

MetabolitName	KEGG ID	HMDB ID
0.583_14	SpermidirC00315	HMDB0001257
0.609_12	PipecolatC00408	HMDB0000070
0.61_146.	L-Lysine C00047	HMDB0000182
0.636_18	2-Phosphoglycerate	HMDB0000362
0.644_18	Nepsilon, C03793	HMDB0001325
0.649_19	2Citrate C00158	HMDB0000094
0.651_89.	L-(+)-Lactic acid	
0.653_13	4(s)-malatC00149	HMDB0000156
0.668_14	1EthanolanC00346	HMDB0000224
0.67_148.	2-HydroxyC02630	HMDB0059655
0.675_14	6OxoglutarC00026	HMDB0000208
0.68_118.	SuccinateC00042	HMDB0000254
0.68_174.	L-arginirC00062	HMDB0000517
0.682_15	5L-HistidiC00135	HMDB0000177
0.69_146.	D-GlutamiC00819	HMDB0003423
0.691_10	5gamma-AmiC00334	HMDB0000112
0.692_10	5L-Serine C00065	HMDB0000187
0.694_16	1L-CARNITIC00318	HMDB0000062
0.696_75.	TrimethylC01104	HMDB0000925
0.698_11	5creatinirC00791	HMDB0000562
0.698_14	6L-GlutamiC00064	HMDB0000641
0.705_11	9L-ThreoniC00188	HMDB0000167
0.708_17	5L-CitrullC00327	HMDB0000904
0.712_13	5D-aspartateC00402	HMDB0006483
0.713_11	7L-Valine C16436	HMDB0000883
0.727_13	1Creatine C00300	HMDB0000064
0.74_147.	L-GlutamiC00025	HMDB0000148
0.747_11	5L-ProlineC00148	HMDB0000162
0.748_15	9N-Acetylvaline	HMDB0011757
0.748_16	1N-methyl-C01046	
0.75_174.	Valylglycine	HMDB0029127
0.75_203.	O-ACETYLC02571	HMDB0000201
0.757_13	5L-aspartateC00049	HMDB0000191
0.807_10	1L-HomoserC00263	HMDB0000719
0.838_30	9N-acetylrc00270	HMDB0000230
0.851_97.	Phosphoric00009	HMDB0001429
0.855_20	5N-Acetyl-C01074	HMDB0000212
0.858_26	6D-mannoseC00275	HMDB0001078
0.994_32	5Cytidine C00055	HMDB0000095
0.998_34	7DeoxyguarC00362	HMDB0001044
1.02_125.	Taurine C00245	HMDB0000251
1.032_89.	Beta-AlarC00099	HMDB0000056
1.04_168.	Uric acidC00366	HMDB0000289
1.087_24	5Cytidine C00475	HMDB0000089
1.108_13	6Allopurinol	HMDB0014581
1.124_12	9O-acetyl-C00979	HMDB0003011
1.124_17	5N-Acetyl-C01042	HMDB0000812
1.16_136.	HypoxanthC00262	HMDB0000157
1.234_15	1Guanine C00242	HMDB0000132
1.239_14	62-Methylglutaric acid	HMDB0000422

1. 254_152	Oxypurine	C07599	HMDB0000786
1. 292_182	Hydroxyphenyl	C03672	HMDB0000755
1. 327_129	PYROGLUTAMIC ACID	C01879	HMDB0000267
1. 375_181	L-Tyrosine	C01536	HMDB0000158
1. 377_131	L-Isoleucine	C00407	HMDB0000172
1. 38_112	Uracil	C00106	HMDB0000300
1. 392_244	Uridine	C00299	HMDB0000296
1. 404_348	Inosine	C00130	HMDB0000175
1. 416_189	N-Acetyl-	C00624	HMDB0001138
1. 476_307	L-Glutathione	C00051	HMDB0000125
1. 591_174	Suberic acid	C08278	HMDB0000893
1. 605_131	L-Norleucine	C01933	HMDB0001645
1. 755_88	Butyric acid	C00246	HMDB0000039
1. 776_131	Leucine	C00123	HMDB0000687
1. 898_267	Adenosine	C00212	HMDB0000050
1. 931_138	Adenine	C00147	HMDB0000034
2. 111_268	Inosine	C00294	HMDB0000195
2. 276_289	Guanosine	C00387	HMDB0000133
2. 506_208	L-Kynurenine	C00328	HMDB0000684
2. 519_284	Xanthosine	C01762	HMDB0000299
2. 577_168	L-Phenylethylamine	C02057	HMDB0000159
2. 721_157	Tiglylglycine		HMDB0000959
2. 772_99	2-Piperidinone		HMDB0011749
3. 002_188	Azelaic acid	C08261	HMDB0000784
3. 046_189	4-Pyridoxal	C00847	HMDB0000017
3. 091_166	Phenylacetic acid	C01479	HMDB0000779
3. 11_219	Pantoic acid	C00864	HMDB0000210
3. 116_204	L-Tryptophan	C00078	HMDB0000929
3. 22_128	Adipic acid	C006104	HMDB0000448
3. 262_148	4-Trimethylaminopropylamine	C01181	HMDB0001161
3. 32_187	Indoleacrylic acid		HMDB0000734
3. 383_148	2-Aminoheptanoate		HMDB0094649
3. 48_297	5'-methylthioadenosine	C00170	HMDB0001173
3. 543_1915	5-hydroxytryptophan	C05635	HMDB0000763
3. 589_191	N-ACETYLMETHANAMINE	C02712	HMDB0011745
3. 738_114	2-Methyl-4-penten-3-one		HMDB0031158
4. 112_147	1H-Indole	C11129	HMDB0061933
4. 197_142	Pimelic acid	C02656	HMDB0000857
4. 295_128	4-Heptenoic acid		HMDB0033793
4. 407_376	Riboflavin	C00255	HMDB0000244
4. 517_204	Homovanillic acid	C05582	HMDB0000118
4. 959_207	N-Acetyl-	C03519	HMDB0000512
5. 175_160	3-Hydroxytryptophan	C16651	HMDB0013899
5. 207_178	Indoleacetic acid	C00954	HMDB0000197
5. 401_144	Caprylic acid	C06423	HMDB0000482
5. 439_152	vanillin	C00642	
6. 278_142	(R)-2-Hydroxycaprylic acid		HMDB0002264
6. 394_224	SEBACIC ACID	C08277	HMDB0000792
7. 024_188	2-Hydroxydecanoate		HMDB0094656
7. 202_188	10-Hydroxyundecanoic acid	C02774	HMDB0244272
7. 316_279	Palmitic acid	C00249	HMDB0000220

7. 659_206 ibuprofen C01588 HMDB0001925
8. 518_278 Linoleic C01595 HMDB0000673
9. 358_302 rac-Glycerol 1-myristate
9. 559_384 25-Hydroxy C15519 HMDB0006247
9. 597_299 Oleate C00712 HMDB0000207
9. 789_356 1-Oleoyl-rac-glycerol HMDB0011567
0. 623_339 a-D-Glucose C01231 HMDB0003514
0. 649_112 3-Furoic acid HMDB0000444
0. 657_260 D-Glucose C00092 HMDB0001401
0. 668_230 D-Ribulose C00199 HMDB0000618
0. 67_566. Uridine C00052 HMDB0000302
0. 675_105 Choline C00114 HMDB0000097
0. 676_76. Glycolic C00160 HMDB0000115
0. 678_106 (2R)-2,3-C00258 HMDB0000139
0. 686_132 3-Ureido C02642 HMDB0000026
0. 7_183. (PHOSPHORYLCHOLINE)
0. 703_276 L-Saccharose C00449 HMDB0000279
0. 735_129 4-Oxoproline C01877
0. 737_89. DL-Alanine C01401 HMDB0062251
0. 763_131 N-Acetylalanine HMDB0000766
0. 763_365 Guanosine C00144 HMDB0001397
0. 787_132 2-hydroxy-4-(methyl) HMDB0037115
0. 823_146 3-Methylglutaric acid HMDB0000752
0. 834_120 4-hydroxy C00156 HMDB0000500
0. 849_126 5-Hydroxy C11101 HMDB0034355
0. 916_276 <U+03A5>- C05282 HMDB0011737
0. 948_165 Methionine C02989 HMDB0002005
0. 971_141 L-Histidine C00860 HMDB0003431
1. 089_145 L-(-)-Met C00073 HMDB0000696
1. 091_164 2-Hydroxy C01772 HMDB0002641
1. 114_122 Nicotinic C00153 HMDB0001406
1. 136_145 N-Acetyl-L-cysteine HMDB0001890
1. 175_97. Caproic acid C01585 HMDB0000535
1. 537_612 L-Glutathione C00127 HMDB0003337
1. 622_85. Piperidine C01746 HMDB0034301
1. 644_304 N-Acetyl- C12270 HMDB0001067
1. 968_162 Paraxanthine C13747 HMDB0001860
10. 031_351 Stearoyl D01947
10. 121_41 Tomatidine C10826 HMDB0034731
10. 133_308 Z, 11Z, 14 C03242 HMDB0002925
10. 272_28 trans-Petroselinic acid
10. 427_3011 (Z), 14 C16525 HMDB0005060
10. 507_38 Cholecalciferol C05443 HMDB0000876
10. 596_35 Docosatrienoic acid HMDB0002823
10. 779_3111 (Z)-Eic C16526 HMDB0002231
11. 128_38 Cholest-4 C00599 HMDB0000921
11. 206_70 Palmitoyl sphingomyelin
11. 459_35 Erucic acid C08316 HMDB0002068
11. 782_75 DL-Dipalmitoylphosphatidylcholine
12. 481_36 Nervonic C08323 HMDB0002368
2. 16_347. 3'-Adenosine C01367 HMDB0003540

2. 335_132 2-Hydroxycaproic acid HMDB0001624
 2. 401_145 6-Oxopiperidine-2-one HMDB0061705
 2. 474_173 Hexanoylglycine HMDB0000701
 2. 517_100 5-valerolactone C02240
 2. 566_228 Prolylleucine
 2. 576_148 trans-Cis-4-Hydroxy-2-pentenoic acid HMDB0000930
 2. 579_155 Arecoline C10129 HMDB0030353
 2. 612_347 Adenosine C00020 HMDB0000045
 2. 629_384 S-Adenosylmethionine C00021 HMDB0000939
 2. 638_297 7-Methylxanthine C20674 HMDB0001107
 2. 698_137 Phenylethylamine C02735 HMDB0001065
 2. 722_106 4-Methylumbelliferone C06730 HMDB0000873
 2. 758_188 Ecgonine
 2. 834_242 Thymidine C00214 HMDB0000273
 2. 835_281 1-Methylxanthine C02494 HMDB0003331
 3. 016_188 Glycyl-L-proline C02155 HMDB0000759
 3. 022_138 Salicylic acid C00805 HMDB0001895
 3. 051_86 Crotonic acid C01771 HMDB0010720
 3. 118_169 Pyridoxal C00314 HMDB0000239
 3. 215_228 Leucylproline
 3. 233_166 DL-alpha-Methoxyphenylacetic acid
 3. 265_122 4-Hydroxyphenylacetic acid HMDB0011718
 3. 321_145 Indole-3-carboxamide C08493 HMDB0029737
 3. 321_204 DL-Tryptophan C00806 HMDB0030396
 3. 324_129 Quinoline C06413 HMDB0033731
 3. 325_159 Indoleacetic acid C00637 HMDB0001190
 3. 415_164 1,5-Anhydrotetracycline C07326 HMDB0002712
 3. 488_173 N-Acetyl-D-alloisoleucine
 3. 503_280 alpha-Aspartylphenylalanine C000706 HMDB0000706
 3. 547_205 Xanthurenic acid C02470 HMDB0000881
 3. 565_128 Heptanoic acid C17714 HMDB0000666
 3. 75_184 2,4-Dinitrophenol C02496
 3. 764_112 Sorbic acid D02411 HMDB0029581
 3. 968_138 3-Acetyl-2,5-dimethylhexanoic acid HMDB0029563
 4. 028_456 Flavin mononucleotide C00061 HMDB0001520
 4. 029_234 Lidocaine C07073 HMDB0014426
 4. 055_214 2-Benzothiazolesulfonic acid
 4. 2_110 (trans,trans-2,4-Heptadienal
 4. 309_119 4-Aminobenzoic acid C00568 HMDB0001392
 4. 33_164 4-Phenylbutyric acid C21793 HMDB0000543
 4. 33_213 Heptafluorobutyric acid HMDB0253102
 4. 361_201 Capryloylglycine HMDB0000832
 4. 376_114 trans-3-Hexenoic acid
 4. 391_198 (-)-Camphanic acid
 4. 519_274 Phenylbenzimidazole sulfonic acid
 4. 604_159 DL-alpha-Aminocaprylic acid HMDB0000991
 4. 665_133 5-Hydroxyindole HMDB0059805
 4. 699_166 Perillic acid C11924 HMDB0004586
 4. 956_139 3-Hydroxyphenylacetic acid C18620 HMDB0013188
 5. 049_196 Loliolide
 5. 108_166 3-(4-Hydroxyphenyl)acetic acid C01744 HMDB0002199

5. 223_122 1-PhenyleC07112 HMDB0032619
 5. 364_166 3-MethoxyphenylacεHMDB0059969
 5. 512_312 tetranor-PGFM
 5. 532_282 Artemisic C09538
 5. 61_230. Dodecanec C02678 HMDB0000623
 5. 701_194 ButylparεD01420 HMDB0032575
 5. 727_162 2-Hydroxy_3_methylHMDB0000407
 5. 728_180 TheophyllC07130 HMDB0001889
 5. 777_166 7-Methylx C16353 HMDB0001991
 5. 792_242 (Z)-2-octylpent-2-enedioic acid
 6. 056_224 Methyl jεC11512 HMDB0036583
 6. 33_594. tiliroside
 6. 395_138 Isophorol C14743 HMDB0031195
 6. 395_170 cis-4-Decenoic aciHMDB0004980
 6. 659_300 13, 14-dihydro-15-keto-tetranor Prostaglandin F1
 6. 847_117 Betaine C00719 HMDB0000043
 6. 898_194 Sedanolic C17002 HMDB0034450
 6. 961_346 Corticost C02140 HMDB0001547
 6. 989_210 Jasmonic C08491 HMDB0032797
 7. 004_280 3, 14-dihydro-15-keto-tetranor Prostaglandin E2
 7. 019_258 Tetradecanedioic εHMDB0000872
 7. 227_278 Triphenylphosphine oxide
 7. 238_370 6-Ketoprc C05961 HMDB0002886
 7. 248_354 ent-Prostaglandin F2a
 7. 352_134 4-Ethylbenzaldehyc HMDB0032024
 7. 353_120 Acetopher C07113 HMDB0033910
 7. 374_282 13, 14-Dihydro-15-keto-tetranor prostaglandin Fla
 7. 392_327 10-Nitrooleate
 7. 392_372 13, 14-Dihydro-19(R)-hydroxy prostaglandin E1
 7. 415_229 N,N-Dimethyldodecylamine N-oxide
 7. 453_170 3-Decenoic acid HMDB0031002
 7. 493_318 15-Deoxy-<U+0394>12, 14-prostaglandin A1
 7. 493_336 Prostaglε C00959 HMDB0002982
 7. 493_376 11 C05959 HMDB0010199
 7. 537_354 (+/-) 5-iPF2a-VI
 7. 539_350 Andrograr C20214
 7. 586_334 15-Deoxy-<U+0394>12, 14-prostaglandin D2
 7. 666_354 ent-8-iso Prostaglandin F2a
 7. 687_218 Nootkator C17914 HMDB0013687
 7. 764_356 Prostaglandin F1
 7. 788_334 Prostaglε C05953 HMDB0002752
 7. 789_312 (+/-) 9-HpODE
 7. 844_353 Prostaglandin F2a 1, 9-lactone
 7. 863_314 trans-10-Heptadecenoic acid
 7. 871_294 13(S)-H01C16316
 7. 875_148 Cuminaldε C06577 HMDB0002214
 7. 973_317 2-Amino-1C12144 HMDB0004610
 7. 975_228 Dibutyl maleate
 7. 988_286 Hexadecar C19615 HMDB0000672
 8. 009_220 (-)-Caryc C16908 HMDB0036789
 8. 011_210 Myristic C06424 HMDB0000806

8.027_368 Isomurolic acid
8.077_296 (+/-) 12(1C14829 HMDB0004705
8.11_461. Psychosine
8.134_324 Lichesterinic acid
8.158_338 13,14-Dihydro prostaglandin E1
8.164_358 13,14-dihydro Prostaglandin Fla
8.225_299 D-Sphingoc C00319 HMDB0000252
8.244_300 Roccellic acid
8.312_376 2-(14,15-Epoxyeic HMDB0013651
8.326_292 12-Oxo p C01226
8.34_301. Sphingani C00836 HMDB0000269
8.34_338. 11-Deoxy prostaglandin F2
8.375_250 2-[(1S,2S,4aR,8aS)-1-hydroxy-4a-methyl-8-methylidene-1,2,3,4,5,6,7,8a-oc
8.46_302. 11-Ketote C14256
8.471_338 (+/-) 8(9)-DiHET
8.509_316 13,14-Dihydro-15-keto Prostaglandin J2
8.51_399. Palmitoylcarnitine
8.544_327 N,N-Dimet C13914 HMDB0013645
8.545_316 Cafestol C09066 HMDB0035710
8.577_287 Lauroyl diethanol HMDB0032358
8.603_336 2-Linoleoyl glycer HMDB0011538
8.712_398 Tris(2-but C14446 HMDB0259275
8.786_408 Cholic ac C00695 HMDB0000619
8.815_326 Roccellaric acid
8.863_318 Prostaglandin F2a 1-11-lactone
8.928_360 (+/-) 11(12)-DiHET
8.936_320 20-Hydrox C14748 HMDB0005998
8.969_302 (+/-) 11(12)-EET
8.969_342 NCGC00384702-01! (2Z,6E,10E)-12-hydroxy-6,10-dimethyl-2-(4-methylpent-3-e
8.997_320 (+/-) 11-HETE
9.032_345 (+/-) 5(6)-EET Ethanolamide
9.039_323 Linoleoyl ethanolamide
9.065_347 0-Arachidonoyl et HMDB0013655
9.088_364 2-Arachidonyl glycerol ether
9.118_310 Ethyl ole C04090
9.219_318 12-Epileukotriene B4
9.32_152. Citral C01499 HMDB0035078
9.33_260. NCGC00381425-01! 8-hydroxy-8-(3-octyloxiran-2-yl)octanoic acid [IIN-based
9.358_284 Glycerol 1-myriste HMDB0304951
9.545_378 2-Arachidic C13856 HMDB0004666
9.545_400 Nordeoxycholic aci HMDB0304947
9.563_453 Glycerophospho-N-palmitoyl ethanolamine
9.667_325 Oleoyl et C20792 HMDB0002088
9.705_281 Oleamide C19670 HMDB0002117
9.838_254 Palmitole C08362 HMDB0003229
9.894_328 Docosahex C06429 HMDB0002183
9.93_327. Stearoyl ethanolamide
9.941_105 Diethanol C06772 HMDB0004437
9.948_304 Arachidol C00219 HMDB0001043
9.999_618 Oleoyl ethylamide
0.582_131 D-Ornithi C00515 HMDB0003374

0.597_123-Methylhistamine HMDB0001861
 0.598_16(N(6)-Methyl C02728 HMDB0002038
 0.605_132 Ornithine C01602
 0.659_29(D-Sedohep C05382 HMDB0001068
 0.682_18(C-Asymmetric C03626 HMDB0001539
 0.683_18(D-Psicose C06468
 0.683_22(Carnosine C00386 HMDB0000033
 0.688_24(L-Cystine C01420 HMDB0000192
 0.689_22(D-(+)-Gal C00124
 0.699_12(Phlorogluc C02183 HMDB0013675
 0.704_2573-Methylcytidine HMDB0240577
 0.706_101(L-allo-Th C05519 HMDB0004041
 0.711_14(Acetylch C01996 HMDB0000895
 0.713_132 Asparagine C00152 HMDB0000168
 0.745_24(L-Anserine C01262 HMDB0000194
 0.746_174 Trans-acc C02341 HMDB0000958
 0.746_20(N-Acetyl- C00140 HMDB0000215
 0.75_117. N-Acetyl glycine HMDB0000532
 0.752_14(4-Guanidine C01035 HMDB0003464
 0.752_18(N6-Acetyl C02727 HMDB0000206
 0.753_16(2-Keto-gl C00940 HMDB0001552
 0.754_27(GLUTARYLCARNITINE HMDB0013130
 0.759_25(Ribothymidine HMDB0000884
 0.761_167 Quinoline C03722 HMDB0000232
 0.774_34(a-Lactose C00243 HMDB0000186
 0.79_275. N2-gamma- C05283 HMDB0011738
 0.791_13(Itaconate C00490 HMDB0002092
 0.792_11(Fumaric C00122 HMDB0000134
 0.806_11(Erythrono-1, 4-lact HMDB0000349
 0.836_18(O-Phosphate C01005 HMDB0000272
 0.837_254 Chrysin C10028 HMDB0036619
 0.871_132 mono-Ethyl malonate HMDB0000576
 0.873_1443-Hydroxy C03761 HMDB0000355
 0.893_174 N-alpha-acetyl-1-epsilon HMDB0006028
 1.083_12(Nicotinic C00253 HMDB0001488
 1.2_177. (Glucosamine C03752
 1.212_15(N-Isovaleryl glycine HMDB0000678
 1.37_161. D-(+)-gluc C00329 HMDB0001514
 1.375_13(Octopamine C04227 HMDB0004825
 1.417_18(Homogentisine C00544 HMDB0000130
 1.807_264 a-Lapachone
 1.838_22(Deoxyuridine C00526 HMDB0000012
 1.905_201 Kanosamine C12212
 10.004_4(D-a-Tocopherol C02477 HMDB0001893
 10.116_4(N-Arachidonic C12271
 10.242_4(7-Oxocholesterol
 10.287_348. 23354
 10.69_284 Stearic C01530 HMDB0000827
 10.74_36(Ursocholanic Acid
 10.991_3(Cholesta-4, 6-dien- HMDB0002394
 12.643_5(C-8 Ceramide-1-phosphate

2.362_134 Ribitol C00474 HMDB0000508
 2.4_132. (Glutaric C00489 HMDB0000661
 2.574_200 4-vinylphenol sulf HMDB0062775
 2.575_174 DL-Argini C02385
 2.578_182 1-Methyl C16359 HMDB0003099
 2.597_157 N-ACETYLPROLINE
 2.612_142 4-Methyl- C04294 HMDB0032985
 2.718_172 N-Acetyl- C02710 HMDB0011756
 2.722_142 3-(2-hydr C01198 HMDB0033752
 2.78_126. Thymine C00178 HMDB0000262
 2.831_181 2-Amino-6-methylmercaptapurine
 2.888_192 Phenothiæ D02601
 2.98_181. L-threo-æ C03290 HMDB0002184
 3.08_316. 13, 14-Dihydro-15-þ HMDB0001244
 3.151_142 Proline þ C10172 HMDB0004827
 3.233_167 Pyridoxal C00250 HMDB0001545
 3.241_252 Alanyltyrosine
 3.321_117 Indole C00463 HMDB0000738
 3.321_142 6-Methylquinoline HMDB0033115
 3.322_114 Skatole C08313 HMDB0000466
 3.324_220 5-Hydroxy C00643 HMDB0000472
 3.462_182 Kynurenic C01717 HMDB0000715
 3.546_212 8-Methoxy C05830 HMDB0060426
 3.566_154 Phenyl ac C00548 HMDB0040733
 3.573_242 Isovaleryl carniti r HMDB0000688
 3.602_144 3-Methylglutaconic HMDB0000522
 3.631_172 ANILINE-2 C06333
 3.698_202 Phosphocþ C00588 HMDB0001565
 3.721_170 Scopoleti C01752 HMDB0034344
 3.78_222. Cytosine C00380 HMDB0000630
 3.788_142 DL-Stachydrine
 3.81_199. Ecgonine-methyl-ester (EME)
 3.967_137 Tyramine C00483 HMDB0000306
 4.157. 110 (S)-Homos C08283 HMDB0033433
 4.002_172 Salsolinol HMDB0005199
 4.034_192 Vanillyln C05584 HMDB0000291
 4.179_132 3-Methoxybenzaldef HMDB0031459
 4.222_112 1H-Benzotriazole HMDB0244873
 4.267_237 Ketamine C07525 HMDB0015352
 4.274_182 1-hydroxyhexanoylæ HMDB0094718
 4.307_182 Gabapentin Related Compound E
 4.411_171 Gabapentin HMDB0005015
 4.514_182 3,5-Dimethoxybenzoic acid
 4.517_164 3,4-Dihydr C10447 HMDB0000423
 4.519_132 4-Toluic C01454 HMDB0029635
 4.617_242 Tiglyl carniti ne HMDB0002366
 4.628_282 3-METHYL-2-OXOVALERATE
 4.733_172 Diacetyl C00741 HMDB0003407
 4.738_162 5-Methoxysalicylic HMDB0001868
 4.8_171. (Metronidæ C07203 HMDB0015052
 4.806_184 Apocynin C11380

