

Metabolomic Data Analysis with MetaboAnalyst 5.0

Name: guest17850890059438804150

May 24, 2021

1 Background

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

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

2 MSEA Overview

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

3 Data Input

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

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

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

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

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

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

4 Data Process

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

| | Query | Match |
|----|-------------|---------------------------------|
| 1 | HMDB0000123 | Glycine |
| 2 | HMDB0014691 | Acetohydroxamic Acid |
| 3 | HMDB0031239 | Ethyl nitrite |
| 4 | HMDB0161401 | NA |
| 5 | HMDB0000925 | Trimethylamine N-oxide |
| 6 | HMDB0142449 | NA |
| 7 | HMDB0140038 | NA |
| 8 | HMDB0012136 | 1-Amino-propan-2-ol |
| 9 | HMDB0062143 | NA |
| 10 | HMDB0031558 | Methyloxirane |
| 11 | HMDB0031652 | Allyl alcohol |
| 12 | HMDB0003366 | Propanal |
| 13 | HMDB0001659 | Acetone |
| 14 | HMDB0144632 | NA |
| 15 | HMDB0062140 | NA |
| 16 | HMDB0034203 | N-(2-Methylpropyl)acetamide |
| 17 | HMDB0031651 | N-(3-Methylbutyl)acetamide |
| 18 | HMDB0062041 | NA |
| 19 | HMDB0012296 | Trimethylaminoacetone |
| 20 | HMDB0031404 | Cyclohexylamine |
| 21 | HMDB0032416 | 2-Methylpiperidine |
| 22 | HMDB0031544 | 3-Methylcyclopentene |
| 23 | HMDB0062716 | NA |
| 24 | HMDB0033971 | 2-Diethylaminoethanol |
| 25 | HMDB0002994 | Erythritol |
| 26 | HMDB0004136 | D-Threitol |
| 27 | HMDB0094689 | NA |
| 28 | HMDB0165469 | NA |
| 29 | HMDB0165470 | NA |
| 30 | HMDB0062640 | NA |
| 31 | HMDB0126088 | NA |
| 32 | HMDB0000710 | 4-Hydroxybutyric acid |
| 33 | HMDB0000442 | (S)-3-Hydroxybutyric acid |
| 34 | HMDB0000357 | 3-Hydroxybutyric acid |
| 35 | HMDB0000336 | (R)-3-Hydroxyisobutyric acid |
| 36 | HMDB0000011 | (R)-3-Hydroxybutyric acid |
| 37 | HMDB0000023 | (S)-3-Hydroxyisobutyric acid |
| 38 | HMDB0000729 | Alpha-Hydroxyisobutyric acid |
| 39 | HMDB0031212 | Ethoxyacetic acid |
| 40 | HMDB0059748 | NA |
| 41 | HMDB0000008 | 2-Hydroxybutyric acid |
| 42 | HMDB0015507 | Gamma Hydroxybutyric Acid |
| 43 | HMDB0000630 | Cytosine |
| 44 | HMDB0031335 | 2-Chloro-1-propanol |
| 45 | HMDB0061966 | NA |
| 46 | HMDB0062141 | NA |
| 47 | HMDB0013716 | Norvaline |
| 48 | HMDB0003355 | 5-Aminopentanoic acid |
| 49 | HMDB0001382 | Vaporole |
| 50 | HMDB0002141 | N-Methyl-a-aminoisobutyric acid |
| 51 | HMDB0015550 | Amyl Nitrite |
| 52 | HMDB0000883 | L-Valine |
| 53 | HMDB0029599 | Glutaral |
| 54 | HMDB0000509 | Senecioic acid |
| 55 | HMDB0001470 | Tiglic acid |
| 56 | HMDB0001862 | 2-Ethylacrylic acid |
| 57 | HMDB0002167 | 3-Methylbutyrolactone |
| 58 | HMDB0031648 | 2,4-Pentanedione |
| 59 | HMDB0033840 | Dihydro-5-methyl-2(3H)-furanone |

