	HMDB0037008	6,8-Epoxy-p-menth-2-ene	HMDB0037008	727469
1106	HMDB0037009	Terpinolene oxide	HMDB0037009	107303
1107	HMDB0037010	(2S,4R)-p-Mentha-1(7),8-dien-2-ol	HMDB0037010	527427
1108	HMDB0037015	p-Mentha-1,8-dien-4-ol	HMDB0037015	527428
1109	HMDB0037017	(R)-p-Mentha-1,8-dien-10-ol	HMDB0037017	527143
1110	HMDB0037024	4-Acetyl-1,4-dimethyl-1-cyclohexene	HMDB0037024	65289
1111	HMDB0037025	Hop ether	HMDB0037025	556518
1112	HMDB0037172	Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran	HMDB0037172	61665
1113	HMDB0037280	Junionone	HMDB0037280	110518
1114	HMDB0037302	xi-p-Mentha-3,8-dien-1-ol	HMDB0037302	783852
1115	HMDB0037303	xi-p-Mentha-1(7),2-dien-4-ol	HMDB0037303	531936
1116	HMDB0038251	xi-Pinol	HMDB0038251	101153
1117	HMDB0038290	Photocitral A	HMDB0038290	102684
1118	HMDB0038557	xi-3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran	HMDB0038557	61275
1119	HMDB0039008	3,4-Epoxy-p-menth-1(7)-ene	HMDB0039008	101409
1120	HMDB0039816	2-Hexylfuran	HMDB0039816	77408
1121	HMDB0040766	Anethofuran	HMDB0040766	586292
1122	HMDB0041011	beta-Cyclocitral	HMDB0041011	9895
1123	HMDB0041013	Isocyclocitral	HMDB0041013	101150
1124	HMDB0041631	3-Thujanone	HMDB0041631	11027
1125	HMDB0059608	(+)-trans-Carveol	HMDB0059608	443178
1126	HMDB0059761	4-(1-Methylethyl)-1-cyclohexene-4-carboxaldehyde	HMDB0059761	124202
1127	HMDB0059827	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	HMDB0059827	38621
1128	HMDB0059838	Camphor	HMDB0059838	159055
1129	HMDB0059875	Carvotanacetone	HMDB0059875	643247
1130	HMDB0059885	p-Menth-1-en-9-al	HMDB0059885	520440
1131	HMDB0061794	NA	NA	NA
1132	HMDB0006291	NA	NA	NA
1133	HMDB0006410	NA	NA	NA
1134	C00808	NA	NA	NA
1135	C00809	NA	NA	NA
1136	C00964	NA	NA	NA
1137	C01123	NA	NA	NA
1138	C01499	NA	NA	NA
1139	C02213	NA	NA	NA
1140	C02452	NA	NA	NA

1141	C02759	NA	NA	NA
1142	C04435	NA	NA	NA
1143	C07271	NA	NA	NA
1144	C09847	NA	NA	NA
1145	C09859	NA	NA	NA
1146	C09885	NA	NA	NA
1147	C09893	NA	NA	NA
1148	C09906	NA	NA	NA
1149	C11387	NA	NA	NA
1150	C11395	NA	NA	NA
1151	C11398	NA	NA	NA
1152	C11401	NA	NA	NA
1153	C11408	NA	NA	NA
1154	C11409	NA	NA	NA
1155	C11412	NA	NA	NA
1156	C11415	NA	NA	NA
1157	C11938	NA	NA	NA
1158	C11941	NA	NA	NA
1159	C11942	NA	NA	NA
1160	C11951	NA	NA	NA
1161	C17623	NA	NA	NA
1162	C18018	NA	NA	NA
1163	C18369	NA	NA	NA
1164	C19081	NA	NA	NA
1165	C20260	NA	NA	NA
1166	C20425	NA	NA	NA
1167	CHEBI:10782	NA	NA	NA
1168	CHEBI:15387	NA	NA	NA
1169	CHEBI:15388	NA	NA	NA
1170	CHEBI:15389	NA	NA	NA
1171	CHEBI:15396	NA	NA	NA
1172	CHEBI:15397	NA	NA	NA
1173	CHEBI:154	NA	NA	NA
1174	CHEBI:15406	NA	NA	NA
1175	CHEBI:15420	NA	NA	NA
1176	CHEBI:155	NA	NA	NA
1177	CHEBI:16431	NA	NA	NA
1178	CHEBI:165	NA	NA	NA
1179	CHEBI:166	NA	NA	NA
1180	CHEBI:168	NA	NA	NA
1181	CHEBI:16980	NA	NA	NA
1182	CHEBI:17546	NA	NA	NA
1183	CHEBI:18481	NA	NA	NA
1184	CHEBI:227	NA	NA	NA
1185	CHEBI:23046	NA	NA	NA
1186	CHEBI:232	NA	NA	NA
1187	CHEBI:23316	NA	NA	NA
1188	CHEBI:23733	NA	NA	NA
1189	CHEBI:24911	NA	NA	NA
1190	CHEBI:26137	NA	NA	NA
1191	CHEBI:26381	NA	NA	NA
1192	CHEBI:26590	NA	NA	NA
1193	CHEBI:27049	NA	NA	NA
1194	CHEBI:29020	NA	NA	NA
1195	CHEBI:29060	NA	NA	NA
1196	CHEBI:35596	NA	NA	NA
1197	CHEBI:35669	NA	NA	NA
1198	CHEBI:35672	NA	NA	NA
1199	CHEBI:36612	NA	NA	NA
1200	CHEBI:36773	NA	NA	NA
1201	CHEBI:37046	NA	NA	NA
1202	CHEBI:37047	NA	NA	NA
1203	CHEBI:41	NA	NA	NA
1204	CHEBI:43812	NA	NA	NA
1205	CHEBI:48697	NA	NA	NA
1206	CHEBI:48933	NA	NA	NA
1207	CHEBI:48934	NA	NA	NA
1208	CHEBI:49150	NA	NA	NA
1209	CHEBI:4999	NA	NA	NA
1210	CHEBI:50040	NA	NA	NA
1211	CHEBI:50043	NA	NA	NA
1212	CHEBI:50045	NA	NA	NA
1213	CHEBI:50046	NA	NA	NA
1214	CHEBI:53177	NA	NA	NA
1215	CHEBI:61551	NA	NA	NA
1216	CHEBI:83263	NA	NA	NA
1217	CHEBI:84970	NA	NA	NA
1218	CHEBI:87568	NA	NA	NA
1219	CHEBI:89872	NA	NA	NA
1220	CHEBI:9577	NA	NA	NA
1221	HMDB0029610	Ascladiol	HMDB0029610	131750
1222	HMDB0059731	2,3-Methyleneglutaric acid	HMDB0059731	123510
1223	HMDB0125064	NA	NA	NA
1224	HMDB0125077	NA	NA	NA
1225	HMDB0140890	NA	NA	NA
1226	HMDB0140891	NA	NA	NA
1227	C04112	NA	NA	NA

1228	C04171	NA	NA	NA
1229	C04558	NA	NA	NA
1230	C04559	NA	NA	NA
1231	C04634	NA	NA	NA
1232	C06210	NA	NA	NA
1233	C06321	NA	NA	NA
1234	C06760	NA	NA	NA
1235	C18311	NA	NA	NA
1236	C20710	NA	NA	NA
1237	CHEBI:15941	NA	NA	NA
1238	CHEBI:16754	NA	NA	NA
1239	CHEBI:16766	NA	NA	NA
1240	CHEBI:28027	NA	NA	NA
1241	CHEBI:28958	NA	NA	NA
1242	CHEBI:36104	NA	NA	NA
1243	CHEBI:37888	NA	NA	NA
1244	CHEBI:37889	NA	NA	NA
1245	CHEBI:48968	NA	NA	NA
1246	CHEBI:48969	NA	NA	NA
1247	CHEBI:58085	NA	NA	NA
1248	CHEBI:75876	NA	NA	NA
1249	CHEBI:89910	NA	NA	NA
1250	CHEBI:90886	NA	NA	NA
1251	HMDB0000798	Oenanthic ether	HMDB0000798	7797
1252	HMDB0000847	Pelargonic acid	HMDB0000847	8158
1253	HMDB0030331	xi-2-Ethylheptanoic acid	HMDB0030331	18648
1254	HMDB0031291	Methyl caprylate	HMDB0031291	8091
1255	HMDB0031480	Heptyl acetate	HMDB0031480	8159
1256	HMDB0031557	4-Methyloctanoic acid	HMDB0031557	62089
1257	HMDB0032042	Butyl 3-methylbutanoate	HMDB0032042	7981
1258	HMDB0032309	3-Heptyl acetate	HMDB0032309	537615
1259	HMDB0032406	5-Methylhexyl acetate	HMDB0032406	221829
1260	HMDB0032454	3-Octyl formate	HMDB0032454	227578
1261	HMDB0034162	Pentyl butanoate	HMDB0034162	10890
1262	HMDB0034165	Propyl hexanoate	HMDB0034165	12293
1263	HMDB0034606	Hexyl propionate	HMDB0034606	88454
1264	HMDB0036234	3-Methylbutyl 2-methylpropanoate	HMDB0036234	519786
1265	HMDB0037143	1-Hydroxy-3-nonanone	HMDB0037143	536257
1266	HMDB0037164	3-(Hydroxymethyl)-2-octanone	HMDB0037164	62148
1267	HMDB0037288	4-Methyl-2-pentyl-1,3-dioxolane	HMDB0037288	15336
1268	HMDB0038040	2-Methylpropyl 3-methylbutanoate	HMDB0038040	11514
1269	HMDB0038603	Octyl formate	HMDB0038603	8176
1270	HMDB0039216	Butyl 2-methylbutanoate	HMDB0039216	61812
1271	HMDB0039219	1-Methylbutyl butanoate	HMDB0039219	43263
1272	HMDB0040221	Isoamyl butyrate	HMDB0040221	7795
1273	HMDB0040295	Butyl pentanoate	HMDB0040295	61137
1274	HMDB0040430	Isopropyl hexanoate	HMDB0040430	16832
1275	HMDB0059822	Ethyl 5-methylhexanoate	HMDB0059822	234290
1276	C01601	NA	NA	NA
1277	CHEBI:29019	NA	NA	NA
1278	CHEBI:37108	NA	NA	NA
1279	CHEBI:86618	NA	NA	NA
1280	CHEBI:87365	NA	NA	NA
1281	CHEBI:87422	NA	NA	NA
1282	CHEBI:87432	NA	NA	NA
1283	CHEBI:87496	NA	NA	NA
1284	CHEBI:87537	NA	NA	NA
1285	CHEBI:87549	NA	NA	NA
1286	CHEBI:87684	NA	NA	NA
1287	HMDB0000555	3-Methyladipic acid	HMDB0000555	699974
1288	HMDB0000857	Pimelic acid	HMDB0000857	385
1289	HMDB0002441	3,3-Dimethylglutaric acid	HMDB0002441	20984
1290	HMDB0029167	2-Methyladipic acid	HMDB0029167	522067
1291	HMDB0029573	Diethyl malonate	HMDB0029573	7761
1292	HMDB0041605	Propyleneglycol diacetate	HMDB0041605	12198
1293	HMDB0059722	Mono-methyl-adipate	HMDB0059722	12328
1294	HMDB0059738	2-Ethylglutaric acid	HMDB0059738	291968
1295	HMDB0059893	Ethyl methyl succinate	HMDB0059893	522068
1296	HMDB0061676	2,2-Dimethylglutaric acid	HMDB0061676	12681
1297	C02656	NA	NA	NA
1298	C04687	NA	NA	NA
1299	C16657	NA	NA	NA
1300	CHEBI:1129201	NA	NA	NA
1301	CHEBI:15566	NA	NA	NA
1302	CHEBI:30531	NA	NA	NA
1303	CHEBI:391281	NA	NA	NA
1304	CHEBI:68459	NA	NA	NA
1305	CHEBI:68502	NA	NA	NA
1306	CHEBI:68503	NA	NA	NA
1307	CHEBI:70855	NA	NA	NA
1308	CHEBI:87360	NA	NA	NA
1309	HMDB0001890	Acetylcysteine	HMDB0001890	12035
1310	C06809	NA	NA	NA
1311	C12876	NA	NA	NA
1312	CHEBI:28939	NA	NA	NA
1313	HMDB0030524	2(3H)-Benzothiazolethione	HMDB0030524	218317
1314	C14437	NA	NA	NA

1315	HMDB0000001	1-Methylhistidine	HMDB0000001	92105
1316	HMDB0000479	Methylhistidine	HMDB0000479	64969
1317	HMDB0004935	NA	NA	NA
1318	HMDB0006703	NA	NA	NA
1319	HMDB0006704	NA	NA	NA
1320	C01152	NA	NA	NA
1321	C03298	NA	NA	NA
1322	CHEBI:27596	NA	NA	NA
1323	CHEBI:50599	NA	NA	NA
1324	CHEBI:50601	NA	NA	NA
1325	CHEBI:70958	NA	NA	NA
1326	CHEBI:70959	NA	NA	NA
1327	CHEBI:70960	NA	NA	NA
1328	CHEBI:70961	NA	NA	NA
1329	CHEBI:75895	NA	NA	NA
1330	HMDB0001112	Glyceraldehyde 3-phosphate	HMDB0001112	439168
1331	HMDB0001473	Dihydroxyacetone phosphate	HMDB0001473	668
1332	HMDB0011735	NA	NA	NA
1333	C00111	NA	NA	NA
1334	C00118	NA	NA	NA
1335	C00661	NA	NA	NA
1336	C12935	NA	NA	NA
1337	C19156	NA	NA	NA
1338	CHEBI:16108	NA	NA	NA
1339	CHEBI:17138	NA	NA	NA
1340	CHEBI:231935	NA	NA	NA
1341	CHEBI:29052	NA	NA	NA
1342	CHEBI:340863	NA	NA	NA
1343	CHEBI:45013	NA	NA	NA
1344	CHEBI:48932	NA	NA	NA
1345	CHEBI:57597	NA	NA	NA
1346	CHEBI:57685	NA	NA	NA
1347	CHEBI:58083	NA	NA	NA
1348	HMDB0000318	3,4-Dihydroxyphenylglycol	HMDB0000318	91528
1349	HMDB0032966	Furaneol acetate	HMDB0032966	61334
1350	HMDB0038760	Herierin III	HMDB0038760	131340
1351	HMDB0038761	Herierin IV	HMDB0038761	131341
1352	HMDB0059756	3,4-Methyleneadipic acid	HMDB0059756	124202
1353	HMDB0132906	NA	NA	NA
1354	HMDB0132907	NA	NA	NA
1355	HMDB0133971	NA	NA	NA
1356	HMDB0133972	NA	NA	NA
1357	HMDB0133982	NA	NA	NA
1358	HMDB0005870	NA	NA	NA
1359	C05576	NA	NA	NA
1360	C06720	NA	NA	NA
1361	C06729	NA	NA	NA
1362	C06731	NA	NA	NA
1363	C07123	NA	NA	NA
1364	C16804	NA	NA	NA
1365	C19495	NA	NA	NA
1366	CHEBI:1387	NA	NA	NA
1367	CHEBI:16100	NA	NA	NA
1368	CHEBI:17641	NA	NA	NA
1369	CHEBI:49008	NA	NA	NA
1370	CHEBI:49009	NA	NA	NA
1371	CHEBI:89898	NA	NA	NA
1372	HMDB0004980	cis-4-Decenoic acid	HMDB0004980	531235
1373	HMDB0010726	trans-Dec-2-enoic acid	HMDB0010726	528272
1374	HMDB0012183	8-Methylnonenoate	HMDB0012183	536595
1375	HMDB0029358	5Z-Octenyl acetate	HMDB0029358	535283
1376	HMDB0029859	Methyl (xi)-3-nonenoate	HMDB0029859	146909
1377	HMDB0030031	(±)-6-Methyl-5-hepten-2-yl acetate	HMDB0030031	87947
1378	HMDB0031002	3-Decenoic acid	HMDB0031002	531235
1379	HMDB0031003	9-Decenoic acid	HMDB0031003	61743
1380	HMDB0031297	2-Octenyl acetate	HMDB0031297	128071
1381	HMDB0031362	Cyclohexylethyl acetate	HMDB0031362	30771
1382	HMDB0031440	Linalool oxide (trans-pyranoid)	HMDB0031440	642778
1383	HMDB0031441	Linalool oxide III	HMDB0031441	642857
1384	HMDB0032119	4-Hydroxy-2,6-dimethyl-7-octen-3-one	HMDB0032119	158402
1385	HMDB0032275	Ethyl 3-octenoate	HMDB0032275	536439
1386	HMDB0032393	2-Methylbutyl 3-methyl-2-butenate	HMDB0032393	113425
1387	HMDB0032452	1-Octen-3-yl acetate	HMDB0032452	17121
1388	HMDB0033203	6-Decanolide	HMDB0033203	62583
1389	HMDB0033377	cis-3-Hexenyl butyrate	HMDB0033377	535243
1390	HMDB0034427	Cyclohexyl butanoate	HMDB0034427	243783
1391	HMDB0034581	2-Hexenyl butanoate	HMDB0034581	535246
1392	HMDB0034880	3-Methyl-2,4-nonanedione	HMDB0034880	529481
1393	HMDB0035122	(S,E)-2,6-Dimethyl-5,7-octadiene-2,3-diol	HMDB0035122	898026
1394	HMDB0035365	Cnidial C	HMDB0035365	26396
1395	HMDB0035837	Citronellal acid	HMDB0035837	10402
1396	HMDB0035839	(E)-3-(Tetrahydro-5,5-dimethyl-2-furanyl)-2-buten-1-ol	HMDB0035839	131751
1397	HMDB0035907	Linalyl oxide	HMDB0035907	22310
1398	HMDB0036099	Lilac alcohol	HMDB0036099	526973
1399	HMDB0036211	Hexyl crotonate	HMDB0036211	535690
1400	HMDB0036990	2,6-Dimethyl-3,7-octadiene-2,6-diol	HMDB0036990	535245
1401	HMDB0036992	1-Cyclopropyl-4-methyl-1,3-cyclohexanediol	HMDB0036992	738151