4.818_168 Vanillic C06672 HMDB0000484
4.891_151 Cathine C08300
4.91_108. Benzyl alc C00556 HMDB0003119
4.915_214 (2S)-2-((1S)-1-Hydroxypentyl)-4-methoxy-2,3-dihydropyran-6-one
4.918_164 2-Deoxy-I C00586
4.921_292 curvularin
5.049_260 3-hydroxy-2-octylpentanedioic acid
5.053_290 Argininos C03406 HMDB0000052
5.081_242 8-acetamido-2-methyl-7-oxononanoic acid
5.46_196. Cantharic C16778
5.514_1912,6-Di-tert-butylpyridine
5.699_242 Lumichron C01727
6.019_252 Hexadecanamide HMDB0012273
6.205_324 NCGC00169827-03! (2E, 4E)-12-hydroxy-13-(hydroxymethyl)-3,5,7-trimethyltet
6.23_288. 2-decyl-3-hydroxypentanedioic acid
6.28_310. Tetranor-PGDM
6.384_242 2-Methylbutyroylc HMDB0000378
6.562_262 3-[4-methyl-1-(2-methylpropanoyl)-3-oxocyclohexyl]butanoic acid
6.62_216. (2R)-2-[(2R, 5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid
6.649_322 2,3-Dinor C14794
6.728_260 falcarin C08449 HMDB0033941
6.729_212 N-(9-oxodecyl)acetamide
6.768_264 (
6.833_162 4-Methoxy C10475 HMDB0032611
6.834_252 Neopterir C05926 HMDB0000845
6.871_3116-Ginger C10462
6.924_334 5-trans-Prostaglandin E2
6.958_322 2,3-Dinor prostaglandin E1
7.022_262 N-(2,6-Dimethylphenyl)-N-(methoxyacetyl) alanine
7.04_334. 13,14-Di C04671 HMDB0002776
7.159_382 11-Dehydr C05964 HMDB0004242
7.196_172 Isobutyl benzoate HMDB0040583
7.206_150 Carvone
7.288_362 3-Methoxy prostaglandin Fla
7.35_136. Phenylac C07086 HMDB0000209
7.353_794 NCGC00380363-01! 8-(2,3-dihydroxy-3-methylbutyl)-5,7-dimethoxy-2-phenyl-2
7.374_157 hyocholic acid HMDB0000760
7.402_250 6,7-bis(hydroxymethyl)-4,9a-dimethyl-2,7,8,9-tetrahydro-1H-benzo[7]annul
7.409_332 8-Isoprostaglandin F1
7.428_232 Radicinin
7.496_302 11 C14606 HMDB0002984
7.528_222 (4,8,8-trimethyldecahydro-1,4-methanoazulen-9-yl)methanol
7.537_292 Gamma-lir C06426 HMDB0003073
7.553_234 Polygodia C09712
7.581_370 19(R)-Hydroxy prostaglandin E1
7.611_322 Avocadyne 4-acetate HMDB0031049
7.624_364 Tetrahydr C05470 HMDB0000903
7.631_292 Nephrosteranic acid
7.634_324 allo-Protolichesterinic acid
7.814_382 1a,1b-Dihomo prostaglandin F2a
7.858_512 taurochol C05122 HMDB0000036

7. 875_436 NCGC00381146-01!2-[5-[2-[2-[5-(2-oxopropyl)oxolan-2-yl]propanoyloxy]buty
7. 913_366 Muroic acid
7. 966_182 Dodecanoic acid HMDB0000638
7. 984_342 (+/-)-9(10)-EpOME
8. 025_366 Pertusaric acid
8. 027_362 Cortisol C00735 HMDB0000063
8. 091_356 Lagochilin
8. 109_220 2,6-Di-tert-butyl-HMDB0013817
8. 127_434 [(2R)-2-[(E,2S,4R)-4,6-dimethyloct-6-en-2-yl]-6-oxo-2,3-dihydropyran-3-yl]
8. 128_204 Prespatane
8. 164_216 12-Hydroxy C08317 HMDB0002059
8. 199_334 15(R)-Prostaglandin D2
8. 223_280 Chaulmoogric Acid
8. 347_328 Avocadene 4-acetate HMDB0031045
8. 349_292 14-(hydroxymethyl)-5,9-dimethyltetracyclo[11.2.1.0
8. 355_290 5a-Dihydro C03917 HMDB0002961
8. 356_326 Nephromopsic acid
8. 384_406 NCGC00385003-01!4-[3-methyl-5-(5,6,7-trihydroxy-1,2,4a,5-tetramethyl-3,4
8. 499_432 Salvinorin A
8. 505_334 (+/-)-CP 47,497-C7-Hydroxy metabolite
8. 581_396 (2Z)-2-[(E)-6-(hydroxymethyl)-2,4,8,10-tetramethyldodec-2-enylidene]-4-n
8. 672_310 Avocadene 2-acetate HMDB0031044
8. 679_396 NCGC00347722-02! (2Z)-2-[(E)-6-(hydroxymethyl)-2,4,8,10-tetramethyldodec-
8. 724_312 NCGC00178646-02!2,4-dihydroxyheptadecyl acetate [IIN-based: Match]
8. 731_166 1-Methyl C16358 HMDB0010738
8. 747_358 Arachidic C06425 HMDB0002212
8. 843_318 5-OxoETE C14732 HMDB0010217
8. 859_266 Lauryl sulfate
8. 879_342 5-[(8aS)-2,5,5,8a-tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-
8. 936_368 Bis(2-ethyl) C03690
9. 055_320 (+)-Aphidicolin
9. 112_338 Senecionin C06176
9. 124_251 (2E,4E)-N-(2-methylpropyl) dodeca-2,4-dienamide
9. 229_320 (8S)-Hydro C14776 HMDB0004679
9. 233_418 NCGC00347722-02! (2Z)-2-[(E)-6-(hydroxymethyl)-2,4,8,10-tetramethyldodec-
9. 239_322 15-OxoEDE
9. 322_302 (+/-)-5(6)-EET
9. 344_390 Hyodeoxycholic acid HMDB0000733
9. 397_300 Retinoate C00777 HMDB0001852
9. 455_406 Methyl Deoxycholate
9. 457_278 Mono(2-ethyl) C03343 HMDB0013248
9. 518_136 Eucalyptol C09844 HMDB0004472
9. 565_319 EICOSAPEN C06428 HMBD01999
9. 715_302 (5R,9S)-5,9-dimethyl-14-methylidene tetracyclo[11.2.1.0
9. 766_321a-Linolenoyl ether HMDB0013624
9. 865_314 (+/-)-9,10-dihydroxy-12Z-octadecenoic acid
9. 891_330 Anandamide C11695 HMDB0004080
9. 893_344 Nor-9-carboxy-d9-THC
9. 941_310 Estriol C05141 HMDB0000153
9. 986_349 Dihomo- Δ^9 C13828 HMDB0013625
0. 553_155 1-Ethyl-3-(dimethyl) HMDB0258121

0.555_200 1,4-Bis(3-aminopropyl)pyridine HMDB0247321
0.565_202 Spermine C00750 HMDB0001256
0.587_102 Cadaverine HMDB0002322
0.595_138 Pentetrazolium HMDB0256296
0.597_116 Temed HMDB0258800
0.6_217.1 beta-Alar C05341
0.603_212 1H-Imidazole-1-ethylamine HMDB0257342
0.604_110 Aminomethanesulfonamide HMDB0248321
0.608_83. Tert-BUTYL ISOCYANIDE HMDB0258845
0.613_197 Methylsulfide C12245
0.615_187 N8-Acetylspermidine HMDB0002189
0.618_167 2,6-Diaminocaproic acid C16397
0.621_108 2-Hydrazinopyridine HMDB0245139
0.621_200 L-Erythrose C21286
0.621_370 D-glycerol C19879
0.622_151 2,2-Dichloro-1,1-dimethylpropane HMDB0245328
0.623_155 N-Methylacetamide C01210
0.625_418 4-[1,1-Dioxo-3-(2-hydroxyethyl)amino]pyridine-2-thione HMDB0257894
0.626_355 Diphosphoglucuronide HMDB0251462
0.627_308 D-Ribulose 1,5-bisphosphate C00345 HMDB0244230
0.629_276 6-Phosphocreatine C00345 HMDB0001316
0.63_190. Azaserine
0.63_274. 1-Phosphocreatine C04037
0.631_210 Galactaric acid C00879 HMDB0000639
0.632_326 Sophoracoumestan B
0.635_220 (-)-threosulfoxide C16597
0.636_206 Glucose ketone HMDB0252777
0.636_236 3,6,7,8-Tetrahydro-2H-pyridin-2-one C21321
0.637_198 Serotonin C00780 HMDB0000259
0.637_342 Ranelic acid HMDB0257107
0.637_410 LMPRO103010027
0.638_115 Thiosulfate HMDB0000257
0.638_135 Sulfoacetic acid HMDB0258590
0.643_387 2-Amino-5-[1-carboxy-2-hydroxyethyl]pyridine-3-carboxamide HMDB0257661
0.643_97. Sulfate HMDB0001448
0.644_155 3-Sulfinoyl-L-alanine HMDB0000996
0.645_222 Radon-222 C16454
0.646_225 2,5-Dichloro-4-oxohex-2-enedioate
0.647_441 Prepacifen C17127
0.648_522 [(2S,3R,4R,5R)-5-(2,3-dichloro-4-oxohex-2-en-1-ylideneamino)pyridin-2-ylideneamino]pyridine-2-carboxamide HMDB0247873
0.65_208. Garcinia acid
0.653_215 3-(Pyridin-2-ylideneamino)pyridine-2-carboxamide HMDB0247198
0.654_859 PC(0-18:0/24:0) HMDB0013423
0.657_121 Polysulfide C19692
0.657_242 5-Phosphocreatine C03366
0.658_234 Benzo[b]furan C20124
0.658_250 Blue pigment C16152
0.66_354. THIODICARB HMDB0259010
0.66_388. Ixoside
0.661_174 cis-Aconitic acid HMDB0000072
0.661_252 3,3'-Dichlorobenzidine HMDB0245999

0.663_177 Pyrophosphate HMDB0000250
0.663_897 PI-Cer(t18:0/22:0(2OH))
0.664_212 beta-(2-Methoxyphenyl)acetic acid HMDB0060557
0.665_231 Benzenesulfonamide HMDB0244954
0.666_220 Glycine glutamate HMDB0252864
0.667_132 Ethylmalonic acid HMDB0000622
0.667_174 Shikimic acid HMDB0003070
0.668_223 N-(2-Methylacryloyl)glycine HMDB0244546
0.668_334 sn-Glycerol 3-phosphate HMDB01225
0.669_203 Lipoamide
0.67_157. (2S)-1,2-Dimethyl-3-oxopropylamine HMDB0257875
0.67_209. 3-thiodimethylarsenopropanoic acid
0.67_247. Doranidazole HMDB0251588
0.67_274. 1-Deoxy-1,2-dioxane-5-carboxamide HMDB0251588
0.671_86. Succinaldehyde HMDB0258537
0.673_189 N-ACETYLGLUTAMATE
0.675_169 Phosphodichloridate HMDB013482
0.675_252 S-(4-Methylphenyl)isothiourea HMDB017242
0.675_264 Benzamide, N-(3R)- HMDB0256659
0.677_222 L-Cystathionine HMDB0000099
0.679_104 Malonic acid HMDB0000691
0.679_120 (2-Hydroxyethoxy)ethylamine HMDB0242471
0.679_121 Tromethamine HMDB007182
0.679_162 Glycerol pyruvate HMDB0252845
0.679_233 Limazocin HMDB0254094
0.68_196. Galactonic acid HMDB0000565
0.682_80. HS03-; H2C11481
0.683_123 Ethyl hydrogen sulfide HMDB0031233
0.683_161 Amino adipic acid HMDB0000510
0.683_198 4-Chloro-7-nitrobenzamide HMDB0246389
0.683_216 2-C-Methyl-2-oxo-1,3-dioxane-5-carboxamide HMDB011434
0.683_244 CGP 52608 HMDB015629
0.684_188 Asparagine butyl ester
0.685_203 Adipoylglycine HMDB0240731
0.686_232 Thr-Leu HMDB0259044
0.687_216 8-Hydroxy-2-deoxy-D-ribose-5-phosphate HMDB017359
0.689_226 Aminopyrrolidine HMDB021109
0.69_252. Orellanin HMDB019959
0.692_186 2-Amino-2-(5-methyl-2-oxopropyl)propanoic acid HMDB0257684
0.692_244 4-Amino-1-(6-aminocyclohex-1-en-1-yl)butane-1,3-dione HMDB0257570
0.693_280 Tos-Ph-CF3 HMDB01964
0.693_324 skimmianin HMDB0258334
0.694_204 2-(2-Oxopropionyl)glycine HMDB0258031
0.696_81. Phosphonic acid HMDB006701
0.697_100 Gyromitrin
0.697_175 (S)-Dimethyl 2-aminopropanoate HMDB0243725
0.697_309 Fluxofenine HMDB018735
0.698_228 Resveratrol HMDB0003747
0.699_123 phosphonoacetaldehyde HMDB0256485
0.699_193 N-Methylglucosamine HMDB0255188
0.699_223 2,2,2-Trifluoro-N-methylacetamide HMDB0254358

0.699_271Rubiadin C10402 HMDB0257354
 0.699_396Fosbretabulin HMDB0252462
 0.701_129(S)-PiperC19782
 0.701_270sorbitol lactate HMDB0258395
 0.702_190Carglumic acid HMDB0015673
 0.702_215sn-GlycerC01233
 0.702_241Pentafluorobenzyl HMDB0256263
 0.702_274N2-SuccirC03296
 0.702_478apiosylskimmin
 0.703_108Furofuran HMDB0252543
 0.704_2708-Quinolinol, 5,7- HMDB0256151
 0.706_282Etoprine HMDB0252116
 0.707_119N,N-Dimethylforman HMDB0255265
 0.707_158Oxiracetam HMDB0255986
 0.707_2052-Acetamido-2,6-di HMDB0259683
 0.707_83.Oxazine HMDB0255970
 0.708_230ThiaburinC11800
 0.708_2585,6,7-Trimethoxycoumarin
 0.708_2723-(2,6-dihydroxyphenyl)-4-hydroxy-6-methyl-3H-2-benzofuran-1-one
 0.71_545.Perfluorooctyl ioc HMDB0256330
 0.711_309Pentafluoropropior HMDB0256269
 0.711_366Kaempferol 3-sulfate HMDB0240539
 0.712_2783-HydroxyC21322
 0.712_87.Vinyl carbamate HMDB0259822
 0.713_176(2S)-2-Amino-3-[(2S)-2-amino-3-oxopropanoate]propanoate HMDB0257605
 0.713_182GalactiticC01697 HMDB0000107
 0.713_73.IminoglycC15809
 0.714_1484-MethylC01180
 0.714_1601-Benzothiepin HMDB0243832
 0.716_317Mitotane HMDB0014786
 0.717_333Costatol;C17103
 0.718_140(1R)-1-Amino-2-sulfamoylpropane-1,2-diol HMDB0242353
 0.719_231Ala-Ala-Ala HMDB0248092
 0.724_235(2R,3R,4R,5R)-2-Amino-3,4-dihydroxybutanoic acid HMDB0255309
 0.727_134mercaptohexanol HMDB0254465
 0.73_243.2-Propylthiazolo[4,5-c]pyridine-5-thione HMDB0245307
 0.73_268.N-Acetylcarnosine HMDB0255058
 0.731_403[(2S,3R,4R,5R)-5-(2S)-2-amino-3-oxopropanoate]propanoate HMDB0257860
 0.732_283Procymidone HMDB0256790
 0.733_2411-(10H-Phenothiazin-10-ylidene)propane-1,2-diol HMDB0244969
 0.733_2652-Hydroxysaclofen HMDB0245169
 0.734_2154-Phosphoric acid HMDB0243082
 0.735_131DL-Norleucine HMDB0251526
 0.736_170N-Nitrosocysteine C19482
 0.736_265(3S,4R,5R)-1,3,4,5-tetrahydro-2H-pyridin-2-one HMDB0243864
 0.736_277(2R,3S,5R)-5-(4,5-dihydro-2H-pyridin-2-yl)propane-2-thione HMDB0257763
 0.737_231TRIAZIQUONE HMDB0259153
 0.737_436PahutoxirC16889
 0.738_2483-(3-(Pyridin-3-yl)propanoate)propanoate HMDB0247644
 0.738_284Articaine HMDB0248628
 0.738_352Penicilloic acid HMDB0060617

0. 739_300 Coronene; C19375
0. 739_384 1-(4-Methylsulfor HMDB0257537
0. 74_246. (2S)-2-(Carboxymet HMDB0260137
0. 74_310. Croconazoc C11096
0. 74_366. Pomaglumetad methi HMDB0256693
0. 741_298 Benzoyl glucuronic HMDB0010324
0. 742_229 5-(L-alanin-3-yl)-2-hydroxy-cis, cis-muconate 6-semialdehyde
0. 743_221 beta-N-Acetylglucoc HMDB0000803
0. 744_258 benzyl styryl sulfi HMDB0249076
0. 744_309 Aceneuramic acid HMDB0259583
0. 744_467 (2S)-2-[[5-[2-[(6 HMDB0248055
0. 745_214 fluorobenzoylpropio HMDB0060951
0. 745_324 Portulacæ C08564
0. 745_327 1-Butyl-3-(1-naphth HMDB0245597
0. 745_366 Acetamide, 2-((2-H HMDB0259959
0. 746_248 Garomefrine HMDB0255774
0. 747_160 3-Methyladipic aci HMDB0000555
0. 747_198 Methylglucamine HMDB0254645
0. 747_238 (2S)-2-[(2-Carboxy HMDB0257920
0. 747_276 D-gamma-Glutamyl-L HMDB0250751
0. 747_308 Penilloic acid HMDB0256237
0. 747_348 Rabeprazole thioet HMDB0244427
0. 747_92. Glycerol HMDB0000131
0. 748_191 N-Isobutyryl-L-cys HMDB0255162
0. 748_218 Ecgonine Ethyl Est HMDB0251685
0. 748_254 Pimonidazole HMDB0256554
0. 748_267 Miserotoxin HMDB0254754
0. 748_426 Cysteine-glutathic HMDB0250707
0. 748_488 Baloxavir HMDB0248854
0. 749_111 Imexon HMDB0253411
0. 749_190 (2R, 6S)-2, 6-Diamir HMDB0242532
0. 749_229 Ergothioneine HMDB0003045
0. 749_384 UVA-1 HMDB0259732
0. 75_101. N, N-Dimethylbutylæ HMDB0255261
0. 75_172. Glycyl-D-proline HMDB0252876
0. 75_177. Anthoplex C16994
0. 75_245. (R)-2-(4-(Tert-but HMDB0247375
0. 751_127 4-Aminohex-5-ynoic HMDB0252607
0. 751_138 Thiazolidine-4-car HMDB0258979
0. 751_148 Isobutyryl glycine HMDB0000730
0. 751_178 beta-D-galactosyl HMDB0249118
0. 751_198 S-(2-Carboxyethyl) HMDB0246645
0. 751_204 [(2S)-6-Amino-1-me HMDB0258077
0. 751_218 (+/-)-(E)-Ethyl-2- HMDB0242267
0. 751_216 [(2S, 3R)-2-Amino- HMDB0257877
0. 751_237 (E)-5-hydroxy-N-[3-[5-[3-[[(E)-5-hydroxy-3-methylpent-2-enoyl] amino] prop
0. 751_328 Cytosine arabinosæ HMDB0243501
0. 751_368 Florbenazine HMDB0252313
0. 752_130 (3R, 4R)-3-Amino-1- HMDB0243603
0. 752_144 ISOVALERYLUREA HMDB0253706
0. 752_188 3h-Adrenaline HMDB0246263

0.752_188 gamma-Glutamylacet HMDB0252618
0.752_188 tetrahydroxybutyli HMDB0258912
0.752_229 2,4-Bis(2-methoxye HMDB0245444
0.752_240 Pirbuterol HMDB0015407
0.752_247 3-Hydroxybutyrylca HMDB0013127
0.752_524 Fedratinib HMDB0247668
0.753_220 1,2-O-Isopropylide HMDB0242729
0.753_232 gamma-Aminobutyric HMDB0252609
0.753_242 3-(3-Methylbut-2-ε HMDB0248907
0.753_244 Butanoyl (2S)-2-an HMDB0257690
0.753_245 4-(E)-Ethyl-2-(E) HMDB0255716
0.753_263 5-Amino-2-[2-amir HMDB0260425
0.754_118 Divinyl sulfone HMDB0251500
0.754_147 2H-Pyran-2-one, tε HMDB0244840
0.754_151 (S)-2-Amino-4-metf HMDB0249989
0.754_151 N-Phenylglycine HMDB0255227
0.754_187 (3R)-3-Hydroxy-N-[HMDB0243607
0.754_197 Tauropine C01616
0.754_228 Pro-leu HMDB0253028
0.754_244 Biotin C00120 HMDB0000030
0.754_251 [(2R,3S,4R,5R)-3,4 HMDB0257777
0.754_266 tubercidin HMDB0259318
0.754_267 Neuraminic acid HMDB0000830
0.754_2810 (6)-Methyl-2'-dec HMDB0255876
0.754_282 Hydroxy-lacosamide HMDB0061146
0.755_134 Pyrazolopyrimidin HMDB0256955
0.755_217 2-(2-Aminopropanyl HMDB0248109
0.755_218 gamma-L-(C03738
0.755_269 (2S)-1-[2-[[(2S)-F HMDB0260136
0.755_272 6,7-DichlC21868
0.755_273 Norgalanthamine HMDB0255738
0.755_275 epsilon-(gamma-Glu HMDB0257624
0.756_179 Fusaric acid HMDB0252556
0.756_260 Biotin sulfoxide HMDB0249229
0.757_116 2-Thiohydantoin HMDB0245322
0.757_189 H-D-Asp(OtBu)-OH HMDB0253009
0.757_207 1-(2-Hydroxyethyl) HMDB0243780
0.757_212 Butethal HMDB0015442
0.758_238 Tyr-Gly HMDB0259337
0.759_249 1-Deoxy-1-morpholi HMDB0243858
0.759_352 4-[2-(5-(C18349
0.759_404 1,2-Diphenyl-4-(2' HMDB0248909
0.76_137. serine thiol HMDB0258249
0.76_291. Glutamine-glutama HMDB0252813
0.761_192 DihydrorflC21888
0.762_10 Pent-2-enoic acid HMDB0256282
0.762_268 HistidinyL-Leucine HMDB0253179
0.763_71. 1-Ethylaziridine HMDB0243874
0.764_207 LigusticiC16987 HMDB0302720
0.764_210 d-Glycero-d-galact HMDB0253107
0.765_216 N-a-Acetyl-L-argir HMDB0004620

0.766_414N-desalkyl delavir HMDB0061021
0.766_78.mercapto-ethanol HMDB0254463
0.768_218Ser-Leu HMDB0258242
0.769_141Aminoethanol phosph HMDB0248314
0.77_427.ADP HMDB0001341
0.771_214Sulfaguanidine HMDB0258573
0.772_199Ecgonine methyl ester HMDB0006406
0.772_2001-(2-Hydroxyethoxy) HMDB0247200
0.774_238Keto-3-deoxy-D-mari HMDB0244292
0.775_1444-Ethoxy-4-oxobut- HMDB0246416
0.775_178Benzo[b]thiophene- HMDB0249004
0.776_172Glycylproline HMDB0000721
0.777_1383-Nitroaniline HMDB0245944
0.779_1342,3-Dihydroxypropy HMDB0243948
0.78_118.Benzofurc14512
0.78_352.4,4'-Dihydroxytetri HMDB0244814
0.782_148D-Digitoxose HMDB0251279
0.784_354(4R,6S)-6-[(E)-2- HMDB0250011
0.787_108Thiomorpholine HMDB0259017
0.793_121N-Methyl-o-toluidi HMDB0255183
0.795_1871-(2-Hydroxyethyl) HMDB0246690
0.797_2612-Hydroxyisovalery HMDB0240421
0.799_247N-SuccinyC05931
0.799_308Convicine HMDB0250445
0.804_138Dapansutrile HMDB0250857
0.804_3317-Chloro-N-[3-(2-r HMDB0247240
0.809_161Alanine glyoxylate HMDB0248103
0.812_266Chlorfenethol HMDB0250094
0.813_301Benoxaprofen HMDB0248956
0.822_260Proline glutamate HMDB0256798
0.823_278Dimethenamid HMDB0251377
0.825_292Ethylenediaminetet HMDB0257824
0.829_259Glycerophosphoseri HMDB0252850
0.83_409.methionine aspartc HMDB0254530
0.832_2402,6-dihydroxyanthraquinone
0.832_249S-Acetyldihydrolipoamide-E
0.832_278(2R,3S)-Piscidic c HMDB0030809
0.832_317N-GlycolyC04336
0.833_177Alanine lactate HMDB0248104
0.834_158Cysteine sulfinic HMDB0250705
0.834_188DL-Homocysteic aci HMDB0251520
0.836_1384-Aminoacetophenor HMDB0246623
0.836_207DihydroliC00579
0.836_330NS 1608; C13835
0.836_3312'-Deoxyadenosine HMDB0245534
0.836_542HypericirC07606 HMDB0034271
0.837_2378-Amino-c21333
0.837_3342-(alpha-C10517
0.837_418N-(3-(5-Chloro-1H- HMDB0256648
0.843_2745-epi-ValC21204
0.845_2082,6-DimetC10331 HMDB0029673

0.847_2112-[Carbamimidoyl (r HMDB0257852
0.849_2243-Amino-5-(3-thiof HMDB0257535
0.85_302. Quercetin C00389 HMDB0005794
0.851_1912-Amino-εC21247
0.853_18ε2-Aminobicyclo[3.1 HMDB0244794
0.855_237Drazoxolc C18929
0.857_27ε5-epi-ValC17693
0.859_50εmyricitrin
0.86_108. Quinone C00472 HMDB0003364
0.86_137. TrigonellC01004 HMDB0000875
0.86_169. (1-Hydroxy-3-oxopi HMDB0242284
0.86_246. Haematommic Acid, Ethyl Ester
0.861_29C Sultiamε HMDB0258622
0.865_31ε5, 9:7, 10a-Dimethar HMDB0246673
0.866_23ε (4R)-3-((2S)-3-Mer HMDB0259957
0.867_17εGlycerophosphoric HMDB0252849
0.869_23εSulbactam HMDB0258566
0.872_23C [(3R)-3, 4, 5-Trihyc HMDB0260227
0.874_20εLipoamideC00248
0.876_28εFosthiazεC18402
0.877_29εPanfuran C19289
0.879_201Creatinine lactate HMDB0250531
0.88_227. triclofos HMDB0259185
0.88_267. Guanidine, (4-chlc HMDB0244397
0.881_23C N1-AcetylC20921
0.881_301 (5-Acetamido-3, 4, ε HMDB0252741
0.883_24ε TETRAHYDROURIDINE HMDB0258911
0.885_29ε1-PyrenylC18269
0.887_20C Cysteine-S-sulfate HMDB0000731
0.89_299. FenbendazC21876
0.901_35ε Calmagite HMDB0249561
0.911_111Hydroxyme C06455
0.923_14ε3, 4-Dehyc C04445
0.928_1342-Carboxyoxypromar HMDB0257720
0.929_88. Ethylene carbonate HMDB0252067
0.93_98. (Moniliformin HMDB0254845
0.945_94. Dimethyl sulfone HMDB0004983
0.946_38εmonophospho-n-acet HMDB0254870
0.947_16εButanoic acid, 2, ε HMDB0243949
0.947_18εSecnidazole HMDB0258202
0.948_161Carboxybetaine HMDB0249655
0.953_1472-Methylthiazolidi HMDB0246657
0.965_264Phenyl 1-hydroxy-ε HMDB0256421
0.967_24ε4-Amino-5-hydroxy- HMDB0258026
0.972_12ε2, 3, 5-Hexanetrione HMDB0245435
0.978_25ε2-Amino-9-[4-hydr HMDB0244320
0.984_231N-Acetyl- C05539
1.001_221Chloridazon
1.017_79. Methanesulfinic ac HMDB0254519
1.018_14ε4-Oxogluc C05572
1.024_18εTobramycin, inactivated by phosphorylated 2''