| | | |
|-----|-------------|----------------------------------|
| 60 | HMDB0031178 | Dihydro-2-methyl-3(2H)-furanone |
| 61 | HMDB0031602 | 4-Pentenoic acid |
| 62 | HMDB0031598 | 2,3-Pentanedione |
| 63 | HMDB0033978 | Ethyl acrylate |
| 64 | HMDB0032385 | Methyl methacrylate |
| 65 | HMDB0029608 | Angelica acid |
| 66 | HMDB0032351 | Isopropenyl acetate |
| 67 | HMDB0035143 | Dihydro-3-methyl-2(3H)-furanone |
| 68 | HMDB0032459 | 2-Pentenoic acid |
| 69 | HMDB0180166 | NA |
| 70 | HMDB0170858 | NA |
| 71 | HMDB0132474 | NA |
| 72 | HMDB0129418 | NA |
| 73 | HMDB0130837 | NA |
| 74 | HMDB0149276 | NA |
| 75 | HMDB0163712 | NA |
| 76 | HMDB0163713 | NA |
| 77 | HMDB0163714 | NA |
| 78 | HMDB0059606 | NA |
| 79 | HMDB0000043 | Betaine |
| 80 | HMDB0039806 | NA |
| 81 | HMDB0031431 | Dipropyl sulfide |
| 82 | HMDB0029579 | Diisopropyl sulfide |
| 83 | HMDB0011601 | 3-Methylcytosine |
| 84 | HMDB0004339 | 2-O-Methylcytosine |
| 85 | HMDB0002894 | 5-Methylcytosine |
| 86 | HMDB0172056 | NA |
| 87 | HMDB0172059 | NA |
| 88 | HMDB0172058 | NA |
| 89 | HMDB0172057 | NA |
| 90 | HMDB0159225 | NA |
| 91 | HMDB0159223 | NA |
| 92 | HMDB0159222 | NA |
| 93 | HMDB0159224 | NA |
| 94 | HMDB0005785 | Indole-3-carbinol |
| 95 | HMDB0030204 | 1-(2-Furanylmethyl)-1H-pyrrole |
| 96 | HMDB0040009 | NA |
| 97 | HMDB0040011 | NA |
| 98 | HMDB0011664 | 3-Methylene-indolenine |
| 99 | HMDB0033731 | Quinoline |
| 100 | HMDB0034244 | Isoquinoline |
| 101 | HMDB0161116 | NA |
| 102 | HMDB0161115 | NA |
| 103 | HMDB0163679 | NA |
| 104 | HMDB0061652 | 3-hydroxyhexanoic acid |
| 105 | HMDB0171222 | NA |
| 106 | HMDB0165043 | NA |
| 107 | HMDB0165041 | NA |
| 108 | HMDB0165042 | NA |
| 109 | HMDB0163681 | NA |
| 110 | HMDB0163682 | NA |
| 111 | HMDB0163680 | NA |
| 112 | HMDB0000525 | 5-Hydroxyhexanoic acid |
| 113 | HMDB0000624 | D-Leucic acid |
| 114 | HMDB0040409 | NA |
| 115 | HMDB0000665 | Leucinic acid |
| 116 | HMDB0000746 | Hydroxyisocaproic acid |
| 117 | HMDB0001624 | 2-Hydroxycaproic acid |
| 118 | HMDB0032158 | (+/-)-1-Acetoxy-1-ethoxyethane |
| 119 | HMDB0032456 | Paraldehyde |
| 120 | HMDB0001975 | 2-Ethyl-2-Hydroxybutyric acid |
| 121 | HMDB0033851 | 4,4-Dimethoxy-2-butanone |
| 122 | HMDB0000409 | (5R)-5-Hydroxyhexanoic acid |
| 123 | HMDB0000317 | 2-Hydroxy-3-methylpentanoic acid |
| 124 | HMDB0012843 | 6-Hydroxyhexanoic acid |
| 125 | HMDB0059770 | NA |
| 126 | HMDB0041844 | NA |
| 127 | HMDB0029166 | 2-Methyl-3-hydroxyvaleric acid |
| 128 | HMDB0165040 | NA |
| 129 | HMDB0010718 | (R)-3-Hydroxyhexanoic acid |
| 130 | HMDB0062045 | NA |
| 131 | HMDB0062118 | NA |
| 132 | HMDB0128943 | NA |
| 133 | HMDB0132477 | NA |
| 134 | HMDB0129097 | NA |
| 135 | HMDB0168839 | NA |
| 136 | HMDB0128916 | NA |
| 137 | HMDB0012233 | Glutarate semialdehyde |
| 138 | HMDB0029172 | 3-keto-2-Methylbutyrate |
| 139 | HMDB0001865 | 2-Oxovaleric acid |
| 140 | HMDB0000310 | Methylacetoacetic acid |
| 141 | HMDB0031643 | Ethyl pyruvate |
| 142 | HMDB0000019 | Alpha-ketoisovaleric acid |
| 143 | HMDB0003771 | 2-Methylacetoacetic acid |
| 144 | HMDB0000720 | Levulinic acid |
| 145 | HMDB0034466 | Acetoxyacetone |
| 146 | HMDB0128917 | NA |