1402	HMDB0037021	trans-p-Menth-2-ene-1,4-diol	HMDB0037021	300085
1403	HMDB0037116	delta-Decalactone	HMDB0037116	12810
1404	HMDB0037217	xi-5-Hexyldihydro-2(3H)-furanone	HMDB0037217	12813
1405	HMDB0037497	Ethyl (E)-2-octenoate	HMDB0037497	535276
1406	HMDB0037632	xi-Tetrahydro-3-pentyl-2H-pyran-2-one	HMDB0037632	122977
1407	HMDB0038744	9-Hydroxygeraniol	HMDB0038744	136194
1408	HMDB0039149	(+)-6-Hydroxy-2,6-dimethyl-7-octen-4-one	HMDB0039149	522417
1409	HMDB0039768	5-Decenoic acid	HMDB0039768	536259
1410	HMDB0039795	Ethyl 4Z-octenoate	HMDB0039795	535279
1411	HMDB0040194	Methyl 2-nonenoate	HMDB0040194	535738
1412	HMDB0040208	2-Propenyl heptanoate	HMDB0040208	8878
1413	HMDB0040213	cis-3-Hexenyl isobutyrate	HMDB0040213	535253
1414	HMDB0040330	Menthone lactone	HMDB0040330	62349
1415	HMDB0040530	Isopentyl 3-methyl-2-butenate	HMDB0040530	92570
1416	HMDB0040726	(±)-cis-Linalyl oxide	HMDB0040726	642857
1417	HMDB0040727	(±)-trans-Linalyl oxide	HMDB0040727	643225
1418	HMDB0041012	6-Decenoic acid	HMDB0041012	536259
1419	HMDB0041630	NA	NA	NA
1420	HMDB0059610	2-Exo-hydroxy-1,8-cineole	HMDB0059610	685738
1421	HMDB0059852	2-Hydroxycineol	HMDB0059852	529885
1422	C03092	NA	NA	NA
1423	C04433	NA	NA	NA
1424	C07276	NA	NA	NA
1425	C09790	NA	NA	NA
1426	C16462	NA	NA	NA
1427	C17621	NA	NA	NA
1428	C18020	NA	NA	NA
1429	C18027	NA	NA	NA
1430	C18066	NA	NA	NA
1431	C18202	NA	NA	NA
1432	C19082	NA	NA	NA
1433	C20326	NA	NA	NA
1434	CHEBI:15662	NA	NA	NA
1435	CHEBI:16271	NA	NA	NA
1436	CHEBI:17219	NA	NA	NA
1437	CHEBI:18515	NA	NA	NA
1438	CHEBI:32380	NA	NA	NA
1439	CHEBI:32381	NA	NA	NA
1440	CHEBI:35811	NA	NA	NA
1441	CHEBI:37809	NA	NA	NA
1442	CHEBI:50243	NA	NA	NA
1443	CHEBI:50244	NA	NA	NA
1444	CHEBI:50250	NA	NA	NA
1445	CHEBI:50251	NA	NA	NA
1446	CHEBI:50465	NA	NA	NA
1447	CHEBI:50466	NA	NA	NA
1448	CHEBI:50467	NA	NA	NA
1449	CHEBI:59623	NA	NA	NA
1450	CHEBI:61200	NA	NA	NA
1451	CHEBI:64235	NA	NA	NA
1452	CHEBI:82759	NA	NA	NA
1453	CHEBI:87325	NA	NA	NA
1454	CHEBI:87327	NA	NA	NA
1455	CHEBI:87575	NA	NA	NA
1456	CHEBI:88534	NA	NA	NA
1457	CHEBI:88903	NA	NA	NA
1458	CHEBI:90956	NA	NA	NA
1459	HMDB0012289	Tetrahydrodipicolinate	HMDB0012289	440179
1460	C03972	NA	NA	NA
1461	C12108	NA	NA	NA
1462	C17356	NA	NA	NA
1463	CHEBI:29514	NA	NA	NA
1464	CHEBI:32975	NA	NA	NA
1465	CHEBI:32976	NA	NA	NA
1466	CHEBI:71963	NA	NA	NA
1467	CHEBI:864	NA	NA	NA
1468	HMDB0000721	Glycylproline	HMDB0000721	301362
1469	HMDB0011178	Prolylglycine	HMDB0011178	642670
1470	CHEBI:356329	NA	NA	NA
1471	CHEBI:356660	NA	NA	NA
1472	CHEBI:49185	NA	NA	NA
1473	CHEBI:61695	NA	NA	NA
1474	CHEBI:61696	NA	NA	NA
1475	CHEBI:70744	NA	NA	NA
1476	CHEBI:73594	NA	NA	NA
1477	CHEBI:73779	NA	NA	NA
1478	HMDB0060015	Phenol sulphate	HMDB0060015	74426
1479	C00850	NA	NA	NA
1480	C02180	NA	NA	NA
1481	C12849	NA	NA	NA
1482	CHEBI:27905	NA	NA	NA
1483	CHEBI:32354	NA	NA	NA
1484	CHEBI:71047	NA	NA	NA
1485	CHEBI:71049	NA	NA	NA
1486	HMDB0000517	L-Arginine	HMDB0000517	6322
1487	HMDB0003416	D-Arginine	HMDB0003416	71070
1488	C00062	NA	NA	NA

1489	C00792	NA	NA	NA
1490	C02385	NA	NA	NA
1491	CHEBI:15816	NA	NA	NA
1492	CHEBI:16467	NA	NA	NA
1493	CHEBI:29016	NA	NA	NA
1494	HMDB0013223	Butyrylcholine	HMDB0013223	17233
1495	HMDB0029936	(2S,4R,5S)-Muscarine	HMDB0029936	507949
1496	C07473	NA	NA	NA
1497	CHEBI:327449	NA	NA	NA
1498	CHEBI:522933	NA	NA	NA
1499	HMDB0000044	Ascorbic acid	HMDB0000044	546700
1500	HMDB0006355	D-Glucurono-6,3-lactone	HMDB0006355	272433
1501	HMDB0031193	1,2,3-Propanetricarboxylic acid	HMDB0031193	14925
1502	HMDB0014273	NA	NA	NA
1503	HMDB0029945	NA	NA	NA
1504	C00072	NA	NA	NA
1505	C02670	NA	NA	NA
1506	C03217	NA	NA	NA
1507	C03289	NA	NA	NA
1508	C03387	NA	NA	NA
1509	C04053	NA	NA	NA
1510	C04349	NA	NA	NA
1511	C04471	NA	NA	NA
1512	C06033	NA	NA	NA
1513	C06430	NA	NA	NA
1514	C06440	NA	NA	NA
1515	C19806	NA	NA	NA
1516	C20364	NA	NA	NA
1517	CHEBI:100148	NA	NA	NA
1518	CHEBI:15623	NA	NA	NA
1519	CHEBI:15624	NA	NA	NA
1520	CHEBI:16278	NA	NA	NA
1521	CHEBI:17039	NA	NA	NA
1522	CHEBI:17208	NA	NA	NA
1523	CHEBI:17782	NA	NA	NA
1524	CHEBI:17801	NA	NA	NA
1525	CHEBI:18268	NA	NA	NA
1526	CHEBI:28745	NA	NA	NA
1527	CHEBI:29073	NA	NA	NA
1528	CHEBI:41893	NA	NA	NA
1529	CHEBI:45969	NA	NA	NA
1530	CHEBI:51384	NA	NA	NA
1531	CHEBI:51438	NA	NA	NA
1532	CHEBI:51440	NA	NA	NA
1533	CHEBI:55433	NA	NA	NA
1534	CHEBI:55463	NA	NA	NA
1535	CHEBI:62479	NA	NA	NA
1536	CHEBI:73681	NA	NA	NA
1537	HMDB0000158	L-Tyrosine	HMDB0000158	6057
1538	HMDB0001119	4-Hydroxy-4-(3-pyridyl)-butanoic acid	HMDB0001119	438
1539	HMDB0002184	L-Threo-3-Phenylserine	HMDB0002184	123141
1540	HMDB0003831	Beta-Tyrosine	HMDB0003831	440311
1541	HMDB0006050	o-Tyrosine	HMDB0006050	91482
1542	HMDB0059720	NA	NA	NA
1543	HMDB0060280	NA	NA	NA
1544	HMDB0000647	NA	NA	NA
1545	C00082	NA	NA	NA
1546	C01536	NA	NA	NA
1547	C03290	NA	NA	NA
1548	C04368	NA	NA	NA
1549	C06420	NA	NA	NA
1550	C19579	NA	NA	NA
1551	C19712	NA	NA	NA
1552	C20807	NA	NA	NA
1553	CHEBI:16795	NA	NA	NA
1554	CHEBI:16939	NA	NA	NA
1555	CHEBI:17895	NA	NA	NA
1556	CHEBI:18186	NA	NA	NA
1557	CHEBI:278475	NA	NA	NA
1558	CHEBI:28479	NA	NA	NA
1559	CHEBI:32763	NA	NA	NA
1560	CHEBI:32776	NA	NA	NA
1561	CHEBI:32787	NA	NA	NA
1562	CHEBI:44303	NA	NA	NA
1563	CHEBI:47990	NA	NA	NA
1564	CHEBI:57901	NA	NA	NA
1565	CHEBI:57956	NA	NA	NA
1566	CHEBI:58315	NA	NA	NA
1567	CHEBI:58570	NA	NA	NA
1568	CHEBI:78290	NA	NA	NA
1569	CHEBI:91037	NA	NA	NA
1570	CHEBI:91038	NA	NA	NA
1571	CHEBI:91041	NA	NA	NA
1572	HMDB0036117	(1'R)-Nepetalic acid	HMDB0036117	123132
1573	HMDB0036998	(S)-Oleuropeic acid	HMDB0036998	123137
1574	HMDB0039052	(4S,8R)-8,9-Dihydroxy-p-menth-1(6)-en-2-one	HMDB0039052	731208
1575	HMDB0039710	1-Acetylcyclohexyl acetate	HMDB0039710	62017

1576	HMDB0040883	(E)-10-Oxo-8-decenoic acid	HMDB0040883	124315
1577	C03843	NA	NA	NA
1578	C04718	NA	NA	NA
1579	C06066	NA	NA	NA
1580	C11405	NA	NA	NA
1581	C11419	NA	NA	NA
1582	C19079	NA	NA	NA
1583	C19084	NA	NA	NA
1584	C20324	NA	NA	NA
1585	CHEBI:29064	NA	NA	NA
1586	CHEBI:37287	NA	NA	NA
1587	CHEBI:37291	NA	NA	NA
1588	CHEBI:37379	NA	NA	NA
1589	CHEBI:64264	NA	NA	NA
1590	CHEBI:64274	NA	NA	NA
1591	CHEBI:64899	NA	NA	NA
1592	CHEBI:70741	NA	NA	NA
1593	CHEBI:87777	NA	NA	NA
1594	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	HMDB0031062	129711
1595	HMDB0031063	(Z)-3-Methyl-4-decenoic acid	HMDB0031063	131751
1596	HMDB0031087	trans-2-Hexyl-1-cyclopropaneacetic acid	HMDB0031087	543595
1597	HMDB0031272	Ethyl (E)-2-nonenolate	HMDB0031272	122775
1598	HMDB0031406	Ethyl 3-cyclohexylpropionate	HMDB0031406	61466
1599	HMDB0031691	cis-3-Hexenyl pentanoate	HMDB0031691	536768
1600	HMDB0031843	2,3-Undecanedione	HMDB0031843	61404
1601	HMDB0032308	(E)-3-Heptenyl 2-methylpropanoate	HMDB0032308	643713
1602	HMDB0032320	3-Hexenyl 2-methylbutyrate	HMDB0032320	616510
1603	HMDB0032396	Methyl 2-decenoate	HMDB0032396	536806
1604	HMDB0032404	6-Methyl-5-hepten-2-one propyleneglycol acetal	HMDB0032404	109257
1605	HMDB0032453	cis-3-Octenyl propionate	HMDB0032453	208363
1606	HMDB0032461	Pent-2-enyl hexanoate	HMDB0032461	536314
1607	HMDB0032489	Prenyl caproate	HMDB0032489	173534
1608	HMDB0032534	trans-2-Hexenyl 2-methylbutyrate	HMDB0032534	535245
1609	HMDB0033371	Citronellyl formate	HMDB0033371	7778
1610	HMDB0033724	Undecylenic acid	HMDB0033724	5634
1611	HMDB0034428	Cyclohexyl 3-methylbutanoate	HMDB0034428	287439
1612	HMDB0034429	Cyclohexyl pentanoate	HMDB0034429	73772
1613	HMDB0036140	5-Hexyldihydro-5-methyl-2(3H)-furanone	HMDB0036140	285097
1614	HMDB0036784	6-Hexyltetrahydro-2H-pyran-2-one	HMDB0036784	61204
1615	HMDB0037106	(x)-1-Nonen-3-yl acetate	HMDB0037106	169364
1616	HMDB0037185	Rhodinyl formate	HMDB0037185	61092
1617	HMDB0037225	Methyl citronellate	HMDB0037225	61290
1618	HMDB0037309	5-Hexyldihydro-4-methyl-2(3H)-furanone	HMDB0037309	106756
1619	HMDB0038273	2-Hexenyl valerate	HMDB0038273	535297
1620	HMDB0038274	2-Hexenyl isovalerate	HMDB0038274	535246
1621	HMDB0038277	cis-3-Hexenyl 2-methylbutanoate	HMDB0038277	536506
1622	HMDB0038278	cis-3-Hexenyl 3-methylbutanoate	HMDB0038278	536768
1623	HMDB0038311	xi-gamma-Undecalactone	HMDB0038311	7714
1624	HMDB0038906	5-Octenyl propanoate	HMDB0038906	110414
1625	HMDB0040593	2-Propenyl octanoate	HMDB0040593	20219
1626	C12295	NA	NA	NA
1627	C13422	NA	NA	NA
1628	C13823	NA	NA	NA
1629	C13910	NA	NA	NA
1630	C19420	NA	NA	NA
1631	CHEBI:31676	NA	NA	NA
1632	CHEBI:35045	NA	NA	NA
1633	CHEBI:39449	NA	NA	NA
1634	CHEBI:39450	NA	NA	NA
1635	CHEBI:39451	NA	NA	NA
1636	CHEBI:39452	NA	NA	NA
1637	CHEBI:39453	NA	NA	NA
1638	CHEBI:39454	NA	NA	NA
1639	CHEBI:48944	NA	NA	NA
1640	CHEBI:59624	NA	NA	NA
1641	CHEBI:87312	NA	NA	NA
1642	CHEBI:87689	NA	NA	NA
1643	HMDB0030988	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	HMDB0030988	131751
1644	HMDB0030992	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	HMDB0030992	131751
1645	C14112	NA	NA	NA
1646	CHEBI:78208	NA	NA	NA
1647	HMDB0000734	Indoleacrylic acid	HMDB0000734	537504
1648	CHEBI:90333	NA	NA	NA
1649	HMDB0002203	3-Hydroxycapric acid	HMDB0002203	531279
1650	HMDB0010725	(R)-3-Hydroxydecanoic acid	HMDB0010725	531279
1651	HMDB0033201	9-Hydroxydecanoic acid	HMDB0033201	457523
1652	HMDB0033574	(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	HMDB0033574	738097
1653	HMDB0033640	7-Methyl-3-methylene-1,6,7-octanetriol	HMDB0033640	106076
1654	HMDB0034783	cis-p-Menthane-1,7,8-triol	HMDB0034783	126863
1655	HMDB0038186	2,6-Dimethyl-7-octene-2,3,6-triol	HMDB0038186	152414
1656	HMDB0039470	(1S,2S,4R,8R)-p-Menthane-1,2,9-triol	HMDB0039470	738097
1657	HMDB0039668	2-Hexyl-1,3-dioxan-5-ol	HMDB0039668	74361
1658	HMDB0039669	2-Hexyl-1,3-dioxolane-4-methanol	HMDB0039669	15571
1659	HMDB0039893	(1R,2R,4S)-p-Menthane-1,2,8-triol	HMDB0039893	186702
1660	HMDB0040329	xi-5-Hydroxydecanoic acid	HMDB0040329	1825
1661	HMDB0041600	Ethyl (±)-3-hydroxyoctanoate	HMDB0041600	110975
1662	C02774	NA	NA	NA

1663	C18067	NA	NA	NA
1664	CHEBI:132983	NA	NA	NA
1665	CHEBI:17409	NA	NA	NA
1666	CHEBI:37371	NA	NA	NA
1667	CHEBI:50451	NA	NA	NA
1668	CHEBI:64265	NA	NA	NA
1669	CHEBI:64269	NA	NA	NA
1670	CHEBI:78951	NA	NA	NA
1671	HMDB0012710	3-Dehydroquinic acid	HMDB0012710	439351
1672	HMDB0059927	NA	NA	NA
1673	C00944	NA	NA	NA
1674	C04049	NA	NA	NA
1675	C05601	NA	NA	NA
1676	C06201	NA	NA	NA
1677	CHEBI:17947	NA	NA	NA
1678	CHEBI:51822	NA	NA	NA
1679	CHEBI:73089	NA	NA	NA
1680	CHEBI:87773	NA	NA	NA
1681	CHEBI:915	NA	NA	NA
1682	HMDB0029915	D-4-O-Methyl-myo-inositol	HMDB0029915	NA
1683	HMDB0029916	NA	NA	NA
1684	HMDB0029965	Methyl beta-D-glucopyranoside	HMDB0029965	445238
1685	HMDB0031437	(-)-Bornesitol	HMDB0031437	NA
1686	HMDB0031449	Sequoiitol	HMDB0031449	439990
1687	HMDB0033816	Mytilitol	HMDB0033816	NA
1688	HMDB0034219	D-Pinitol	HMDB0034219	0
1689	HMDB0034221	L-Quebrachitol	HMDB0034221	0
1690	HMDB0034222	NA	NA	NA
1691	HMDB0062564	NA	NA	NA
1692	C03365	NA	NA	NA
1693	C03619	NA	NA	NA
1694	C03659	NA	NA	NA
1695	C03660	NA	NA	NA
1696	C03844	NA	NA	NA
1697	C05163	NA	NA	NA
1698	C06352	NA	NA	NA
1699	C06353	NA	NA	NA
1700	C08257	NA	NA	NA
1701	CHEBI:111	NA	NA	NA
1702	CHEBI:113524	NA	NA	NA
1703	CHEBI:15975	NA	NA	NA
1704	CHEBI:17540	NA	NA	NA
1705	CHEBI:18173	NA	NA	NA
1706	CHEBI:18266	NA	NA	NA
1707	CHEBI:18427	NA	NA	NA
1708	CHEBI:20741	NA	NA	NA
1709	CHEBI:28310	NA	NA	NA
1710	CHEBI:28548	NA	NA	NA
1711	CHEBI:28762	NA	NA	NA
1712	CHEBI:320055	NA	NA	NA
1713	CHEBI:320061	NA	NA	NA
1714	CHEBI:37209	NA	NA	NA
1715	CHEBI:37656	NA	NA	NA
1716	CHEBI:37657	NA	NA	NA
1717	CHEBI:43943	NA	NA	NA
1718	CHEBI:55507	NA	NA	NA
1719	CHEBI:64171	NA	NA	NA
1720	CHEBI:73918	NA	NA	NA
1721	HMDB0031517	(R)-3-Hydroxy-5-phenylpentanoic acid	HMDB0031517	111062
1722	HMDB0031984	2,5-Dimethoxy-4-(2-propenyl)phenol	HMDB0031984	110525
1723	HMDB0032575	Butylparaben	HMDB0032575	7184
1724	HMDB0032590	Zingerone	HMDB0032590	31211
1725	HMDB0034206	Ethyl 4-methylphenoxyacetate	HMDB0034206	404728
1726	HMDB0034990	4-Methoxybenzyl propanoate	HMDB0034990	61417
1727	HMDB0036432	Isobutyl salicylate	HMDB0036432	6873
1728	HMDB0037271	2,6-Dimethoxy-4-(1-propenyl)phenol	HMDB0037271	535290
1729	HMDB0040730	Butyl salicylate	HMDB0040730	16330
1730	HMDB0041194	Methoxyeugenol	HMDB0041194	226486
1731	HMDB0041505	5-Hydroxy-2-benzyl-1,3-dioxane	HMDB0041505	78476
1732	HMDB0041506	2-Benzyl-5-hydroxymethyl-1,3-dioxolane	HMDB0041506	21895
1733	HMDB0041666	3-Hydroxyphenyl-valeric acid	HMDB0041666	105597
1734	HMDB0059898	Ethyl 4-ethoxybenzoate	HMDB0059898	90232
1735	HMDB0059940	NA	NA	NA
1736	HMDB0059941	NA	NA	NA
1737	HMDB0059942	NA	NA	NA
1738	HMDB0059943	NA	NA	NA
1739	HMDB0059944	NA	NA	NA
1740	HMDB0059945	NA	NA	NA
1741	HMDB0124918	NA	NA	NA
1742	HMDB0126161	NA	NA	NA
1743	HMDB0126162	NA	NA	NA
1744	HMDB0126163	NA	NA	NA
1745	HMDB0126262	NA	NA	NA
1746	HMDB0126462	NA	NA	NA
1747	HMDB0126463	NA	NA	NA
1748	HMDB0126464	NA	NA	NA
1749	HMDB0126465	NA	NA	NA