1. 031_282 3-[[(2R)-2-AcetamiHMDB0247775
1. 038_71. Oxazoline HMDB0255973
1. 059_159 (2R, 4S)-PyrrolidirHMDB0242583
1. 083_258 (2R)-8-ethyl-7-hydroxy-5-methoxy-2-methyl-2, 3-dihydrochromen-4-one
1. 085_218 1, 4-ButanediphosphHMDB0244204
1. 088_238 3, 5-DihydroxybenzHMDB0240373
1. 089_239 Sulfanegen HMDB0258580
1. 089_248 ThionazirC19036
1. 089_281 4-Hydroxy-5-(2, 3, 4HMDB0260278
1. 109_668 beta-nicotinamide HMDB0249146
1. 115_272 Pyridine N-oxide HMDB0061177
1. 116_124 4-Methyl-1H-pyrrolHMDB0246501
1. 116_250 gamma-GlutamylcystHMDB0001049
1. 119_294 3, 4-Bis(carboxymetHMDB0258023
1. 119_297 Teroxirone HMDB0258835
1. 12_388. Repenol
1. 12_78. (pyridinyl HMDB0256969
1. 122_157 Benzenesulfonamide HMDB0248984
1. 124_249 Norepinephrine sulHMDB0002062
1. 124_568 dTDP-4-hyC21348
1. 124_578 dTDP-D-glcC06017
1. 134_261 HymexazolC11104
1. 136_200 AesculetiC09263 HMDB0030819
1. 152_136 Medina HMDB0254633
1. 152_136 2-HydroxyacetopherHMDB0245150
1. 161_218 Meprobamate HMDB0014515
1. 169_188 2-((3, 5-DihydroxyHMDB0244908
1. 169_218 L-Alanyl-C20957
1. 175_200 (3S, 8As)-7-hydroxyHMDB0253728
1. 183_312 1-SulfooxymethylpyHMDB0244010
1. 184_324 [(2S, 3R, 4R, 5R)-5-(HMDB0247871
1. 188_120 Oxazolo[5, 4-B]pyriHMDB0255974
1. 192_152 Mercaptopurine HMDB0015167
1. 197_246 2, 4-Bis(εC19972
1. 212_308 FenamiphcC18659
1. 235_207 S-(2-HydrC14876
1. 244_260 4-Thiouridine HMDB0246588
1. 248_179 S-CarboxyC03727 HMDB0029415
1. 251_109 Imidazooxazole HMDB0253423
1. 256_220 s-Nitroso-n-acetylHMDB0250051
1. 281_368 2-S-GlutεC14862
1. 289_378 DIMBOA-Glc HMDB0029710
1. 291_128 Methylendiglyoxal HMDB0254631
1. 291_192 Isocitric acid HMDB0000193
1. 292_156 cis-Aconitic anhyHMDB0250284
1. 317_289 Tabtoxin;C20917
1. 317_504 J Acid urea HMDB0244554
1. 32_189. Citramide HMDB0250304
1. 327_278 CardiospeC08328
1. 328_258 2-methoxy-5-methyl-3-(2-methylbut-3-en-2-yl)chromen-4-one
1. 33_267. Piridronic acid HMDB0256596

1.331_357 Florfenicol HMDB0252314
1.336_258 Pelubiprofen HMDB0256212
1.341_219 O-Succinyl C01118
1.342_88. N-Nitrosomethylethylamine (NMEA)
1.343_290 Glutamic acid glut HMDB0252808
1.356_232 Kinetin C08272 HMDB0012245
1.36_181. Thiocyclam HMDB0259009
1.361_187 (1R, 4R, 5S, 6R)-4-Amino-2,3,4,5-tetrahydro-1H-2,3,4-triazole HMDB0242337
1.364_339 Glutathione thiol HMDB0252822
1.371_378 Fluprednisolone HMDB0252404
1.372_283 N2-Acetyl C12987
1.374_258 Ethoxzolamide HMDB0014456
1.379_334 Aramite; C19019
1.382_204 Diethyl C04586
1.384_342 Thiophanate-methyl HMDB0259025
1.385_181 Pyridostigmine HMDB0014685
1.405_370 Conopodopiepicrin
1.41_463. Pivampicillin HMDB0015542
1.412_143 N-Ethylmaleamic acid HMDB0255136
1.421_263 Alanine lactate py HMDB0248105
1.426_266 1-(3-Chlorophenyl) HMDB0260231
1.455_414 Chlorimur C10943
1.457_100 Succinic C19524
1.508_199 3-(2-Hydroxyethyl) HMDB0245773
1.582_306 2-Protocæ C04524
1.583_346 4-Fluoro-1-[2-[(4-Hydroxyphenyl)amino]ethyl]piperazine HMDB0258003
1.59_127. Penem HMDB0256222
1.631_304 (5S)-5-hydroxy-1,7-diphenylheptan-3-one
1.638_278 Fluorescamine HMDB0252357
1.641_536 Mecapregfilgrastim HMDB0254391
1.642_240 Dinoterb; C18671
1.643_268 8,9-Dihydro-8-(1H-imidazol-2-yl)octan-3-one HMDB0244406
1.644_304 IPSP; C19000
1.645_389 Cyclothiazide HMDB0014744
1.646_572 genipin 1-gentiobioside HMDB0252678
1.647_739 Batefenterol HMDB0248878
1.667_304 9-(Formylloxymethyl)octan-3-one HMDB0258038
1.723_305 Sealdin HMDB0258197
1.766_173 L-Proline, 1-acetyl HMDB0253913
1.79_369. Thioflosulide HMDB0259011
1.798_190 Allo-hydroxycitric acid HMDB0259498
1.831_185 Diethyldithiophosphoric acid HMDB0061736
1.847_162 1,5,6-Trihydroxyheptan-2-one HMDB0255346
1.852_321 Diclofensine HMDB0251206
1.853_129 Epigoitrin HMDB0251849
1.876_363 [(2R, 5R)-5-(2-Aminoethyl)-2,3,4,5-tetrahydro-1H-imidazole] HMDB0257693
1.891_188 alpha-Acetyllysine HMDB0247927
1.905_152 N1-Methyl-2-pyridone HMDB0004193
1.971_88. tetrahydrothiophene HMDB0258909
10_574. 4,8-Diethyl-10,12,14,16-tetrazadecalin [iso2]
10.001_27 ent-kaurane HMDB0251824

10.001_5E DG (16:1 (9Z)/14:1 (9Z)) HMDB0007125
10.004_3E alpha-N-(3-hydroxyhexadecanoyl)-L-ornithine
10.004_5E Octaethyleneglycol HMDB0246126
10.005_6E N-(3-(hexadecanoyloxy)-heptadecanoyl)-L-ornithine
10.009_3C (4-oxido-2,3,5,6,7,8-hexahydro-1H-pyrrolizin-4-ium-1-yl)methyl 2,3-dihydro-11Z-octacosenoic acid
10.013_5I 15-nonacosylresorcinol
10.02_39I N-stearoyl taurine
10.021_7E PC (0-20:0/18:3 (9Z)) HMDB0013440
10.022_3C Nerisopam HMDB0255544
10.023_4C Adunctin A
10.024_6C LysoPI (0:0/18:0) HMDB0061704
10.029_4E Octillool HMDB0255888
10.029_6E Cer (t18:1 (6OH)/23:0 (2OH))
10.032_3E [(8R,9S,13S,14S,17S)] HMDB0257965
10.033_2E 2-Octadecanone, 3- HMDB0245276
10.033_3E 2-Hydroxy-22-methyltetracosanoic acid
10.033_7E LMGL05020003
10.034_34 20-oxo-heneicosanoic acid
10.034_4E (E)-8-(2-(4-(Diphenylamino)phenyl)butyl)octadecanoic acid HMDB0259910
10.042_5E 1-(2-methoxy-6Z-heptadecenyl)-sn-glycero-3-phosphoserine
10.043_4E Eicosopentanoic acid HMDB0251724
10.045_5I PG (18:0/0:0)
10.046_4E Norselic acid D
10.052_57 Cer (d14:2 (4E,6E)/22:1 (13Z) (2OH))
10.053_5E Milbemycin beta2 HMDB0254728
10.057_5E 1-O-Palmitoyl-2-O-Phosphatidylcholine HMDB0251102
10.058_5E PE (22:1 (13Z)/0:0)
10.059_4C Cholestane-2,3-diol HMDB0250163
10.06_49E Cer (d15:1/16:0)
10.061_6E Concanamycin HMDB0250429
10.066_5E FAHFA (18:1 (9Z)/3-0-18:0)
10.067_3E (Z)-3-(1,2-Dihydroxy-3-oxo-1-phenylethyl)propanoic acid HMDB0255948
10.076_6C Cer (d18:2 (4E,8Z)/20:0 (2OH[R]))
10.077_3E N-(4-Fluorophenyl)acetamide HMDB0244857
10.084_5E Cer (d18:1 (4E)/15:0 (2OH))
10.086_77 Distearoyl phosphatidylcholine HMDB0251484
10.087_5E (2-Acetyloxy-3-oxo-1-phenylethyl)propanoic acid HMDB0242460
10.091_37 Docosatetraenylethanolamine HMDB0251564
10.094_3E Piperonyl sulfoxide HMDB0258607
10.096_3E 2-hydroxy behenic acid
10.097_47 30-methyl-, 21Z-hentriaconten-31-olactone
10.11_484 Lanoceric acid
10.111_77 PG (18:0/18:1 (11Z)) HMDB0010603
10.113_5E PG (20:1 (11Z)/0:0)
10.114_9C (3'-sulfo)Galbeta-Cer (d18:1/24:1 (15Z) (2OH))
10.116_44 MG (0:0/24:1 (15Z)) HMDB0011559
10.116_57 LysoPC (22:1 (13Z)) HMDB0010399
10.117_3E Docosapentaenoic acid HMDB0006528
10.117_5I 1,2-DimyrC16667
10.117_6E OHHdiA-PE

10.118_4Iridal HMDB0253581
10.118_5Cer(d18:2/15:0)
10.118_71,2-Dioleoyl-sn-g1HMDB0244089
10.119_57Cer(d18:2/18:0(20H))
10.119_6PA(20:0/15:1(9Z))
10.12_50FAHFA(16:1(9Z)/9-0-16:0)
10.121_5232,35-anhydrobacteriohopan-11-ene-tetrol
10.124_41Mycolipanic acid (C26)
10.124_4LysoPC(16:1(9Z)/0:HMDB0010383
10.124_72PE(0-16:0/20:5(5Z,8Z,11Z,14Z,17Z))
10.125_74PE(18:3(6Z,9Z,12Z)/18:0)
10.125_77PE(0-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
10.127_52DG(12:0/17:1(9Z)/0:0)[iso2]
10.133_42Semiplenamide D
10.139_32Lesquerolic acid
10.15_25(-)-SolerC16782
10.151_41Type III cyanolipid 22:0 ester
10.154_43alpha,7alpha-Dih, HMDB0000359
10.157_4Cocr#28
10.163_4Mycocerosic acid (C29)
10.165_54Norgarmultinone B
10.166_4ErucylphosphocholiHMDB0251925
10.169_372-hydroxy-tricosanoic acid
10.173_4PA(19:0/0:0)
10.173_5Xymarginatin
10.176_3N-myristoyl glutamine
10.177_61C-ToxiferC09246
10.181_42CPA(18:0)
10.184_51FAHFA(16:0/8-0-16:0)
10.188_28Nonadecanal
10.188_34Selachyl alcohol HMDB0258210
10.188_383-(6-(DimethylamirHMDB0244848
10.189_3818Z-Heptacosen-10-one
10.19_51Cer(t15:0/16:0)
10.191_29TridemorfC11285
10.193_4Tridecyl palmitoleate
10.194_4Lignoceric acid benzyl ester
10.195_4(S)-25-Hydroxy-14,16-hentriacontanedione
10.195_5Cer(t26:1(8E)/10:0(20H[R]))
10.197_5Cer(t18:1(60H)/17:0(20H))
10.203_4N(4)-Oleylcytosine HMDB0255284
10.209_8CP(16:0/22:6(4Z,7Z)HMDB0012362
10.215_5DG(14:0/18:1(11Z)/HMDB0007014
10.225_3Arterolane HMDB0248627
10.225_52Cer(d18:1/15:0)
10.231_163,4-MethylenedioxyHMDB0032613
10.232_5232,35-anhydrobacteriohopaneterol
10.237_52FAHFA(15:0/15-0-18:0)
10.239_44(1R,3S,5E)-5-[(2E)HMDB0260074
10.239_5(11-Oxoceromelissic acid
10.24_36(5beta-Cholanic aciHMDB0247018

10.24_55FAHFA(18:2/15-0-18:2)
10.241_44(2R,3S,4R,5R)-5-(2,4-dioxypyrimidin-1-yl)-4-hydroxy-2-(hydroxymethyl)oxo
10.242_38N-palmitoleyl glutamine
10.244_6DG(19:1(9Z)/16:1(9Z)/0:0)[iso2]
10.246_362-oxo-tricosanoic acid
10.246_38Erucicoyl-EA
10.246_67DG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/0:0)[iso2]
10.249_34Betyl alcohol HMDB0248884
10.256_341,2-Ethandiol morHMDB0252073
10.259_68Teasterone 3-myristate
10.261_397-oxo-cholestenone
10.265_44Alnespirone HMDB0248173
10.265_6C Squafosacin C
10.267_56Tenofovir exalide, HMDB0250380
10.268_55DG(13:0/18:1(9Z)/0:0)[iso2]
10.269_4828-methyl-29-nonacosanolactone
10.273_42Mycolipanic acid (C27)
10.276_42Bourgeanic acid
10.277_61DG(14:0/22:5(4Z,7Z)HMDB0007032
10.278_68DG(19:1(9Z)/22:3(10Z,13Z,16Z)/0:0)[iso2]
10.284_68Lysine-containing siolipin
10.285_53FAHFA(16:0/6-0-18:0)
10.286_36Flugestone HMDB0252333
10.286_64OHODA-PA
10.289_62PG(13:0/12:0)
10.289_88PI(16:0/20:4(5Z,8Z)HMDB0009789
10.296_38Docosa-2,4,6,8-tetHMDB0251563
10.296_58Cer(d18:1(4E)/18:0(3OH))
10.31_2679-Octadecen-1-ami HMDB0244390
10.315_38MG(20:0/0:0/0:0)[rac]
10.316_4217-Estradiol cyclcHMDB0247180
10.329_81PS(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
10.344_411-(cis-13-DocosencHMDB0254855
10.349_3825-Azacholesterol
10.364_57LysoPC(22:0/0:0) HMDB0010398
10.371_58DG(12:0/19:0/0:0)[iso2]
10.381_5133-methyl-24Z-tetratriaconten-34-olactone
10.39_608LysoPC(24:1(15Z)/C)HMDB0010406
10.399_48Dehydrotumulosic εHMDB0250960
10.401_44MessageniC08631
10.419_4311-keto-Octacosanoic acid
10.42_6161-(9,14-dimethyl-pentadecanoyl)-2-(8-[1]-ladderane-octanyl)-sn-glycerol
10.421_77PS(P-20:0/16:0)
10.424_57Annopurpuricin E
10.441_88PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:4(7Z,10Z,13Z,16Z))
10.45_524FAHFA(15:0/11-0-18:0)
10.451_56Cer(d18:1(4E)/17:0(3OH))
10.453_4427-Hydroxyoctacosanoic acid
10.454_68PG(15:0/12:0)
10.46_48C Cetyl palmitate HMDB0249838
10.495_77PS(P-18:0/18:1(9Z))

10.5_530. Epoxymuric08484
10.507_405Alpha-Cholestan-3Beta-01-6-One
10.507_42Valactamide E putative
10.514_52Cer(m18:0/16:0)
10.515_4723Z-dotriacontenoic acid
10.523_591-(2-methoxy-18Z-pentacosenyl)-sn-glycero-3-phosphoethanolamine
10.526_86(3'-sulfo)Galbeta-Cer(d18:1/22:0)
10.527_77PG(16:0/20:4(5Z, 8Z)HMDB0010580
10.535_5334-methyl-25Z-pentatriaconten-35-olactone
10.536_38Behenoyl-EA
10.539_56DG(18:0/14:0/0:0) HMDB0007153
10.562_63Cer(d16:2(4E, 6E)/24:0(20H))
10.566_40Nervonoyl-EA
10.577_88(3'-sulfo)Galbeta-Cer(d18:1/24:1(15Z))
10.578_72PE(0-16:0/20:2(11Z, 14Z))
10.581_43Diglyceryl monooleinHMDB0251281
10.6_494. tritriacontanoic acidHMDB0259286
10.6_823. (3'-sulfo)Galbeta-Cer(d18:1/18:0(20H))
10.614_38Cholest-5-EN-3-oneHMDB0246773
10.617_421-Hydroxyvitamin I HMDB0243905
10.617_46Dehydroeburicoic acidHMDB0250950
10.624_79PS(P-18:0/20:4(5Z, 8Z, 11Z, 14Z))
10.637_40Cetylmannoside HMDB0249840
10.642_52Cetyl recinoleate HMDB0249839
10.644_53FAHFA(18:0/13-0-16:0)
10.65_4141-0-(2R-hydroxy-4Z-docosenyl)-sn-glycerol
10.65_49231-methyl-32-dotriacontalactone
10.678_59CoixenolideC17566
10.7_623. Cer(d18:1(4E)/21:0(30H))
10.701_60LysoPC(24:0/0:0) HMDB0010405
10.712_414, 7beta-Dimethyl-4HMDB0244713
10.714_39(8S, 9S, 10R, 13R, 14S)HMDB0260186
10.721_83PS(22:6(4Z, 7Z, 10Z, HMDB0012444
10.732_63LysoPC(26:1(5Z)/0:HMDB0029220
10.742_58LMGLO2030026
10.757_67SM(d18:1/14:0) HMDB0012097
10.768_67DimyristoylphosphatidylcholineHMDB0244821
10.773_63Cer(d18:1/23:0) HMDB0000950
10.775_66Cer(d18:2/24:0(20H))
10.801_4630-hydroxy-triacontanoic acid
10.802_83PE(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
10.805_73PE(14:0/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
10.806_70PG(18:3(6Z, 9Z, 12Z)/13:0)
10.807_68PG(14:0/15:0)
10.82_609Cer(t18:1(60H)/20:0)
10.821_70PE(16:0/16:0(9Cp))
10.823_70PE-Cer(d16:2(4E, 6E)/21:0)
10.845_52octadecyl heptadecanoate
10.86_753PC(14:1(9Z)/20:3(9Z)HMDB0007914
10.86_761PE(16:1(9Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
10.879_81PE(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/20:4(5Z, 8Z, 11Z, 14Z))

10.887_50 Cer (d18:1/14:0) HMDB0011773
10.902_72 PC (18:2 (9Z, 12Z) / 14:0) HMDB0008130
10.906_54 LMFA07011175
10.915_77 PC (20:4 (8Z, 11Z, 14Z) HMDB0008463
10.937_41 Lignoceroyl-EA
10.937_73 PE (16:0/20:5 (5Z, 8Z, 11Z, 14Z, 17Z))
10.948_60 Cer (d16:1/23:0) HMDB0249814
10.95_53 2-Hexadec-7-enylol HMDB0255384
10.962_52 Cer (d16:2 (4E, 6E) / 18:0)
10.963_78 PE (18:2 (9Z, 12Z) / 22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
10.978_69 1,2-Dipalmitoyl-r- HMDB0246972
11.008_78 PS (18:2 (9Z, 12Z) / 18:0) HMDB0012400
11.029_74 GlcAbeta-Cer (d18:1/18:0)
11.03_46 Cholesterol sulfat HMDB0000653
11.034_56 FAHFA (15:0/21:0-21:0)
11.041_81 PE (22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z) / 20:1 (11Z))
11.071_69 GalCer (d18:1/16:0)
11.118_81 PS (20:4 (5Z, 8Z, 11Z, 14Z) HMDB0012433
11.123_41 Corbisterol
11.129_78 PC (18:3 (6Z, 9Z, 12Z) HMDB0008166
11.136_72 GlcCer (d16:2 (4E, 6E) / 20:0)
11.153_83 PS (22:6 (4Z, 7Z, 10Z, 13Z) HMDB0012445
11.154_74 LMGPO2080008
11.179_43 (-)-alpha-Tocopherol HMDB0242201
11.209_38 [(3S, 8R, 9S, 10R, 13S) HMDB0257762
11.209_80 PC (22:6 (4Z, 7Z, 10Z, 13Z) HMDB0008725
11.21_70 PC (15:0/15:0) HMDB0007934
11.224_83 PE (22:4 (7Z, 10Z, 13Z, 16Z) / 22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
11.242_76 PE (P-16:0/22:6 (4Z, 7Z, 10Z, 12E, 16Z, 19Z) (140H))
11.243_78 2-[5-[2-[2-[5-[2-[2-[5-[2-[2-[5-(2-hydroxybutyl)oxolan-2-yl]propanoyloxy
11.271_73 PC (16:0/16:1 (9Z)) HMDB0007969
11.278_39 17-(3-Pyridyl)-5,11 HMDB0244761
11.278_72 SM (d18:1/18:1 (9Z)) HMDB0012101
11.29_78 PE (18:1 (9Z) / 22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
11.29_81 Fulvyne D
11.299_68 PE (12:0/20:1 (11Z))
11.315_78 PC (20:4 (5Z, 8Z, 11Z, 14Z) HMDB0008429
11.315_80 1-(7Z-Hexadecenoyl) HMDB0260236
11.347_73 PE (18:4 (6Z, 9Z, 12Z, 15Z) / 18:0)
11.389_80 PC (22:5 (7Z, 10Z, 13Z) HMDB0008692
11.399_74 Termitomycesphin E
11.402_60 Cer (d16:0/23:0)
11.404_78 LMGPO6030030
11.408_40 4-Methylcholest-7- HMDB0246507
11.408_58 Gondoyl-linoleate
11.408_75 Soybean lecithin HMDB0258399
11.409_36 (5Z, 7E)-9,10-Seco- HMDB0245858
11.409_76 PE (18:3 (6Z, 9Z, 12Z) / 20:2 (11Z, 14Z))
11.409_81 PE (20:2 (11Z, 14Z) / 22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
11.413_38 Epicholesterol HMDB0251842
11.417_71 PE (16:0/18:2 (9Z, 12Z))

11.418_78 Isorangiformic acid
11.42_79 PG(22:1(11Z)/15:0)
11.422_78 PC(20:5(5Z, 8Z, 11Z, HMDB0008523
11.431_77 Gamithromycin HMDB0252606
11.432_68 PC(14:0/P-16:0) HMDB0007895
11.432_70 SM(d18:0/16:0) HMDB0010168
11.434_76 PC(O-16:1(9Z)/20:4 HMDB0013415
11.441_56 Cer(d18:1/18:1(11Z) HMDB0011774
11.446_74 GlcCer(d18:1(8E)/18:0(2OH[R]))
11.454_74 PE(P-16:0/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
11.471_81 PC(17:2(9Z, 12Z)/22:5 HMDB0256158
11.478_56 Linoleyl arachidate
11.489_71 PE(13:0/21:0)
11.493_58 Gondoyl-linolenate
11.496_57 Cer(m18:0/20:0)
11.502_61 Cer(t18:1(6OH)/19:0(2OH))
11.505_77 PC(22:6(4Z, 7Z, 10Z, HMDB0008722
11.516_84 PE(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/22:1(11Z))
11.52_77 LMGP02080003
11.52_79 3'-sulfoGalbeta-Cer(d18:1/16:0(2OH))
11.54_74 PE(20:3(8Z, 11Z, 14Z)/16:0)
11.542_79 PC(O-16:0/22:6(4Z, HMDB0013409
11.543_67 PE(P-18:0/14:1(9Z))
11.547_69 PC(O-14:0/16:0) HMDB0013341
11.565_78 PC(16:0/20:3(5Z, 8Z) HMDB0007980
11.601_72 GlcCer(d14:1/22:0)
11.608_75 PG(O-16:0/19:0)
11.613_69 PE(O-16:0/18:3(9Z, 12Z, 15Z))
11.643_82 PE(22:4(7Z, 10Z, 13Z, 16Z)/20:1(11Z))
11.644_77 LMGP02080002
11.65_74 PE(P-18:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))
11.663_55 Cer(d18:1/17:0)
11.678_76 1-O-Hexadecyl-2-ar HMDB0243975
11.692_86 PG(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
11.713_72 PE(O-16:0/20:4(5Z, 8Z, 11Z, 14Z))
11.751_83 PC(20:4(8Z, 11Z, 14Z) HMDB0008473
11.764_83 PI(16:0/18:1(11Z)) HMDB0009782
11.783_73 SM(d18:0/18:1(9Z)) HMDB0012089
11.799_81 PE(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/20:3(8Z, 11Z, 14Z))
11.804_79 PC(15:0/22:6(4Z, 7Z) HMDB0007958
11.807_83 LacCer(d14:0/18:0)
11.854_75 PC(18:0/16:1(9Z)) HMDB0008035
11.867_47 PE(P-19:1(12Z)/0:0)
11.894_711-Hexadec C13877
11.902_73 PC(18:4(6Z, 9Z, 12Z, HMDB0008258
11.909_50 LysoPC(P-18:1(9Z)/ HMDB0010408
11.911_80 PC(16:0/22:4(7Z, 10Z) HMDB0007988
11.937_78 PC(18:0/18:2(9Z, 12Z) HMDB0008039
11.952_76 1-Octadec C21480
11.973_74 1,2-Dioleoyl-sn-g3l HMDB0244088
11.974_83 PC(22:5(7Z, 10Z, 13Z) HMDB0008694