| | | |
|-----|-------------|-----------------------------------|
| 147 | HMDB0129096 | NA |
| 148 | HMDB0129098 | NA |
| 149 | HMDB0168838 | NA |
| 150 | HMDB0177210 | NA |
| 151 | HMDB0169666 | NA |
| 152 | HMDB0177209 | NA |
| 153 | HMDB0171727 | NA |
| 154 | HMDB0032356 | N-Lactoyl ethanolamine |
| 155 | HMDB0039499 | NA |
| 156 | HMDB0031658 | L-2-Amino-5-hydroxypentanoic acid |
| 157 | HMDB0039790 | NA |
| 158 | HMDB0038974 | NA |
| 159 | HMDB0039789 | NA |
| 160 | HMDB0000786 | Oxypurinol |
| 161 | HMDB0000292 | Xanthine |
| 162 | HMDB0001182 | 6,8-Dihydroxypurine |
| 163 | HMDB0000744 | Malic acid |
| 164 | HMDB0031518 | D-Malic acid |
| 165 | HMDB0000156 | L-Malic acid |
| 166 | HMDB0032872 | Velcorin |
| 167 | HMDB0061971 | NA |
| 168 | HMDB0166738 | NA |
| 169 | HMDB0164724 | NA |
| 170 | HMDB0165094 | NA |
| 171 | HMDB0165096 | NA |
| 172 | HMDB0165095 | NA |
| 173 | HMDB0165097 | NA |
| 174 | HMDB0166737 | NA |
| 175 | HMDB0031484 | 2-Heptenoic acid |
| 176 | HMDB0038962 | NA |
| 177 | HMDB0031500 | Methyl 2E-hexenoate |
| 178 | HMDB0166739 | NA |
| 179 | HMDB0029314 | Isopentenyl acetate |
| 180 | HMDB0031477 | 3,4-Heptanedione |
| 181 | HMDB0031476 | 2,3-Heptanedione |
| 182 | HMDB0031504 | Methyl (Z)-3-hexenoate |
| 183 | HMDB0031603 | Ethyl 4-pentenoate |
| 184 | HMDB0040214 | NA |
| 185 | HMDB0031342 | Cyclohexanecarboxylic acid |
| 186 | HMDB0038271 | NA |
| 187 | HMDB0031174 | 4-Methyl-5-hexanolide |
| 188 | HMDB0031681 | Dihydro-5-propyl-2(3H)-furanone |
| 189 | HMDB0033793 | 4-Heptenoic acid |
| 190 | HMDB0031593 | 5-Methyl-2,3-hexanedione |
| 191 | HMDB0039819 | NA |
| 192 | HMDB0166736 | NA |
| 193 | HMDB0173760 | NA |
| 194 | HMDB0173761 | NA |
| 195 | HMDB0173762 | NA |
| 196 | HMDB0173763 | NA |
| 197 | HMDB0180322 | NA |
| 198 | HMDB0180323 | NA |
| 199 | HMDB0029165 | 1,3-Diacetylpropane |
| 200 | HMDB0031351 | Cyclohexyl formate |
| 201 | HMDB0032460 | 4-Pentenyl acetate |
| 202 | HMDB0032391 | 3-Methyl-3-butenyl acetate |
| 203 | HMDB0030330 | 1-Methoxy-3-methylene-2-pentanone |
| 204 | HMDB0059876 | NA |
| 205 | HMDB0040591 | NA |
| 206 | HMDB0145113 | NA |
| 207 | HMDB0145114 | NA |
| 208 | HMDB0145115 | NA |
| 209 | HMDB0145125 | NA |
| 210 | HMDB0145116 | NA |
| 211 | HMDB0094649 | 2-Amino-heptanoic acid |
| 212 | HMDB0001161 | 4-Trimethylammonibutanoic acid |
| 213 | HMDB0006831 | 3-Dehydroxycarnitine |
| 214 | HMDB0000895 | Acetylcholine |
| 215 | HMDB0013811 | 1-Nitroheptane |
| 216 | HMDB0041477 | NA |
| 217 | HMDB0031660 | Dibutyl sulfide |
| 218 | HMDB0240251 | NA |
| 219 | HMDB0061880 | NA |
| 220 | HMDB0059659 | Trans-3-hydroxy-L-proline |
| 221 | HMDB0002113 | 3-Hydroxy-L-proline |
| 222 | HMDB0000783 | Propionylglycine |
| 223 | HMDB0000766 | N-Acetyl-L-alanine |
| 224 | HMDB0000725 | 4-Hydroxyproline |
| 225 | HMDB0036576 | NA |
| 226 | HMDB0001149 | 5-Aminolevulinic acid |
| 227 | HMDB0002104 | L-Glutamic gamma-semialdehyde |
| 228 | HMDB0006055 | 4-Hydroxy-L-proline |
| 229 | HMDB0060460 | cis-4-Hydroxy-D-proline |
| 230 | HMDB0006272 | 5-Amino-2-oxopentanoic acid |
| 231 | HMDB0177404 | NA |
| 232 | HMDB0014389 | Mesalazine |
| 233 | HMDB0164041 | NA |