1750	HMDB0126466	NA	NA	NA
1751	HMDB0132270	NA	NA	NA
1752	HMDB0133190	NA	NA	NA
1753	HMDB0133191	NA	NA	NA
1754	HMDB0133192	NA	NA	NA
1755	HMDB0133193	NA	NA	NA
1756	HMDB0133194	NA	NA	NA
1757	HMDB0133463	NA	NA	NA
1758	HMDB0133484	NA	NA	NA
1759	HMDB0133515	NA	NA	NA
1760	HMDB0133538	NA	NA	NA
1761	HMDB0141323	NA	NA	NA
1762	C17497	NA	NA	NA
1763	C20342	NA	NA	NA
1764	CHEBI:39359	NA	NA	NA
1765	CHEBI:68657	NA	NA	NA
1766	CHEBI:86551	NA	NA	NA
1767	CHEBI:86562	NA	NA	NA
1768	CHEBI:87513	NA	NA	NA
1769	HMDB0000529	5Z-Dodecenoic acid	HMDB0000529	531237
1770	HMDB0010729	trans-Dodec-2-enoic acid	HMDB0010729	528272
1771	HMDB0029585	Methyl 10-undecenoate	HMDB0029585	8138
1772	HMDB0029763	Allyl nonanoate	HMDB0029763	61410
1773	HMDB0031683	xi-Dihydro-5-octyl-2(3H)-furanone	HMDB0031683	16821
1774	HMDB0032214	cis-4-Decenyl acetate	HMDB0032214	535283
1775	HMDB0032235	2,6-Dimethyl-5-heptenal propyleneglycol acetal	HMDB0032235	441537
1776	HMDB0032248	11-Dodecenoic acid	HMDB0032248	125207
1777	HMDB0033378	cis-3-Hexenyl hexanoate	HMDB0033378	535254
1778	HMDB0034160	(±)-Citronellyl acetate	HMDB0034160	9017
1779	HMDB0034844	Citronellyl acetate	HMDB0034844	670868
1780	HMDB0036182	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	HMDB0036182	106080
1781	HMDB0037186	Rhodinyl acetate	HMDB0037186	8833
1782	HMDB0037305	Methyl 9-undecenoate	HMDB0037305	117456
1783	HMDB0037329	Ethyl 2-decenoate	HMDB0037329	546390
1784	HMDB0037498	1-Ethenylhexyl butanoate	HMDB0037498	27892
1785	HMDB0037742	xi-5-Dodecanolide	HMDB0037742	12844
1786	HMDB0037813	3-Heptyldihydro-5-methyl-2(3H)-furanone	HMDB0037813	61990
1787	HMDB0038081	2-Octenyl butyrate	HMDB0038081	124355
1788	HMDB0038269	Hexyl 2E-hexenoate	HMDB0038269	643586
1789	HMDB0038895	7-Hexyl-2-oxepanone	HMDB0038895	61835
1790	HMDB0038924	2-Hexenyl hexanoate	HMDB0038924	535297
1791	HMDB0039220	Ethyl 4-decenoate	HMDB0039220	536258
1792	HMDB0040158	Hexyl 2-methyl-3-pentenoate	HMDB0040158	715871
1793	HMDB0040163	Hexyl 2-methyl-4-pentenoate	HMDB0040163	573511
1794	HMDB0040361	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene	HMDB0040361	535243
1795	HMDB0041264	(±)-Menthyl acetate	HMDB0041264	220674
1796	HMDB0041449	[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde	HMDB0041449	61401
1797	C09870	NA	NA	NA
1798	C12298	NA	NA	NA
1799	C16825	NA	NA	NA
1800	C16947	NA	NA	NA
1801	CHEBI:1030421	NA	NA	NA
1802	CHEBI:1115857	NA	NA	NA
1803	CHEBI:37162	NA	NA	NA
1804	CHEBI:37207	NA	NA	NA
1805	CHEBI:38371	NA	NA	NA
1806	CHEBI:38372	NA	NA	NA
1807	CHEBI:38373	NA	NA	NA
1808	CHEBI:38374	NA	NA	NA
1809	CHEBI:38375	NA	NA	NA
1810	CHEBI:38376	NA	NA	NA
1811	CHEBI:38377	NA	NA	NA
1812	CHEBI:38378	NA	NA	NA
1813	CHEBI:38379	NA	NA	NA
1814	CHEBI:38380	NA	NA	NA
1815	CHEBI:38381	NA	NA	NA
1816	CHEBI:70478	NA	NA	NA
1817	CHEBI:750110	NA	NA	NA
1818	CHEBI:83044	NA	NA	NA
1819	CHEBI:86595	NA	NA	NA
1820	CHEBI:87324	NA	NA	NA
1821	CHEBI:87338	NA	NA	NA
1822	CHEBI:87493	NA	NA	NA
1823	HMDB0032424	2-(4-Methyl-5-thiazolyl)ethyl propionate	HMDB0032424	299333
1824	CHEBI:61550	NA	NA	NA
1825	HMDB0032662	(S)-9-Hydroxy-10-undecenoic acid	HMDB0032662	104653
1826	HMDB0036029	Clarycet	HMDB0036029	574833
1827	HMDB0037179	3-Nonanon-1-yl acetate	HMDB0037179	126784
1828	CHEBI:132854	NA	NA	NA
1829	CHEBI:78953	NA	NA	NA
1830	CHEBI:79123	NA	NA	NA
1831	HMDB0000638	Dodecanoic acid	HMDB0000638	3893
1832	HMDB0030998	Ethyl decanoate	HMDB0030998	8048
1833	HMDB0032310	2-Heptyl butyrate	HMDB0032310	89307
1834	HMDB0032440	Nonanal propyleneglycol acetal	HMDB0032440	95572
1835	HMDB0033619	Hexyl hexanoate	HMDB0033619	22873
1836	HMDB0034128	Isopropyl nonanoate	HMDB0034128	119911

1837	HMDB0034136	Octyl butanoate	HMDB0034136	61030
1838	HMDB0034137	Octyl 2-methylpropanoate	HMDB0034137	61024
1839	HMDB0035410	(R)-Dihydrocitronellol acetate	HMDB0035410	30249
1840	HMDB0036225	Pentyl heptanoate	HMDB0036225	61415
1841	HMDB0040166	Decyl acetate	HMDB0040166	8167
1842	HMDB0059868	Isobutyl octanoate	HMDB0059868	79582
1843	C02679	NA	NA	NA
1844	CHEBI:201659	NA	NA	NA
1845	CHEBI:30805	NA	NA	NA
1846	CHEBI:84889	NA	NA	NA
1847	CHEBI:85059	NA	NA	NA
1848	CHEBI:87380	NA	NA	NA
1849	CHEBI:87430	NA	NA	NA
1850	CHEBI:87527	NA	NA	NA
1851	HMDB0032306	Diethyl oxalpropionate	HMDB0032306	97750
1852	HMDB0033092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	HMDB0033092	101414
1853	C04067	NA	NA	NA
1854	CHEBI:16879	NA	NA	NA
1855	HMDB0032443	3-Hydroxynonyl acetate	HMDB0032443	234237
1856	HMDB0061654	NA	NA	NA
1857	CHEBI:71005	NA	NA	NA
1858	CHEBI:77419	NA	NA	NA
1859	CHEBI:78956	NA	NA	NA
1860	CHEBI:79126	NA	NA	NA
1861	HMDB0060013	O-methoxycatechol-O-sulphate	HMDB0060013	22473
1862	CHEBI:133460	NA	NA	NA
1863	CHEBI:85537	NA	NA	NA
1864	HMDB0000929	L-Tryptophan	HMDB0000929	6305
1865	HMDB0013609	D-Tryptophan	HMDB0013609	9060
1866	HMDB0013840	3-Hydroxymethylantipyrine	HMDB0013840	123963
1867	HMDB0014892	Ethotoin	HMDB0014892	3292
1868	HMDB0030396	(±)-Tryptophan	HMDB0030396	1148
1869	HMDB0060533	Nirvanol	HMDB0060533	91480
1870	HMDB0060878	4-Hydroxyantipyrine	HMDB0060878	98889
1871	HMDB0060967	S-nirvanol	HMDB0060967	654081
1872	C00078	NA	NA	NA
1873	C00525	NA	NA	NA
1874	C00806	NA	NA	NA
1875	C07839	NA	NA	NA
1876	C10968	NA	NA	NA
1877	C14916	NA	NA	NA
1878	CHEBI:16296	NA	NA	NA
1879	CHEBI:16828	NA	NA	NA
1880	CHEBI:27897	NA	NA	NA
1881	CHEBI:32713	NA	NA	NA
1882	CHEBI:32724	NA	NA	NA
1883	CHEBI:32729	NA	NA	NA
1884	CHEBI:4888	NA	NA	NA
1885	CHEBI:51053	NA	NA	NA
1886	CHEBI:51054	NA	NA	NA
1887	CHEBI:57719	NA	NA	NA
1888	CHEBI:57912	NA	NA	NA
1889	CHEBI:5862	NA	NA	NA
1890	CHEBI:60359	NA	NA	NA
1891	CHEBI:60360	NA	NA	NA
1892	CHEBI:64554	NA	NA	NA
1893	HMDB0059752	NA	NA	NA
1894	HMDB0060016	Pyrogallol-1-O-sulphate	HMDB0060016	541106
1895	HMDB0060018	Pyrogallol-2-O-sulphate	HMDB0060018	920136
1896	CHEBI:89613	NA	NA	NA
1897	CHEBI:89615	NA	NA	NA
1898	HMDB0030762	Ethyl trans-p-methoxycinnamate	HMDB0030762	528178
1899	HMDB0031729	Phenylmethylglycidic ester	HMDB0031729	6501
1900	HMDB0031973	(2R,5R)-(E)-2-(2-Phenylethenyl)-1,3-dioxan-5-ol	HMDB0031973	131751
1901	HMDB0032348	Isoeugenyl acetate	HMDB0032348	876160
1902	HMDB0033594	Cuelure	HMDB0033594	19137
1903	HMDB0034122	Aceteugenol	HMDB0034122	7136
1904	HMDB0034135	Isoeugenol acetate	HMDB0034135	171513
1905	HMDB0035071	Verimol I	HMDB0035071	109326
1906	HMDB0041410	2,3-Dihydro-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	HMDB0041410	125316
1907	HMDB0127763	NA	NA	NA
1908	HMDB0132972	NA	NA	NA
1909	HMDB0132974	NA	NA	NA
1910	HMDB0132975	NA	NA	NA
1911	HMDB0132976	NA	NA	NA
1912	HMDB0132977	NA	NA	NA
1913	HMDB0132987	NA	NA	NA
1914	HMDB0135898	NA	NA	NA
1915	C04000	NA	NA	NA
1916	C10476	NA	NA	NA
1917	C12458	NA	NA	NA
1918	C14567	NA	NA	NA
1919	CHEBI:16079	NA	NA	NA
1920	CHEBI:259672	NA	NA	NA
1921	CHEBI:31111	NA	NA	NA
1922	CHEBI:86583	NA	NA	NA
1923	HMDB0013825	4-(1,1,3,3-Tetramethylbutyl)-phenol	HMDB0013825	8814

1924	HMDB0031737	delta-Methylionone	HMDB0031737	537219
1925	HMDB0031738	3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	HMDB0031738	537217
1926	HMDB0032397	Methyl-delta-ionone	HMDB0032397	546391
1927	HMDB0032528	NA	NA	NA
1928	HMDB0035245	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one	HMDB0035245	537108
1929	HMDB0035631	alpha-Irone	HMDB0035631	537100
1930	HMDB0036023	Etaspirene	HMDB0036023	222190
1931	HMDB0036024	10-Isopropyl-2,7-dimethyl-1-oxaspiro[4.5]deca-3,6-diene	HMDB0036024	202686
1932	HMDB0038130	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	HMDB0038130	537521
1933	HMDB0061831	(Z)-alpha-Irone	HMDB0061831	643114
1934	HMDB0133179	NA	NA	NA
1935	C09690	NA	NA	NA
1936	C11350	NA	NA	NA
1937	C14132	NA	NA	NA
1938	C14205	NA	NA	NA
1939	CHEBI:10284	NA	NA	NA
1940	CHEBI:34432	NA	NA	NA
1941	CHEBI:88618	NA	NA	NA
1942	CHEBI:88921	NA	NA	NA
1943	HMDB0032797	Jasmonic acid	HMDB0032797	528116
1944	HMDB0032871	Sedanonic acid	HMDB0032871	123670
1945	HMDB0033102	Dihydro-3-(2-octenyl)-2,5-furandione	HMDB0033102	536268
1946	HMDB0037104	(R)-8-Acetoxy-carvotanacetone	HMDB0037104	538920
1947	HMDB0037135	1-Benzyloxy-1-(2-methoxyethoxy)ethane	HMDB0037135	222351
1948	HMDB0037642	4-(Butoxy methyl)-2-methoxyphenol	HMDB0037642	508414
1949	HMDB0037735	Isoamyl 2-furonpropionate	HMDB0037735	538506
1950	HMDB0037816	Dihydro-3-(1-octenyl)-2,5-furandione	HMDB0037816	536272
1951	HMDB0041573	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	HMDB0041573	216308
1952	C08491	NA	NA	NA
1953	C16317	NA	NA	NA
1954	CHEBI:18292	NA	NA	NA
1955	CHEBI:18435	NA	NA	NA
1956	CHEBI:84246	NA	NA	NA
1957	HMDB0029707	2-Amino-3,4-dimethylimidazo[4,5-f]quinoline	HMDB0029707	62274
1958	C19254	NA	NA	NA
1959	HMDB0031017	10-Undecenyl acetate	HMDB0031017	61035
1960	HMDB0031028	Methyl (E)-2-dodecenoate	HMDB0031028	637723
1961	HMDB0031741	Coniferan	HMDB0031741	62240
1962	HMDB0032792	(±)-(E)-3-Methyl-4-decen-1-yl acetate	HMDB0032792	101416
1963	HMDB0034286	Ethyl 10-undecenoate	HMDB0034286	12729
1964	HMDB0037187	Rhodinyl propionate	HMDB0037187	7781
1965	HMDB0037226	Citronellyl propionate	HMDB0037226	8834
1966	HMDB0037626	1-Ethylhexyl tiglate	HMDB0037626	131752
1967	HMDB0037907	2,6,10,10-Tetramethyl-1-oxaspiro[4.5]decan-6-ol	HMDB0037907	65428
1968	HMDB0038078	1,1-Diethoxy-2,6-nonadiene	HMDB0038078	208387
1969	HMDB0039805	4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	HMDB0039805	131752
1970	HMDB0040451	Oxacyclotetradecan-2-one	HMDB0040451	15596
1971	C18206	NA	NA	NA
1972	CHEBI:87153	NA	NA	NA
1973	HMDB0000682	Indoxyl sulfate	HMDB0000682	10258
1974	HMDB0003309	NA	NA	NA
1975	CHEBI:43355	NA	NA	NA
1976	HMDB0030984	5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	HMDB0030984	103759
1977	HMDB0030985	alpha-Carboxy-delta-decalactone	HMDB0030985	131751
1978	HMDB0030986	2-Carboxy-5,7-dimethyl-4-octanolide	HMDB0030986	131751
1979	HMDB0010727	3-Oxododecanoic acid	HMDB0010727	439717
1980	HMDB0037398	4-Acetoxy-2-hexyltetrahydrofuran	HMDB0037398	61457
1981	C02367	NA	NA	NA
1982	CHEBI:18037	NA	NA	NA
1983	CHEBI:78977	NA	NA	NA
1984	CHEBI:79164	NA	NA	NA
1985	HMDB0000910	Tridecanoic acid	HMDB0000910	12530
1986	HMDB0029552	Ethyl undecanoate	HMDB0029552	12327
1987	HMDB0031018	Methyl dodecanoate	HMDB0031018	8139
1988	HMDB0032211	Decanal propyleneglycol acetal	HMDB0032211	95397
1989	HMDB0034140	Octyl 3-methylbutanoate	HMDB0034140	228769
1990	HMDB0036217	Pentyl octanoate	HMDB0036217	61185
1991	HMDB0036219	Octyl 2-methylbutyrate	HMDB0036219	520455
1992	HMDB0037311	Decyl propionate	HMDB0037311	229385
1993	HMDB0038729	3-Methylbutyl octanoate	HMDB0038729	16255
1994	HMDB0059900	Propyl decanoate	HMDB0059900	121739
1995	HMDB0061828	9-Methyldodecanoic acid	HMDB0061828	528264
1996	HMDB0061829	Isopropyl dodecanoic acid	HMDB0061829	16833
1997	C04780	NA	NA	NA
1998	C16640	NA	NA	NA
1999	C17076	NA	NA	NA
2000	CHEBI:15720	NA	NA	NA
2001	CHEBI:45919	NA	NA	NA
2002	CHEBI:75084	NA	NA	NA
2003	CHEBI:77359	NA	NA	NA
2004	CHEBI:84872	NA	NA	NA
2005	CHEBI:86973	NA	NA	NA
2006	CHEBI:87386	NA	NA	NA
2007	CHEBI:87494	NA	NA	NA
2008	CHEBI:87536	NA	NA	NA
2009	HMDB0012204	Zeatin	HMDB0012204	449093
2010	C00371	NA	NA	NA