11. 999_5fCer(d18:0/18:1(9Z)HMDB0011763
12. 018_77MGDG(18:2(9Z, 12Z)/18:2(9Z, 12Z))
12. 019_5gDG(20:1(11Z)/14:0/HMDB0007385
12. 021_77Termitomycesphin F
12. 026_7gPE(22:1(11Z)/18:4(6Z, 9Z, 12Z, 15Z))
12. 047_81PC(22:6(4Z, 7Z, 10Z, HMDB0008752
12. 09_73zSM(d18:0/18:0) HMDB0012087
12. 094_71PC(P-16:0/16:0) HMDB0011206
12. 098_77G1cCer(d16:1(4E)/22:0(20H))
12. 099_5gCer(d16:2(4E, 6E)/22:0)
12. 099_77PE(P-18:0/22:6(4Z, HMDB0011394
12. 111_84PE(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/22:0)
12. 141_6zDG(18:4(6Z, 9Z, 12Z, 15Z)/20:3(8Z, 11Z, 14Z)/0:0) [iso2]
12. 141_741, 2-DistearoylphosHMDB0251629
12. 142_74PE-Cer(d16:1(4E)/24:0)
12. 148_67PE(P-20:0/12:0)
12. 164_74PC(16:0/P-18:1(11Z)HMDB0007996
12. 17_79fPC(18:3(9Z, 12Z, 15Z)HMDB0256165
12. 177_7gG1cCer(d16:2(4E, 6E)/24:0(20H))
12. 178_77PE(P-20:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))
12. 206_7gPC(O-18:1(9Z)/20:4HMDB0013432
12. 208_77PC(18:1(9Z)/17:0) HMDB0256160
12. 211_6fDiarachidonyl diglHMDB0251476
12. 218_7c1-HexadecC13878
12. 242_7z2-Htcptmn
12. 243_7ePC(O-18:1(11Z)/18:HMDB0013425
12. 243_8ePC(20:1(11Z)/22:5HMDB0008319
12. 245_71PE(O-16:0/19:0)
12. 246_81PC(22:2(13Z, 16Z)/1HMDB0008594
12. 269_7fPE(O-18:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))
12. 275_7gPC(18:2(9Z, 12Z)/1fHMDB0256163
12. 279_7fMGDG(16:0/18:2(9Z, 12Z))
12. 279_8zPE(22:1(11Z)/20:3(8Z, 11Z, 14Z))
12. 296_7ePE(18:0/20:3(8Z, 11Z, 14Z))
12. 308_7zPE(P-18:0/18:2(9Z, 12Z))
12. 317_74PC(O-18:1(9Z)/16:0HMDB0013426
12. 321_87PS(22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))
12. 324_7fGalCer(d18:2/22:0)
12. 325_74Azitromycin HMDB0249627
12. 327_7fTG(14:1(9Z)/15:1(9Z)/18:3(9Z, 12Z, 15Z)) [iso6]
12. 375_7cPE(P-20:0/14:0)
12. 386_7fG1cCer(d21:1(8E) (9Me)/15:0(20H[R]))
12. 391_57Cer(d19:1/18:0)
12. 391_77PC(18:0/P-18:1(11Z)HMDB0008062
12. 401_7gPC(O-18:0/20:4(8Z, HMDB0013420
12. 434_64PA(P-20:0/13:0)
12. 435_641, 3-Di-(cC13845
12. 436_84PS(18:1(9Z)/22:0)
12. 44_80fTG(13:0/18:3(6Z, 9Z, 12Z)/18:3(6Z, 9Z, 12Z)) [iso3]
12. 444_7zPE(P-20:0/16:1(9Z))
12. 457_7fPE(P-20:0/18:3(9Z, 12Z, 15Z))

12. 486_8εPS(20:3(8Z, 11Z, 14Z)/20:1(11Z))
12. 488_7εLMGL05010003
12. 492_8εSemduramiC22197
12. 501_8εPC(20:3(8Z, 11Z, 14Z)HMDB0011201
12. 545_7εPE-NMe(18:0/18:0)
12. 566_7εLoroxanthin ester/ Loroxanthin dodecenoate
12. 572_7εSM(d18:1/22:1(13Z)HMDB0012104
12. 575_7εSM(d18:1/20:0) HMDB0012102
12. 607_3εLinaprazan HMDB0254096
12. 631_81PG(22:2(13Z, 16Z)/17:1(9Z))
12. 634_34Naloxazone HMDB0255434
12. 64_35ε1alpha, 5εC14960
12. 646_3εsufac#1
12. 649_7εPC(22:1(13Z)/14:0)HMDB0008558
12. 651_37Androstane-3, 17-diHMDB0247995
12. 661_71PC(P-18:0/14:1(9Z)HMDB0011237
12. 714_74Stearoyl-oleoyl-ph HMDB0256188
12. 717_77(3'-sulfo)Galbeta-Cer(d18:1/16:0)
12. 743_81PE(22:2(13Z, 16Z)/19:0)
12. 748_74PC(0-16:1(9Z)/18:εHMDB0013413
12. 75_55C Octenidine HMDB0255907
12. 761_77PC(18:2(9Z, 12Z)/17HMDB0256162
12. 774_7εGalCer(d18:2/23:0)
12. 779_7εPE(0-20:0/18:1(9Z))
12. 78_86εPC(22:2(13Z, 16Z)/εHMDB0008605
12. 789_77GlcCer(t15:0(14Me)/21:0(2OH[R]))
12. 794_77PC(16:0/19:0) HMDB0256153
12. 815_6εDG(22:6(4Z, 7Z, 10Z, HMDB0007767
12. 815_6εDG(20:4(5Z, 8Z, 11Z, 14Z)/22:5(7Z, 10Z, 13Z, 16Z, 19Z)/0:0) [iso2]
12. 815_7C PA(P-18:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))
12. 831_77PE(P-20:0/20:4(5Z, 8Z, 11Z, 14Z))
12. 853_57phenolic phthiocerol
12. 854_5εCer(d18:1/20:0) HMDB0004951
12. 855_6εbacteriohopane-32, 33-diol-34, 35-dicarbamate
12. 858_313-oxo-nonadecanoic acid
12. 858_8εPE(22:1(11Z)/22:0)
12. 862_61Cer(d16:2(4E, 6E)/24:0)
12. 862_81PE(P-20:0/22:2(13Z, 16Z))
12. 865_5εCer(t18:0/17:0(2OH))
12. 881_6C LysoPI(18:0/0:0) HMDB0240261
12. 885_5ε5-OxoaverC11978
13. 376_27C16 Sphinganine
14. 165_2εLaurocapram HMDB0253992
2. 074_1412, 4-Dimethyl-1, 3-c HMDB0245693
2. 079_1444-Hydroxycyclohexy HMDB0001988
2. 082_551Haloperidol glucur HMDB0060904
2. 084_314Fluorapacin HMDB0247537
2. 167_277trans-2-[C19232
2. 182_171terrein
2. 255_36εTryptophan 2-C-mar HMDB0240296
2. 323_14ε2-(2-Aminophenyl)-HMDB0244917

2.338_261 Pinacidil pyridine HMDB0256557
2.366_435 2-[Acridin-9-yl]an HMDB0255367
2.382_244 (5R,6S)-3-(Amino HMDB0248479
2.386_2714-Amino-N-(3-chlor HMDB0247648
2.387_270 Clitidine C19977
2.393_296 Medinoter C19068
2.397_114 Ethane-1,1,2-tricε HMDB0257799
2.397_249 Gallic acid 3-sulf HMDB0240519
2.4_316. ε Phosmet HMDB0256463
2.401_234 p-N,N-(Di C13681
2.402_303 Resorufin benzyl ε HMDB0257167
2.454_326 1-[2-(1,3-benzodioxol-5-yl)-3-methyl-1-benzofuran-5-yl]propane-1,2-diol
2.478_167 Phosphoenolpyruvic HMDB0000263
2.503_310 (1,7,8-trihydroxy-3-methyl-2,3,4,7-tetrahydro-1H-benzo[a]anthracen-12-one
2.507_254 Bis(2-hydroxyethyl HMDB0249245
2.555_168 Dephostatin HMDB0251017
2.556_2144-Acetamidobenzene HMDB0246327
2.56_309. Pro-Pro-Pro HMDB0256689
2.562_388 dUDP HMDB0001000
2.568_197 HC Red Nc C19430
2.576_331 Dibenz(b,f)(1,4)ox HMDB0256187
2.577_366 (1'S,3R,3'R,5R,6'R,7'S)-5-(furan-3-yl)-3',6',7'-trimethyl-9'-oxaspiro[ox
2.58_186. alpha-AMINO-3-HYDF HMDB0248356
2.58_232. Pyrene-4, C18251
2.61_280. Simendan HMDB0258295
2.613_172 5,6-dihydropenicillic acid
2.613_294 Kelatorphan HMDB0253779
2.614_262 NCGC00384489-01!2-phenylfuro[2,3-h]chromen-4-one [IIN-based: Match]
2.629_169 5-Hydroxydopamine HMDB0004817
2.696_278 Dihydratanshinone HMDB0251332
2.709_377 (2S)-2-(Butanoyl)an HMDB0252946
2.71_266. N-(4-Aminobenzoyl) HMDB0255007
2.721_76. Cyclohexa-1,2,4,5- HMDB0248980
2.737_299 D-4' -Phos C03492
2.744_498 Bis-gammε C03646
2.756_249 S-[(3R,3As,6S,6aS) HMDB0253932
2.762_249 2',3'-Didehydro-2' HMDB0245542
2.764_135 9h-Purin-9-amine HMDB0247703
2.766_124 Tris(hydroxymethyl) HMDB0259280
2.778_237 L-Glutamic acid 5- HMDB0250759
2.795_2814-Chloro-3-ethoxy- HMDB0246385
2.81_124. Phenylmethanediol HMDB0256441
2.811_96. 2,3-Dimethylfuran HMDB0245403
2.816_220 N-hydroxy-L-tryptc HMDB0255152
2.834_298 6-Methylthioinosir HMDB0242752
2.855_573 CMP-2-ket C21384
2.865_267 Citrinin C16765 HMDB0041857
2.87_221. N-Acetyl-S-(3-hyd HMDB0245906
2.873_210 2,4-diacetylphloroglucinol
2.874_303 NOTA HMDB0255756
2.879_310 gamma-Glutamyltyrc HMDB0011741

2. 885_160 2-Methyladipic acid HMDB0029167
 2. 886_188 3-(3-Oxobutanoyloxy) HMDB0258085
 2. 894_239 2'-Deoxy-2'-methyl HMDB0245533
 2. 903_287 Nitrobenzylmercaptan HMDB0255643
 2. 921_135 Carbamothioic acid HMDB0249607
 2. 922_181 Dihydroxyethylidene HMDB0251344
 2. 941_390 L-Alanyl-C20925
 2. 942_267 Oxycarboxylic acid C10956
 2. 96_329 Valclavan C06668
 2. 961_217 Tyramine-O-sulfate HMDB0006409
 2. 964_208 Isoquinolinesulfone HMDB0253686
 2. 974_297 (3, 4, 5-trihydroxy-6-methyloxan-2-yl) 2-(methylamino)benzoate
 2. 988_158 4, 7-Dioxoheptanoic acid HMDB0246616
 2. 991_305 Hpmpa HMDB0253216
 2. 994_175 Aryl sulfide C00850
 3. 022_130 3-Hydroxy-3-methyl HMDB0257911
 3. 053_277 Decahydro-6-(phosphoryl) HMDB0254231
 3. 075_325 Trichloroethanol ξ HMDB0042049
 3. 096_399 Difloxacin HMDB0251259
 3. 101_435 Neoxaline C22172
 3. 103_258 L-enantiomer HMDB0253884
 3. 109_185 (2S)-2-Amino-3-(4-hydroxyphenyl) HMDB0257983
 3. 109_311 Val-pro-pro HMDB0253034
 3. 109_491 3-{4-[(6, 7-Dimethyl-2-oxo-1, 2, 3, 4-tetrahydro-1H-benzothiazol-5-yl)amino]phenyl}propanoic acid HMDB0249994
 3. 111_272 5-S-Cysteinyl-dopa HMDB0246842
 3. 112_397 1-(4-Acetyl-2-pyrrolidinyl)ethanone HMDB0250045
 3. 12_430 Aliarin 4'-methyl ether
 3. 131_246 2, 4-Diacetylphenol C20424
 3. 151_158 Betonicine HMDB0029412
 3. 167_205 Tert-Butyl (2-(2-hydroxyethyl)amino)acetate HMDB0244567
 3. 171_141 Icofungipen HMDB0253367
 3. 181_232 Pyrene-1, C18258
 3. 185_206 Monoethylglycine, x HMDB0060656
 3. 194_200 Fumaryl acetoacetate HMDB0252519
 3. 204_385 Succinyladenosine HMDB0000912
 3. 213_215 Indanidine HMDB0253447
 3. 22_110 Hydroquinone C00530 HMDB0002434
 3. 22_203 Cystathionine ketide HMDB0002015
 3. 233_302 2-(3-hydroxy-5-methoxyphenoxy)-6-(hydroxymethyl)oxane-3, 4, 5-triol
 3. 238_175 Sulfanilic acid HMDB0258581
 3. 262_270 {5-(5-Nitro-2-furyl)oxy}acetic acid HMDB0243768
 3. 263_168 2, 2-Dihydroxy-2-propanol HMDB0258145
 3. 272_314 N-(N-(3-Carboxyoxymethyl)phenyl)acetamide HMDB0247379
 3. 277_354 Barucainide HMDB0248876
 3. 282_138 3-Hydroxybenzylhydrazide HMDB0245893
 3. 286_209 1, 1, 2-Trimethyl-1H-imidazole HMDB0246655
 3. 289_518 26, 26, 27, 27, 27-hexafluoro-1 α , 25-dihydroxy-16, 17, 23, 23, 24, 24-hexadecane
 3. 29_241 2, 3, 5-Trimethyl-6-hydroxy-2-pyrone HMDB0250599
 3. 319_187 Deprenyl
 3. 321_158 1-Benzylimidazole HMDB0243836
 3. 326_175 4-Methoxy-2-naphthylamine HMDB0246491

3. 326_204 1,2-Propanediol, ε HMDB0245961
3. 329_222 N5-PhenylC20843
3. 33_220. 2,4-Diamino-6,7-di HMDB0060724
3. 332_142 2-Methylidene-4-(c HMDB0257753
3. 346_268 9-(2-Aminopurin-9- HMDB0260431
3. 353_134 Trimethylolpropane HMDB0259243
3. 354_172 Toluene-4C06677
3. 355_194 alpha-(4-Pyridyl-1 HMDB0248183
3. 36_200. 3-[(1R,2S C21087
3. 368_198 alpha-[3-C19581
3. 383_254 Paracetamol cystei HMDB0256120
3. 387_164 Tetra-methoxypropa HMDB0258866
3. 391_236 Hexobarbital HMDB0015444
3. 391_238 7-Amino-4-hydroxy- HMDB0243485
3. 403_204 methyl orsellinate
3. 41_369. fleroxacin HMDB0252299
3. 414_186 Calcium r C18379
3. 415_328 L-Proline, 1-(1-L- HMDB0253022
3. 416_391 2-(Glutamate C21374
3. 431_266 gamma-Glutamate C20926
3. 438_268 3-Hydroxybenzo(a) r HMDB0248998
3. 446_268 3-(5-Acetamido-2- r HMDB0255408
3. 447_266 Fructose 6-phosphate HMDB0000124
3. 464_208 3-[(1-Car C20772
3. 471_116 5-Aminopropionate C00990
3. 485_218 4-Methylpiperidine C03837 HMDB0032989
3. 489_312 4-hydroxy-8-methoxy-5-methyl-3-(3-methylbut-2-enyl)chromen-2-one
3. 499_196 Dihydroferulic acid HMDB0062121
3. 52_294. Tanshinone IIA HMDB0258715
3. 529_197 Desglymidodrine HMDB0060558
3. 535_156 N-(3-(Dimethylamino)propyl)acetamide HMDB0246231
3. 55_215. Propionylcarnitine HMDB0013124
3. 551_298 (S)-methyl alpha-D-glucosaminide
3. 555_322 Isoderricin A
3. 56_140. Cyclohepta-1,3,5-triene HMDB0250645
3. 566_208 3-[(1-Carboxyvinyl)oxy]benzoic acid
3. 567_156 4,5-dihydroxy-3-propylcyclopent-2-en-1-one
3. 574_206 Pheneturide HMDB0256403
3. 575_156 9-Hydroxynon-2-ene HMDB0257844
3. 581_262 Propylphenylalanine
3. 586_278 L-Tyrosine C04201
3. 586_296 Flunixin HMDB0252340
3. 594_84. Diketene HMDB0251360
3. 595_222 4-Benzyl-2-methyl- HMDB0258758
3. 608_297 (2R,5S)-2-(6-Amino-2-methyl-2H-pyridin-5-yl)ethane-1-thiol HMDB0257557
3. 622_131 indol-2-one HMDB0253466
3. 624_191 2,4-Thiazolidinedione HMDB0244750
3. 627_198 (Carbamoylamino)propylamine HMDB0257890
3. 642_101 Pentanamide C01842 HMDB0256275
3. 645_312 Pentaleno(1,6a-c) r HMDB0247731
3. 647_198 2-Oxopropanoic acid C11497

3. 654_564 Butyloxycarbonyl-1 HMDB0247808
3. 657_162 2-Oxo-5-n C17211
3. 665_240 3-(3,4,5-Trimethoxy HMDB0030254
3. 674_331 N'-Acetyl-3-chloro HMDB0257530
3. 677_274 ascr#7
3. 68_187. N-Heptanoylglycine HMDB0013010
3. 687_285 Leu-Gly-FC01833
3. 705_155 Norfenefrine HMDB0255737
3. 711_242 Diethylene glycol HMDB0251246
3. 719_165 Phthalamic acid HMDB0256499
3. 721_252 Hexazinone HMDB0253153
3. 726_279 Imepitoin HMDB0253409
3. 727_186 1,2-Cyclohexanedic HMDB0253138
3. 755_510 Sarcoehrendin A
3. 756_175 p-Menthan-3-ol HMDB0035765
3. 758_210 3',5'-Dideoxythymi HMDB0246113
3. 759_245 N-[4-(4-Methyl-6-c HMDB0250023
3. 76_210. Phenazine-2,3-dian HMDB0256396
3. 761_305 Aditoprim HMDB0248017
3. 768_220 Propionamide, 3-ar HMDB0252178
3. 769_235 Piperic Acid
3. 772_301 Isofebrifugine HMDB0253633
3. 774_342 Clozapine N-oxide HMDB0060900
3. 779_225 5-(4-Hydroxybenzyl HMDB0247358
3. 782_128 Polylysine HMDB0256678
3. 784_111 Policapram HMDB0256664
3. 795_182 (S)-3-(2-Methylphe HMDB0247880
3. 796_217 0-Propanc C03017
3. 805_224 Alongside HMDB0248179
3. 809_234 1-Acetyl-2-(3-pyrr HMDB0244295
3. 818_228 (2S)-3-Hydroxy-1-[HMDB0257791
3. 825_447 Cyflumetc C18517
3. 826_192 2-(Trifluoromethoxy HMDB0243914
3. 827_170 Penicillic acid HMDB0256217
3. 833_216 7-Methoxy-2,3-dihy HMDB0247267
3. 839_267 S-(+)-apomorphine HMDB0257375
3. 85_260. gamma-Glutamylleuc HMDB0011171
3. 857_361 Ofloxacin HMDB0015296
3. 866_200 Cladosporacid E
3. 87_198. 5-(4-methyl-5-oxo-2H-furan-3-yl)pentanoic acid
3. 877_247 Forchlorf C18604 HMDB0252436
3. 882_207 5-Hydroxy-6-methoxy HMDB0246803
3. 887_126 1-Cyclohexene-1-cis HMDB0243852
3. 889_202 METAMITR C10930 HMDB0254501
3. 895_205 N-Lactoylleucine HMDB0062176
3. 895_212 7-Deoxylc C20790
3. 898_166 Isopeanol
3. 905_212 2,4-Diaminoazobenz HMDB0245446
3. 907_176 2-Isopropylmalic acid HMDB0000402
3. 91_179. Umbelliferone C09315 HMDB0029865
3. 92_221. (2R)-2-Acetamido-5- HMDB0258091

3.924_293 Islatravir HMDB0253596
 3.925_203 N-Acetyl-S-allylcysteine HMDB0240543
 3.942_309 Metixene HMDB0014484
 3.949_340 methyl 2,8-dihydroxy-6-(hydroxymethyl)-9-oxo-1,2-dihydroanthene-1-carboxylate
 3.968_252 5-Ethynyl-2'-deoxythymidine HMDB0246787
 3.972_158 trans-4-Hydroxycyclohexanone HMDB0000909
 3.975_249 Macromomycin B HMDB0254293
 3.977_372 (Ac)2-L-IC03326
 3.98_158.1,4-Naphthoquinone HMDB0244221
 3.981_144 3-Hydroxypropyl methylcarbamate HMDB0245905
 3.981_257 N-Tert-butyl-1-(2-hydroxyethyl)pyrrolidine HMDB0244399
 3.982_294 Lidofenin HMDB0254082
 3.984_238 Velaresol HMDB0259776
 3.986_273 Glutaconylcarnitine HMDB0013129
 3.989_262 Phaseolic acid
 3.99_264. LID_265.1546_9.2
 3.991_170 2',4'-Dihydroxyacetophenone HMDB0029659
 4_259.033 Glucosamine 6-sulfate HMDB0000592
 4.002_140 5,5-Dimethyl-1,3-cyclohexanedione HMDB0251369
 4.008_154 Milameline HMDB0254718
 4.013_164 Thymoquinone HMDB0034732
 4.034_372 [(1S,3aR,5R,5aR,8aR,9S,9aR)-1,5,8a-trimethyl-2,8-dioxo-3a,4,5,5a,9,9a-hexahydro-1H-benzo[5,6]cyclohepta[1,2-b]pyridine-2,8-dione] HMDB0244411
 4.045_226 3-Carboxy-4-methylphenol HMDB0244411
 4.054_272 Asperitaconic acid B
 4.078_172 7-methyl-4-oxooctanoic acid
 4.083_178 Nikethamide HMDB0255604
 4.089_173 Quinoline-4-carboxamide HMDB0257047
 4.089_176 Cladinose HMDB0250311
 4.098_219 N-Deschlorobenzoylserine HMDB0013988
 4.098_281 Hydroxylacetone HMDB021883
 4.112_202 Diethyl malonate HMDB004067
 4.121_273 [(1S,2S,4S,5S)-2-(1-hydroxyethyl)-4,5-dihydro-1H-imidazole-5-carboxamide] HMDB0260215
 4.126_214 Methyl 2-cyanoacetate HMDB001223
 4.128_244 (5E)-3,4,9-trihydroxy-2-propyl-2,3,4,7,8,9-hexahydrooxecine-10-one
 4.131_194 Dihydromyristicin
 4.134_137 o-Phenetidine HMDB0255863
 4.144_276 Daumone HMDB0250877
 4.146_146 2-(Tetrahydrofuran-2-yl)ethanol HMDB0252869
 4.147_392 Dehydrorotenone
 4.154_244 epsilon-(Hexanoyl)lysine HMDB0251888
 4.158_224 2,6-Diamino-9-(2-hydroxyethyl)purine HMDB0246998
 4.158_232 Naphthoxylactic acid HMDB0255452
 4.161_269 2-(1-hydroxy-1-methoxy-3-methylbutyl)-6-methyl-5H-[1,3]dioxolo[4,5-c]pyridine
 4.172_209 4-oxo-5-phenylpentanoic acid
 4.173_271 Pentritinol HMDB0256293
 4.177_257 2-Hexenoylcarnitine HMDB0013161
 4.178_182 Methyl Orsellinate
 4.178_199 L-Anticarinone C20941
 4.179_181 Glufosinate HMDB0252799
 4.182_204 1,4,8,11-Tetraoxadecane HMDB0244226
 4.184_333 10-Acetoxydecanal HMDB0248002