| | | |
|-----|-------------|---|
| 234 | HMDB0059749 | NA |
| 235 | HMDB0001972 | 3-Aminosalicylic acid |
| 236 | HMDB0014378 | Aminosalicylic Acid |
| 237 | HMDB0001476 | 3-Hydroxyanthranilic acid |
| 238 | HMDB0059811 | NA |
| 239 | HMDB0012289 | Tetrahydrodipicolinate |
| 240 | HMDB0001280 | 2-Aminomuconic acid semialdehyde |
| 241 | HMDB0031670 | 1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione |
| 242 | HMDB0028696 | Alanyl-Serine |
| 243 | HMDB0029032 | Serylalanine |
| 244 | HMDB0145395 | NA |
| 245 | HMDB0029061 | Threoninyl-Glycine |
| 246 | HMDB0028851 | Glycyl-Threonine |
| 247 | HMDB0169117 | NA |
| 248 | HMDB0125105 | NA |
| 249 | HMDB0038987 | NA |
| 250 | HMDB0032029 | 2-Isopropylphenol |
| 251 | HMDB0032149 | 1-Methoxy-2,4-dimethylbenzene |
| 252 | HMDB0032625 | 4-Propylphenol |
| 253 | HMDB0029667 | 2,3,6-Trimethylphenol |
| 254 | HMDB0039782 | NA |
| 255 | HMDB0038986 | NA |
| 256 | HMDB0032624 | 2-Propylphenol |
| 257 | HMDB0038988 | NA |
| 258 | HMDB0032621 | (2-Methoxyethyl)benzene |
| 259 | HMDB0038985 | NA |
| 260 | HMDB0031312 | Benzyl ethyl ether |
| 261 | HMDB0033962 | 3-Phenyl-1-propanol |
| 262 | HMDB0031627 | 1-Phenyl-1-propanol |
| 263 | HMDB0034378 | (Δ^5)-1-(4-Methylphenyl)ethanol |
| 264 | HMDB0031628 | 2-Phenyl-1-propanol |
| 265 | HMDB0038984 | NA |
| 266 | HMDB0032544 | 2,4,6-Trimethylphenol |
| 267 | HMDB0031446 | p-Isopropylphenol |
| 268 | HMDB0032441 | Nona-2,4,6-trienal |
| 269 | HMDB0059896 | NA |
| 270 | HMDB0169118 | NA |
| 271 | HMDB0156380 | NA |
| 272 | HMDB0000259 | Serotonin |
| 273 | HMDB0001046 | Cotinine |
| 274 | HMDB0156382 | NA |
| 275 | HMDB0156381 | NA |
| 276 | HMDB0156383 | NA |
| 277 | HMDB0040299 | NA |
| 278 | HMDB0029727 | 5-Ethyl-2,3-dimethylpyrazine |
| 279 | HMDB0040000 | NA |
| 280 | HMDB0041252 | NA |
| 281 | HMDB0015644 | Betahistine |
| 282 | HMDB0036584 | NA |
| 283 | HMDB0036808 | NA |
| 284 | HMDB0014918 | Phenelzine |
| 285 | HMDB0032276 | 2-Ethyl-3,(5 or 6)-dimethylpyrazine |
| 286 | HMDB0041253 | NA |
| 287 | HMDB0036809 | NA |
| 288 | HMDB0037151 | NA |
| 289 | HMDB0030410 | L-2-Amino-3-methylenehexanoic acid |
| 290 | HMDB0004827 | Proline betaine |
| 291 | HMDB0038949 | NA |
| 292 | HMDB0032332 | Hydroxylated lecithin |
| 293 | HMDB0145430 | NA |
| 294 | HMDB0128078 | NA |
| 295 | HMDB0134039 | NA |
| 296 | HMDB0135273 | NA |
| 297 | HMDB0135648 | NA |
| 298 | HMDB0135274 | NA |
| 299 | HMDB0135275 | NA |
| 300 | HMDB0035243 | 1-Phenyl-1,2-propanedione |
| 301 | HMDB0000930 | trans-Cinnamic acid |
| 302 | HMDB0000567 | Cinnamic acid |
| 303 | HMDB0036626 | NA |
| 304 | HMDB0040986 | (E)-3-(4-Hydroxyphenyl)-2-propenal |
| 305 | HMDB0031725 | (E)-3-(2-Hydroxyphenyl)-2-propenal |
| 306 | HMDB0032947 | Di-2-furanylmethane |
| 307 | HMDB0062407 | NA |
| 308 | HMDB0004992 | Benzocaine |
| 309 | HMDB0001007 | 3-Pyridinebutanoic acid |
| 310 | HMDB0059934 | NA |
| 311 | HMDB0033589 | Ethyl 2-aminobenzoate |
| 312 | HMDB0033485 | Gentiatibetine |
| 313 | HMDB0034169 | Methyl N-methylanthranilate |
| 314 | HMDB0006044 | Norsalsolinol |
| 315 | HMDB0000159 | L-Phenylalanine |
| 316 | HMDB0159744 | NA |
| 317 | HMDB0062402 | NA |
| 318 | HMDB0155168 | NA |
| 319 | HMDB0029455 | Ginkgotoxin |
| 320 | HMDB0000068 | Epinephrine |