2011	C15545	NA	NA	NA
2012	CHEBI:15333	NA	NA	NA
2013	CHEBI:16522	NA	NA	NA
2014	CHEBI:46570	NA	NA	NA
2015	HMDB0041942	N-Acetyl-S-(N-methylcarbamoyl)cysteine	HMDB0041942	108218
2016	C11490	NA	NA	NA
2017	CHEBI:77702	NA	NA	NA
2018	HMDB0010325	Ethyl glucuronide	HMDB0010325	183921
2019	HMDB0125202	NA	NA	NA
2020	HMDB0131286	NA	NA	NA
2021	C02655	NA	NA	NA
2022	CHEBI:17901	NA	NA	NA
2023	CHEBI:62111	NA	NA	NA
2024	CHEBI:87248	NA	NA	NA
2025	HMDB0002056	Monoisobutyl phthalic acid	HMDB0002056	92272
2026	HMDB0013247	Monobutylphthalate	HMDB0013247	8575
2027	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	HMDB0029226	302841
2028	HMDB0029470	Isodillapiole	HMDB0029470	114359
2029	HMDB0030725	Dillapiol	HMDB0030725	10231
2030	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	HMDB0031668	765513
2031	HMDB0033776	Apiole	HMDB0033776	10659
2032	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	HMDB0034056	532185
2033	HMDB0037130	Piperonyl isobutyrate	HMDB0037130	62580
2034	HMDB0037681	Vanillin isobutyrate	HMDB0037681	539829
2035	HMDB0038563	(Z)-3-(2,4,5-Trimethoxyphenyl)-2-propenal	HMDB0038563	469067
2036	HMDB0041379	2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	HMDB0041379	728008
2037	HMDB0094660	Diethyl phthalic acid	HMDB0094660	6781
2038	HMDB0127824	NA	NA	NA
2039	HMDB0131283	NA	NA	NA
2040	HMDB0131284	NA	NA	NA
2041	HMDB0131285	NA	NA	NA
2042	HMDB0135689	NA	NA	NA
2043	HMDB0135900	NA	NA	NA
2044	HMDB0135904	NA	NA	NA
2045	HMDB0135906	NA	NA	NA
2046	C10429	NA	NA	NA
2047	C10449	NA	NA	NA
2048	C14175	NA	NA	NA
2049	C19228	NA	NA	NA
2050	C20225	NA	NA	NA
2051	CHEBI:1156602	NA	NA	NA
2052	CHEBI:34698	NA	NA	NA
2053	CHEBI:47905	NA	NA	NA
2054	CHEBI:544678	NA	NA	NA
2055	CHEBI:73715	NA	NA	NA
2056	CHEBI:78250	NA	NA	NA
2057	CHEBI:86899	NA	NA	NA
2058	CHEBI:90038	NA	NA	NA
2059	HMDB0000560	Goshuyic acid	HMDB0000560	531240
2060	HMDB0030426	Linalyl isobutyrate	HMDB0030426	6532
2061	HMDB0030427	Linalyl butyrate	HMDB0030427	62321
2062	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	HMDB0031015	643820
2063	HMDB0032053	alpha-Terpineol butanoate	HMDB0032053	578423
2064	HMDB0032342	Isobornyl isobutyrate	HMDB0032342	112645
2065	HMDB0032524	Terpinyl isobutyrate	HMDB0032524	522673
2066	HMDB0036424	Allyl undecylenate	HMDB0036424	61412
2067	HMDB0037814	2-Propenyl cyclohexanepentanoate	HMDB0037814	61407
2068	HMDB0038246	Bornyl butyrate	HMDB0038246	97897
2069	HMDB0038259	Neryl butyrate	HMDB0038259	535216
2070	HMDB0038260	Geranyl 2-methylpropanoate	HMDB0038260	536599
2071	HMDB0039129	NA	NA	NA
2072	CHEBI:70719	NA	NA	NA
2073	CHEBI:72000	NA	NA	NA
2074	HMDB0000499	5-Tetradecenoic acid	HMDB0000499	528274
2075	HMDB0000521	5Z-Tetradecenoic acid	HMDB0000521	531240
2076	HMDB0002000	Myristoleic acid	HMDB0002000	528111
2077	HMDB0005051	Tsuzuic acid	HMDB0005051	531239
2078	HMDB0010732	trans-Tetra-dec-2-enoic acid	HMDB0010732	528273
2079	HMDB0030921	(R)-14-Methylxacyclotetradecan-2-one	HMDB0030921	543405
2080	HMDB0031029	Ethyl (E)-2-dodecenoate	HMDB0031029	112875
2081	HMDB0031073	12-Methyl-13-tridecanolide	HMDB0031073	534607
2082	HMDB0032152	Acetaldehyde di-cis-3-hexenyl acetal	HMDB0032152	536776
2083	HMDB0032321	2-Hexenyl octanoate	HMDB0032321	536513
2084	HMDB0034561	Houttuynin	HMDB0034561	144433
2085	HMDB0037188	Rhodinyl butyrate	HMDB0037188	61093
2086	HMDB0037189	Rhodinyl isobutyrate	HMDB0037189	61085
2087	HMDB0037227	Citronellyl butyrate	HMDB0037227	8835
2088	HMDB0037228	Citronellyl isobutyrate	HMDB0037228	60985
2089	HMDB0037369	Butyl 2-decenoate	HMDB0037369	546390
2090	HMDB0037633	xi-Tetrahydro-3-nonyl-2H-pyran-2-one	HMDB0037633	684594
2091	HMDB0038056	delta-Tetradecalactone	HMDB0038056	520296
2092	HMDB0040228	1,1-Diethoxy-3,7-dimethyl-2,6-octadiene	HMDB0040228	577203
2093	HMDB0062243	7Z-tetradecenoic acid	HMDB0062243	531240
2094	HMDB0062248	9E-tetradecenoic acid	HMDB0062248	531240
2095	HMDB0094671	Heptyl cyclohexane carboxylic acid	HMDB0094671	229794
2096	C08322	NA	NA	NA
2097	CHEBI:131381	NA	NA	NA

2098	CHEBI:27781	NA	NA	NA
2099	CHEBI:37271	NA	NA	NA
2100	CHEBI:37273	NA	NA	NA
2101	CHEBI:37274	NA	NA	NA
2102	CHEBI:38331	NA	NA	NA
2103	CHEBI:53206	NA	NA	NA
2104	CHEBI:61366	NA	NA	NA
2105	CHEBI:61367	NA	NA	NA
2106	CHEBI:70716	NA	NA	NA
2107	CHEBI:87147	NA	NA	NA
2108	CHEBI:87152	NA	NA	NA
2109	CHEBI:87291	NA	NA	NA
2110	HMDB0035881	11-Hydroxy-9-tridecenoic acid	HMDB0035881	531836
2111	HMDB0036139	Menthone 1,2-glyceryl ketal	HMDB0036139	162184
2112	HMDB0037212	Menthyl lactate	HMDB0037212	62151
2113	HMDB0040004	Menthone 1,3-glyceryl ketal	HMDB0040004	106791
2114	CHEBI:78979	NA	NA	NA
2115	CHEBI:79165	NA	NA	NA
2116	HMDB0000806	Myristic acid	HMDB0000806	11005
2117	HMDB0002221	2,6,10-Trimethylundecanoic acid	HMDB0002221	304776
2118	HMDB0031072	12-Methyltridecanoic acid	HMDB0031072	520298
2119	HMDB0032318	Hexanal octane-1,3-diol acetal	HMDB0032318	526993
2120	HMDB0032548	Undecanal propyleneglycol acetal	HMDB0032548	229153
2121	HMDB0033788	Ethyl dodecanoate	HMDB0033788	7800
2122	HMDB0034461	Heptyl heptanoate	HMDB0034461	69350
2123	HMDB0036216	Hexyl octanoate	HMDB0036216	14228
2124	HMDB0037312	Decyl butanoate	HMDB0037312	229387
2125	HMDB0037495	3-Methylbutyl nonanoate	HMDB0037495	522676
2126	HMDB0038034	Nonyl isovalerate	HMDB0038034	546391
2127	HMDB0038969	Dodecyl acetate	HMDB0038969	8205
2128	HMDB0059865	Isobutyl decanoate	HMDB0059865	121738
2129	HMDB0061781	10-Methyltridecanoic acid	HMDB0061781	222518
2130	C06424	NA	NA	NA
2131	C13798	NA	NA	NA
2132	CHEBI:23580	NA	NA	NA
2133	CHEBI:28875	NA	NA	NA
2134	CHEBI:34491	NA	NA	NA
2135	CHEBI:43722	NA	NA	NA
2136	CHEBI:542954	NA	NA	NA
2137	CHEBI:87427	NA	NA	NA
2138	CHEBI:87490	NA	NA	NA
2139	CHEBI:87570	NA	NA	NA
2140	CHEBI:90062	NA	NA	NA
2141	HMDB0062720	Thymol Sulfate	HMDB0062720	124563
2142	HMDB0133674	NA	NA	NA
2143	CHEBI:82911	NA	NA	NA
2144	HMDB0002335	Aspartyl-L-proline	HMDB0002335	170612
2145	HMDB0028761	Aspartyl-Proline	HMDB0028761	146476
2146	HMDB0029013	Prolyl-Aspartate	HMDB0029013	383887
2147	HMDB0029756	(1R,2S,3R)-2-Acetyl-4(5)-(1,2,3,4-tetrahydroxybutyl)imidazole	HMDB0029756	180624
2148	HMDB0031701	1-(gamma-Glutamylamino)cyclopropanecarboxylic acid	HMDB0031701	131751
2149	HMDB0039110	(2S,3'S)-alpha-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid	HMDB0039110	141011
2150	CHEBI:18317	NA	NA	NA
2151	CHEBI:41988	NA	NA	NA
2152	CHEBI:74756	NA	NA	NA
2153	HMDB0036133	3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol	HMDB0036133	536259
2154	HMDB0061655	3-hydroxytridecanoic acid	HMDB0061655	531274
2155	CHEBI:78980	NA	NA	NA
2156	CHEBI:79166	NA	NA	NA
2157	CHEBI:84852	NA	NA	NA
2158	HMDB0030582	Dillapional	HMDB0030582	924758
2159	HMDB0030858	Austdiol	HMDB0030858	352023
2160	HMDB0033096	Apional	HMDB0033096	994277
2161	HMDB0040407	(S)-2,3-Dihydro-7-hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid	HMDB0040407	591742
2162	HMDB0128676	NA	NA	NA
2163	HMDB0137293	NA	NA	NA
2164	C09313	NA	NA	NA
2165	C09958	NA	NA	NA
2166	CHEBI:28126	NA	NA	NA
2167	CHEBI:67369	NA	NA	NA
2168	CHEBI:71303	NA	NA	NA
2169	CHEBI:86582	NA	NA	NA
2170	HMDB0030254	3-(3,4,5-Trimethoxyphenyl)propanoic acid	HMDB0030254	64860
2171	HMDB0038627	Ethyl 3,4,5-trimethoxybenzoate	HMDB0038627	231162
2172	HMDB0041756	Isopropyl 3-(3,4-dihydroxyphenyl)-2-hydroxypropanoate	HMDB0041756	442345
2173	HMDB0061112	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid	HMDB0061112	123979
2174	HMDB0062776	NA	NA	NA
2175	HMDB0125802	NA	NA	NA
2176	HMDB0125804	NA	NA	NA
2177	HMDB0127748	NA	NA	NA
2178	HMDB0127826	NA	NA	NA
2179	HMDB0128672	NA	NA	NA
2180	HMDB0128705	NA	NA	NA
2181	HMDB0128721	NA	NA	NA
2182	HMDB0142074	NA	NA	NA
2183	CHEBI:41254	NA	NA	NA
2184	CHEBI:583580	NA	NA	NA

2185	CHEBI:87585	NA	NA	NA
2186	HMDB0029765	9-Pentadecenoic acid	HMDB0029765	636514
2187	HMDB0032347	Isobutyl 10-undecenoate	HMDB0032347	79457
2188	HMDB0034455	Exaltolide	HMDB0034455	235414
2189	HMDB0036426	Butyl undecylenate	HMDB0036426	61027
2190	HMDB0037190	Rhodinyl isovalerate	HMDB0037190	162045
2191	HMDB0037211	Menthyl isovalerate	HMDB0037211	119900
2192	HMDB0037229	Citronellyl pentanoate	HMDB0037229	61416
2193	HMDB0038954	Citronellyl isovalerate	HMDB0038954	111440
2194	HMDB0039715	Auberganol	HMDB0039715	851579
2195	HMDB0040997	15,5-Farnesanolide	HMDB0040997	131753
2196	C17676	NA	NA	NA
2197	CHEBI:75087	NA	NA	NA
2198	CHEBI:75089	NA	NA	NA
2199	CHEBI:75090	NA	NA	NA
2200	CHEBI:78992	NA	NA	NA
2201	CHEBI:79000	NA	NA	NA
2202	CHEBI:87148	NA	NA	NA
2203	CHEBI:87151	NA	NA	NA
2204	CHEBI:87377	NA	NA	NA
2205	HMDB0000826	Pentadecanoic acid	HMDB0000826	13849
2206	HMDB0030469	Methyl tetradecanoate	HMDB0030469	31284
2207	HMDB0032250	Dodecyl propionate	HMDB0032250	80354
2208	HMDB0032328	Hexyl nonanoate	HMDB0032328	81045
2209	HMDB0036218	Heptyl octanoate	HMDB0036218	61342
2210	HMDB0036220	Octyl heptanoate	HMDB0036220	521326
2211	HMDB0037306	Pentyl decanoate	HMDB0037306	550768
2212	HMDB0038907	3-Methylbutyl decanoate	HMDB0038907	75320
2213	HMDB0040998	7(14)-Farnesene-9,12-diol	HMDB0040998	131753
2214	HMDB0041588	2,6,10-Trimethyldodecanoic acid	HMDB0041588	157651
2215	HMDB0059820	Isopropyl laurate	HMDB0059820	25068
2216	HMDB0059833	Ethyl tridecanoate	HMDB0059833	119908
2217	HMDB0061707	13-Methylmyristic acid	HMDB0061707	151014
2218	C16537	NA	NA	NA
2219	C16665	NA	NA	NA
2220	CHEBI:32361	NA	NA	NA
2221	CHEBI:39250	NA	NA	NA
2222	CHEBI:39251	NA	NA	NA
2223	CHEBI:42504	NA	NA	NA
2224	CHEBI:447965	NA	NA	NA
2225	CHEBI:87330	NA	NA	NA
2226	HMDB0124975	NA	NA	NA
2227	HMDB0125166	NA	NA	NA
2228	HMDB0127985	NA	NA	NA
2229	HMDB0128093	NA	NA	NA
2230	HMDB0134054	NA	NA	NA
2231	HMDB0028866	Hydroxypropyl-Isoleucine	HMDB0028866	611573
2232	HMDB0028867	Hydroxypropyl-Leucine	HMDB0028867	217775
2233	HMDB0028908	Isoleucylhydroxyproline	HMDB0028908	611588
2234	HMDB0028930	Leucylhydroxyproline	HMDB0028930	208478
2235	HMDB0002261	2-Hydroxymyristic acid	HMDB0002261	1563
2236	HMDB0010731	(R)-3-Hydroxy-tetradecanoic acid	HMDB0010731	528826
2237	HMDB0032417	3-(L-Menthoxyl)-2-methylpropane-1,2-diol	HMDB0032417	167348
2238	HMDB0059850	Ethyl 3-hydroxydodecanoate	HMDB0059850	575843
2239	HMDB0061656	3-Hydroxytetradecanoic acid	HMDB0061656	531286
2240	C13790	NA	NA	NA
2241	CHEBI:37374	NA	NA	NA
2242	CHEBI:42539	NA	NA	NA
2243	CHEBI:59270	NA	NA	NA
2244	CHEBI:77168	NA	NA	NA
2245	CHEBI:78989	NA	NA	NA
2246	CHEBI:85148	NA	NA	NA
2247	CHEBI:85934	NA	NA	NA
2248	CHEBI:85937	NA	NA	NA
2249	HMDB0000413	3-Hydroxydodecanedioic acid	HMDB0000413	166633
2250	HMDB0031696	Dibutyl malate	HMDB0031696	95385
2251	CHEBI:78812	NA	NA	NA
2252	HMDB0028829	Glutamylthreonine	HMDB0028829	699803
2253	HMDB0029159	gamma-Glutamylthreonine	HMDB0029159	538611
2254	CHEBI:133747	NA	NA	NA
2255	CHEBI:73510	NA	NA	NA
2256	CHEBI:74857	NA	NA	NA
2257	CHEBI:82968	NA	NA	NA
2258	HMDB0035293	Norambreinolide	HMDB0035293	61129
2259	HMDB0037631	3-Methyl-alpha-ionyl acetate	HMDB0037631	643746
2260	HMDB0037712	[2,2-Bis(2-methylpropoxy)ethyl]benzene	HMDB0037712	71544
2261	C16503	NA	NA	NA
2262	CHEBI:22340	NA	NA	NA
2263	CHEBI:80535	NA	NA	NA
2264	HMDB0030668	1-(2,4,6-Trimethoxyphenyl)-1,3-butanedione	HMDB0030668	531727
2265	HMDB0038551	Methyl 3,4,5-trimethoxycinnamate	HMDB0038551	735846
2266	HMDB0125460	NA	NA	NA
2267	HMDB0137142	NA	NA	NA
2268	C18541	NA	NA	NA
2269	C20207	NA	NA	NA
2270	CHEBI:69472	NA	NA	NA
2271	CHEBI:70192	NA	NA	NA