4. 193_233 4-[(2, 4-Dihydroxy-HMDB0246316
4. 197_133 1, 2-Benzisothiazol-HMDB0244057
4. 197_243 4-Hydroxycyclonidine-HMDB0060555
4. 225_317 Suberoyl-L-carniti-HMDB0240724
4. 225_357 Tolrestat-C01621
4. 229_283 Triethylene glycol-HMDB0244334
4. 234_303 Isocordoin
4. 25_194. 2-Nonyl-1H-imidaz-HMDB0246914
4. 252_227 N-(3-oxo-heptanoyl)-homoserine lactone
4. 253_253 Meteloidi-C10861
4. 256_153 8-hydroxy-5, 6-Octadienoic acid
4. 262_282 2-Aminoac-C00939
4. 265_243 Trimecaine HMDB0259231
4. 267_162 ISOSAFROLE HMDB0253689
4. 271_213 Lucerastat HMDB0254192
4. 273_223 9-methoxycarbonyldec-9-enoic acid
4. 273_253 (2, 6-Diaminopurine HMDB0250896
4. 283_143 Anisole, p-propenyl-HMDB0248443
4. 284_233 (2S)-2-[(1S, 2R)-1, 2-dihydroxypentyl]-4-methoxy-2, 3-dihydropyran-6-one
4. 286_273 Tenax GC HMDB0258813
4. 29_326. 4-amino-2-hydroxy-5-[[1-hydroxy-1-(5-oxo-6-bicyclo[4. 1. 0]hept-3-enyl)pro
4. 29_386. Fulvinervin B
4. 296_113 Cyclohexanecarbonyl-HMDB0250650
4. 3_254. 13, 4-dimethyl-5-carboxyethyl-2-furanbutanoic acid
4. 303_284 4-[3, 4, 5-Trihydroxymethyl]-2-methyl-5-hydroxy-2-furanbutanoic acid
4. 303_283 Cladosporester C
4. 306_343 Violacein HMDB0259831
4. 314_253 N-D-Glucc-C03142
4. 316_243 ascr#9
4. 324_333 Dimefuror-C18783
4. 33_169. 1, 1, 1, 2, 3, 3, 3-Heptamethyl-2, 2, 4, 4-tetrahydro-1, 3-dioxane-5-carboxylic acid
4. 334_201 Penicillanic acid HMDB0256227
4. 344_313 Meclofenac-C02996
4. 346_193 Dethiobacillin-C01909 HMDB0003581
4. 348_153 2-Azaspiro[4. 5]decane-2, 3-dione
4. 348_213 Guanadrel HMDB0014371
4. 348_283 Etazolate HMDB0251990
4. 36_269. 4-(3'-Methylamino)-2, 2, 4, 4-tetrahydro-1, 3-dioxane-5-carboxylic acid
4. 367_193 Anemonin; C16913
4. 368_381 Benthiavone; C18415
4. 369_343 Erybraedin E
4. 375_121 2-Ethenyl-1-oxidopyridine-4-carboxylic acid
4. 377_343 Cefradine HMDB0015428
4. 39_170. Methylglyoxal-bis-(2-aminoethyl)-amine
4. 396_214 Pantheric Acid C
4. 4_261. 1N-[2-(5-Methoxy-1H-imidazol-2-yl)ethyl]pyrrolidine
4. 403_183 Harman C09209 HMDB0035196
4. 406_203 2-(5-Fluoropentyl)-2-methyl-5-hydroxy-2, 2, 4, 4-tetrahydro-1, 3-dioxane-5-carboxylic acid
4. 409_213 N,N'-Diphenylethylamine
4. 415_283 methyl 2-ethyl-4-[(3R, 4R, 5S)-5-hydroxy-4, 5-dimethyl-2-oxooxolan-3-yl]-2-oxo-1, 2, 3, 4-tetrahydro-1, 2, 4-triazole-5-carboxylic acid
4. 43_242. C20822; (C20822)

4. 44_286. Kushenin HMDB0253835
4. 441_272 6, 7-Dimethoxy-2- (r HMDB0247128
4. 459_276 Triphenyl C14549
4. 463_310 Acromelic C19949
4. 465_189 2, 4-Dichl C06670
4. 466_210 2, 4-Diacε C21896
4. 473_299 TRIADIMEFON HMDB0259142
4. 482_277 1-(1-hydroxybutyl)-1, 3, 4, 5, 6, 7-hexahydro-2-benzofuran-4, 5, 6, 7-tetrol
4. 483_241 (1R, 4R, 5S)-1-[(1S) HMDB0242338
4. 486_408 Montirelin HMDB0254874
4. 487_211 mescaline HMDB0254474
4. 494_289 1-Tert-butyl 4-ethyl HMDB0244604
4. 502_268 3, 4-dimethyl-5-carboxyethyl-2-furanpentanoic acid
4. 518_350 Clitidine C08429
4. 529_178 5-Hydroperoxypent- HMDB0256717
4. 542_158 5, 6-Dimethyl-2, 3- (r HMDB0246643
4. 548_110 Hexa-2, 4-dienedial HMDB0254943
4. 553_259 Celgosivir HMDB0249792
4. 561_349 (3R, 4S)-2-[6- (Cyc HMDB0243620
4. 562_224 1-Methyl- C16038 HMDB0041008
4. 569_230 2-(6-hydroxyhexyl)-3-methylidenebutanedioic acid
4. 574_509 Lysyl-aspartyl-glu HMDB0247848
4. 581_331 Melochin C10727
4. 584_151 2-Amino-1-phenyl p HMDB0256426
4. 587_214 Methyl 2- C04130
4. 588_276 Meisoindigo HMDB0254414
4. 591_416 Dipfluzine HMDB0251442
4. 599_222 Diethylbenzenedicε HMDB0258113
4. 601_119 Cyclohexanemethylε HMDB0250653
4. 62_294. 5' -N-Methylcarboxε HMDB0246883
4. 628_198 Glu-P-1; C19244
4. 636_250 2-[4-(2-Carboxy-2- HMDB0257843
4. 641_379 8H-Purin-8-one, 7- HMDB0259448
4. 647_369 Angiotens C20973
4. 65_256. 4-O-methylolivetolcarboxylic acid
4. 666_291 5-Hydroxylysinoic acid HMDB0246805
4. 676_278 Leucylphenylalanine HMDB0013243
4. 705_164 Phenylalanine amic acid HMDB0253026
4. 707_241 ((2R, 3S)-3-Amino-ε HMDB0242228
4. 713_168 Methylhexahydrophthalic acid HMDB0254649
4. 715_169 Piperidine C17730
4. 715_252 Amdoxovir HMDB0248284
4. 728_251 Ac-Tyr-OEt C01657
4. 731_406 Palomid 529 HMDB0256093
4. 732_238 N7-(2-Carbamoyl-2- HMDB0255307
4. 739_341 Propiconazole HMDB0256825
4. 744_189 1-Methylpiperidine HMDB0243943
4. 744_220 Carbamoyl piperidine C18923
4. 744_281 Caffeine, 8-((3-methyl- HMDB0247409
4. 748_141 Tropine HMDB0259297
4. 752_249 3-Amino-Beta-Pinene

4. 752_27(1-(4-Fluorophenyl) HMDB0248995
4. 752_29(Tetraethyl pyrophosphate) HMDB0258824
4. 752_39(2R, 3S, 4S, 5R, 6R)-2-(hydroxymethyl)-6-[4-(4-hydroxy-2, 6, 6-trimethylcyclohexyl)oxy]propanoic acid HMDB0259505
4. 752_43(N, N-Dimethyl-5-(1H-imidazol-2-yl)pentan-1-amine) HMDB0259505
4. 752_59(Delphinidin) C08677
4. 752_61(Rotigaptide) HMDB0257314
4. 753_18(L-Valine, N-(2-hydroxyethyl)carbamoyl) HMDB0253927
4. 753_241(6S)-2-Amino-6-[1-(1H-imidazol-2-yl)ethyl]hexanoic acid HMDB0257929
4. 753_261(Cytochrome c) HMDB0246767
4. 753_28(Azvidine) HMDB0248824
4. 754_12(4-Dihydrocollidine) HMDB0246411
4. 754_12(2, 4-octadienal) HMDB0246411
4. 754_151(-)-Norephedrine HMDB0243518
4. 755_27(Mopidralazine) HMDB0254879
4. 759_28(Probenecid) HMDB0015166
4. 77_414. Neoisosteric C10707
4. 771_411(Magon) HMDB0246903
4. 774_26(Cernuine; C09860) HMDB0246903
4. 801_39(BENZOYLARGININE) HMDB0249046
4. 802_17(8, 8a-Diepiswainson) HMDB0247470
4. 802_39(Ketanserin) HMDB0253783
4. 803_23(9-(3, 4-Dihydroxybutyl)phenyl)propanoic acid HMDB0247573
4. 805_14(Triethyl orthoformate) HMDB0259190
4. 811_377(2R, 3R, 4S, 5S, 6R)-2-[3-hydroxy-2-(4-hydroxy-3-methoxyphenyl)propoxy]-6-(hydroxymethyl)hexanoic acid HMDB0257402
4. 823_14(S-Methyl N, N-Diethylacetamide) HMDB0257402
4. 833_18(N-ALPHA-ACETYL) LYSINE
4. 835_17(2-hydroxy pelargonic acid) HMDB0257402
4. 85_312. Ethyl 4-methyl-5-oxo-2-pentenoate HMDB0260031
4. 854_34(2-Methylene-5-(2, 5-Dioxotetrahydrofuran-3-yl)-6-oxo-1, 10-Dimethylbicyclo[2.2.1]heptane) HMDB0257402
4. 869_22(4-Hydroxy-3', 4'-dihydroxyacetophenone) HMDB0041679
4. 869_27(Tenascin C) HMDB0257402
4. 874_28(methyl 3-(3, 4-dihydroxy-5-phenyloxolan-2-yl)-3-hydroxypropanoate) HMDB0257402
4. 886_25(Hexenoylcarnitine) HMDB0253155
4. 889_18(Dimethyl pimelimidate) HMDB0251389
4. 897_11(2-Amino-3-methylpentanoic acid) HMDB0257959
4. 899_27(Creatine glutamate) HMDB0250524
4. 902_17(4-Piperidinol, 1-yl) HMDB0243489
4. 916_29(3, 5-Dihydroxyphenyl) HMDB0240452
4. 917_12(2-Methyl) C07214
4. 917_30(Clofarabine) HMDB0014769
4. 918_28(Nicaraven) HMDB0255579
4. 92_200. Hydralazine acetate HMDB0060606
4. 924_32(10-(Phosphonoxy)decane) HMDB0247525
4. 943_26(1, 2, 6-Diamino-3, 5-dimethylimidazole) HMDB0259620
4. 953_29(Corrole) HMDB0250458
4. 962_22(Glycerol 1, 2-dimethyl ether) HMDB0252838
4. 974_16(3, 5-Dimethylphenyl) HMDB0244732
4. 974_31(N-(3-Chlorophenyl)acetamide) HMDB0248054
4. 986_20(3, 4-Methylenedioxyphenyl) HMDB0254369
4. 987_27(Tezampanel) HMDB0258944
4. 99_98. (2-Pentenedial) HMDB0252802

4. 994_2062-(3-Pentylphenyl) HMDB0244924
5. 002_254C75 trans HMDB0249518
5. 011_288Nifuratel HMDB0255596
5. 013_228Traumatic acid HMDB0000933
5. 018_2744-Alanylaminointi HMDB0246333
5. 021_259Propylparaben sulf HMDB0240718
5. 037_229N-(3-oxo-hexanoyl)-homoserine thiolactone
5. 039_1542,6-Dihydroxy-4-Methoxytoluene
5. 049_3162,3,4,5-tetranor-thromboxane B1
5. 053_330(2S,3R,4S,5S,6R)-2-[[(1S,4aR,7aS)-7-(hydroxymethyl)-1,4a,5,7a-tetrahydro
5. 056_1742-Amino-4-[carbami HMDB0255374
5. 056_248Monocyclohexyl pht HMDB0254852
5. 056_3287-Hydroxy graniset HMDB0247255
5. 057_146Glycylsarcosine HMDB0252887
5. 058_166(R)-2-Hydroxy-2H-1 HMDB0038318
5. 06_340. Glycyl-1-histidyl- HMDB0252882
5. 067_348(2S,3R,4S,5S,6R)-2-[4-(3-hydroxybutyl)phenoxy]-6-(hydroxymethyl)oxane-3,
5. 083_3001-[4,5-bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-
5. 086_3222-Hydroxyphenylacetate HMDB0240440
5. 099_280(E)-2-(hydroxymethyl)-3-(3-oxo-5-propan-2-yl-4,5,6,7-tetrahydro-1H-2-ben
5. 125_2783-Hydroxyhexanoyl HMDB0013131
5. 128_231Butyrylcarnitine HMDB0002013
5. 137_2082-(1-hydroxyethyl)-4-(2-hydroxypropyl)-2H-furan-5-one
5. 137_219aniracetam HMDB0248441
5. 139_147N-Methyl-DL-aspartate HMDB0255174
5. 141_228Prenalterol HMDB0256762
5. 146_2842-Hydroxy-4-[(1R)- HMDB0258463
5. 148_318Hexaconazole C18466
5. 151_30611-dimethylarsinoyl-undecanoic acid
5. 152_3305-Hydroxy Dantrolene HMDB0246799
5. 154_194Temozolomide HMDB0014991
5. 185_304Cedpht HMDB0251608
5. 186_284Phenylethyl 2-Glucoside
5. 187_269N-(3-oxo-decanoyl)-homoserine lactone
5. 193_2583-oxo-C9-HSL
5. 216_2041-Hydroxycyclohexane HMDB0247678
5. 223_237Pyrido[3, C19516
5. 223_2885-(4-Methylphenyl) HMDB0257964
5. 225_218Hexaminolevulinate HMDB0253144
5. 235_1475-Methoxyindole HMDB0246822
5. 246_338C8-sterol isomerase inhibitor Naegleria fowleri Ameobia 1
5. 251_258N-[4-(5- N C19273
5. 267_348Crisnatol HMDB0250538
5. 27_191. Juarezic Acid
5. 271_237N-acetyl-O-methyltyrosine
5. 284_1391-Indolizine C16697
5. 295_318(+)-Neomycin C04165
5. 304_276Etidocaine HMDB0252097
5. 306_268Ripazepan C19518
5. 31_278. Raxofelast HMDB0257115
5. 324_282Cadiamine C10756

5.325_224 Jasmonic acid methyl HMDB0253727
5.326_338 N-[[(2S, 3S, 4R, 5R)- HMDB0257719
5.333_244 MCPA-thioethyl HMDB0254367
5.336_196 Phenol A HMDB0256407
5.339_268 Methyl parathion HMDB0256125
5.349_326 3-[4-Hydroxy-3-[3- HMDB0257654
5.354_270 (2S, 3R, 4R, 5S, 6S)-ε HMDB0243491
5.367_246 3-Hydroxydodecanoic HMDB0000413
5.367_314 Resiquimod HMDB0257161
5.376_318 Gardiquimod HMDB0252643
5.383_177 Dihomomet C17217
5.389_238 2, 3-Dihydroxypropyl HMDB0257749
5.392_291 Cyproconazole HMDB0250696
5.398_310 Lersivirine HMDB0254020
5.399_170 Dendryphielic acid B
5.399_341 Cyclacillin HMDB0015135
5.401_108 Vinylcyclohexene HMDB0244016
5.401_286 Avadomide HMDB0249718
5.402_228 Metoxuror C11011
5.402_246 D-Kynurer C01718 HMDB0250769
5.403_166 Cyromazir C14147 HMDB0029862
5.404_278 2-Nitrobenzanthrone HMDB0245254
5.406_408 Nifekalant HMDB0255595
5.41_227. N-OCTANOYL-L-HOMOSE HMDB0255213
5.419_130 2-hydroxy-Heptan-3-one
5.419_229 (E)-3-(2-(1H-Tetra HMDB0244544
5.423_229 butenoylcarnitine HMDB0249460
5.429_218 12-amino-dodecanoic acid
5.434_237 viloxazine HMDB0259807
5.44_254. Butanoic acid, [(c HMDB0245609
5.445_172 9-Oxonone C16322
5.447_262 Clonixin HMDB0250352
5.449_186 Cyclohexyl propan- HMDB0250658
5.457_322 Neamine HMDB0255495
5.466_394 Nigakilac C17036
5.478_424 L-Prolinamide, gly HMDB0253912
5.479_188 Methyprylon HMDB0015239
5.481_137 Pyrrole, 2-pentyl HMDB0256996
5.481_168 1-Methoxy C10452 HMDB0034121
5.488_318 6-Hydroxyemedastir HMDB0060785
5.496_244 Veliparib HMDB0259777
5.539_188 Chrysanthemic Acid
5.542_200 3Z-Hexenyl 2R-hydroxy-3-methylbutyrate
5.559_298 PSEUDO-ANISATIN
5.56_252. NCGC00179744-02! (2S)-2-[(1S, 2R)-1, 2-dihydroxypentyl]-4-methoxy-2, 3-dihyd
5.567_142 4-ene-Valproic acid HMDB0013897
5.567_214 Curvulalide
5.568_336 Tephrowatsin B
5.581_291 Befunolol HMDB0248930
5.586_200 Dimethyl suberimide HMDB0251407
5.586_202 DL-Alanyl-DL-leucine HMDB0251509

5. 588_22 Rimiterol HMDB0257235
5. 589_30 tetra(methoxymethyl)melamine (putative)
5. 596_25 Lacosamide HMDB0253940
5. 597_30 Azapropazone HMDB0248765
5. 61_160. 5,6-undecadien-8,10-diyne-1-ol
5. 621_31 Propamide HMDB0256810
5. 623_25 L-Pyrrolyl C16138
5. 624_32 D-Valacyclovir HMDB0259521
5. 624_33 Riboprime HMDB0257214
5. 629_18 Leucine butyl ester
5. 635_26 Batatasin III HMDB0030636
5. 64_241. (E, 2S, 3R)-5-[3-hydroxy-2-(hydroxymethyl)phenyl]pent-4-ene-2,3-diol
5. 681_26 Deoxyqinghaosu HMDB0251012
5. 684_32 Propentofylline HMDB0256822
5. 692_39 Methyl 4-[(E)-2-(HMDB0257579
5. 693_16 Pseudoephedrine HMDB0001943
5. 702_25 Phomalone
5. 708_27 (1,5-Dihydro-7-(1-HMDB0259407
5. 719_34 (-)-erythro-Anethc HMDB0033067
5. 722_14 Poly(lactic acid-c HMDB0256668
5. 722_16 7-Methylguanine HMDB0000897
5. 725_28 4-Carbethoxyhexaf HMDB0244812
5. 727_20 6-hydroxy-4-Undecanolide
5. 728_18 pyrrolobenzodiazep HMDB0257005
5. 728_19 Caffeine C07481 HMDB0001847
5. 731_21 (2,8-Phenazinediamine
5. 734_13 Formyl 3-hydroxybu HMDB0257659
5. 74_132. Oxalacetic acid HMDB0000223
5. 745_16 3-(2-Hydroxy-1-me HMDB0255680
5. 748_19 Cycluron; C19109
5. 75_202. Theobromi C07480 HMDB0002825
5. 76_248. Micheliolide HMDB0254704
5. 763_25 Desmethyl rizatrip HMDB0244626
5. 764_29 11-(6-Oxo-C15433
5. 765_26 5-Chloro-2'-deoxy HMDB0250110
5. 771_18 10-Hydroxy-2-dece HMDB0244269
5. 773_20 (2,6R-Dimethyl-2E-octen-1,8-dioic acid
5. 777_36 Pramanicin
5. 779_30 Therafectin HMDB0248335
5. 779_32 6-[(1R, 2R, 3S, 5S)- HMDB0256370
5. 781_19 10-Hydroxy-2-oxabi HMDB0255348
5. 794_27 3-Hydroxytetradec HMDB0000394
5. 798_31 Glycerol C13870 HMDB0031094
5. 8_360. 11-O-(8R-hydroxy-8-methyl-3Z,9-decadienoyl)-beta-D-glucopyranose
5. 803_24 (N-Hydroxy phip HMDB0255150
5. 806_31 Indicine-N-oxide HMDB0253458
5. 806_32 (2S, 3S, 4S, 5S)-2-(HMDB0255782
5. 816_34 3-hydroxy-6-[[(E)-3-hydroxy-2,4-dimethylhept-4-enoyl]amino]-2,4-dimethyl
5. 823_35 Dimethylsphingosir HMDB0251406
5. 835_29 Indicine HMDB0253457
5. 843_22 3,5-dihydroxydecanoic acid

5.846_298 alpha-Artemether HMDB0248189
 5.849_2512-Nitrophenyl octyl HMDB0245262
 5.849_378 Cumi-101 HMDB0250589
 5.863_268 4,6-dihydroxy-4-(hydroxymethyl)-3,4a,8,8-tetramethyl-5,6,7,8a-tetrahydro
 5.868_308 1-Oxononan-4-yl (Z) HMDB0255339
 5.877_378 Cynisin HMDB0250382
 5.882_198 N-Formyl-dl-phenyl HMDB0255143
 5.889_291 Perlapine HMDB0256346
 5.908_358 Lobeline Hydrochloride
 5.909_212 Nontrial HMDB0255710
 5.939_128 4-Trimethylaminobutyl HMDB0246589
 5.951_308 (3,6,9-trimethylidene-2-oxo-3a,4,5,6a,7,8,9a,9b-octahydroazuleno[4,5-b]f
 5.951_328 Deoxyaminopteroic HMDB0244853
 5.952_308 Norcocaethylene HMDB0255728
 5.955_240 Budralazine HMDB0249426
 5.957_248 (6R,7R)-6-Methoxy- HMDB0258050
 5.958_218 1-Benzyl-4-(chloro HMDB0243834
 5.971_292 Benzoyl L-arginine HMDB0249040
 5.98_229. Icaridin HMDB0253340
 5.981_268 Rizatriptan HMDB0015088
 5.981_287 Gabazine HMDB0252568
 5.989_254 (E)-2-(hydroxymethyl)-3-[3-(hydroxymethyl)-6-propan-2-ylcyclohex-2-en-1-
 5.989_261 Bufuralol HMDB0249434
 6.003_302 Gemcabene HMDB0252669
 6.011_341 Dodecenoylcarnitine HMDB0251567
 6.013_388 12-hydroxyjasmonic acid 12-O-beta-D-glucoside
 6.028_207 THURFYL NICOTINATE HMDB0259050
 6.031_228 Tigloidir C10868
 6.033_288 1,4-dihydroxy-6,6,9a-trimethyl-4,5,5a,7,8,9-hexahydro-1H-benzo[e][2]benz
 6.04_321. 3-[[3-Methoxy-5-(1 HMDB0246613
 6.041_264 (-)-Abscisic acid HMDB0243505
 6.043_194 2-(1-Adamantyl)-1, HMDB0257906
 6.043_242 Ieodomycin A
 6.067_284 [5-hydroxy-3-(hydroxymethyl)-2-oxo-6-propan-2-ylcyclohex-3-en-1-yl] 3-me
 6.069_112 (2E)-2-Heptenal HMDB0033827
 6.092_348 Coenzyme C04628
 6.097_208 Propoxur HMDB0256832
 6.098_278 N-Ethyl-N-(2-hydrox HMDB0255133
 6.103_268 Deoxydihydro-arten HMDB0060570
 6.104_178 Ethanone, 1-(4-but HMDB0246227
 6.106_204 Idazoxan HMDB0253375
 6.108_240 Cropropamide HMDB0250543
 6.115_1512-Aminoadamantane HMDB0245006
 6.115_178 Ephedrine methyl ε HMDB0251838
 6.115_218 Ethyl butylacetyl ε HMDB0246904
 6.115_271 Ciadox HMDB0250601
 6.121_382 Sumarotene HMDB0258626
 6.128_342 NCGC00169827-03! (2E,4E)-12-hydroxy-13-(hydroxymethyl)-3,5,7-trimethyl tet
 6.13_170. Furfural C14280
 6.13_302. Dehydrosiphonochalynol
 6.138_354 5-hydroperoxy-7-[3,5-epidioxy-2-(2-octenyl)-cyclopentyl]-6-heptenoic aci

6. 145_306 6-Hydroxy-8-methylHMDB0244793
6. 147_332 Floctafenic acid HMDB0252309
6. 161_283 Tris(2-chloroethyl)HMDB0259276
6. 165_297 NCGC00380135-01! (3aS, 6S, 7R, 8aR)-8-hydroxy-6, 8-dimethyl-3-methylidenespir
6. 169_323 isoxazolyl penicilHMDB0253713
6. 178_242 1, 5-DiphenylcarbazHMDB0244234
6. 179_146 Pentacyclo(5. 4. 0. (HMDB0246677
6. 179_182 Methyl 4, 8-decadienHMDB0034708
6. 179_316 (E)-N-(3-(3-(4-FluHMDB0249490
6. 181_164 3-Butyl-4-methylpHMDB0249476
6. 181_214 3-OxododecC02367
6. 181_330 Rhodamine 110 HMDB0257198
6. 192_1712 Cyclooctyl-2-hycHMDB0245091
6. 198_210 2-Nonyl-1, 4-dioxirHMDB0255390
6. 201_287 Prosopinine
6. 22_356. Rolofylline HMDB0257295
6. 222_273 Pyrodone HMDB0256988
6. 224_241 N-(7-methyloctanoyl)homoserine lactone
6. 235_267 Diethyl 2, 4, 6-trinHMDB0260367
6. 245_283 alpha-HydroxymetoHMDB0060994
6. 252_308 2, 2'-Azobis(4-metHMDB0244704
6. 254_184 CyclopropaneoctancHMDB0250676
6. 256_20111-AminoC19325
6. 258_180 3, 7-DimethylbicyclHMDB0260264
6. 262_182 Dacarbazine HMDB0014989
6. 264_362 Thyrotropin-releaHMDB0259062
6. 276_2513-(2-Furoyl)quinoHMDB0245772
6. 277_231 EglinazirC19102
6. 299_412 LMPK12060045
6. 3_310. 2 Bacillamidin C
6. 303_197 Estreptoquinasa HMDB0258508
6. 307_319 Thalassotalic acid C
6. 311_264 5-HydroxyC17747
6. 318_306 (4E, 6E)-2-(hydroxymethyl)-3-(3-methoxy-3-oxopropyl)deca-4, 6-dienoic acid
6. 319_177 Pelletierine Hydrochloride
6. 32_271. 4-oxo-4-(3-oxodecan-2-ylamino)butanoic acid
6. 325_386 (Z)-7-[(1R, 2R, 3R, 5HMDB0244520
6. 326_292 8-(2-hydroxy-3-methoxy-3-methylbutyl)-7-methoxychromen-2-one
6. 332_154 2-Nonenal, 4-oxo- HMDB0245270
6. 335_164 5-Ethyl-3-methyl-2E, 4E, 6E-nonatriene
6. 341_136 2E, 4Z, 6Z-Nonatrienal
6. 347_163 3-MethylsulfinylpHMDB0006095
6. 348_342 Penicillin K HMDB0256231
6. 353_252 SugetriolC17502
6. 365_198 4-(4-MethylcycloheHMDB0253742
6. 368_220 PentamethylchromarHMDB0256272
6. 375_311 Noberastine HMDB0255678
6. 375_312 Albendazole 2-amirHMDB0248115
6. 377_331 Prizidilol HMDB0256780
6. 378_227 N-Octanoyl-L-homoserine lactone
6. 382_290 5-(2-Chloroethyl)-HMDB0246718

6. 384_1123, 5-Cyclohexadiene HMDB0246048
 6. 384_232 NCGC00381044-0113, 6-diphenylcyclohexane-1,2-diol [IIN-based on: CCMSLIBC
 6. 392_287 N-(3-Methyl-1,1-di HMDB0255486
 6. 392_336 Phenobenz C19090
 6. 394_230 Dibutyl succinate HMDB0251173
 6. 394_292 N(4)-Acetylsulfadi HMDB0244494
 6. 394_305 Atherospe C09347
 6. 396_322 Sulprofos HMDB0258619
 6. 396_360 oscr#22
 6. 402_242 (2S)-2-Amino-4-(2- HMDB0246396
 6. 442_2373-(Cyclohexylaminc HMDB0247339
 6. 445_326 Etomoxir HMDB0252113
 6. 446_322 4-[(2R,5R)-5-(6-An HMDB0257574
 6. 446_327 Diclobutrazol HMDB0251205
 6. 455_235 Norketobemidone HMDB0255743
 6. 465_297 (1R,2E,7R,10E,12S,13S,15R)-12,15-dihydroxy-7-methyl-8-oxabicyclo[11.3.0]
 6. 476_294 3-Undec-1-enylbenz HMDB0260258
 6. 479_214 12-oxo-dodecanoic acid
 6. 483_375 4-(2-(3-(Cyclopent HMDB0249743
 6. 484_325 18-Nitrooctadeca- HMDB0257646
 6. 502_142 Menotrophin HMDB0254444
 6. 503_182 N(2),N(2),N(4),N(6 HMDB0245343
 6. 509_344 [(8S,9S,13S,14S,17 HMDB0258033
 6. 51_292. Trichoderonin HMDB0259176
 6. 518_342 2,3-Dinor-6-keto- HMDB0002277
 6. 521_222 3,5-Diisopropylsal HMDB0246059
 6. 523_297 N-(3-oxododecanoyl) homoserine lactone
 6. 528_310 N-(Dimethylamino) n HMDB0247659
 6. 538_315 Butoctami C12946
 6. 557_232 Atractylenolide I HMDB0248707
 6. 557_237 Biopterin HMDB0000468
 6. 565_226 Cyclo(L-1C20514
 6. 565_3011-[[Z)-[5-(Hydrox HMDB0260010
 6. 577_345 5-Nitroxystearic ε HMDB0246831
 6. 587_332 (2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-[4-(hydroxymethyl)-1-propan-2-ylcyc
 6. 608_185 2-(Diethylamino) et HMDB0244939
 6. 611_158 1-Phenyl-1-cyclohex HMDB0243990
 6. 618_176 5,6,7,8-1C14111
 6. 619_96. Methylenecyclohexε HMDB0254637
 6. 625_301 (+)-Isofebrifugine HMDB0242253
 6. 637_182 (+)-geosmin
 6. 638_562 Cucurbitacin IIa HMDB0246992
 6. 644_415 2,4-dihydroxy-5-methoxy-1'',6'',8''-trimethyldispiro[bis(oxolane)-3,2':5
 6. 65_289. Dyclonine HMDB0014783
 6. 65_426. [(6E,10Z)-10-(acetyloxymethyl)-6-formyl-3-methylidene-2-oxo-3a,4,5,8,9,1
 6. 651_307 Betaxolol HMDB0014341
 6. 651_322 Cytosporone B HMDB0250727
 6. 651_408 2-Naphthalenol, 1- HMDB0259580
 6. 652_359 Lavoltidine HMDB0254182
 6. 652_425 Coelenterazine HMDB0250397
 6. 658_211 Elaekani C10592

6. 659_285 arabinosyl-2-fluor HMDB0248556
6. 66_229. Dihydrojasmonic ac HMDB0033601
6. 66_303. Pyrimidopurinone HMDB0256981
6. 66_314. Fenleuton HMDB0252203
6. 674_352 3-[(E)-3,4-dihydroxy-3,5-dimethylhept-1-enyl]-7,8-dihydroxy-7-methyl-8,8
6. 675_416 Elarofiban HMDB0251734
6. 681_314 (2R,3R,4S,5S,6R)-2-[(2E)-4-ethenyl-2,5-dimethylhexa-2,5-dienoxy]-6-(hydr
6. 69_314. 2S-hydroxy-3-(10Z-tetradecenoyloxy)-propanoic acid
6. 693_315 Decanoylcarnitine HMDB0000651
6. 694_422 1H-2-Benzopyran-6- HMDB0256656
6. 695_392 Penicildione D
6. 696_387 4'-hydroxytrazodor HMDB0061060
6. 701_241 Valeroidi C10869
6. 702_205 Indolelactic acid HMDB0000671
6. 709_305 3-hydroxyoctanoyl HMDB0061634
6. 711_254 2-Acetylamino phenol HMDB0240369
6. 712_250 Nardosinone HMDB0255460
6. 712_412 Asebotoxin HMDB0248654
6. 718_195 [3-(2-Aminopropyl) HMDB0257571
6. 721_226 Pentobarbital HMDB0014457
6. 723_170 Sobrepin HMDB0258357
6. 725_228 Glyphosate C18564
6. 726_312 LMPK12110104
6. 728_316 Emerin HMDB0251772
6. 728_80. 1,3,5-Hexatriene HMDB0251502
6. 729_196 Chrysanthemic Acid, Ethyl Ester
6. 729_215 Pyrimidin C03169
6. 729_228 11-Hydroxy-9-tridecenoic acid
6. 729_315 Pipethiadene HMDB0256582
6. 738_126 2-Octenal HMDB0030961
6. 745_145 Valpromide HMDB0259756
6. 745_306 2,3,5,10,15,17,18, HMDB0255398
6. 753_148 Anethole HMDB0030837
6. 758_272 3-methyl-tetradecanedioic acid
6. 763_134 Indan-1-yl C01710 HMDB0059601
6. 763_294 Pyrifenoxy C18804
6. 766_384 20-Trihydroxy-leukotriene-B4
6. 767_244 Dimethyl (3,3-dimethyl HMDB0247330
6. 767_272 5-methyl-tetradecanedioic acid
6. 772_354 Prostasin HMDB0256860
6. 791_310 (9-Oxo-11-(3-pentyl) HMDB0246689
6. 793_410 Isoforskolin HMDB0253641
6. 797_382 Sarcostir C17770
6. 801_294 NCGC00169318-02! (E)-7-(4-methoxy-5-methyl-6-oxopyran-2-yl)-5-methyloct-6
6. 804_338 18-hydroxy-18-oxo-dinorleukotriene B4
6. 805_436 Polhovoli C09532
6. 806_357 Enecadin HMDB0251807
6. 809_396 PGF2alpha-11-acetate
6. 809_468 3,17-Androstane diol HMDB0010321
6. 817_255 N-decanoyl-homoserine lactone
6. 821_325 (3R)-(3alpha,4alpha) HMDB0260151

6.823_1882-tridecene-4,7-diyal
6.824_17(Aethusin;C08395
6.826_128 Isobutyl acrylate HMDB0253609
6.845_2989'-desmethylgranis HMDB0061061
6.854_292 Lerisetron HMDB0254019
6.862_2143,3'-Diaminobenzic HMDB0245998
6.863_241 NCGC00385536-01! (2E,4E)-N-(1,3-dihydroxy-3-methylpentan-2-yl)-2-methylhe
6.864_326 Chembl4238926 HMDB0256196
6.865_333 Nolomirole HMDB0255699
6.87_363.6-[1-(3,5,5,8,8-Pe HMDB0254073
6.877_303 1-(5-Methoxy-2,3- HMDB0260241
6.891_37(C Mutanamide
6.892_309 N-(7Z-tetradecenoyl)-homoserine lactone
6.898_222 Noruron; C19111
6.903_324 12-oxo-14,18-dihydroxy-9Z,13E,15Z-octadecatrienoic acid
6.907_442 RHODAMINE 6G HMDB0257199
6.909_328 10-Nitrolinoleic ε HMDB0005049
6.91_190. trans-beta-damascenone
6.914_208 Dimethylmethoxy c HMDB0259688
6.92_247. dehydrocostus lact HMDB0250946
6.936_376 7,8,17-trihydroxy- HMDB0247298
6.943_281 N-octanoyl histidine
6.946_306 (9a-hydroxy-3,8a-dimethyl-5-methylidene-2-oxo-4,4a,6,7,8,9-hexahydrobenz
6.955_352 7-[(1R,2R,3R)-3-Hy HMDB0247796
6.957_378 Pentosidine HMDB0003933
6.96_356. NCGC00380990-01! (2E,4E)-12-hydroxy-13-(hydroxymethyl)-14-methoxy-3,5,7-t
6.968_311 2-trans,4-cis-Decε HMDB0013325
6.978_172 4-Amino-2,2,6,6-tε HMDB0246342
6.978_360 (8S,9S,10R,13S,14ε HMDB0246907
6.993_44(C Exiguaflavanone G
7.012_299 5-Amino-N'-[2-(2-c HMDB0253825
7.013_270 9-Anilinoacridine HMDB0247580
7.013_45(C Chaksine;C09940
7.015_218 Germacrone HMDB0252704
7.016_40(C Atractylc C17860
7.017_128 Azulene HMDB0248822
7.018_14(C 5-Phenyl- C17717
7.018_182 1,2-Diphenylethane HMDB0244093
7.02_349. Pancopride HMDB0256106
7.023_408 N-(9,12-octadecadienoyl)-glutamine
7.033_268 Dansyl chloride HMDB0250846
7.042_338 Bacillamidin D
7.061_246 Geranylhy C10793
7.064_268 0-(N-Phthalimido) ε HMDB0255867
7.064_279 Graveolir C10689
7.065_247 1-Nitropyrene HMDB0243967
7.068_168 2-Methyl C20243
7.068_348 Sebacyl-L-carniti HMDB0240726
7.07_302. Terizidone HMDB0258834
7.081_296 10-Deoxyn C11993
7.082_296 Graphinor C09674

7.089_396 NCGC00347750-02! (E, 2S, 3R, 4R, 5S)-4-acetyloxy-2-amino-3, 5, 14-trihydroxyico
 7.095_418 Phyllanthin HMDB0256511
 7.105_266 Nevirapine HMDB0014383
 7.105_312 13-L-Hydroperoxyli HMDB0003871
 7.114_247 Methoxetamine HMDB0254541
 7.123_251 Dihydroalprenolol HMDB0251293
 7.134_208 4-Heptyloxyphenol HMDB0246434
 7.135_216 Isofuranodiene HMDB0253643
 7.135_338 Idebenone HMDB0253376
 7.143_346 oscr#20
 7.146_424 CAPERATIC ACID
 7.148_176 3, 5, 7-Trimethyl-2E, 4E, 6E, 8E-decatetraene
 7.148_386 Rangiformic acid
 7.155_274 (4aS)-6, 7-dihydroxy-1, 1, 4a-trimethyl-3, 4, 10, 10a-tetrahydro-2H-phenanthre
 7.159_184 r-limonene HMDB0257077
 7.162_98. Hexenal HMDB0253154
 7.164_236 Heptyl p-C14718
 7.164_298 Esmolol HMDB0014333
 7.168_492 Sordarin HMDB0242737
 7.173_257 N-lauroyl glycine
 7.173_412 3-Deoxycaryoptinol
 7.175_266 (8aR, 12S, 12aR)-12-hydroxy-4-methyl-4, 5, 6, 7, 8, 8a, 12, 12a-octahydro-1H-3-be
 7.185_392 N'-(6-Oxo-5-prop- HMDB0256069
 7.193_336 Ethyl 2-[2-(diethy HMDB0258088
 7.193_402 Cinitapride HMDB0015698
 7.199_390 Mevastatin
 7.199_428 Lotrafiban HMDB0254173
 7.202_424 HT-2 Toxin HMDB0253219
 7.203_236 KOBUSONE
 7.206_328 albocycline
 7.209_417 Sphingofungin E
 7.209_448 Glutathic C16566
 7.213_454 Lunarine
 7.216_84. Tetrahydrofuranyl n HMDB0245228
 7.217_220 SANTALOL HMDB0257480
 7.22_311. 3-oxo-C13-HSL
 7.222_330 (9, 12, 13-TriHOME HMDB0004708
 7.227_136 (+)-Limor C06099 HMDB0003375
 7.241_290 4-Androstene-3, 17- HMDB0246370
 7.242_287 Valproylcarnitine HMDB0259757
 7.242_448 N-[5-Methyl-8-(4-n HMDB0258014
 7.245_356 2E, 4E, 6E, 8E, 10E, 12E, 14E, 16E, 18E, 20E, 22E. 24E, 26E-hexacosadodecaenal
 7.246_386 (+)-Eudes C10561
 7.246_408 Melatonin glucuror HMDB0060830
 7.247_328 9-hydroperoxy-12, 13-epoxy-10-octadecenoic acid
 7.248_406 Benzoyl-DL-arginir HMDB0257846
 7.249_404 bhos#26
 7.25_506. Mucronine C10009
 7.251_322 (5E)-2-heptyl-3, 4, 7-trihydroxy-2, 3, 4, 7, 8, 9-hexahydrooxecin-10-one
 7.253_226 Diethylamino nonar HMDB0260404
 7.254_268 Petroraspaillyne B2

7.255_322 Decylubiquinone HMDB0250928
7.256_370 N-[1'-(Aminocarbonyl)-2,3-dimethyl-2E,4E,6E,8E-decatetraene]acetamide HMDB0255030
7.257_190 7-Ethyl-3,5-dimethyl-2E,4E,6E,8E-decatetraene
7.259_174 Capillanone C17783
7.259_209 Bamethan HMDB0248857
7.26_192. Ibufenac HMDB0253333
7.26_231. Fenfluramine HMDB0252200
7.266_326 1-[2,3-Dimethyl-2-oxo-1-phenylethyl]piperazine HMDB0247708
7.268_255 3-hydroxy-5,5,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-2-carboxylic acid
7.269_402 Telocinobufagin HMDB0258793
7.27_444. Bufotalin HMDB0249432
7.271_484 LMST05010036
7.272_346 Sorbitan laurate
7.274_350 Thromboxane A3 HMDB0259049
7.276_224 NCGC00380330-0112-(6-methyl-7-oxooctyl)-2H-furan-5-one [IIN-based: Match]
7.276_226 1,3-Butyleneglycol HMDB0244160
7.277_270 (10S)-Juvicic acid C16506
7.284_224 tetradec-5-ynoic acid
7.285_284 Tetranorprostanediol HMDB0258926
7.286_254 Prohydrocinnonolide C18538
7.286_306 7-beta-Hydroxyepibatidine HMDB0259631
7.286_342 2,3-Dinor-TXB1 HMDB0245413
7.286_348 trihydroxy-4-pregnane HMDB0259218
7.286_452 Sarcoehrendin I
7.287_312 Arteether HMDB0242731
7.287_340 Terguride HMDB0258831
7.288_266 Juvenate HMDB0253743
7.288_442 L-Ascorbic acid C20340
7.288_460 5beta-hydroxybufotalin
7.292_212 (Z)-7-Dodecenyl formate
7.292_262 Homosalate HMDB0253209
7.295_337 Istamyacin C17982
7.296_280 12-Hydroxyheptadecanoic acid HMDB0244447
7.296_334 Dihydroxy (3Alpha,12Alpha)Pregnan-20-One
7.296_410 Sterol 3-C03641
7.297_248 (4E,7E,10E,13E)-Heptacosane HMDB0253125
7.299_374 1-dimethylarsinoyl-octadecane
7.305_648 1-(O-alpha-D-galactopyranosyl)-(1,3R,27S,29R)-triacontanetetrol
7.307_400 bonactin
7.31_229. Xestoaminol C
7.315_355 4-(4'-Chlorobenzyl)pyridine HMDB0253775
7.317_70. 2-Methyl-1-butene HMDB0245210
7.332_197 N-allyldecylamine HMDB0255079
7.342_659 Aridanin; C08922
7.351_488 1-Ethyl-5-(5-piperidyl)pyridine HMDB0258323
7.352_104 Styrene HMDB0034240
7.352_204 alpha-Caryophyllene HMDB0248192
7.352_264 3-(3-Hydroxy-4-methyl-2-pyrone-5-yl)propanoic acid HMDB0246020
7.352_266 (E)-5-(4-methoxy-5-methyl-6-oxopyran-2-yl)-3-methylhex-4-enoic acid
7.352_282 Bis(2-methoxyethyl)amine HMDB0249246
7.352_360 ascr#22

7.352_386 eudesmin
 7.353_355 5-[(E)-3-hydroxybut-1-enyl]-4-[4-[(E)-3-oxobut-1-enyl]anilino]oxolan-2-ol
 7.353_416 6-Amino-ε-C20773
 7.354_284 karalicin
 7.355_237 Ambazone HMDB0248279
 7.356_228 Antigastrin HMDB0248486
 7.357_454 Hydroxy thaxtomin A
 7.358_382 Licoricorin C17765
 7.358_431 Tropolone A HMDB0255800
 7.358_461 21-hydroxy-10-methoxy-1,4,14,19,19-pentamethyl-2,7,18-trioxapentacyclo[1.3.0.0^{2,7}.0^{4,14}.0^{19,19}.0]hept-1-ene
 7.359_229 ent-Lamivudine HMDB0251826
 7.359_384 schisandrin C HMDB0258167
 7.363_481 LMPK12010431
 7.364_429 Sarpogrelate HMDB0257502
 7.366_313 N-(4-Methylphenyl)acetamide HMDB0255014
 7.366_828 Triglutamate folate HMDB0259214
 7.368_300 Tetranor-PGF1α
 7.373_236 2-hexyl-5-propyl-resorcinol
 7.373_240 2,5-dimethyl-2E-tridecenoic acid
 7.375_649 OHODiA-PE
 7.376_241 (4E,6E,d14:2) sphingosine
 7.376_405 Aminopentol HMDB0248328
 7.377_256 Lyngbic acid
 7.392_302 (1R,4Ar,7S)-1,4a,7-trimethyl-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid HMDB0242332
 7.397_401 (2S,3R,4R)-2-Amino-3,4-dihydroxybutanoic acid HMDB0242536
 7.399_352 N6-goshuyoyl lysine
 7.401_452 2-(3-(4-((1H-Indazol-3-ylidene)amino)phenyl)butyl)propanoic acid HMDB0247641
 7.404_188 Plumbagin HMDB0256646
 7.41_330. Dehydroepiandrosterone HMDB0250951
 7.411_342 Ergonovir C07543 HMDB0015383
 7.412_334 3,4-Dihexylphthalic anhydride HMDB0258114
 7.414_373 Dodecanedioylcarnitine HMDB0013327
 7.417_304 16β-Hydroxydehydroepiandrosterone HMDB0244758
 7.42_231. Suberylglycine HMDB0000953
 7.424_352 Acetylportentol
 7.426_338 NCGC00380990-01 (2E,4E)-12-hydroxy-13-(hydroxymethyl)-14-methoxy-3,5,7-trimethyl-2,3,4,5-tetrahydro-2H-pyridine-2-thione
 7.428_263 Cytidine, 5-chloro-2'-deoxy-5'-O-(3-thiophenyl)thio- HMDB0252181
 7.428_324 2'-Deoxy-5'-O-(3-thiophenyl)thio-2'-thiothymidine HMDB0251638
 7.428_397 5-(4-acetyloxy-3-hydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydronaphthalen-1-yl)propanoic acid
 7.432_296 methyl 2-[4-ethenyl-2,6-dihydroxy-3-(3-hydroxyprop-1-en-2-yl)-4-methylcyclohexane-1-carboxylate] HMDB0251638
 7.432_516 LMST01031078
 7.435_205 N-Desethienylethyl-1,2,3,4-tetrahydroquinoline-5-carboxamide HMDB0060843
 7.438_390 5-chloro-2,4-dihydroxy-6-methyl-3-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl]propanoic acid
 7.44_262. 2-Hydroxy-1,2,3,4-tetrahydroquinoline-5-carboxamide C16264
 7.443_206 β-Carotene C20157 HMDB0012897
 7.445_222 3-(3'-Methyl-2-thiophenyl)propanoic acid C17215
 7.447_240 Mycinonic acid III
 7.453_270 (E)-2-decylpent-2-enedioic acid
 7.455_382 Tetramethylchromarolone HMDB0258916
 7.459_428 2-glyceryl-PGF2α
 7.461_278 5-(hexa-5-en-1,3-dien-1-yl)-5'-(prop-1-en-1-yl)-2,2'-bithiophene

7.461_382 NCGC00180835-03!2-[5-[2-[2-[5-(2-hydroxybutyl)oxolan-2-yl]propanoyloxy]p
7.465_163 Normephedrone HMDB0255719
7.469_238 6-Chloro-C21867
7.47_185. Dodecylamine HMDB0251571
7.472_329 Commendamide
7.473_224 Aurantoic acid
7.474_460 (1R, 3E, 5R, 7S, 11R, 12R, 13S, 14S)-1, 13-bis(acetyloxy)-3, 6, 6, 14-tetramethyl-1
7.474_478 Diflucortolone val HMDB0251261
7.475_413 Isoconazole HMDB0253623
7.48_462. Dokdolipid A
7.486_162 4, 10-undecadiynal
7.495_318 (2E, 4E, 8E)-7, 13-dihydroxy-4, 8, 12-trimethyltetradeca-2, 4, 8-trienoic acid
7.504_221 N, N, O-Tridesmethyl HMDB0060850
7.509_408 [6, 10a-dihydroxy-4-(hydroxymethyl)-4, 7, 11b-trimethyl-9-oxo-1, 2, 3, 4a, 5, 6,
7.519_374 [(1R, 2S, 3S, 4R, 4aS)-2, 3-dihydroxy-3, 4a, 8, 8-tetramethyl-4-[(E)-3-oxobut-1-
7.524_346 Spenolimyc17970
7.53_313. Decenoylcarnitine HMDB0250918
7.531_320 Arginylphenylalanine HMDB0257190
7.542_301 (2R, 3R)-2-Aminoocit HMDB0242634
7.55_309. Methadone C07163 HMDB0014477
7.566_254 3-hydroxy-1a, 5-bis(hydroxymethyl)-5, 6b-dimethyl-1, 3, 3a, 4, 6, 6a-hexahydroc
7.57_298. QUINALPHOS HMDB0257033
7.571_404 6|A-Hydroxy-7|A-(1 HMDB0246665
7.573_276 teadenol A
7.577_466 5alpha-Androstan-1 HMDB0246662
7.581_404 bhas#26
7.583_242 6-oxo-tetradecanoic acid
7.59_386. 2-[5-[2-[2-[5-(2-hydroxypropyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-
7.593_288 3, 12-dihydroxy palmitic acid
7.595_356 Prostaglandin F1a HMDB0002685
7.597_285 Spisulosine HMDB0258433
7.598_300 Heptadecanedioic acid
7.598_432 Pseudolaric acid-F HMDB0242611
7.599_428 1(3)-glyceryl-PGF2alpha
7.601_328 9-epi-9-F1c-PhytoP
7.601_388 ascr#26
7.607_245 Curium HMDB0250595
7.608_350 (5S, 12R, 18R)-5, 12, HMDB0257670
7.609_188 Irene HMDB0253579
7.612_238 jaeschkeanadiol
7.623_307 Cletoquine HMDB0250320
7.624_269 Zedoarondiol HMDB0036448
7.624_323 Tetranor-(+)-S-14 HMDB0258924
7.625_251 (4S, 5Z, 6S)-4-(2-methoxy-2-oxoethyl)-5-[2-[(E)-3-phenylprop-2-enoyl]oxyet
7.625_400 2-(4-Allyl-2, 6-din HMDB0030828
7.63_287. C17 Sphinganine
7.631_466 N-(1-((Cyanomethyl HMDB0245747
7.634_282 Fumagillol HMDB0252515
7.644_288 (8S, 9R, 10S, 13S, 14S HMDB0260183
7.645_339 Bursopoietin HMDB0249448
7.646_271 N-LAUROYLSARCOSINE HMDB0255165

7.669_2486-Chloro-2,3,4,9-t HMDB0246699
7.684_358 Amopyroquine HMDB0248347
7.685_134 Tert-butylbenzene HMDB0258847
7.685_258 3,7-Epoxy caryophyllan-6-one
7.686_307 Dihydrocæ C16952 HMDB0038457
7.691_120 2-Ethyltc C14572
7.703_444 Nitromifene HMDB0255655
7.71_274 Nandrolone HMDB0002725
7.715_122 Phenetole HMDB0252021
7.719_228 NCGC00385536-01! (2E,4E)-N-(1,3-dihydroxy-3-methylpentan-2-yl)-2-methylhe
7.728_254 Methyl 7-oxo-11E-tetradecenoate
7.728_438 (-)-Fusicoplagin A
7.734_384 4,4'-Bis(2-hydroxy HMDB0248812
7.736_448 icos#3
7.739_387 2-Hydroxymyristoyl HMDB0013166
7.74_268 2-(N-butylformamido)-N-cyclohexylbutanamide
7.743_420 1-Piperidinyloxy, HMDB0248372
7.743_426 1(3)-glyceryl-PGH2
7.744_288 N-(dodecanoyl)-homoserine lactone
7.746_352 15-Keto-prostaglar HMDB0004240
7.748_248 Heptadecæ C16343
7.752_462 Trichomonacid HMDB0252900
7.753_242 7-Oxotetradecanoic acid
7.754_431 Sphingofungin D
7.766_196 4Z-Tridecenal
7.767_268 methyl palmitoleate
7.773_258 (2S,6R,8aS)-6-(2-hydroxypropan-2-yl)-8a-methyl-4-methylidene-1,2,3,4a,5,
7.775_424 Adifoline C09020
7.776_357 N-palmitoyl threonine
7.788_298 8E-Heptadecenedioic acid
7.788_527 Dihydropi C15755
7.792_300 8-methyl-hexadecanedioic acid
7.796_402 2-(4-(3-(4-Acetyl- HMDB0247399
7.797_351 N-(3-oxo-9Z-hexadecenoyl)-homoserine lactone
7.802_214 Monolinuron HMDB0254863
7.802_278 6-Nitrochrysene HMDB0247097
7.803_242 2-(4-Amino-2-chlor HMDB0246686
7.805_222 7-propyltheophylline
7.806_218 2-Hydroxydecanedic HMDB0000424
7.818_444 2-glyceryl-6-keto-PGF1alpha
7.82_276. shogaol
7.821_446 Methyl (2R,3R)-2-[HMDB0247861
7.823_220 Precocene II HMDB0256742
7.823_298 Nvp dpp 728 dihydr HMDB0255823
7.827_477 Etimicin HMDB0252101
7.838_311 N-tetradecanoyl-homoserine lactone
7.858_358 Pracinostat HMDB0256722
7.865_310 (E)-4-[(1R,2S,3S,4R,8aS)-2,3,4-trihydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,
7.867_431 (E,2S,3R,4R,5S)-4-acetyloxy-2-amino-3,5,14-trihydroxyicos-6-enoic acid
7.873_296 (1R,2S,7R,9R,10R,11 HMDB0260070
7.875_118 beta-Methylstyrene HMDB0249142