2272	CHEBI:81817	NA	NA	NA
2273	CHEBI:86898	NA	NA	NA
2274	HMDB0000477	7Z,10Z-Hexadecadienoic acid	HMDB0000477	139321
2275	HMDB0029351	Geranyl hexanoate	HMDB0029351	125713
2276	HMDB0030429	Linalyl hexanoate	HMDB0030429	564550
2277	HMDB0031086	(Z)-7-Hexadecen-1,16-olide	HMDB0031086	536570
2278	HMDB0032340	Isoambrettolide	HMDB0032340	535529
2279	HMDB0037805	D6-Ambrettolide	HMDB0037805	586960
2280	HMDB0038255	Geranyl 2-ethylbutyrate	HMDB0038255	924758
2281	HMDB0039131	Ethyl (Z,Z)-5,8-tetradecadienoate	HMDB0039131	131752
2282	C16795	NA	NA	NA
2283	CHEBI:61671	NA	NA	NA
2284	CHEBI:61675	NA	NA	NA
2285	CHEBI:77522	NA	NA	NA
2286	CHEBI:86142	NA	NA	NA
2287	CHEBI:86147	NA	NA	NA
2288	HMDB0029604	Lubiminol	HMDB0029604	744277
2289	HMDB0035780	8-Hydroxy-4(6)-lactarene-5,14-diol	HMDB0035780	141098
2290	HMDB0036053	(3beta,9beta)-7-Drimene-3,11,12-triol	HMDB0036053	144330
2291	HMDB0036866	7-Drimene-11,12,14-triol	HMDB0036866	144330
2292	HMDB0037197	Kessyl glycol	HMDB0037197	123048
2293	HMDB0040276	5-Acetoxydihydrotheaspirane	HMDB0040276	93838
2294	C17603	NA	NA	NA
2295	C17606	NA	NA	NA
2296	C17608	NA	NA	NA
2297	C17610	NA	NA	NA
2298	C18538	NA	NA	NA
2299	CHEBI:67346	NA	NA	NA
2300	HMDB0002186	Hypogeic acid	HMDB0002186	531839
2301	HMDB0003229	Palmitoleic acid	HMDB0003229	445638
2302	HMDB0010735	Trans-Hexa-dec-2-enoic acid	HMDB0010735	528274
2303	HMDB0012328	Palmitelaidic acid	HMDB0012328	528274
2304	HMDB0031053	(E)-6-Hexadecenoic acid	HMDB0031053	528274
2305	HMDB0031145	5-Dodecylidihydro-2(3H)-furanone	HMDB0031145	97747
2306	HMDB0031711	15-Hexadecanolide	HMDB0031711	543385
2307	HMDB0032638	(Z)-5-Hexadecenoic acid	HMDB0032638	131053
2308	HMDB0033791	(E)-3-Hexadecenoic acid	HMDB0033791	535537
2309	HMDB0035877	(Z)-13-Hexadecenoic acid	HMDB0035877	531241
2310	HMDB0037647	(E)-11-Hexadecenoic acid	HMDB0037647	531241
2311	HMDB0038958	Citronellyl hexanoate	HMDB0038958	114416
2312	HMDB0041422	(Z)-14-Methyl-6-pentadecenoic acid	HMDB0041422	875089
2313	HMDB0060082	NA	NA	NA
2314	C08362	NA	NA	NA
2315	CHEBI:28716	NA	NA	NA
2316	CHEBI:35464	NA	NA	NA
2317	CHEBI:35465	NA	NA	NA
2318	CHEBI:37252	NA	NA	NA
2319	CHEBI:59265	NA	NA	NA
2320	CHEBI:72004	NA	NA	NA
2321	CHEBI:76244	NA	NA	NA
2322	CHEBI:86140	NA	NA	NA
2323	CHEBI:87146	NA	NA	NA
2324	HMDB0030993	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	HMDB0030993	131751
2325	HMDB0036143	Monomenthyl succinate	HMDB0036143	101990
2326	CHEBI:76281	NA	NA	NA
2327	HMDB0000592	Glucosamine 6-sulfate	HMDB0000592	72361
2328	HMDB0001481	N-Sulfo-D-glucosamine	HMDB0001481	439388
2329	C01075	NA	NA	NA
2330	C04132	NA	NA	NA
2331	CHEBI:16702	NA	NA	NA
2332	CHEBI:743540	NA	NA	NA
2333	CHEBI:84776	NA	NA	NA
2334	HMDB0032857	Glycerol tripropanoate	HMDB0032857	8763
2335	CHEBI:88153	NA	NA	NA
2336	HMDB0011170	gamma-Glutamylisoleucine	HMDB0011170	228850
2337	HMDB0011171	gamma-Glutamylleucine	HMDB0011171	151023
2338	HMDB0028822	Glutamylisoleucine	HMDB0028822	981385
2339	HMDB0028823	Glutamylleucine	HMDB0028823	985650
2340	HMDB0029152	NA	NA	NA
2341	HMDB0029153	NA	NA	NA
2342	CHEBI:68433	NA	NA	NA
2343	CHEBI:68434	NA	NA	NA
2344	CHEBI:73506	NA	NA	NA
2345	CHEBI:74531	NA	NA	NA
2346	HMDB0030327	Perlolyrine	HMDB0030327	160179
2347	C09231	NA	NA	NA
2348	C20280	NA	NA	NA
2349	C20281	NA	NA	NA
2350	CHEBI:610215	NA	NA	NA
2351	HMDB0030997	Cyclohexaneundecanoic acid	HMDB0030997	192796
2352	HMDB0031046	9E-Heptadecenoic acid	HMDB0031046	531244
2353	HMDB0040888	2,4-Heptadecanedione	HMDB0040888	116363
2354	HMDB0060038	10Z-Heptadecenoic acid	HMDB0060038	531243
2355	HMDB0061858	7-Hexadecenoic acid, methyl ester	HMDB0061858	140298
2356	HMDB0062437	9Z-Heptadecenoic acid	HMDB0062437	528274
2357	C12100	NA	NA	NA
2358	C16536	NA	NA	NA

2359	CHEBI:75094	NA	NA	NA
2360	CHEBI:75097	NA	NA	NA
2361	CHEBI:75098	NA	NA	NA
2362	CHEBI:78448	NA	NA	NA
2363	CHEBI:84156	NA	NA	NA
2364	CHEBI:84328	NA	NA	NA
2365	HMDB0002259	Heptadecanoic acid	HMDB0002259	10465
2366	HMDB0031067	(S)-14-Methylhexadecanoic acid	HMDB0031067	22207
2367	HMDB0034131	Nonyl octanoate	HMDB0034131	589365
2368	HMDB0037372	3-Methylbutyl dodecanoate	HMDB0037372	61386
2369	HMDB0040392	Isopropyl tetradecanoate	HMDB0040392	8042
2370	HMDB0040598	(±)-11-Methylhexadecanoic acid	HMDB0040598	531229
2371	HMDB0059870	Ethyl pentadecanoate	HMDB0059870	38762
2372	HMDB0061859	Methyl hexadecanoic acid	HMDB0061859	8181
2373	C16995	NA	NA	NA
2374	CHEBI:32365	NA	NA	NA
2375	CHEBI:70850	NA	NA	NA
2376	CHEBI:84874	NA	NA	NA
2377	CHEBI:85057	NA	NA	NA
2378	CHEBI:87343	NA	NA	NA
2379	HMDB0010734	(R)-3-Hydroxy-hexadecanoic acid	HMDB0010734	155697
2380	HMDB0031057	2-Hydroxyhexadecanoic acid	HMDB0031057	125759
2381	HMDB0061658	3-Hydroxyhexadecanoic acid	HMDB0061658	109894
2382	HMDB0112184	5-Hydroxyhexadecanoic acid	HMDB0112184	531276
2383	HMDB0112185	7-Hydroxyhexadecanoic acid	HMDB0112185	155697
2384	HMDB0112186	8-Hydroxyhexadecanoic acid	HMDB0112186	155697
2385	HMDB0112187	9-Hydroxyhexadecanoic acid	HMDB0112187	155697
2386	HMDB0112188	10-Hydroxyhexadecanoic acid	HMDB0112188	155697
2387	HMDB0112189	11-Hydroxyhexadecanoic acid	HMDB0112189	301389
2388	HMDB0112190	12-Hydroxyhexadecanoic acid	HMDB0112190	155697
2389	HMDB0112191	13-Hydroxyhexadecanoic acid	HMDB0112191	155697
2390	HMDB0112192	6-Hydroxyhexadecanoic acid	HMDB0112192	123989
2391	C18218	NA	NA	NA
2392	CHEBI:37248	NA	NA	NA
2393	CHEBI:37250	NA	NA	NA
2394	CHEBI:38247	NA	NA	NA
2395	CHEBI:55328	NA	NA	NA
2396	CHEBI:65101	NA	NA	NA
2397	CHEBI:75785	NA	NA	NA
2398	CHEBI:75972	NA	NA	NA
2399	CHEBI:75977	NA	NA	NA
2400	CHEBI:78998	NA	NA	NA
2401	CHEBI:83935	NA	NA	NA
2402	CHEBI:83937	NA	NA	NA
2403	HMDB0002697	19-Norandrosterone	HMDB0002697	954875
2404	HMDB0004590	19-Nor-5-androstenediol	HMDB0004590	990024
2405	HMDB0005886	19-Noretiocholanolone	HMDB0005886	140092
2406	HMDB0006547	Stearidonic acid	HMDB0006547	531250
2407	HMDB0032464	Phenethyl decanoate	HMDB0032464	112733
2408	HMDB0032672	4,8,12,15-Octadecatetraenoic acid	HMDB0032672	131751
2409	HMDB0034382	(E,E)-11,13-Octadecadien-9-ynoic acid	HMDB0034382	131751
2410	HMDB0062677	17beta-hydroxy-5beta-estran-3-one	HMDB0062677	216342
2411	C16300	NA	NA	NA
2412	C19042	NA	NA	NA
2413	CHEBI:32389	NA	NA	NA
2414	CHEBI:32408	NA	NA	NA
2415	CHEBI:32409	NA	NA	NA
2416	CHEBI:32410	NA	NA	NA
2417	CHEBI:32411	NA	NA	NA
2418	CHEBI:36412	NA	NA	NA
2419	CHEBI:39243	NA	NA	NA
2420	CHEBI:529214	NA	NA	NA
2421	CHEBI:72953	NA	NA	NA
2422	CHEBI:84935	NA	NA	NA
2423	CHEBI:86135	NA	NA	NA
2424	CHEBI:86506	NA	NA	NA
2425	CHEBI:87333	NA	NA	NA
2426	HMDB0001388	alpha-Linolenic acid	HMDB0001388	528093
2427	HMDB0003073	gamma-Linolenic acid	HMDB0003073	528093
2428	HMDB0030962	Calendic acid	HMDB0030962	528281
2429	HMDB0030963	Punicic acid	HMDB0030963	123094
2430	HMDB0030964	Linolenelaidic acid	HMDB0030964	860
2431	C06426	NA	NA	NA
2432	C06427	NA	NA	NA
2433	C07289	NA	NA	NA
2434	C08315	NA	NA	NA
2435	C08364	NA	NA	NA
2436	C15201	NA	NA	NA
2437	CHEBI:10275	NA	NA	NA
2438	CHEBI:16423	NA	NA	NA
2439	CHEBI:27432	NA	NA	NA
2440	CHEBI:28661	NA	NA	NA
2441	CHEBI:38382	NA	NA	NA
2442	CHEBI:38383	NA	NA	NA
2443	CHEBI:38384	NA	NA	NA
2444	CHEBI:38386	NA	NA	NA
2445	CHEBI:38387	NA	NA	NA

2446	CHEBI:38388	NA	NA	NA
2447	CHEBI:38389	NA	NA	NA
2448	CHEBI:38396	NA	NA	NA
2449	CHEBI:38403	NA	NA	NA
2450	CHEBI:38413	NA	NA	NA
2451	CHEBI:44602	NA	NA	NA
2452	CHEBI:48907	NA	NA	NA
2453	CHEBI:61673	NA	NA	NA
2454	CHEBI:61676	NA	NA	NA
2455	CHEBI:86136	NA	NA	NA
2456	CHEBI:86148	NA	NA	NA
2457	CHEBI:8638	NA	NA	NA
2458	HMDB0000673	Linoleic acid	HMDB0000673	528045
2459	HMDB0003797	Bovinic acid	HMDB0003797	528064
2460	HMDB0005047	(9E,11E)-Octadecadienoic acid	HMDB0005047	528279
2461	HMDB0005048	(10E,12Z)-Octadecadienoic acid	HMDB0005048	528280
2462	HMDB0006270	Linoelaidic acid	HMDB0006270	528245
2463	HMDB0029800	Mangiferic acid	HMDB0029800	643902
2464	HMDB0030430	Linalyl caprylate	HMDB0030430	61435
2465	HMDB0031051	Ethyl 2E,4Z-hexadecadienoate	HMDB0031051	888340
2466	HMDB0031097	5-Octadecynoic acid	HMDB0031097	531269
2467	HMDB0062238	6Z,9Z-octadecadienoic acid	HMDB0062238	531248
2468	HMDB0062784	Octadecadienoate	HMDB0062784	531245
2469	C01595	NA	NA	NA
2470	C04056	NA	NA	NA
2471	C08282	NA	NA	NA
2472	C08321	NA	NA	NA
2473	C08459	NA	NA	NA
2474	CHEBI:17351	NA	NA	NA
2475	CHEBI:24993	NA	NA	NA
2476	CHEBI:27939	NA	NA	NA
2477	CHEBI:28801	NA	NA	NA
2478	CHEBI:32798	NA	NA	NA
2479	CHEBI:36025	NA	NA	NA
2480	CHEBI:36331	NA	NA	NA
2481	CHEBI:38362	NA	NA	NA
2482	CHEBI:38394	NA	NA	NA
2483	CHEBI:38401	NA	NA	NA
2484	CHEBI:38402	NA	NA	NA
2485	CHEBI:44526	NA	NA	NA
2486	CHEBI:61389	NA	NA	NA
2487	CHEBI:61391	NA	NA	NA
2488	CHEBI:6673	NA	NA	NA
2489	CHEBI:75108	NA	NA	NA
2490	CHEBI:82749	NA	NA	NA
2491	CHEBI:83063	NA	NA	NA
2492	CHEBI:86141	NA	NA	NA
2493	HMDB0060994	alpha-Hydroxymetoprolol	HMDB0060994	114962
2494	C10263	NA	NA	NA
2495	CHEBI:2617	NA	NA	NA
2496	HMDB0060593	Alpha-dihydroartemisinin	HMDB0060593	456410
2497	HMDB0061088	Dihydroartemisinin (DHA)	HMDB0061088	713168
2498	CHEBI:207229	NA	NA	NA
2499	HMDB0035473	Avocadyne	HMDB0035473	301518
2500	HMDB0038685	Muricatacin	HMDB0038685	100167
2501	C13792	NA	NA	NA
2502	C13946	NA	NA	NA
2503	C14996	NA	NA	NA
2504	CHEBI:78999	NA	NA	NA
2505	CHEBI:79175	NA	NA	NA
2506	HMDB0000827	Stearic acid	HMDB0000827	5281
2507	HMDB0029811	Ethyl hexadecanoate	HMDB0029811	12366
2508	HMDB0031066	16-Methylheptadecanoic acid	HMDB0031066	21859
2509	HMDB0061946	Hexyl dodecanoate	HMDB0061946	94454
2510	C01530	NA	NA	NA
2511	C20356	NA	NA	NA
2512	CHEBI:1305874	NA	NA	NA
2513	CHEBI:28842	NA	NA	NA
2514	CHEBI:65084	NA	NA	NA
2515	CHEBI:84896	NA	NA	NA
2516	CHEBI:84932	NA	NA	NA
2517	CHEBI:85218	NA	NA	NA
2518	HMDB0060995	10-alpha-methoxy-9,10-dihydrolysergol	HMDB0060995	107927
2519	C20410	NA	NA	NA
2520	CHEBI:40149	NA	NA	NA
2521	CHEBI:67248	NA	NA	NA
2522	CHEBI:68464	NA	NA	NA
2523	CHEBI:90609	NA	NA	NA
2524	HMDB0000153	Estriol	HMDB0000153	5756
2525	HMDB0000338	2-Hydroxyestradiol	HMDB0000338	247304
2526	HMDB0000347	16b-Hydroxyestradiol	HMDB0000347	68929
2527	HMDB0000356	17-Epiestriol	HMDB0000356	256737
2528	HMDB0000431	16,17-Epiestriol	HMDB0000431	212522
2529	HMDB0005896	4-Hydroxyestradiol	HMDB0005896	528236
2530	HMDB0040864	O-Geranylvannillin	HMDB0040864	644428
2531	HMDB0060353	2-Polyprenyl-3-methyl-6-methoxy-1,4-benzoquinone	HMDB0060353	109022
2532	HMDB0060999	4-hydroxystradiol	HMDB0060999	1743

2533	HMDB0062741	7alpha-hydroxyestradiol	HMDB0062741	259693
2534	HMDB0003962	NA	NA	NA
2535	C03935	NA	NA	NA
2536	C05141	NA	NA	NA
2537	C05301	NA	NA	NA
2538	C14209	NA	NA	NA
2539	C15385	NA	NA	NA
2540	CHEBI:1150237	NA	NA	NA
2541	CHEBI:16784	NA	NA	NA
2542	CHEBI:27974	NA	NA	NA
2543	CHEBI:28744	NA	NA	NA
2544	CHEBI:38236	NA	NA	NA
2545	CHEBI:62845	NA	NA	NA
2546	CHEBI:62847	NA	NA	NA
2547	CHEBI:62848	NA	NA	NA
2548	CHEBI:87593	NA	NA	NA
2549	CHEBI:87598	NA	NA	NA
2550	CHEBI:87620	NA	NA	NA
2551	HMDB0004667	13-HODE	HMDB0004667	644301
2552	HMDB0004670	alpha-Dimorphecolic acid	HMDB0004670	531283
2553	HMDB0004701	9,10-Epoxyoctadecenoic acid	HMDB0004701	624615
2554	HMDB0004702	12,13-EpOME	HMDB0004702	535642
2555	HMDB0010223	NA	NA	NA
2556	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	HMDB0029796	446121
2557	HMDB0029978	Avenoleic acid	HMDB0029978	755360
2558	HMDB0029998	12-Hydroxy-8,10-octadecadienoic acid	HMDB0029998	131750
2559	HMDB0061708	NA	NA	NA
2560	HMDB0062652	(10E,12Z)-9-HODE	HMDB0062652	528294
2561	HMDB0112194	NA	NA	NA
2562	HMDB0006939	NA	NA	NA
2563	C08318	NA	NA	NA
2564	C08368	NA	NA	NA
2565	C14762	NA	NA	NA
2566	C14767	NA	NA	NA
2567	C14825	NA	NA	NA
2568	C14826	NA	NA	NA
2569	C19617	NA	NA	NA
2570	CHEBI:27706	NA	NA	NA
2571	CHEBI:28932	NA	NA	NA
2572	CHEBI:34154	NA	NA	NA
2573	CHEBI:34494	NA	NA	NA
2574	CHEBI:34496	NA	NA	NA
2575	CHEBI:38299	NA	NA	NA
2576	CHEBI:38300	NA	NA	NA
2577	CHEBI:595882	NA	NA	NA
2578	CHEBI:72639	NA	NA	NA
2579	CHEBI:72651	NA	NA	NA
2580	CHEBI:78730	NA	NA	NA
2581	CHEBI:86022	NA	NA	NA
2582	HMDB0013622	10Z-Nonadecenoic acid	HMDB0013622	531251
2583	HMDB0035575	4,6-Nonadecanediene	HMDB0035575	917131
2584	C00174	NA	NA	NA
2585	C03425	NA	NA	NA
2586	C13787	NA	NA	NA
2587	C13838	NA	NA	NA
2588	CHEBI:27542	NA	NA	NA
2589	CHEBI:34811	NA	NA	NA
2590	CHEBI:37527	NA	NA	NA
2591	CHEBI:61456	NA	NA	NA
2592	CHEBI:78443	NA	NA	NA
2593	CHEBI:83050	NA	NA	NA
2594	CHEBI:83051	NA	NA	NA
2595	HMDB0010736	3-Oxo-octadecanoic acid	HMDB0010736	528300
2596	HMDB0030979	9-Oxo-octadecanoic acid	HMDB0030979	308383
2597	HMDB0030980	10-Oxo-octadecanoic acid	HMDB0030980	361941
2598	HMDB0030981	11-Oxo-octadecanoic acid	HMDB0030981	531290
2599	HMDB0031127	5-Hexyltetrahydro-2-furanooctanoic acid	HMDB0031127	536566
2600	HMDB0034074	5-Oxo-octadecanoic acid	HMDB0034074	85548
2601	HMDB0034297	Ricinoleic acid	HMDB0034297	528294
2602	HMDB0061650	9,10-Epoxyoctadecanoic acid	HMDB0061650	160610
2603	C00869	NA	NA	NA
2604	C08365	NA	NA	NA
2605	C13791	NA	NA	NA
2606	C19418	NA	NA	NA
2607	C19616	NA	NA	NA
2608	CHEBI:28592	NA	NA	NA
2609	CHEBI:30820	NA	NA	NA
2610	CHEBI:45478	NA	NA	NA
2611	CHEBI:50576	NA	NA	NA
2612	CHEBI:75828	NA	NA	NA
2613	CHEBI:79002	NA	NA	NA
2614	CHEBI:79178	NA	NA	NA
2615	CHEBI:79312	NA	NA	NA
2616	CHEBI:85639	NA	NA	NA
2617	CHEBI:85641	NA	NA	NA
2618	CHEBI:85661	NA	NA	NA
2619	HMDB0015500	Allylestrenol	HMDB0015500	235905

2620	HMDB0029816	Cardanoldiene	HMDB0029816	535611
2621	C12811	NA	NA	NA
2622	C15420	NA	NA	NA
2623	C15431	NA	NA	NA
2624	CHEBI:36725	NA	NA	NA
2625	HMDB0000380	2-Hydroxyestradiol-3-methyl ether	HMDB0000380	515
2626	HMDB0000405	2-Methoxyestradiol	HMDB0000405	66414
2627	HMDB0003955	19-Hydroxyandrost-4-ene-3,17-dione	HMDB0003955	252379
2628	HMDB0003959	19-Oxotestosterone	HMDB0003959	704858
2629	HMDB0006771	7a-Hydroxyandrost-4-ene-3,17-dione	HMDB0006771	65542
2630	HMDB0006773	11b-Hydroxyandrost-4-ene-3,17-dione	HMDB0006773	4762
2631	HMDB0006774	16a-Hydroxyandrost-4-ene-3,17-dione	HMDB0006774	440574
2632	HMDB0012782	4-Methoxy-17beta-estradiol	HMDB0012782	68578
2633	HMDB0031038	(2Z,8S,9Z)-2,9-Heptadecadiene-8-hydroxy-4,6-diyne-1-yl acetate	HMDB0031038	131751
2634	HMDB0033125	[8]-Dehydroshogaol	HMDB0033125	131751
2635	HMDB0034028	2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone	HMDB0034028	142366
2636	HMDB0034167	Falcarindiol 3-acetate	HMDB0034167	131751
2637	HMDB0036696	Yucalexin B'11	HMDB0036696	141911
2638	HMDB0039568	Ginsenosyne H	HMDB0039568	157258
2639	HMDB0040927	2-Hexyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan	HMDB0040927	159291
2640	HMDB0041204	Acetylpanaxydol	HMDB0041204	129509
2641	C04676	NA	NA	NA
2642	C05140	NA	NA	NA
2643	C05284	NA	NA	NA
2644	C05290	NA	NA	NA
2645	C05295	NA	NA	NA
2646	C05296	NA	NA	NA
2647	C05302	NA	NA	NA
2648	C14256	NA	NA	NA
2649	C14269	NA	NA	NA
2650	C14337	NA	NA	NA
2651	C14593	NA	NA	NA
2652	C14907	NA	NA	NA
2653	C15072	NA	NA	NA
2654	C15103	NA	NA	NA
2655	C15216	NA	NA	NA
2656	C20693	NA	NA	NA
2657	CHEBI:17347	NA	NA	NA
2658	CHEBI:18084	NA	NA	NA
2659	CHEBI:27576	NA	NA	NA
2660	CHEBI:27582	NA	NA	NA
2661	CHEBI:27768	NA	NA	NA
2662	CHEBI:27967	NA	NA	NA
2663	CHEBI:28955	NA	NA	NA
2664	CHEBI:34572	NA	NA	NA
2665	CHEBI:39115	NA	NA	NA
2666	CHEBI:39118	NA	NA	NA
2667	CHEBI:39119	NA	NA	NA
2668	CHEBI:39120	NA	NA	NA
2669	CHEBI:39121	NA	NA	NA
2670	CHEBI:39122	NA	NA	NA
2671	CHEBI:39135	NA	NA	NA
2672	CHEBI:39136	NA	NA	NA
2673	CHEBI:39137	NA	NA	NA
2674	CHEBI:39138	NA	NA	NA
2675	CHEBI:39139	NA	NA	NA
2676	CHEBI:39140	NA	NA	NA
2677	CHEBI:63783	NA	NA	NA
2678	CHEBI:65580	NA	NA	NA
2679	CHEBI:67190	NA	NA	NA
2680	CHEBI:68789	NA	NA	NA
2681	CHEBI:70566	NA	NA	NA
2682	CHEBI:75172	NA	NA	NA
2683	CHEBI:75308	NA	NA	NA
2684	CHEBI:85549	NA	NA	NA
2685	CHEBI:85575	NA	NA	NA
2686	CHEBI:87571	NA	NA	NA
2687	HMDB0001999	Eicosapentaenoic acid	HMDB0001999	446284
2688	HMDB0003598	Retinyl ester	HMDB0003598	546016
2689	HMDB0015655	Methyltestosterone	HMDB0015655	6010
2690	HMDB0035692	8,15-Isopimaradiene-18-oic acid	HMDB0035692	156277
2691	HMDB0036703	Siderone	HMDB0036703	146816
2692	HMDB0036709	Yucalexin B14	HMDB0036709	141911
2693	HMDB0036775	Yucalexin A16	HMDB0036775	141912
2694	HMDB0036805	8(17),12-Labdadiene-15,16-dial	HMDB0036805	990451
2695	HMDB0036811	Isopimaric acid	HMDB0036811	442048
2696	HMDB0036826	Cascarillone	HMDB0036826	156275
2697	HMDB0038172	8,13-Abietadiene-18-oic acid	HMDB0038172	16040
2698	HMDB0038687	(ent-15beta,16beta)-15,16-Epoxy-3-kauranone	HMDB0038687	131752
2699	HMDB0039486	ent-8(17),13(16),14-Labdatriene-18-oic acid	HMDB0039486	727809
2700	HMDB0041928	Methenolone	HMDB0041928	303770
2701	C02075	NA	NA	NA
2702	C06087	NA	NA	NA
2703	C06428	NA	NA	NA
2704	C07198	NA	NA	NA
2705	C09118	NA	NA	NA
2706	C09148	NA	NA	NA

2707	C09159	NA	NA	NA
2708	C11874	NA	NA	NA
2709	C11888	NA	NA	NA
2710	C11889	NA	NA	NA
2711	C12077	NA	NA	NA
2712	C12083	NA	NA	NA
2713	C14255	NA	NA	NA
2714	C14490	NA	NA	NA
2715	C14588	NA	NA	NA
2716	C14890	NA	NA	NA
2717	C15003	NA	NA	NA
2718	C15008	NA	NA	NA
2719	C15017	NA	NA	NA
2720	C15036	NA	NA	NA
2721	C15070	NA	NA	NA
2722	C15184	NA	NA	NA
2723	C15188	NA	NA	NA
2724	C15259	NA	NA	NA
2725	C15318	NA	NA	NA
2726	C15412	NA	NA	NA
2727	C15460	NA	NA	NA
2728	C20149	NA	NA	NA
2729	C20208	NA	NA	NA
2730	CHEBI:15417	NA	NA	NA
2731	CHEBI:27436	NA	NA	NA
2732	CHEBI:28364	NA	NA	NA
2733	CHEBI:28987	NA	NA	NA
2734	CHEBI:29457	NA	NA	NA
2735	CHEBI:34849	NA	NA	NA
2736	CHEBI:545914	NA	NA	NA
2737	CHEBI:6039	NA	NA	NA
2738	CHEBI:63731	NA	NA	NA
2739	CHEBI:65960	NA	NA	NA
2740	CHEBI:66459	NA	NA	NA
2741	CHEBI:66549	NA	NA	NA
2742	CHEBI:70577	NA	NA	NA
2743	CHEBI:72658	NA	NA	NA
2744	CHEBI:78258	NA	NA	NA
2745	CHEBI:79761	NA	NA	NA
2746	HMDB0001043	Arachidonic acid	HMDB0001043	444899
2747	HMDB0002177	Cis-8,11,14,17-Eicosatetraenoic acid	HMDB0002177	117225
2748	HMDB0006036	Mesterolone	HMDB0006036	15020
2749	HMDB0014996	Drostanolone	HMDB0014996	6011
2750	HMDB0036702	Sideridiol	HMDB0036702	123155
2751	HMDB0036721	ent-17-Hydroxy-16beta-kauran-19-al	HMDB0036721	348185
2752	HMDB0036754	Yucalexin P21	HMDB0036754	141912
2753	HMDB0036829	Copalic acid	HMDB0036829	131752
2754	HMDB0036830	Junicedral	HMDB0036830	131752
2755	HMDB0037824	7,13-Eperudien-15-oic acid	HMDB0037824	131752
2756	HMDB0039687	Oryzalexin S	HMDB0039687	131752
2757	HMDB0039702	Oryzalexin E	HMDB0039702	862894
2758	HMDB0060102	NA	NA	NA
2759	C00219	NA	NA	NA
2760	C09057	NA	NA	NA
2761	C09124	NA	NA	NA
2762	C11897	NA	NA	NA
2763	C14493	NA	NA	NA
2764	C14605	NA	NA	NA
2765	C14956	NA	NA	NA
2766	C15176	NA	NA	NA
2767	C15252	NA	NA	NA
2768	C15367	NA	NA	NA
2769	C17920	NA	NA	NA
2770	C20329	NA	NA	NA
2771	CHEBI:15843	NA	NA	NA
2772	CHEBI:30041	NA	NA	NA
2773	CHEBI:34838	NA	NA	NA
2774	CHEBI:36033	NA	NA	NA
2775	CHEBI:36035	NA	NA	NA
2776	CHEBI:36038	NA	NA	NA
2777	CHEBI:36039	NA	NA	NA
2778	CHEBI:36040	NA	NA	NA
2779	CHEBI:36042	NA	NA	NA
2780	CHEBI:36045	NA	NA	NA
2781	CHEBI:36232	NA	NA	NA
2782	CHEBI:36302	NA	NA	NA
2783	CHEBI:36306	NA	NA	NA
2784	CHEBI:529213	NA	NA	NA
2785	CHEBI:63668	NA	NA	NA
2786	CHEBI:64014	NA	NA	NA
2787	CHEBI:71488	NA	NA	NA
2788	CHEBI:78256	NA	NA	NA
2789	CHEBI:78259	NA	NA	NA
2790	CHEBI:79754	NA	NA	NA
2791	CHEBI:82835	NA	NA	NA
2792	CHEBI:84856	NA	NA	NA
2793	CHEBI:84971	NA	NA	NA

2794	D04947	NA	NA	NA
2795	HMDB0005060	Eicosadienoic acid	HMDB0005060	643984
2796	HMDB0036827	Sclareol	HMDB0036827	521332
2797	HMDB0061864	Dihomolinoleic acid	HMDB0061864	528279
2798	HMDB0062432	8Z,11Z-eicosadienoic acid	HMDB0062432	531252
2799	C09183	NA	NA	NA
2800	C16525	NA	NA	NA
2801	CHEBI:31572	NA	NA	NA
2802	CHEBI:603631	NA	NA	NA
2803	CHEBI:73731	NA	NA	NA
2804	CHEBI:78706	NA	NA	NA
2805	CHEBI:9053	NA	NA	NA
2806	HMDB0011688	Ribose 1,5-bisphosphate	HMDB0011688	140356
2807	C01095	NA	NA	NA
2808	C01151	NA	NA	NA
2809	C01182	NA	NA	NA
2810	CHEBI:16710	NA	NA	NA
2811	CHEBI:17994	NA	NA	NA
2812	CHEBI:28662	NA	NA	NA
2813	CHEBI:28764	NA	NA	NA
2814	CHEBI:4235	NA	NA	NA
2815	CHEBI:68819	NA	NA	NA
2816	CHEBI:79189	NA	NA	NA
2817	HMDB0013623	12(13)Ep-9-KODE	HMDB0013623	528300
2818	HMDB0033505	(9Z,11R,12S,13S,15Z)-12,13-Epoxy-11-hydroxy-9,15-octadecadienoic acid	HMDB0033505	131751
2819	HMDB0035337	Sterebin A	HMDB0035337	131751
2820	HMDB0038484	Auxin b	HMDB0038484	103739
2821	C04785	NA	NA	NA
2822	C07357	NA	NA	NA
2823	C15753	NA	NA	NA
2824	C16321	NA	NA	NA
2825	C16341	NA	NA	NA
2826	C19936	NA	NA	NA
2827	C20704	NA	NA	NA
2828	CHEBI:48905	NA	NA	NA
2829	CHEBI:60961	NA	NA	NA
2830	CHEBI:63237	NA	NA	NA
2831	CHEBI:63238	NA	NA	NA
2832	CHEBI:75615	NA	NA	NA
2833	CHEBI:76236	NA	NA	NA
2834	CHEBI:78908	NA	NA	NA
2835	CHEBI:84180	NA	NA	NA
2836	CHEBI:85474	NA	NA	NA
2837	HMDB0002231	11Z-Eicosenoic acid	HMDB0002231	528276
2838	HMDB0034296	NA	NA	NA
2839	HMDB0034451	Ethyl oleate	HMDB0034451	536443
2840	HMDB0035159	Paullinic acid	HMDB0035159	531251
2841	HMDB0035572	6,8-Icosanedione	HMDB0035572	917011
2842	HMDB0035573	5,7-Icosanedione	HMDB0035573	916988
2843	HMDB0035574	4,6-Icosanedione	HMDB0035574	131751
2844	HMDB0037127	Oleyl acetate	HMDB0037127	536765
2845	HMDB0062436	9Z-Eicosenoic acid	HMDB0062436	528276
2846	C02064	NA	NA	NA
2847	C16526	NA	NA	NA
2848	CHEBI:134474	NA	NA	NA
2849	CHEBI:134475	NA	NA	NA
2850	CHEBI:134479	NA	NA	NA
2851	CHEBI:32419	NA	NA	NA
2852	CHEBI:32422	NA	NA	NA
2853	CHEBI:32425	NA	NA	NA
2854	CHEBI:46274	NA	NA	NA
2855	CHEBI:79014	NA	NA	NA
2856	CHEBI:84940	NA	NA	NA
2857	CHEBI:84942	NA	NA	NA
2858	CHEBI:8504	NA	NA	NA
2859	HMDB0000417	3D,7D,11D-Phytanic acid	HMDB0000417	103808
2860	HMDB0000553	3L,7D,11D-Phytanic acid	HMDB0000553	997284
2861	HMDB0000801	Phytanic acid	HMDB0000801	26840
2862	HMDB0002212	Arachidic acid	HMDB0002212	10467
2863	HMDB0031318	2,2,6,10,14-Pentamethylpentadecanoic acid	HMDB0031318	855991
2864	HMDB0034156	Ethyl stearate	HMDB0034156	8122
2865	HMDB0035672	5-Hydroxy-7-eicosanone	HMDB0035672	131751
2866	HMDB0035673	4-Hydroxy-6-eicosanone	HMDB0035673	131751
2867	HMDB0062520	3,7R,11R,15-tetramethyl-hexadecanoic acid	HMDB0062520	468706
2868	C01607	NA	NA	NA
2869	C06425	NA	NA	NA
2870	CHEBI:16285	NA	NA	NA
2871	CHEBI:28822	NA	NA	NA
2872	CHEBI:84899	NA	NA	NA
2873	CHEBI:84936	NA	NA	NA
2874	CHEBI:87384	NA	NA	NA
2875	HMDB0030263	Rhazidigenine Nb-oxide	HMDB0030263	626805
2876	CHEBI:66012	NA	NA	NA
2877	HMDB0011532	NA	NA	NA
2878	HMDB0011563	NA	NA	NA
2879	HMDB0031008	(+)-15,16-Dihydroxyoctadecanoic acid	HMDB0031008	531276
2880	HMDB0059633	(9S,10S)-9,10-dihydroxyoctadecanoate	HMDB0059633	122352

2881	HMDB0072849	NA	NA	NA
2882	HMDB0072862	NA	NA	NA
2883	HMDB0072865	NA	NA	NA
2884	HMDB0072878	NA	NA	NA
2885	C08314	NA	NA	NA
2886	C15988	NA	NA	NA
2887	C19622	NA	NA	NA
2888	CHEBI:128770	NA	NA	NA
2889	CHEBI:28724	NA	NA	NA
2890	CHEBI:49254	NA	NA	NA
2891	CHEBI:710856	NA	NA	NA
2892	CHEBI:76933	NA	NA	NA
2893	CHEBI:79250	NA	NA	NA
2894	CHEBI:79290	NA	NA	NA
2895	CHEBI:85633	NA	NA	NA
2896	HMDB0013880	S-6-Hydroxywarfarin	HMDB0013880	134272
2897	HMDB0013881	S-4'-Hydroxywarfarin	HMDB0013881	693599
2898	HMDB0013882	R-4'-Hydroxywarfarin	HMDB0013882	693600
2899	HMDB0013883	R-6-Hydroxywarfarin	HMDB0013883	134272
2900	HMDB0013884	R-10-Hydroxywarfarin	HMDB0013884	
2901	HMDB0013885	R-8-Hydroxywarfarin	HMDB0013885	134272
2902	HMDB0013886	R-7-Hydroxywarfarin	HMDB0013886	134272
2903	HMDB0041296	Moracin K	HMDB0041296	118726
2904	HMDB0041297	Moracin L	HMDB0041297	19005
2905	HMDB0140986	NA	NA	NA
2906	HMDB0140987	NA	NA	NA
2907	HMDB0140988	NA	NA	NA
2908	HMDB0140989	NA	NA	NA
2909	HMDB0140990	NA	NA	NA
2910	HMDB0140991	NA	NA	NA
2911	HMDB0140992	NA	NA	NA
2912	HMDB0140993	NA	NA	NA
2913	HMDB0140995	NA	NA	NA
2914	HMDB0142561	NA	NA	NA
2915	HMDB0142603	NA	NA	NA
2916	C18679	NA	NA	NA
2917	CHEBI:67399	NA	NA	NA
2918	HMDB0002183	Docosaehxaenoic acid	HMDB0002183	445580
2919	HMDB0030053	Neogrifolin	HMDB0030053	987442
2920	HMDB0030446	Grifolin	HMDB0030446	537231
2921	HMDB0035185	Retinol acetate	HMDB0035185	102459
2922	HMDB0038908	(Z,Z)-2-Methyl-5-(8,11,14-pentadecatienyl)-1,3-benzenediol	HMDB0038908	131752
2923	C06429	NA	NA	NA
2924	C14586	NA	NA	NA
2925	C15116	NA	NA	NA
2926	C15265	NA	NA	NA
2927	C15299	NA	NA	NA
2928	CHEBI:28125	NA	NA	NA
2929	CHEBI:32095	NA	NA	NA
2930	CHEBI:52681	NA	NA	NA
2931	CHEBI:544843	NA	NA	NA
2932	CHEBI:79767	NA	NA	NA
2933	HMDB0001976	Docosapentaenoic acid (22n-6)	HMDB0001976	644145
2934	HMDB0006528	Docosapentaenoic acid (22n-3)	HMDB0006528	549718
2935	HMDB0032257	Ethyl abietate	HMDB0032257	61182
2936	HMDB0035024	ent-16-Kauren-19-ol acetate	HMDB0035024	537596
2937	HMDB0035581	1-Phenyl-1,3-hexadecanedione	HMDB0035581	199009
2938	HMDB0038909	2-Methyl-5-(8,11-pentadecadienyl)-1,3-benzenediol	HMDB0038909	131752
2939	HMDB0039133	4,8,12,15,19-Docosapentaenoic acid	HMDB0039133	102281
2940	HMDB0039530	Ethyl icosapentate	HMDB0039530	983141
2941	HMDB0060113	NA	NA	NA
2942	C11896	NA	NA	NA
2943	C13364	NA	NA	NA
2944	C15413	NA	NA	NA
2945	C15421	NA	NA	NA
2946	C16184	NA	NA	NA
2947	C16513	NA	NA	NA
2948	CHEBI:30042	NA	NA	NA
2949	CHEBI:53488	NA	NA	NA
2950	CHEBI:546104	NA	NA	NA
2951	CHEBI:65136	NA	NA	NA
2952	CHEBI:84883	NA	NA	NA
2953	HMDB0030935	9,10,13-Trihydroxystearic acid	HMDB0030935	453592
2954	HMDB0034295	Floionolic acid	HMDB0034295	528293
2955	C19621	NA	NA	NA
2956	HMDB0002226	Adrenic acid	HMDB0002226	549718
2957	HMDB0035676	1-Hydroxy-1-phenyl-3-hexadecanone	HMDB0035676	131751
2958	HMDB0035677	3-Hydroxy-1-phenyl-1-hexadecanone	HMDB0035677	131751
2959	HMDB0038910	2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol	HMDB0038910	645220
2960	HMDB0062725	Ethyl Arachidonate	HMDB0062725	536736
2961	C15373	NA	NA	NA
2962	C16527	NA	NA	NA
2963	CHEBI:53487	NA	NA	NA
2964	CHEBI:84873	NA	NA	NA
2965	CHEBI:84876	NA	NA	NA
2966	HMDB0001244	15-Keto-13,14-dihydroprostaglandin A2	HMDB0001244	528304
2967	HMDB0002710	Prostaglandin J2	HMDB0002710	528088