7.875_132 4H-1-Benzopyran HMDB0246704
 7.875_243 4-Amino-1-[(2R,5R)HMDB0257848
 7.875_280 2-hydroxy-4-(hydroxymethyl)-6-(1-hydroxy-3-methylbut-2-enyl)-3-[(E)-prop
 7.875_294 7-methoxy-6-(1,2,3-trihydroxy-3-methylbutyl)chromen-2-one
 7.875_412 Bisindolylmaleimide HMDB0249269
 7.875_414 NCGC00179793-02! 3,4-dimethyl-2,5-bis(3,4,5-trimethoxyphenyl)oxolane [IIN
 7.875_459 methyl 8-hydroxy-4,5,7,10,14,14-hexamethyl-6,17-dioxo-16-oxapentacyclo[1
 7.875_530 (2E,4E)-1-[(2R,6S,14S,22S,25R)-25-(3,3-dimethyloxiran-2-yl)-15-methyl-1,
 7.876_106 Ethylbenzene HMDB0059905
 7.876_164 Sorbitan HMDB0258390
 7.876_452 Chamuvaritin
 7.877_292 17beta-HyC14911
 7.88_171. Chrysanthemyl Alcohol
 7.88_251. cycloguanil HMDB0060974
 7.881_196 Stilbene oxide HMDB0258501
 7.882_166 4E,6E-undecenal
 7.882_219 3-(1-Propyl-3-piperidyl)propanoic acid HMDB0245975
 7.886_345 icos-19-ene-1,2,4-triol
 7.903_224 (2R,5S,8R)-2,8-Dimethyl-2,8-dioxabicyclo[2.2.1]heptane HMDB0257819
 7.91_248. 8-Cyclopentyl-1,3-dioxane HMDB0247431
 7.91_291. s-Triazine, 2-amino HMDB0248038
 7.921_401 [4,5-dihydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-5,6,7,8a-tetrahyd
 7.925_402 ACTINONIN
 7.927_314 9,10-DHOME HMDB0004704
 7.928_353 N-(3-oxo-hexadecanoyl)-homoserine lactone
 7.944_307 Pumiliotoxin A HMDB0256924
 7.947_299 N-(3-hydroxy-dodecanoyl)-homoserine lactone
 7.955_283 N-dodecanoyl-S-homoserine lactone
 7.967_315 NCGC00380344-01! (2E,4E)-N-[2-(4-hydroxyphenyl)ethyl]dodeca-2,4-dienamide
 7.967_330 9,10,13-TriHOME HMDB0004710
 7.968_655 20,21-DiHOME C20595
 7.97_202. alpha-Curc C09649
 7.97_400. Murolic acid
 7.971_258 NCGC00169702-02! (5R)-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)decan-3-one
 7.974_340 3-(4-(4-Chlorophenyl)but-3-en-1-yl)propanoic acid HMDB0253858
 7.975_340 [5-acetyloxy-3-(hydroxymethyl)-2-oxo-6-propan-2-ylcyclohex-3-en-1-yl] 3-
 7.991_213 Tetradecylamine HMDB0258887
 7.996_313 LMSP01080031
 8.004_257 7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-2,3,4,5,6,7,8,8a-octahydronaphtha
 8.005_437 (1S,4S,5R,9S,10R,13R,14R)-14-hydroxy-5,9-dimethyl-14-[[3-methylbutanoyl
 8.01_303. Bornaprolol HMDB0249349
 8.01_313. (+)-Prosc C10167
 8.011_270 2-Hydroxydodecyl n HMDB0245155
 8.011_328 Desloratadine HMDB0015102
 8.011_424 N-(17-hydroxy-9,12-octadecadienoyl)-glutamine
 8.017_344 1,2-Dioctanoylglycine HMDB0244086
 8.018_259 Nortilidine HMDB0255754
 8.019_233 N,O-Didesmethyltriazine HMDB0060851
 8.019_318 5-HEPE HMDB0005081
 8.019_383 N-(3-hydroxy-octadecanoyl)-homoserine lactone
 8.024_208 Caryophyllene [T(-)]

8.027_427 PGF2alpha-dihydroxypropanylamine
8.028_267 Allopumil C20034
8.029_357 5-hydroxypropafenc HMDB0060988
8.03_250. 5-Methylc C02376 HMDB0002894
8.05_196. 6-dodecynoic acid
8.05_264. Heptadeca-2, 4, 6-tri HMDB0253100
8.064_3673, 5-Tetradecadienol HMDB0013331
8.067_335 9-hydroxy-1, 4a-dimethyl-7-propan-2-yl-2, 3, 4, 9, 10, 10a-hexahydrophenanthrene
8.068_325 Cycloxydi C10913
8.076_432 Buclizine HMDB0014498
8.077_282 Tryptophan butyl ester
8.079_280 Deepoxy-deoxynivalin HMDB0250929
8.08_294. Tutin; C09570
8.08_459. Militaric C12333
8.084_308 ent-9-L1-PhytoP
8.086_392 Auda HMDB0248721
8.086_404 N-((1, 2, 3, 5, 6, 7-Hexa HMDB0254364
8.088_250 (+)-12-(Z) C15464
8.088_458 LMST01031185
8.103_340 Gallicynoic acid F
8.103_386 Olodaterol HMDB0255957
8.109_237 N,N-di-n-propylidol HMDB0255249
8.109_262 5-((Z)-undec-3-en-1-yl)resorcinol
8.114_269 SPI_270.2429_14.9
8.118_522 Metabolite M6 HMDB0061034
8.119_506 (2R, 3S, 4S, 5S, 6R)-2-[[7-hydroxy-4-[(Z)-5-hydroxy-3-methylpent-3-enyl]-4a,
8.12_282. 6-Oxabicy C15465
8.12_400. oscr#27
8.124_278 Dibutyl r C14214 HMDB0033244
8.124_444 1(3)-glyceryl-6-keto-PGF1alpha
8.125_367 Tetradecadienoyl c HMDB0258882
8.125_435 Ricolinostat HMDB0244543
8.125_450 Neoglabrescin A
8.126_371 Myristoylcarnitine HMDB0254979
8.126_435 Epanorin
8.126_446 Solacetal B
8.126_449 N-Ethyl-N-(6, 6-dim HMDB0255477
8.127_317 dehydroak C12078 HMDB0061925
8.127_326 2-oxophytanic acid
8.127_357 N-(8-Amino-1-carb HMDB0247737
8.127_419 Roquefort C22171
8.127_447 Hydromorphone-3-gl HMDB0061144
8.127_4514-Hydroxyvalsartan HMDB0013848
8.128_4514-Hydroxypropranolol HMDB0247679
8.128_462 Retinyl beta-glucoside HMDB0010340
8.128_520 Cyasterone HMDB0250618
8.128_656 3-O-(2-O-(2E-decenoyl)-alpha-L-rhamnopyranosyl)-3-hydroxydecanoic acid
8.13_250. Triton X-100 HMDB0259285
8.13_276. Octadeca-2, 4, 6, 8-t HMDB0255898
8.13_328. N6-lauroyl lysine
8.13_340. 15S-HpEDE

8. 131_392 VIPROSTOL HMDB0259834
 8. 135_293, 7-Dimethyl-9-(2, HMDB0250571
 8. 137_348 Carbocyclic thromb HMDB0249633
 8. 138_566 Venustone
 8. 138_576 Foliandrin HMDB0252427
 8. 139_290 (E, E, E)-Geranylger HMDB0247803
 8. 14_370. Glycerylmonooleate HMDB0252857
 8. 142_460 Petrosaspongiolide HMDB0256357
 8. 143_256 4-keto pentadecanoic acid
 8. 144_294 (2E, 4E)-Nonadeca-2 HMDB0242705
 8. 148_358 4-(N-Maleic C13678
 8. 149_188 Nonate HMDB0011717
 8. 151_298 Norethindrone
 8. 152_315 4-hydroxy-8cis-sphingene
 8. 153_214 Metribuzin HMDB0254685
 8. 155_450 methyl (Z)-6-(3, 7- HMDB0254559
 8. 155_460 Prednisolone hemis HMDB0245744
 8. 157_592 1, 25-Dihydroxyvit HMDB0244154
 8. 158_249 N-Desmethyltramad HMDB0061007
 8. 163_379 N-(3-oxo-11Z-octadecenoyl)-homoserine lactone
 8. 171_312 (9Z, 12E)-15, 16-dihydroxyoctadeca-9, 12-dienoic acid
 8. 175_352 1-Monolinolenoyl-ri HMDB0252853
 8. 18_355. N-[3-(1, 3-Dioxois HMDB0259635
 8. 184_401 NCGC00385827-01!7-[[(1S, 4aS, 6S, 8aR)-6-hydroxy-5, 5, 8a-trimethyl-2-methyl
 8. 188_357 Bacillamidin B
 8. 196_227 Pentadecylamine HMDB0243828
 8. 201_339 (1R, 4aS, 5R, 8aS)-5-(5-hydroxy-3-methylpentyl)-1, 4a-dimethyl-6-methylidene
 8. 205_331 Acid Ar HMDB0259636
 8. 206_338 1H-Imidazole-4-car HMDB0248071
 8. 207_333 Andolast HMDB0248393
 8. 207_359 Trehalose C01083 HMDB0000975
 8. 217_353 Anandamide (20:1, n-9)
 8. 222_396 methyl 8-[3, 5-epidioxy-2-(3-hydroperoxy-1-pentenyl)-cyclopentyl]-octanoa
 8. 226_309 Dicyclomine HMDB0014942
 8. 23_240. (1R, 2R)-3-oxo-2-pentyl-cyclopentanebutanoic acid
 8. 23_264. Octadeca-9, 12-dier HMDB0247717
 8. 23_380. LMST04060006
 8. 234_2512, 4-Dodecadienamic HMDB0259472
 8. 234_426 2-glyceryl-PGE2
 8. 237_428 (2R, 2' R, 4a' S, 6' S, 7' R, 8a' S)-7-formyl-4, 7'-dihydroxy-6-(hydroxymethyl)-2' ,
 8. 241_415 3-Hydroxyhexadecar HMDB0013336
 8. 244_397 Hexadecenoylcarnit HMDB0253127
 8. 246_398 TRPM8 antagonist HMDB0259304
 8. 25_290. Octyl 4-methoxycir HMDB0061861
 8. 255_341 N-(1, 3-Dihydroxyoc HMDB0247781
 8. 261_194 Oxidized C03527
 8. 266_233 Meptazinol HMDB0254458
 8. 269_304 2-Hydroxyestriol HMDB0245157
 8. 3_269. 1Declopramide HMDB0250921
 8. 3_285. 1Letrozole C08163 HMDB0015141
 8. 301_300 Roccellic Acid

8. 612_35 N-(6-Aminopyridin- HMDB0256368
8. 614_22 9-Tetradecenoic ac HMDB0258881
8. 615_24 C14 sphingosine
8. 62_211. 211A Decahydroquinoline cis
8. 627_27 3-(7'-Met C17231
8. 632_35 Ferutinin HMDB0252237
8. 632_43 Tris(2-ethylhexyl) HMDB0259278
8. 638_52 C22-epi-Hippurin-1
8. 64_372. Cesamet HMDB0249827
8. 651_52 Hemiasterlin HMDB0253082
8. 652_3014-[(4-Aminophenyl) HMDB0252507
8. 653_19 Dodecanamide HMDB0251566
8. 655_33 1-(2-methylpropylidene)-4-(propan-2-yl)-1H, 2H, 3H, 4H, 6H-piperazino[2, 1-b]
8. 659_23 Khellin C09010 HMDB0253797
8. 659_35 3-hydroxydodecanoyl HMDB0061638
8. 659_53 Uncariursanic acid
8. 661_39 (2-Acetyloxy-3-hy HMDB0242459
8. 663_41 Heptadecanoyl carr HMDB0006210
8. 663_414 ascr#29
8. 667_26 Sclareol oxide HMDB0258180
8. 667_29 Carbinoxamine HMDB0014886
8. 667_45 Byrsonic acid
8. 677_40 Androstane-3, 17-di HMDB0249623
8. 679_44 ascr#33
8. 685_23 C2-Gonen HMDB0245136
8. 697_35 Pantheric Acid A
8. 704_32 L-2-Hydro C02982
8. 706_42 isopropyl unoprost HMDB0253677
8. 709_31 10, 11-dihydroxy stearic acid
8. 712_35 Trioctylamine HMDB0259251
8. 713_39 latrunculin B HMDB0253990
8. 714_47 triterpenoids HMDB0259282
8. 723_38 8-(3, 4-Dimethoxypl HMDB0244693
8. 727_36 Propantheline HMDB0014920
8. 729_29 Phoxim HMDB0256498
8. 729_82. Cyclohexene HMDB0250655
8. 731_38 Eszopiclone HMDB0014546
8. 735_34 N-Acetylsphingani HMDB0249513
8. 736_29 Spiroxamine HMDB0258432
8. 736_39 9alpha-Fl C14638
8. 741_19 Sodium or C19298
8. 741_26 Mebeverine alcohol HMDB0254390
8. 741_33 C4-(2, 6-Dimethylhe HMDB0260274
8. 741_43 3alpha, 7alpha, 12alpha-Trihydroxy-5beta-23E-cholestan-26-oic acid
8. 742_42 Gallamonum HMDB0252596
8. 744_35 monoolein
8. 767_34 trans-2-Dodecenoyl HMDB0013326
8. 772_46 Scymnol HMDB0258186
8. 773_43 Kurarinone HMDB0253834
8. 783_44 Neotokorogenin
8. 794_54 Milbemycin beta1 HMDB0254727

8. 796_49 Homaline; C10599
8. 799_36 FAHFA (10:0/3-0-12:1 (5Z)
8. 804_18 Isopropyl 4-hydroxy HMDB0253675
8. 806_36 2alpha, 3epsilon C15322
8. 806_44 3-Epilupeol
8. 811_42 Cholic Acid, Methyl Ester
8. 838_29 13-OxoODE HMDB0004668
8. 844_27 bakuchiol HMDB0248849
8. 845_34 Pexacerfont HMDB0256359
8. 846_41 Eplerenone HMDB0014838
8. 848_38 methyl 9-butylperoxy-10, 12-octadecadienoate
8. 85_208. 8E, 10Z-Tetradecadienal
8. 855_30 2-[2-(4-Nonylphenyl) HMDB0255709
8. 856_32 Avocadoene 1-acetate HMDB0031043
8. 858_30 Clavepictine B
8. 858_40 (2S)-2-phenyl-7-[(2S, 3R, 4S, 5S, 6R)-3, 4, 5-trihydroxy-6-(hydroxymethyl) oxan
8. 859_33 Difucol Hexamethyl Ether
8. 862_55 Integerre C10006
8. 864_37 LITHOCHOL-11-ENIC ACID
8. 869_43 Varanic acid HMDB0002195
8. 871_29 Epiandrosterone
8. 871_36 Clinprost HMDB0250326
8. 871_60 00V-PG
8. 874_27 2, 3-Dihydroxypropyl HMDB0245396
8. 878_26 Cryptophycin C10139
8. 879_32 15beta-Hydroxydescurvone HMDB0060707
8. 885_48 (1R, 3S, 5Z)-5-[(2Z) HMDB0260077
8. 89_636. Fasciculic acid B HMDB0036438
8. 896_29 N, N-Dimethyloctadecane HMDB0255266
8. 902_39 N-Hexanoylsphingosine HMDB0249517
8. 906_55 Vecuronium HMDB0015432
8. 907_56 Vitamin D3 glucoside HMDB0259846
8. 913_22 Xestoaminol B
8. 913_47 LMST01031102
8. 92_276. (3R)-10, 13-Dimethyl HMDB0246254
8. 921_40 1, 2-Didecane C03199
8. 924_61 Phorbol 12-myristate HMDB0244744
8. 927_22 6-Acryloyl-2-dimethyl HMDB0247971
8. 927_35 2-(2-hydroxybut-3-en-2-yl)-3a, 6, 6, 9a-tetramethyl-2, 4, 5, 5a, 7, 8, 9, 9b-octah
8. 93_284. LYNESTRENOL HMDB0254258
8. 933_31 7-(2-hydroxypropan-2-yl)-1, 4a-dimethyl-2, 3, 4, 9, 10, 10a-hexahydrophenanthr
8. 934_34 N-palmitoyl serine
8. 938_30 3beta-Hydroxycholesterol C22103
8. 941_28 Tetradecylglycidate HMDB0258888
8. 943_31 17-Propyl C14933
8. 943_38 Misoprostol HMDB0015064
8. 944_46 (1S, 2S, 6R, 15S, 16R) HMDB0260098
8. 949_38 3-oxo-tetracosanoic acid
8. 95_438. 1alpha, 25-dihydroxy-26, 27-dimethyl-20, 21, 22, 22, 23, 23-hexadehydrovitamin
8. 954_21 Tridecanamide
8. 958_37 13, 14-dihydroxy-docosanoic acid

8.96_448. [(2E, 6Z, 10Z)-7, 11-bis(acetyloxymethyl)-3, 15-dimethylhexadeca-2, 6, 10, 14-t
8.965_506 Penicisteroid A
8.965_514 Butyryl trihexyl c HMDB0247498
8.965_536 Turkesterone 22-acetonide
8.969_428 PE (0:0/14:0)
8.969_558 3-O-alpha-L-rhamnopyranosyl-3-hydroxy-5Z-tetradecenoyl-3-hydroxydecanoic
8.97_358. Rislenemdaz HMDB0257242
8.973_257 Lauric isopropanolamide
8.974_438 27-Nor-cholestane-pentol
8.979_296 Methyl octadec-11- HMDB0254604
8.992_298 [5-hydroxy-3-(hydroxymethyl)-2-oxo-6-propan-2-ylcyclohex-3-en-1-yl] 3-me
8.992_302 NCGC00169348-03! (3Z)-3-[[5-(2-methylbut-3-en-2-yl)-1H-imidazol-4-yl]meth
8.992_316 oscr#15
8.992_330 AB-Pinaca HMDB0247743
8.993_308 Delpazolid HMDB0250974
9.005_490 Osimertinib HMDB0248778
9.009_228 (E, E)-2, 4-Decadienoic isobutylamide
9.016_430 Bicalutamide HMDB0015260
9.017_432 (1S, 3R, 5Z)-5-[(2E) HMDB0260101
9.017_518 Chletric acid
9.029_516 (Z)-2-((3R, 4S, 8S, 9S)- HMDB0260210
9.036_574 Phorbol-12-monomyr HMDB0256457
9.04_454. Testosterone buci HMDB0258857
9.043_458 Arachidyl carniti HMDB0006460
9.053_324 (2R, 4aR, 7S, 8S, 8aR)-8-[(Z)-5-hydroxy-3-methylpent-3-enyl]-4, 4, 7, 8a-tetra
9.054_286 (8R, 9R, 10R, 13S, 14S) HMDB0257608
9.055_436 (3beta, 5alpha, 12beta) HMDB0244290
9.062_467 Buprenorfi C08007 HMDB0015057
9.065_271 Delmopinol HMDB0250973
9.071_278 (6E)-2, 6, 10-trimethyldodeca-6, 11-diene-2, 3, 10-triol
9.073_466 Certonardosterol K
9.081_368 Octadecyl fumarate
9.081_428 Piriprost HMDB0256603
9.087_530 Acinospesigenin A
9.091_404 1, 25-Dihydroxy-19- HMDB0244153
9.091_420 6-Ethylchenodeoxy HMDB0247056
9.092_346 3-[(Z)-heptadec-10-enyl]benzene-1, 2-diol
9.092_451 Cytochalasin J
9.101_307 Tebuconaz C18489 HMDB0258762
9.106_342 Aloxistatin HMDB0248182
9.108_478 Homocastasterone HMDB0253202
9.11_291. Ketocaine HMDB0253788
9.111_351 Estradiol sulfamat HMDB0251667
9.114_234 7Z, 11Z, 13E-Hexadecatrienal
9.121_498 N(4)-Octadecyl-1-epsilon HMDB0248147
9.128_428 Arlace1 HMDB0248603
9.144_446 Didecyl phthalate HMDB0251217
9.146_3616-(6-(3r-Hydroxy-1 HMDB0244441
9.149_508 Galactocerebroside HMDB0249909
9.152_288 Diazoxon HMDB0251156
9.152_304 Flupirtine HMDB0252403

9. 153_286 ZOLAZEPAM HMDB0260040
9. 153_304 Istamyacin C17984
9. 16_379. C18-Sphingosine 1- HMDB0247790
9. 16_418. Dinonyl phthalate HMDB0251424
9. 16_466. 6alpha-HyC15803
9. 161_282 NCGC00384809-01!5-[5-hydroxy-3-(hydroxymethyl)pentyl]-8a-(hydroxymethyl)
9. 161_427 Cer(d12:0/14:0)
9. 163_488 Esculentic acid (I HMDB0035782
9. 169_497 Cer(d18:0/13:0)
9. 176_493 (2R)-2-[[(9Z)-Hexa HMDB0245288
9. 177_515 (3E, 5S, 7R, 8R, 11E, 13S, 15R, 16R)-3, 5, 7, 11, 13, 15-hexamethyl-8, 16-bis(1, 3-oxa
9. 189_424 Bis(7-methyloctyl) HMDB0244746
9. 192_451 PE(0:0/16:1(9Z))
9. 193_376 Camptothecin
9. 195_308 Icosa-2, 6-dienoic HMDB0260426
9. 195_372 B-Norchole C15378
9. 203_292 Methyl linolenate HMDB0254600
9. 206_374 19-norcholestanol
9. 208_378 Pantheric Acid B
9. 21_227. Halaminol A
9. 21_286. Methyl 16-hydroxy HMDB0254562
9. 213_406 Oblatone G
9. 216_384 Estradiol enanthate HMDB0251964
9. 216_525 LysoPE(22:6(4Z, 7Z, HMDB0011526
9. 217_402 Saphenamycin C12311
9. 219_586 Triethylene glycol HMDB0248490
9. 221_369 cis-5-Tetradecenoic HMDB0002014
9. 223_506 Iriomotec C20009
9. 228_836 Simvastatin HMDB0005007
9. 229_426 Phospho-epsilon C19913
9. 229_857 PS(22:4(7Z, 10Z, 13Z, 16Z)/20:5(5Z, 8Z, 11Z, 14Z, 17Z))
9. 23_501. Glycerophospho-N- HMDB0252848
9. 23_555. Cer(t18:0/16:0)
9. 231_366 3beta-HyC15417
9. 235_523 4-Chloro-2-nitrobenzene HMDB0249542
9. 236_462 3-dehydroecdysone
9. 237_294 2E-Phytanal
9. 237_298 Methyl palmoxirate HMDB0254605
9. 237_594 destruxin A
9. 239_616 Nonoxynol-9 HMDB0015680
9. 239_638 Filipin II HMDB0252258
9. 24_198. Hexyl 2E-hexenoate
9. 24_529. Rocuronium HMDB0014866
9. 241_152 4, 8-Dimethyl-1, 3(E), 7-nonatriene
9. 241_572 Dmap-ethyl-paf HMDB0251534
9. 242_484 LMST01010328
9. 243_322 (3S, 4R)-(6S, 7R)-Diepoxy-9Z-heneicosene
9. 247_511 Cer(d18:0/14:0) HMDB0011759
9. 268_476 Emetamine C09420
9. 271_306 9R, 10S-Epoxy-3Z, 6Z-heneicosadiene
9. 271_486 3-O-(alpha-L-rhamnopyranosyl-(1-2)-alpha-L-rhamnopyranosyl)-3-hydroxydec

9. 272_324 18:1 (5Z) (9Me, 13Me, 17Me)
9. 277_567 Penitrem D HMDB0256240
9. 278_537 C16-Ceramide HMDB0249508
9. 286_362 Adipostatin I
9. 286_396 FAHFA (14:1 (7Z) 1/3-0-10:0)
9. 286_481 LysoPC (15:0/0:0) HMDB0010381
9. 289_587 Cer (d18:0/20:4) HMDB0240729
9. 291_986 PIM1 (19:0/14:0)
9. 292_484 Stigmatel C12150
9. 293_132 Dicyclopentadiene HMDB0251216
9. 294_207 N-Desmethyl tapent HMDB0060611
9. 294_543 LysoPC (20:4 (5Z, 8Z, HMDB0010395
9. 303_813 PI-Cer (t18:0/16:0 (20H))
9. 306_464 Trihydroxycoprosta HMDB0002163
9. 309_350 2-(5-hexadecylfuran-2-yl)-acetic acid
9. 309_422 (5Z, 9Z)-2-methoxy-hexacosadienoic acid
9. 312_502 Crustecdysone HMDB0030180
9. 314_138 Phorone HMDB0245519
9. 318_519 LysoPC (18:2 (9Z, 12Z) HMDB0010386
9. 32_140. Non-2-enal HMDB0255708
9. 32_326. Heneicosylic acid
9. 32_544. 11alpha-Hemiglutaryloxy-1, 25-dihydroxyvitamin D3
9. 324_529 3, 6-dibenzyl-9-[(2, 3-diamino-1, 2-dihydroindol-3-yl)methyl]-1, 4, 7-triazon
9. 326_204 9Z, 13-Tetradecadien-11-ynal
9. 326_523 Cer (d18:0/15:0)
9. 328_253 Palmitoleamide HMDB0256086
9. 329_221 (2E, 4E)-1-(Pyrroli HMDB0242647
9. 329_309 N-Benzyl-9-(tetra HMDB0245639
9. 329_343 2-[4-[4-(4-Carbami HMDB0252929
9. 331_169 Nitramine C10163
9. 332_277 4-(Dodecylamino) P HMDB0256035
9. 332_527 PE (22:5 (7Z, 10Z, 13Z, 16Z, 19Z) /0:0)
9. 332_590 Coenzyme Q6
9. 333_353 4-(4-(4-Fluorophenyl) HMDB0244845
9. 334_352 9-Octadecenyl 3-methylbutanoate
9. 334_377 7-[(3S, 4S)-3-(Benz HMDB0244396
9. 335_353 2-(1, 3-Dimethyl-2, HMDB0253057
9. 335_477 VAPIPROST HMDB0259765
9. 336_416 24, 25-Dihydroxyvit HMDB0000430
9. 337_337 NCGC00385530-02! (E)-5-(1, 2, 4a, 5-tetramethyl-7-oxo-3, 4, 8, 8a-tetrahydro-2H
9. 338_218 2, 6, 10-Trimethyl-(E, E)-2, 6, 10, 12-tridecatetraene
9. 339_273 Ibafloracin HMDB0253322
9. 342_193 1-(2, 4, 6-Trimethyl HMDB0246512
9. 342_302 tributyrilglycerol HMDB0259168
9. 342_343 Schizone C17638
9. 344_352 2, 2-Dimet C15055
9. 344_370 Docosane C19625
9. 347_253 N-[1-(4-methoxy-6-oxopyran-2-yl)-2-methylbutyl]acetamide
9. 348_210 10Z, 12Z-Tetradecadien-1-ol
9. 351_552 2, 11, 20, 29, 37, 38, 39 HMDB0260022
9. 358_386 Butyryl timolol HMDB0249485

9. 358_576 1-(O-alpha-D-glucopyranosyl)-(1, 3S, 25R)-hexacosanetriol
9. 358_577 35-aminobacteriohopane-30, 31, 32, 33, 34-pentol
9. 36_374. 12, 14-Pentacosadiynoic acid
9. 364_432 7-[(1R, 2R, 3R, 5S)-]HMDB0244526
9. 366_545 Cholyhistidine HMDB0242389
9. 369_454 27-Norcholestanehexol
9. 369_480 Cryptocycin C17880
9. 372_236 11Z, 13E-Hexadecadienal
9. 372_336 13, 16-Docosadienoic acid HMDB0244521
9. 373_452 2-Hydroxy-24-keto-octacosanolide
9. 375_585 Cer (d18:0/18:0(2OH))
9. 38_434. 6-Deoxotetracycline C15799
9. 381_548 Cholesteryl glucoside HMDB0250186
9. 384_348 Roxatidine acetate HMDB0015695
9. 385_295 Pizotifen HMDB0256623
9. 386_376 5-Nonadecyl-1, 3-bisphosphatidylcholine HMDB0030956
9. 387_505 PE (20:3 (5Z, 8Z, 11Z) / 0:0)
9. 388_338 Brassidic acid HMDB0249369
9. 389_452 (8S, 9S, 10R, 13R, 14S) Hexacosane HMDB0260189
9. 39_472. ascr#38
9. 393_535 Cer (d18:0/16:0) HMDB0011760
9. 394_565 LysoPC (22:5 (7Z, 10Z) / 0:0) HMDB0010403
9. 398_334 11-hydroxy-12-chloro-octadecanoic acid
9. 41_506. Amoritin
9. 417_395 C19 Sphingosine-1-phosphate
9. 419_371 n-docosahexaenoyl carnitine HMDB0255128
9. 419_446 3-Dehydroxycorticosterone C16497
9. 42_468. Antcin B HMDB0248458
9. 425_362 LMPK15030053
9. 427_411 0-leylcarnitine HMDB0255949
9. 429_385 N-palmitoyl dopamine
9. 429_616 DG (22:4 (7Z, 10Z, 13Z) / 0:0) HMDB0007675
9. 433_340 2-oxo-heneicosanoic acid
9. 434_474 20-Epi-Eldecalcitol HMDB0245562
9. 436_300 Octadecaneperoxydic acid HMDB0255896
9. 436_795 GlcCer (d18:1 (8Z) / 22:0 (2OH[R]))
9. 443_644 PI (22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z) / 0:0)
9. 444_328 Methyl 8-[3-(2-hydroxyoctadecyl)]-octadecanoate HMDB0246127
9. 447_390 Adipostatin J
9. 447_414 Tetracosanoic acid, 15, 16-dihydroxy-, methyl ester
9. 449_406 1alpha, 25-dihydroxy-19-nor-22-oxavitamin D3 / 1alpha, 25-dihydroxy-19-nor-22-oxavitamin D3
9. 453_387 N-linoleoyl taurine
9. 453_545 LysoPC (20:3 (5Z, 8Z) / 0:0) HMDB0010393
9. 455_411 N-arachidonoyl taurine
9. 455_620 PI (20:4 (5Z, 8Z, 11Z) / 0:0) HMDB0256523
9. 457_398 Lauroyl peroxide HMDB0253994
9. 459_377 Pyrimidinofuran C18603
9. 459_506 (20S)-24-Hydroxy-19-norgeminivitamin D3
9. 461_528 Pachymic acid HMDB0256070
9. 462_565 PS (22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z) / 0:0)
9. 463_394 2-Methyl-2-(4, 8, 12-dimethyltridecyl)propane-1-thiol HMDB0258110

9. 463_396 FAHFA (10:0/3-0-14:1 (7Z))
9. 463_598 (8S, 9S, 10R, 13S, 14S) HMDB0260191
9. 471_579 PS (22:1 (11Z) /0:0)
9. 473_486 Cholesteryl hemisuccinate HMDB0250187
9. 476_545 17-Aminogeldanamycin HMDB0259661
9. 48_444. oscr#34
9. 48_556. PG (22:6 (4Z, 7Z, 10Z, 13Z, 16Z, 19Z) /0:0)
9. 481_517 LysoPC (18:3 (9Z, 12Z) HMDB0010388
9. 483_378 TRIMOPROSTIL HMDB0259247
9. 483_495 LysoPC (16:0/4:2:30) HMDB0010382
9. 484_479 PE (18:1 (11Z) /0:0)
9. 484_482 Certonardosterol M
9. 484_593 Povpc HMDB0256712
9. 485_400 1-O-(2R-methoxy-4Z-eicosenyl)-sn-glycerol
9. 485_527 Cer (t18:0/14:0)
9. 488_167 Thymol C09908 HMDB0001878
9. 488_181 N-Ethyl trans-2-cis-6-nonadienamide
9. 488_406 15-(3,4-dimethyl-5-pentylfuran-2-yl)-pentadecanoic acid
9. 488_551 LMFA08020287
9. 489_335 Hydroxychloroquine HMDB0015549
9. 489_408 17-oxo-20Z-hexacosenoic acid
9. 489_562 Campesterol glucoside
9. 49_291. 17beta-An C15356
9. 49_418. Cholesterol-5beta-HMDB0250177
9. 49_462. 2alpha-(3-Hydroxyphenyl) HMDB0254341
9. 491_392 4-Methyl-3-heptyl linoleate
9. 491_478 25(R)-Hydroxyprotocatechuic acid HMDB0245691
9. 491_518 (20S)-24-Hydroxygeminin vitamin D3
9. 492_432 Cathaster C15790
9. 494_532 PG (20:4 (5Z, 8Z, 11Z, 14Z) /0:0)
9. 496_195 3-(1-Aminoethyl)acetic acid HMDB0245767
9. 501_426 Dioctyl sebacate HMDB0251115
9. 502_648 Uvaricin; C08572
9. 503_237 4-Keto-2-C21573
9. 504_514 [1-(3,3-Dimethyl-2-oxopropyl)oxy]propanoic acid HMDB0248142
9. 506_180 8Z, 10E-Dodecadienal
9. 507_155 Cyclopropanecarboxylic acid HMDB0250674
9. 507_379 Sudan Red 7B HMDB0258561
9. 508_178 2-Cyclohexylideneacetone HMDB0245090
9. 509_127 N-Cyclohexylformamide HMDB0255105
9. 509_192 beta-Jonone HMDB0249136
9. 509_311 13-Azaprostanoic acid HMDB0244503
9. 51_178. 6-Ethyl-4-methyl-3E, 5E, 7E-decatriene
9. 511_279 Linoleamide
9. 512_552 Montalicin A
9. 514_223 Carylophyllene Oxide
9. 514_244 (8R, 9R, 10S, 13S, 14S) HMDB0260170
9. 515_150 (3E)-4,8-C21795
9. 516_169 Lupinine
9. 517_617 Sulfobacin A
9. 518_424 terpestacin

9. 52_361. N-Arachidonoylglyc HMDB0005096
9. 52_414. beta-SitcC01753 HMDB0000852
9. 52_642. PA(P-16:0/17:2(9Z, 12Z))
9. 521_183 TecostaniC09989
9. 521_628 Telocinobufagin-3-(14-hydroxymyristate)
9. 522_529 PE(0:0/22:4(7Z, 10Z, 13Z, 16Z))
9. 524_518 Mayolene-15
9. 525_390 1,25-dihydroxy-2,4-dinor-1,3-secovitamin D3 / 1,25-dihydroxy-2,4-dinor-1
9. 525_538 DG(16:1(9Z)/14:0/ HMDB0007124
9. 527_508 LMST01031065
9. 529_442 Testosterone decar HMDB0258859
9. 53_420. Cholestanetriol HMDB0250165
9. 54_472. Theonellasterol D
9. 543_154 Geraniol C09871 HMDB0005812
9. 547_286 9-cis retinol HMDB0247586
9. 55_451. PE(16:1(9Z)/0:0)
9. 555_521 LysoPC(18:1(9Z)/0: HMDB0002815
9. 557_279 (HMDB0033435
9. 558_493 Dasabuvir HMDB0250872
9. 562_356 N-(6,8-Difluoro-2- HMDB0245742
9. 562_568 N-(15-methyl-3-(13-methyl-4Z-tetradecenoyloxy)-hexadecanoyl)-glycine
9. 563_324 1,4a-dimethyl-6-methylidene-5-[(2E)-3-methylpenta-2,4-dienyl]-3,4,5,7,8,
9. 564_318 3,6,9-Tricosatriene
9. 565_293 Monohydroxyperhexi HMDB0061155
9. 566_354 Tricosanoic acid HMDB0001160
9. 571_507 Cytochalasin H1
9. 573_266 5'-Amino-5'-deoxyε HMDB0246876
9. 573_434 29:2(5Z, 9Z)
9. 573_502 Streptotol C19785
9. 576_354 Polypropylene HMDB0255988
9. 576_450 6-Deoxocε C15802
9. 578_354 Glyceryl monolinol HMDB0242115
9. 579_314 2-hydroxy-nonadecanoic acid
9. 584_571 LysoPC(22:4(7Z, 10Z HMDB0010401
9. 589_336 14Z-Tricosene-10-one
9. 593_334 6,7-Epoxy-3Z, 9Z-tricosadiene
9. 596_508 PC(17:2(9Z, 12Z)/0: HMDB0256157
9. 597_314 Clomipran C06918 HMDB0015372
9. 598_344 3beta-Cyc C14979
9. 598_380 15-oxo-18Z-tetracosenoic acid
9. 598_392 (3R, 5S, 6R, 7R, 8S, 9S HMDB0248866
9. 599_512 Tripelargonin HMDB0259260
9. 609_556 Demecarium HMDB0015079
9. 611_238 Methyl 9-tetradecyl HMDB0254572
9. 614_124 Hexahydroindan HMDB0253139
9. 614_350 20:2(5Z, 9Z) (11Me, 15Me, 19Me)
9. 614_448 (1Ar, 3S, 4aS, 7S, 8aS HMDB0242305
9. 616_363 N-palmitoyl taurine
9. 617_138 Pinane HMDB0256559
9. 619_232 Gonane HMDB0252914
9. 619_308 9R, 10S-Epoxy-6Z-heneicosene

9. 62_346. Nor-Dolichol-[13-22]
9. 62_350. 15-tetracosenal
9. 621_49C Aragusteroketal
9. 622_224R-cucujolide III
9. 622_268Heptadec-2-enoic acid HMDB0253101
9. 622_56DG(12:0/20:4(5Z, 8Z, 11Z, 14Z)/0:0) [iso2]
9. 624_512Bis-(tetramethyl ether) HMDB0259422
9. 625_4325-Tricosyl-1, 3-ether HMDB0038524
9. 626_2527-Hexadecynoic acid HMDB0247253
9. 626_542 (5-D-ribonyl)hopane
9. 629_553Topostin B553
9. 629_637Cer(d18:1(4E)/22:0(3OH))
9. 639_5041alpha, 25-Dihydroxy-2-[3'-(methoxymethoxy)propylidene]-19-norvitamin D3
9. 642_437LysoPE(P-16:0/0:0) HMDB0011152
9. 645_572LysoPI(16:0/0:0) HMDB0061695
9. 645_68C(PA(20:5(5Z, 8Z, 11Z, 14Z, 17Z)/15:0))
9. 646_238Pentaethylene glycol HMDB0256256
9. 651_50220alpha-acetoxy-hopane-6alpha, 22-diol
9. 657_509LysoPC(17:0/0:0) HMDB0012108
9. 659_72. Butanone HMDB0000474
9. 663_44C(MG(24:1(15Z)/0:0/0:0)) HMDB0011589
9. 665_531(2S)-2-Cyclopentyl HMDB0258043
9. 668_44613' hydroxy-alpha-tocopherol
9. 672_408delta-heptacosanalactone
9. 672_479LysoPC(P-16:0/0:0) HMDB0010407
9. 684_484PG(16:0/0:0)
9. 691_46C(Lexacalcitol) HMDB0254070
9. 692_448(3beta, 5alpha, 6beta, 24R)-Stigmastane-3, 5, 6-triol
9. 698_4666alpha-Hydroxycastasterone
9. 701_326Promegestone HMDB0256802
9. 701_55C(Cholestanyl glucoside)
9. 701_6724alpha-Phorbol 12, HMDB0246703
9. 702_222Patchoulol HMDB0256142
9. 702_506(20R)-24-Hydroxy-19-norgeminivitamin D3
9. 702_522DG(12:0/17:2(9Z, 12Z)/0:0) [iso2]
9. 705_477PE(0:0/18:2(9Z, 12Z))
9. 705_504Mayolene-14
9. 706_246Estrane HMDB0251974
9. 706_578cis-corossolone
9. 707_608Squamostatin D
9. 712_55C(DG(13:0/18:2(9Z, 12Z)/0:0) [iso2])
9. 713_148EctocarpeC16993
9. 714_389N-oleoyl taurine
9. 714_43C(Nirtetralin) HMDB0255627
9. 719_348N-(2-Hydroxyethyl) HMDB0260372
9. 72_630. DG(19:1(9Z)/18:3(9Z, 12Z, 15Z)/0:0) [iso2]
9. 723_558DG(12:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z)/0:0) [iso2]
9. 727_43619-oxo-22Z-octacosenoic acid
9. 727_528ELV-N34
9. 727_57C(HR1917; 4C15343)
9. 727_586(1R, 6R, 10S, 11R, 13S, 15R)-1, 6-dihydroxy-8-(hydroxymethyl)-4, 12, 12, 15-tetra

9. 728_508 DG (14:1 (9Z)/14:1 (9Z)/0:0)
9. 729_486 N-(2'-(4-benzenesulfonamide)-ethyl) arachidonoyl amine
9. 73_330. 3-Palmitoyl-sn-glycero-3-phosphatidylcholine HMDB0245964
9. 73_598. LysoPI (18:1 (9Z)/0:0) HMDB0061693
9. 731_454 (R)-3-(1-oxo-2-(2-oxoethyl)ethyl)butanoic acid HMDB022000
9. 731_525 NCGC00381435-01!13-dodecan-2-yl-6-(1-hydroxyethyl)-3-(hydroxymethyl)-12-oxododecanoate HMDB022000
9. 732_416 gamma-Tocopherol HMDB0001492
9. 734_438 27-Oxo-octacosanoic acid
9. 736_400 Cochliobolin A HMDB0250395
9. 738_534 DG (12:0/18:3 (9Z, 12Z, 15Z)/0:0) [iso2]
9. 739_671 Dipalmitoyl-sn-glycero-3-phosphatidylcholine HMDB0257984
9. 74_544. 6alpha,16beta-diacetoxy-hopan-22-ol
9. 74_578. DG (15:1 (9Z)/18:1 (9Z)/0:0) [iso2]
9. 741_319 1-(1-Acetyl-piperidin-4-yl)ethanone HMDB0259461
9. 742_508 FAHFA (16:1 (9Z)/13:0-16:0)
9. 743_410 3-oxohexacosanoic acid
9. 743_602 DG (17:2 (9Z, 12Z)/18:2 (9Z, 12Z)/0:0) [iso2]
9. 745_677 Cer(d18:2/25:0 (20H))
9. 745_716 2,3-Bis(sn-3'-phosphatidyl)-sn-glycero-3-phosphatidylcholine HMDB024638
9. 749_510 DG (12:0/16:1 (9Z)/0:0) [iso2]
9. 75_704. Flavuxant C22057
9. 751_606 Muricin-I
9. 752_576 DG (13:0/20:3 (8Z, 11Z, 14Z)/0:0) [iso2]
9. 753_525 PS (18:1 (9Z)/0:0)
9. 755_278 Octadeca-8,10,12-triene HMDB0246901
9. 755_524 DG (13:0/16:1 (9Z)/0:0) [iso2]
9. 756_622 Squamocin-V
9. 757_472 Cortistatin A HMDB0250469
9. 758_356 4-[[1-(1,3-benzodioxol-5-yl)propan-2-yl]-4,5-dimethoxy-2-prop-2-enyl]cyclohexane HMDB0256816
9. 764_337 Propanidid HMDB0256816
9. 766_510 PG (18:1 (9Z)/0:0)
9. 78_338. Glycidyl C19426
9. 783_450 Nuciferonic Acid
9. 789_607 PON-PE
9. 79_507. PE (20:1 (11Z)/0:0)
9. 793_410 Famitinib HMDB0252164
9. 795_197 Dibenzylamine HMDB0251169
9. 797_428 5-[1,2,4a-trimethyl-5-(3-methylbutanoyloxymethyl)-2,3,4,7,8,8a-hexahydro-1H-benzodioxol-5-yl]propan-2-yl]propanoate HMDB0251169
9. 797_575 PS (22:4 (7Z, 10Z, 13Z, 16Z)/0:0)
9. 804_380 3-Methyl-3-butenyl eicosanoate
9. 814_525 2-Lysophosphatidylcholine HMDB0258493
9. 819_395 2,2-Dimethyl-N-(2-hydroxyethyl)acetamide HMDB0250221
9. 825_481 Palmitoyl Ara-C HMDB0256087
9. 83_359. Eptastigmine HMDB0251892
9. 849_475 Cer(d14:2 (4E, 6E)/16:0)
9. 849_484 Aztequynol A
9. 85_503. PE (20:3 (8Z, 11Z, 14Z)/0:0)
9. 854_549 1-(9Z-Eicosenoyl)-HMDB0243798
9. 861_609 PHHdiA-PE
9. 863_479 PE (18:1 (9Z)/0:0)
9. 863_625 Rhizoxin HMDB0257197

9. 864_5411-(2-methoxy-octadecanyl)-sn-glycero-3-phosphoserine
9. 865_569 Methyl 2-(3-(((3-(HMDB0248790
9. 868_527 PE(0:0/22:5(4Z, 7Z, 10Z, 13Z, 16Z))
9. 871_438 PA(18:0/0:0)
9. 872_538 PE(0:0/22:2(13Z, 16Z))
9. 877_414 alpha-N-(3-hydroxyoctadecanoyl)-L-ornithine
9. 885_450 PA(19:1(9Z)/0:0)
9. 886_382 Persin
9. 889_269 Capsi-amiC17515
9. 889_344 Solutol HS 15 HMDB0258368
9. 889_396 Hexacosanoic acid HMDB0002356
9. 889_399 L-Palmitic C02990
9. 89_368. (2-((3,5-Di-*t*-butyl HMDB0242455
9. 891_450 Coprocholic acid HMDB0000601
9. 893_328 (9E, 12E)-N-(2-Hydroxy HMDB0247196
9. 893_328 Acaranoic acid
9. 894_384 Mycolipanoic acid (C24)
9. 896_367 N-Acetyl-S-trans, *t* HMDB0247773
9. 896_396 (9S, 10S)-10-hydroxy-9-(phosphonoxy)octadecanoic acid
9. 897_678 PA(P-16:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))
9. 901_418 CPA(18:1(9Z))
9. 903_394 PA(P-16:0/0:0)
9. 907_314 3-Hydroxy-11-methyl-stearic acid
9. 907_398 Mitragynin C09226 HMDB0041933
9. 908_422 PA(17:1(9Z)/0:0)
9. 911_488 Hydroxyethyl myristic HMDB0244501
9. 911_529 PE(22:4(7Z, 10Z, 13Z, 16Z)/0:0)
9. 914_438 1,4-Bis((*p*-propyl HMDB0248499
9. 914_441 Leukotriene E3
9. 915_298 (12R)-12-Hydroxyoc HMDB0242322
9. 929_308 Sclareol C09183 HMDB0036827
9. 929_388 5alpha-Cholesterol HMDB0000908
9. 931_406 26:2(5Z, 9Z) (25Me)
9. 932_356 Tetracosahexaenic HMDB0258879
9. 933_378 Arachidonoylmorpholine
9. 934_658 2-(3, 7, 11, 15, 19, 23 HMDB0247795
9. 935_414 2-[2-[(1R, 2R)-1-(8 HMDB0253353
9. 936_466 29-Oxotriacontanoic acid
9. 938_328 Steryl st C02195
9. 938_468 PE(0-18:1(9Z)/0:0)
9. 939_424 LMST04010261
9. 94_456. DG(12:0/12:0/0:0) [iso2]
9. 943_464 PA(20:1(11Z)/0:0)
9. 943_484 DG(13:0/13:0/0:0)
9. 943_624 Xylopien
9. 944_248 3,7-Diethyl-11-methyltrideca-1,3,6,10-tetraene
9. 944_280 9S,10R-Epoxy-6Z-nonadecene
9. 944_468 Nonacosane-1,29-dioic acid
9. 944_541 Cer(t18:1(6OH)/14:0(2OH))
9. 945_466 4-[3-[4-(Diphenyl HMDB0251609
9. 946_540 DG(14:0/16:0/0:0) HMDB0007011

9.946_567 1-Heneicosanoyl-glycerol HMDB0243883
9.947_486 17beta, 21beta-epoxy-16alpha-ethoxyhopan-3beta-ol
9.95_536. DG (14:1 (9Z)/16:1 (9Z)) HMDB0007041
9.954_446 Linolenyl laurate
9.954_556 Cer (t18:1 (6OH)/15:0 (20H))
9.955_486 30, 32-dihydroxy-2b-methyl-bishomohopane
9.956_707 Cer (d18:1 (4E)/27:0 (30H))
9.96_450. 2-Dodecyl-3-oxooctanoic acid HMDB0255380
9.967_516 1alpha, 25-dihydroxy-2beta-(6-hydroxyhexyl) vitamin D3 / 1alpha, 25-dihydroxy-2beta-(6-hydroxyhexyl) vitamin D3
9.971_316 1-O-Hexacosanoic acid C13859
9.987_304 Aleuritic acid
9.99_379. Ateviridine HMDB0248697
9.99_564. DG (18:2 (9Z, 12Z)/14:0 (0Z)) HMDB0007240
9.99_716. Menaquinone 8 HMDB0254435
9.991_366 3-oxo-tricosanoic acid
9.992_366 N-(4-(4-Methyl-1-piperidyl)phenyl)acetamide HMDB0252901
9.993_336 Xamoterol C11775
9.993_604 DG (17:0/18:3 (9Z, 12Z, 15Z)/0:0) [iso2]
9.994_586 Mayolene-20
9.995_331 (E)-2-(3-(Naphthalen-1-yl)propyl)acetic acid HMDB0249179
9.995_616 lup-20 (29)-en-3
9.996_416 Carboceric acid
9.998_337 13-Docosenamide HMDB0244507
9.999_292 3, 4-Epoxy-6Z, 9Z-eicosadiene
9.999_596 DG (20:3 (8Z, 11Z, 14Z)) HMDB0007472

[1,6,7,8,8a-hexahydro-2H-naphthalen-1-yl)pentoxy]-4-oxobutanoic acid [IIN-based on:

2-enylidene]-4-methylpentanedioic acid [IIN-based on: CCMSLIB00000847318]

[propyl]oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoyloxy]propyl]oxolan-2-

lehydrovitamin D3 / 26, 26, 26, 27, 27, 27-hexafluoro-1alpha, 25-dihydroxy-16, 17, 23, 23, 2

o[4, 5, 6, 8a-tetrahydro-3aH-cyclohepta[b]furan-7, 5'-oxolane]-2, 2'-dione [IIN-based:

rimethyl-14-oxotetradeca-2,4-dienoic acid [IIN-based on: CCMSLIB00000847299]

hylidene]-6-[(2S, 3R, 4S, 5S, 6R)-3, 4, 5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-

8,8-trimethyl-3-methylidene-2,4,5,6,7,8a-hexahydro-1H-naphthalen-2-yl]oxy]-6-(hyd

dene-3, 4, 4a, 6, 7, 8-hexahydro-1H-naphthalen-1-yl]methoxy]chromen-2-one [IIN-based o

5', 5', 8a' -tetramethyl-3', 4', 4a', 5', 6', 7', 8', 8a' -octahydro-2'H, 3H-spiro[benzofuran

D3 / 1alpha, 25-dihydroxy-26, 27-dimethyl-20, 21, 22, 22, 23, 23-hexadehydrocholecalciferol

-5,6-dimethyl-3,4,4a,6,7,8-hexahydronaphthalene-1-carboxylic acid [IIN-based on:

[1-naphthalen-1-yl)-3-methylpent-2-enoic acid [IIN-based on: CCMSLIB00000847550]

methyl-9-propan-2-yl-1-oxa-4,7,10-triazacyclotridecane-2,5,8,11-tetrone [IIN-base

14, 24-hexadehydrocholecalciferol

troxymethyl)oxane-3,4,5-triol

[2,1'-naphthalen]-6'-yl acetate