2968	HMDB0002752	Prostaglandin A2	HMDB0002752	528088
2969	HMDB0004234	12-Keto-leukotriene B4	HMDB0004234	528087
2970	HMDB0004236	Prostaglandin B2	HMDB0004236	528814
2971	HMDB0004238	Delta-12-Prostaglandin J2	HMDB0004238	528088
2972	HMDB0005073	Leukotriene B5	HMDB0005073	528312
2973	HMDB0012824	5-Oxo-6-trans-leukotriene B4	HMDB0012824	534815
2974	HMDB0012850	7 ¹ -Carboxy-gamma-chromanol	HMDB0012850	134159
2975	HMDB0035286	Crispanone	HMDB0035286	131751
2976	HMDB0035878	8alpha-8-Hydroxy-12-oxo-13-abieten-18-oic acid	HMDB0035878	245310
2977	HMDB0036760	(ent-16betaOH)-16,17-Dihydroxy-9(11)-kauren-19-oic acid	HMDB0036760	738192
2978	HMDB0036763	(ent-6alpha,7alpha)-6,7-Dihydroxy-16-kauren-19-oic acid	HMDB0036763	146354
2979	HMDB0036828	Dehydropinifolic acid	HMDB0036828	225687
2980	HMDB0041055	Phytocassane B	HMDB0041055	851400
2981	HMDB0060046	15d PGD2	HMDB0060046	131769
2982	HMDB0060054	bicyclo-PGE2	HMDB0060054	528304
2983	HMDB0060095	Prostaglandin-c2	HMDB0060095	528088
2984	HMDB0062298	15-deoxy-PGD2	HMDB0062298	528305
2985	HMDB0062423	5-oxo-12-HETE	HMDB0062423	105687
2986	HMDB0062486	5,12-dihydroxy-6,8,10,14,17-eicosapentaenoic acid	HMDB0062486	531298
2987	HMDB0062524	NA	NA	NA
2988	HMDB0005078	NA	NA	NA
2989	HMDB0005086	NA	NA	NA
2990	HMDB0012825	NA	NA	NA
2991	C05949	NA	NA	NA
2992	C05953	NA	NA	NA
2993	C05954	NA	NA	NA
2994	C05955	NA	NA	NA
2995	C05957	NA	NA	NA
2996	C05958	NA	NA	NA
2997	C09125	NA	NA	NA
2998	C09150	NA	NA	NA
2999	C11876	NA	NA	NA
3000	C14504	NA	NA	NA
3001	C14815	NA	NA	NA
3002	C14913	NA	NA	NA
3003	C15159	NA	NA	NA
3004	C18173	NA	NA	NA
3005	CHEBI:130073	NA	NA	NA
3006	CHEBI:27485	NA	NA	NA
3007	CHEBI:27555	NA	NA	NA
3008	CHEBI:27814	NA	NA	NA
3009	CHEBI:27820	NA	NA	NA
3010	CHEBI:28099	NA	NA	NA
3011	CHEBI:28130	NA	NA	NA
3012	CHEBI:64095	NA	NA	NA
3013	CHEBI:65462	NA	NA	NA
3014	CHEBI:68865	NA	NA	NA
3015	CHEBI:68866	NA	NA	NA
3016	CHEBI:72666	NA	NA	NA
3017	CHEBI:76966	NA	NA	NA
3018	CHEBI:78909	NA	NA	NA
3019	CHEBI:85552	NA	NA	NA
3020	CHEBI:88493	NA	NA	NA
3021	CHEBI:90996	NA	NA	NA
3022	HMDB0030358	Aspidospermatine	HMDB0030358	626678
3023	C09019	NA	NA	NA
3024	C09041	NA	NA	NA
3025	C09139	NA	NA	NA
3026	C10940	NA	NA	NA
3027	HMDB0002265	14,15-DiHETrE	HMDB0002265	528314
3028	HMDB0002311	8,9-DiHETrE	HMDB0002311	528314
3029	HMDB0002314	11,12-DiHETrE	HMDB0002314	528314
3030	HMDB0002343	5,6-DHET	HMDB0002343	528314
3031	HMDB0002995	12-Keto-tetrahydro-leukotriene B4	HMDB0002995	528312
3032	HMDB0012504	10,11-dihydro-leukotriene B4	HMDB0012504	534814
3033	HMDB0012838	6,7-dihydro-12-epi-LTB4	HMDB0012838	534815
3034	HMDB0035379	Sterebin E	HMDB0035379	131751
3035	HMDB0060106	15-Hydroperoxyeicosa-8Z,11Z,13E-trienoate	HMDB0060106	131769
3036	HMDB0002330	NA	NA	NA
3037	HMDB0002342	NA	NA	NA
3038	HMDB0002351	NA	NA	NA
3039	HMDB0004675	NA	NA	NA
3040	HMDB0004676	NA	NA	NA
3041	HMDB0011139	NA	NA	NA
3042	C02165	NA	NA	NA
3043	C06088	NA	NA	NA
3044	C09205	NA	NA	NA
3045	C14772	NA	NA	NA
3046	C14773	NA	NA	NA
3047	C14774	NA	NA	NA
3048	C14775	NA	NA	NA
3049	CHEBI:15647	NA	NA	NA
3050	CHEBI:2766	NA	NA	NA
3051	CHEBI:63966	NA	NA	NA
3052	CHEBI:63969	NA	NA	NA
3053	CHEBI:63970	NA	NA	NA
3054	CHEBI:63974	NA	NA	NA

3055	CHEBI:65463	NA	NA	NA
3056	CHEBI:65789	NA	NA	NA
3057	CHEBI:78859	NA	NA	NA
3058	CHEBI:78860	NA	NA	NA
3059	CHEBI:84174	NA	NA	NA
3060	CHEBI:85477	NA	NA	NA
3061	HMDB0002068	Erucic acid	HMDB0002068	528111
3062	HMDB0002884	Cetoleic acid	HMDB0002884	528277
3063	HMDB0031013	Catelaic acid	HMDB0031013	531254
3064	HMDB0032470	Phytyl acetate	HMDB0032470	642853
3065	HMDB0035566	7,9-Docosanediene	HMDB0035566	538711
3066	HMDB0035567	6,8-Docosanediene	HMDB0035567	917011
3067	HMDB0035568	5,7-Docosanediene	HMDB0035568	861179
3068	HMDB0035569	4,6-Docosanediene	HMDB0035569	131751
3069	HMDB0062659	N-butyl Oleate	HMDB0062659	535434
3070	C08316	NA	NA	NA
3071	CHEBI:28792	NA	NA	NA
3072	CHEBI:32428	NA	NA	NA
3073	CHEBI:82946	NA	NA	NA
3074	CHEBI:84862	NA	NA	NA
3075	CHEBI:84864	NA	NA	NA
3076	CHEBI:84870	NA	NA	NA
3077	HMDB0030591	Dihydro-O-methylsterigmatocystin	HMDB0030591	532188
3078	HMDB0129366	NA	NA	NA
3079	HMDB0129367	NA	NA	NA
3080	HMDB0129392	NA	NA	NA
3081	C03944	NA	NA	NA
3082	C10090	NA	NA	NA
3083	C17473	NA	NA	NA
3084	CHEBI:66807	NA	NA	NA
3085	CHEBI:67400	NA	NA	NA
3086	CHEBI:72678	NA	NA	NA
3087	CHEBI:81115	NA	NA	NA
3088	CHEBI:8617	NA	NA	NA
3089	HMDB0033786	Plastoquinone 3	HMDB0033786	131751
3090	HMDB0039762	1,1'-[1,11-Undecanediylbis(oxy)]bisbenzene	HMDB0039762	713438
3091	C07628	NA	NA	NA
3092	C15186	NA	NA	NA
3093	HMDB0030340	Piperolein B	HMDB0030340	215802
3094	HMDB0033959	Isopiperolein B	HMDB0033959	160418
3095	CHEBI:534866	NA	NA	NA
3096	HMDB0031465	Methyl-[10]-shogaol	HMDB0031465	917211
3097	HMDB0033897	Ginkgoic acid	HMDB0033897	531760
3098	HMDB0034944	Siderol	HMDB0034944	123155
3099	HMDB0036722	ent-17-Acetoxy-16b-kauran-19-al	HMDB0036722	536366
3100	HMDB0041001	Volemolide	HMDB0041001	145846
3101	HMDB0041302	(R)-3,4-Dihydro-8-hydroxy-3-tridecyl-1H-2-benzopyran-1-one	HMDB0041302	714242
3102	C10794	NA	NA	NA
3103	C11898	NA	NA	NA
3104	C14976	NA	NA	NA
3105	CHEBI:50436	NA	NA	NA
3106	CHEBI:91274	NA	NA	NA
3107	HMDB0029683	2-Hydroxy-6-pentadecylbenzoic acid	HMDB0029683	167551
3108	HMDB0035477	Tridecyl phloretate	HMDB0035477	131751
3109	HMDB0036801	ent-16b,19-Kauranediol 19-acetate	HMDB0036801	630219
3110	HMDB0112069	NA	NA	NA
3111	HMDB0112073	NA	NA	NA
3112	C10759	NA	NA	NA
3113	C14919	NA	NA	NA
3114	HMDB0002341	8-iso-15-keto-PGE2	HMDB0002341	534777
3115	HMDB0002664	Prostaglandin E3	HMDB0002664	528093
3116	HMDB0003034	Prostaglandin D3	HMDB0003034	528226
3117	HMDB0003175	15-Keto-prostaglandin E2	HMDB0003175	528071
3118	HMDB0010410	Resolvin E1	HMDB0010410	250633
3119	HMDB0012552	12-Oxo-20-hydroxy-leukotriene B4	HMDB0012552	534814
3120	HMDB0012588	15-Epi-lipoxin B5	HMDB0012588	534814
3121	HMDB0012590	15-Oxo-lipoxin A4	HMDB0012590	534814
3122	HMDB0012641	20-oxo-leukotriene B4	HMDB0012641	644983
3123	HMDB0013040	Prostaglandin H3	HMDB0013040	101600
3124	HMDB0036701	(ent-6alpha,7alpha,12alpha)-6,7,12-Trihydroxy-16-kauran-19-oic acid	HMDB0036701	131752
3125	HMDB0037593	Oryzalic acid A	HMDB0037593	131752
3126	HMDB0038693	Oryzalic acid B	HMDB0038693	131752
3127	HMDB0060096	5,12,18R-TriHEPE	HMDB0060096	131769
3128	HMDB0062297	9S-hydroxy-11,15-dioxo-5Z,13E-prostadienoic acid	HMDB0062297	528072
3129	HMDB0062300	15-oxo-5S,6R-dihydroxy-7E,9E,11Z,13E-eicosatetraenoic acid	HMDB0062300	529218
3130	HMDB0062616	(5S)-hydroperoxy-18-hydroxy-EPE	HMDB0062616	593855
3131	C00427	NA	NA	NA
3132	C04707	NA	NA	NA
3133	C04758	NA	NA	NA
3134	C04835	NA	NA	NA
3135	C06439	NA	NA	NA
3136	C13802	NA	NA	NA
3137	C18171	NA	NA	NA
3138	C18176	NA	NA	NA
3139	C18848	NA	NA	NA
3140	C20214	NA	NA	NA
3141	CHEBI:15547	NA	NA	NA

3142	CHEBI:15554	NA	NA	NA
3143	CHEBI:15556	NA	NA	NA
3144	CHEBI:15557	NA	NA	NA
3145	CHEBI:28031	NA	NA	NA
3146	CHEBI:34939	NA	NA	NA
3147	CHEBI:63979	NA	NA	NA
3148	CHEBI:63992	NA	NA	NA
3149	CHEBI:65408	NA	NA	NA
3150	CHEBI:66394	NA	NA	NA
3151	CHEBI:68871	NA	NA	NA
3152	CHEBI:68872	NA	NA	NA
3153	CHEBI:68873	NA	NA	NA
3154	CHEBI:81559	NA	NA	NA
3155	CHEBI:91287	NA	NA	NA
3156	HMDB0006059	20-Carboxy-leukotriene B4	HMDB0006059	528087
3157	HMDB0012549	12-oxo-10,11-dihydro-20-COOH-LTB4	HMDB0012549	534814
3158	HMDB0012551	12-oxo-20-dihydroxy-leukotriene B4	HMDB0012551	534814
3159	HMDB0036863	Anhydrocinnzeylanol	HMDB0036863	730997
3160	HMDB0037062	Sporotrichiol	HMDB0037062	131752
3161	HMDB0004235	NA	NA	NA
3162	C05950	NA	NA	NA
3163	C08758	NA	NA	NA
3164	C15438	NA	NA	NA
3165	CHEBI:27562	NA	NA	NA
3166	CHEBI:79937	NA	NA	NA
3167	HMDB0002368	Nervonic acid	HMDB0002368	528112
3168	HMDB0029799	(E)-2-Tetracosenoic acid	HMDB0029799	644026
3169	HMDB0035559	10,12-Tetracosanedione	HMDB0035559	131751
3170	HMDB0035560	7,9-Tetracosanedione	HMDB0035560	861179
3171	HMDB0035561	6,8-Tetracosanedione	HMDB0035561	131751
3172	HMDB0035562	5,7-Tetracosanedione	HMDB0035562	131751
3173	HMDB0035563	4,6-Tetracosanedione	HMDB0035563	131751
3174	C08323	NA	NA	NA
3175	C15398	NA	NA	NA
3176	CHEBI:44247	NA	NA	NA
3177	CHEBI:84888	NA	NA	NA
3178	CHEBI:84891	NA	NA	NA
3179	HMDB0031941	8'-Episesaminone	HMDB0031941	534626
3180	HMDB0034119	Sesamolin	HMDB0034119	585998
3181	HMDB0035527	Glycyrrhizaflavonol A	HMDB0035527	531776
3182	HMDB0036555	Glycyrrhizaisoflavone A	HMDB0036555	105471
3183	HMDB0038398	Gancaonin P	HMDB0038398	548196
3184	HMDB0038900	2,3-Dehydrokievitol	HMDB0038900	442573
3185	HMDB0038932	Justisolin	HMDB0038932	979950
3186	HMDB0039731	Neouralenol	HMDB0039731	532011
3187	HMDB0039732	Uralenol	HMDB0039732	531512
3188	HMDB0132502	NA	NA	NA
3189	HMDB0132503	NA	NA	NA
3190	HMDB0137144	NA	NA	NA
3191	C10887	NA	NA	NA
3192	C20452	NA	NA	NA
3193	CHEBI:65611	NA	NA	NA
3194	CHEBI:67538	NA	NA	NA
3195	CHEBI:70489	NA	NA	NA
3196	CHEBI:71356	NA	NA	NA
3197	HMDB0029782	6-Epi-7-isocucurbitic acid glucoside	HMDB0029782	131750
3198	HMDB0000381	Allolithocholic acid	HMDB0000381	534776
3199	HMDB0000713	Isoallolithocholic acid	HMDB0000713	94228
3200	HMDB0000717	Isolithocholic acid	HMDB0000717	164853
3201	HMDB0000761	Lithocholic acid	HMDB0000761	9903
3202	HMDB0002431	12b-Hydroxy-5b-cholanoic acid	HMDB0002431	528381
3203	HMDB0002492	7a-Hydroxy-5b-cholanic acid	HMDB0002492	447718
3204	C03990	NA	NA	NA
3205	C17658	NA	NA	NA
3206	CHEBI:16325	NA	NA	NA
3207	CHEBI:542339	NA	NA	NA
3208	CHEBI:73676	NA	NA	NA
3209	CHEBI:81253	NA	NA	NA
3210	HMDB0036893	Gibberellin A75	HMDB0036893	145831
3211	HMDB0037056	8-Oxodiacetoxyscirpenol	HMDB0037056	131752
3212	HMDB0038328	(S)-Bitalin A 12-glucoside	HMDB0038328	853910
3213	HMDB0038450	Gibberellin A86	HMDB0038450	101663
3214	HMDB0040899	Methyl helianthenoate A glucoside	HMDB0040899	131752
3215	HMDB0030760	Pteroside B	HMDB0030760	739817
3216	HMDB0035166	Cinn cassiol C	HMDB0035166	148415
3217	HMDB0035840	Deacetylisovaltrate	HMDB0035840	131751
3218	HMDB0041228	6b-Angeloyl-3b,8b,9b-trihydroxy-7(11)-eremophilen-12,8-olide	HMDB0041228	131753
3219	HMDB0126521	NA	NA	NA
3220	C08756	NA	NA	NA
3221	C17643	NA	NA	NA
3222	CHEBI:66622	NA	NA	NA
3223	CHEBI:66623	NA	NA	NA
3224	HMDB0010343	Ibuprofen glucuronide	HMDB0010343	922784
3225	HMDB0035201	4,8-Diacetyl-T2-tetrol	HMDB0035201	100227
3226	HMDB0038916	7alpha,8alpha-Dihydroxycalonectrin	HMDB0038916	557474
3227	HMDB0039811	Cyclocalopin B	HMDB0039811	731184
3228	HMDB0060919	NA	NA	NA

3229	HMDB0132958	NA	NA	NA
3230	HMDB0140970	NA	NA	NA
3231	C03033	NA	NA	NA
3232	CHEBI:68930	NA	NA	NA
3233	HMDB0031676	5a,6a-Epoxy-7E-megastigmene-3a,9e-diol 3-glucoside	HMDB0031676	131751
3234	HMDB0036318	9,13-Dihydroxy-4-megastigmen-3-one 9-glucoside	HMDB0036318	727915
3235	HMDB0036846	Icariside B8	HMDB0036846	145399
3236	HMDB0038306	5a,6a-Epoxy-7E-megastigmene-3b,9e-diol 9-glucoside	HMDB0038306	131752
3237	HMDB0040614	Dihydoroseoside	HMDB0040614	161969
3238	C17452	NA	NA	NA
3239	HMDB0030564	trans-Piceid	HMDB0030564	528171
3240	HMDB0030565	(Z)-Resveratrol 4'-glucoside	HMDB0030565	131751
3241	HMDB0031422	cis-Piceid	HMDB0031422	101784
3242	HMDB0036294	(E)-2-Glucosyl-3,4',5-trihydroxystilbene	HMDB0036294	138517
3243	HMDB0135201	NA	NA	NA
3244	C10275	NA	NA	NA
3245	C10823	NA	NA	NA
3246	CHEBI:336507	NA	NA	NA
3247	CHEBI:76155	NA	NA	NA
3248	CHEBI:8198	NA	NA	NA
3249	HMDB0002356	Hexacosanoic acid	HMDB0002356	10469
3250	HMDB0035628	6-Hydroxy-8-hexacosanone	HMDB0035628	131751
3251	HMDB0060125	NA	NA	NA
3252	CHEBI:31009	NA	NA	NA
3253	CHEBI:84063	NA	NA	NA
3254	CHEBI:84905	NA	NA	NA
3255	HMDB0000447	7a,12a-Dihydroxy-3-oxo-4-cholenoic acid	HMDB0000447	528399
3256	HMDB0014372	Lovastatin	HMDB0014372	53232
3257	HMDB0038152	Lucidone C	HMDB0038152	141094
3258	C07074	NA	NA	NA
3259	C15568	NA	NA	NA
3260	CHEBI:40303	NA	NA	NA
3261	CHEBI:49269	NA	NA	NA
3262	CHEBI:68416	NA	NA	NA
3263	HMDB0011555	NA	NA	NA
3264	HMDB0011556	NA	NA	NA
3265	HMDB0011585	NA	NA	NA
3266	HMDB0011586	NA	NA	NA
3267	HMDB0012517	11'-Carboxy-gamma-chromanol	HMDB0012517	534814
3268	C14624	NA	NA	NA
3269	HMDB0000312	3alpha,7alpha,12beta-Trihydroxy-5beta-cholanoic acid	HMDB0000312	528386
3270	HMDB0000320	3a,4b,7a-Trihydroxy-5b-cholanoic acid	HMDB0000320	534776
3271	HMDB0000326	1b,3a,12a-Trihydroxy-5b-cholanoic acid	HMDB0000326	534776
3272	HMDB0000330	3a,4b,12a-Trihydroxy-5b-cholanoic acid	HMDB0000330	308061
3273	HMDB0000364	3a,6a,7b-Trihydroxy-5b-cholanoic acid	HMDB0000364	528385
3274	HMDB0000371	1,3,12-Trihydroxycholelan-24-oic acid	HMDB0000371	208493
3275	HMDB0000376	3b,7a,12a-Trihydroxy-5a-Cholanoic acid	HMDB0000376	528387
3276	HMDB0000390	3a,7b,12b-Trihydroxy-5b-cholanoic acid	HMDB0000390	528387
3277	HMDB0000395	3b,7b,12a-Trihydroxy-5b-cholanoic acid	HMDB0000395	528387
3278	HMDB0000404	2b,3a,7a-Trihydroxy-5b-cholanoic acid	HMDB0000404	528384
3279	HMDB0000414	1b,3a,7a-Trihydroxy-5b-cholanoic acid	HMDB0000414	528384
3280	HMDB0000415	3a,6b,7b-Trihydroxy-5b-cholanoic acid	HMDB0000415	528385
3281	HMDB0000419	3b,7a,12a-Trihydroxy-5b-cholanoic acid	HMDB0000419	528387
3282	HMDB0000427	3b,7b,12a-Trihydroxy-5a-Cholanoic acid	HMDB0000427	528387
3283	HMDB0000432	3a,7b,12a-Trihydroxy-5a-Cholanoic acid	HMDB0000432	129
3284	HMDB0000505	Allocholic acid	HMDB0000505	160636
3285	HMDB0000506	alpha-Muricholic acid	HMDB0000506	528385
3286	HMDB0000527	6a,12a-Dihydroxylithocholic acid	HMDB0000527	228335
3287	HMDB0000619	Cholic acid	HMDB0000619	221493
3288	HMDB0000760	Hyochoic acid	HMDB0000760	131750
3289	HMDB0000865	Muricholic acid	HMDB0000865	119473
3290	HMDB0000917	Ursocholic acid	HMDB0000917	122340
3291	HMDB0006053	NA	NA	NA
3292	C00695	NA	NA	NA
3293	C01558	NA	NA	NA
3294	C04661	NA	NA	NA
3295	C17644	NA	NA	NA
3296	C17647	NA	NA	NA
3297	C17649	NA	NA	NA
3298	C17650	NA	NA	NA
3299	C17654	NA	NA	NA
3300	C17657	NA	NA	NA
3301	C17667	NA	NA	NA
3302	C17668	NA	NA	NA
3303	C17726	NA	NA	NA
3304	C17727	NA	NA	NA
3305	C17737	NA	NA	NA
3306	CHEBI:134216	NA	NA	NA
3307	CHEBI:16359	NA	NA	NA
3308	CHEBI:36240	NA	NA	NA
3309	CHEBI:803879	NA	NA	NA
3310	CHEBI:85490	NA	NA	NA
3311	CHEBI:88105	NA	NA	NA
3312	CHEBI:89219	NA	NA	NA
3313	HMDB0011470	NA	NA	NA
3314	HMDB0011500	NA	NA	NA
3315	CHEBI:84299	NA	NA	NA

3316	HMDB0012607	18-Carboxy-dinor-LTE4	HMDB0012607	534814
3317	CHEBI:74017	NA	NA	NA
3318	HMDB0002829	Androsterone glucuronide	HMDB0002829	114833
3319	HMDB0004484	Etiocholanolone glucuronide	HMDB0004484	443078
3320	HMDB0006203	5-alpha-Dihydrotestosterone glucuronide	HMDB0006203	442633
3321	HMDB0010365	3-alpha-hydroxy-5-alpha-androstane-17-one 3-D-glucuronide	HMDB0010365	534804
3322	C111135	NA	NA	NA
3323	C111136	NA	NA	NA
3324	CHEBI:28832	NA	NA	NA
3325	CHEBI:37451	NA	NA	NA
3326	CHEBI:83024	NA	NA	NA
3327	CHEBI:89417	NA	NA	NA
3328	HMDB0000036	Taurocholic acid	HMDB0000036	6675
3329	HMDB0000889	Tauroursocholic acid	HMDB0000889	212522
3330	HMDB0000922	Taurallocholic acid	HMDB0000922	123590
3331	HMDB0000932	Tauro-b-muricholic acid	HMDB0000932	168408
3332	HMDB0011637	Taurohyocholate	HMDB0011637	131750
3333	C05122	NA	NA	NA
3334	C15516	NA	NA	NA
3335	CHEBI:28865	NA	NA	NA
3336	CHEBI:52022	NA	NA	NA
3337	HMDB0038847	Apigenin 7-[rhamnosyl-(1->2)-galacturonide]	HMDB0038847	143097
3338	HMDB0041129	6"-O-(3-Hydroxy-3-methylglutaroyl)astragalin	HMDB0041129	237572
3339	HMDB0041719	Daidzin 4'-O-glucuronide	HMDB0041719	131753
3340	HMDB0127121	NA	NA	NA
3341	HMDB0127122	NA	NA	NA
3342	HMDB0127170	NA	NA	NA
3343	HMDB0127171	NA	NA	NA
3344	HMDB0127234	NA	NA	NA
3345	HMDB0127235	NA	NA	NA
3346	HMDB0127275	NA	NA	NA
3347	HMDB0127276	NA	NA	NA
3348	HMDB0127295	NA	NA	NA
3349	HMDB0127296	NA	NA	NA
3350	HMDB0116652	NA	NA	NA
3351	HMDB0116688	NA	NA	NA

4 Pathway Analysis

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

4.1 Pathway Library

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

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

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

4.2 Over Representation Analysis

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

- Fishers'Exact test
- Hypergeometric Test

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

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

4.3 Pathway Topology Analysis

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

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

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

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

5 Pathway Analysis Result

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

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

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

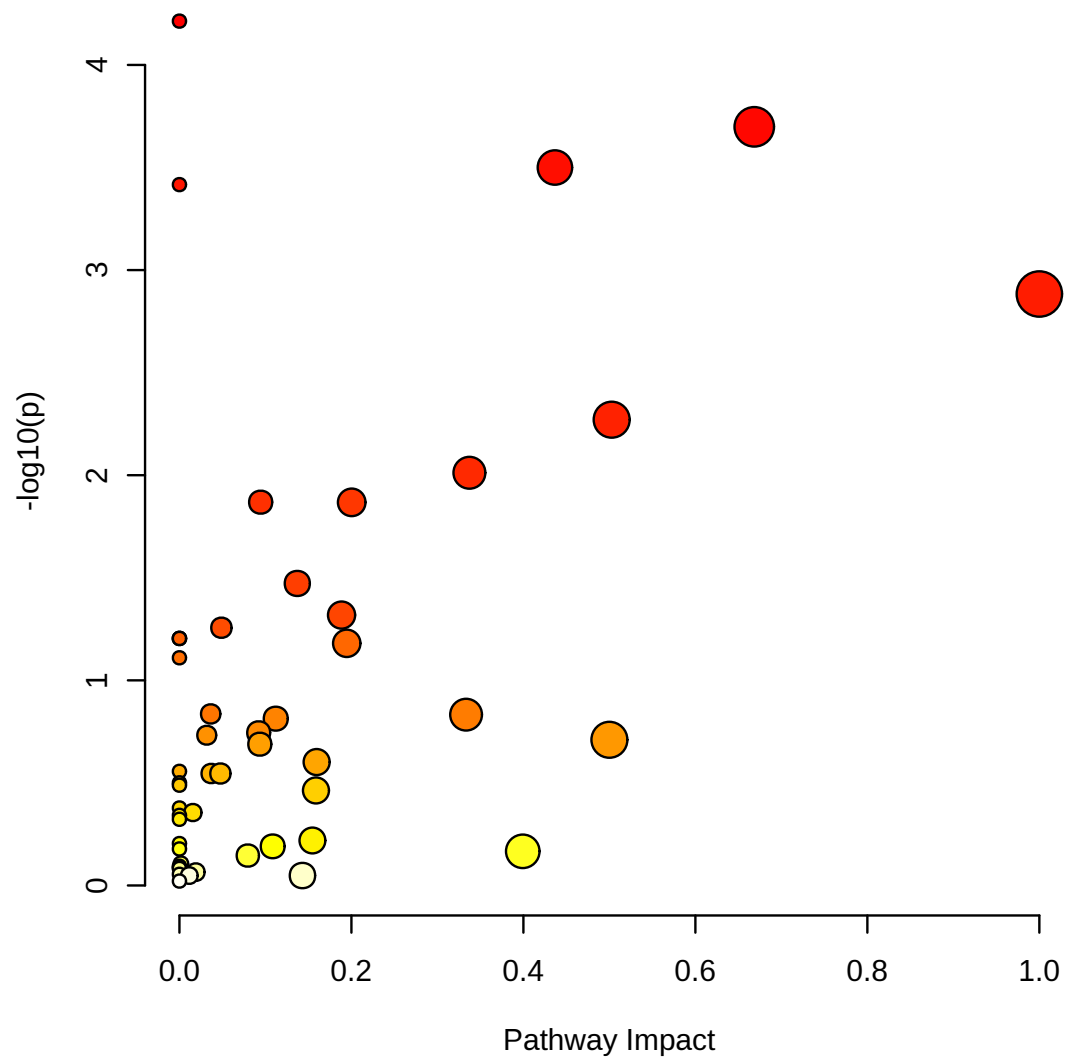


Figure 1: Summary of Pathway Analysis

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

Table 2: Result from Pathway Analysis

	Total	Expected	Hits	Raw p	-log10(p)	Holm adjust	FDR	Impact
D-Amino acid metabolism	15	0.79	6	6.11E-05	4.21E+00	4.89E-03	4.89E-03	0.00
Glycine, serine and threonine metabolism	33	1.74	8	2.00E-04	3.70E+00	1.58E-02	7.66E-03	0.67
Arachidonic acid metabolism	44	2.32	9	3.16E-04	3.50E+00	2.47E-02	7.66E-03	0.44
Biosynthesis of unsaturated fatty acids	36	1.90	8	3.83E-04	3.42E+00	2.95E-02	7.66E-03	0.00
Linoleic acid metabolism	5	0.26	3	1.31E-03	2.88E+00	9.94E-02	2.09E-02	1.00
Glyoxylate and dicarboxylate metabolism	32	1.69	6	5.36E-03	2.27E+00	4.02E-01	7.15E-02	0.50
Arginine and proline metabolism	36	1.90	6	9.73E-03	2.01E+00	7.20E-01	1.11E-01	0.34
Steroid hormone biosynthesis	87	4.58	10	1.35E-02	1.87E+00	9.88E-01	1.21E-01	0.09
Alanine, aspartate and glutamate metabolism	28	1.48	5	1.36E-02	1.87E+00	9.88E-01	1.21E-01	0.20
Arginine biosynthesis	14	0.74	3	3.37E-02	1.47E+00	1.00E+00	2.70E-01	0.14
Histidine metabolism	16	0.84	3	4.81E-02	1.32E+00	1.00E+00	3.30E-01	0.19
Valine, leucine and isoleucine degradation	40	2.11	5	5.54E-02	1.26E+00	1.00E+00	3.30E-01	0.05
Valine, leucine and isoleucine biosynthesis	8	0.42	2	6.25E-02	1.20E+00	1.00E+00	3.30E-01	0.00
Phenylalanine metabolism	8	0.42	2	6.25E-02	1.20E+00	1.00E+00	3.30E-01	0.00
Taurine and hypotaurine metabolism	8	0.42	2	6.25E-02	1.20E+00	1.00E+00	3.30E-01	0.00
Tyrosine metabolism	42	2.21	5	6.60E-02	1.18E+00	1.00E+00	3.30E-01	0.19
Ascorbate and aldarate metabolism	9	0.47	2	7.76E-02	1.11E+00	1.00E+00	3.65E-01	0.00
Pyrimidine metabolism	39	2.06	4	1.46E-01	8.36E-01	1.00E+00	6.15E-01	0.04
alpha-Linolenic acid metabolism	13	0.69	2	1.47E-01	8.33E-01	1.00E+00	6.15E-01	0.33
Glycolysis / Gluconeogenesis	26	1.37	3	1.54E-01	8.13E-01	1.00E+00	6.15E-01	0.11
Glutathione metabolism	28	1.48	3	1.80E-01	7.45E-01	1.00E+00	6.73E-01	0.09
Butanoate metabolism	15	0.79	2	1.85E-01	7.32E-01	1.00E+00	6.73E-01	0.03
Phenylalanine, tyrosine and tryptophan biosynthesis	4	0.21	1	1.95E-01	7.10E-01	1.00E+00	6.78E-01	0.50
Glycerolipid metabolism	16	0.84	2	2.05E-01	6.89E-01	1.00E+00	6.82E-01	0.09
Cysteine and methionine metabolism	33	1.74	3	2.50E-01	6.02E-01	1.00E+00	8.01E-01	0.16
Nitrogen metabolism	6	0.32	1	2.78E-01	5.56E-01	1.00E+00	8.13E-01	0.00
Fructose and mannose metabolism	20	1.05	2	2.85E-01	5.46E-01	1.00E+00	8.13E-01	0.04
Pantothenate and CoA biosynthesis	20	1.05	2	2.85E-01	5.46E-01	1.00E+00	8.13E-01	0.05
Thiamine metabolism	7	0.37	1	3.16E-01	5.00E-01	1.00E+00	8.65E-01	0.00
Propanoate metabolism	22	1.16	2	3.24E-01	4.89E-01	1.00E+00	8.65E-01	0.00
Pentose phosphate pathway	23	1.21	2	3.44E-01	4.63E-01	1.00E+00	8.88E-01	0.16
Biotin metabolism	10	0.53	1	4.19E-01	3.78E-01	1.00E+00	1.00E+00	0.00
Primary bile acid biosynthesis	46	2.42	3	4.41E-01	3.56E-01	1.00E+00	1.00E+00	0.02
Fatty acid biosynthesis	47	2.48	3	4.55E-01	3.42E-01	1.00E+00	1.00E+00	0.00
Inositol phosphate metabolism	30	1.58	2	4.76E-01	3.23E-01	1.00E+00	1.00E+00	0.00
Retinol metabolism	17	0.90	1	6.04E-01	2.19E-01	1.00E+00	1.00E+00	0.15
Ubiquinone and other terpenoid-quinone biosynthesis	18	0.95	1	6.25E-01	2.04E-01	1.00E+00	1.00E+00	0.00
Pentose and glucuronate interconversions	19	1.00	1	6.45E-01	1.91E-01	1.00E+00	1.00E+00	0.11
Selenocompound metabolism	20	1.05	1	6.64E-01	1.78E-01	1.00E+00	1.00E+00	0.00
beta-Alanine metabolism	21	1.11	1	6.82E-01	1.66E-01	1.00E+00	1.00E+00	0.40
Pyruvate metabolism	23	1.21	1	7.15E-01	1.46E-01	1.00E+00	1.00E+00	0.08
Lipoic acid metabolism	28	1.48	1	7.83E-01	1.06E-01	1.00E+00	1.00E+00	0.00
Lysine degradation	30	1.58	1	8.06E-01	9.37E-02	1.00E+00	1.00E+00	0.00
Porphyryn metabolism	31	1.63	1	8.16E-01	8.81E-02	1.00E+00	1.00E+00	0.00
Sphingolipid metabolism	32	1.69	1	8.26E-01	8.29E-02	1.00E+00	1.00E+00	0.00
Glycerophospholipid metabolism	36	1.90	1	8.61E-01	6.51E-02	1.00E+00	1.00E+00	0.02
Fatty acid degradation	39	2.06	1	8.82E-01	5.45E-02	1.00E+00	1.00E+00	0.00
Tryptophan metabolism	41	2.16	1	8.95E-01	4.84E-02	1.00E+00	1.00E+00	0.14
Purine metabolism	70	3.69	2	8.95E-01	4.83E-02	1.00E+00	1.00E+00	0.01
Drug metabolism - cytochrome P450	55	2.90	1	9.52E-01	2.15E-02	1.00E+00	1.00E+00	0.00

6 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "compd.vec<-c(\"HMDB0000042\", \"HMDB0003344\", \"HMDB0002165\", \"C00033\", \"C00266\", \"CHEBI:1536
[3] "mSet<-Setup.MapData(mSet, compd.vec);"
[4] "mSet<-CrossReferencing(mSet, \"hmdb\");"
[5] "mSet<-CreateMappingResultTable(mSet)"
[6] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[7] "mSet<-SetMetabolomeFilter(mSet, F);"
[8] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[9] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA, NA, NA )"
[10] "mSet<-SaveTransformedData(mSet)"
[11] "mSet<-PreparePDFReport(mSet, \"guest5869009112759895119\")\n"
```

The report was generated on Fri Aug 2 03:46:11 2024 with R version 4.2.2 (2022-10-31), OS system: Linux.