| | | |
|-----|-------------|---|
| 321 | HMDB0000819 | Normetanephrine |
| 322 | HMDB0002832 | Methylnoradrenaline |
| 323 | HMDB0015652 | Levonordefrin |
| 324 | HMDB0062515 | NA |
| 325 | HMDB0061679 | NA |
| 326 | HMDB0154785 | NA |
| 327 | HMDB0000232 | Quinolinic acid |
| 328 | HMDB0033161 | 2,6-Pyridinedicarboxylic acid |
| 329 | HMDB0185628 | NA |
| 330 | HMDB0001330 | 2-Amino-3-carboxymuconic acid semialdehyde |
| 331 | HMDB0062578 | NA |
| 332 | HMDB0060260 | NA |
| 333 | HMDB0001552 | 2-Keto-glutaramic acid |
| 334 | HMDB0000289 | Uric acid |
| 335 | HMDB0166108 | NA |
| 336 | HMDB0171094 | NA |
| 337 | HMDB0172092 | NA |
| 338 | HMDB0062005 | NA |
| 339 | HMDB0124926 | NA |
| 340 | HMDB0168664 | NA |
| 341 | HMDB0150437 | NA |
| 342 | HMDB0125528 | NA |
| 343 | HMDB0137457 | NA |
| 344 | HMDB0146870 | NA |
| 345 | HMDB0146889 | NA |
| 346 | HMDB0166106 | NA |
| 347 | HMDB0166109 | NA |
| 348 | HMDB0182861 | NA |
| 349 | HMDB0166107 | NA |
| 350 | HMDB0183905 | NA |
| 351 | HMDB0183904 | NA |
| 352 | HMDB0036907 | NA |
| 353 | HMDB0029660 | 2',6'-Dihydroxyacetophenone |
| 354 | HMDB0029657 | 2,4'-Dihydroxyacetophenone |
| 355 | HMDB0029659 | 2',4'-Dihydroxyacetophenone |
| 356 | HMDB0029658 | 2',3'-Dihydroxyacetophenone |
| 357 | HMDB0032594 | 2-(Hydroxymethyl)benzoic acid |
| 358 | HMDB0033003 | 1-(5-Methyl-2-furanyl)-1,2-propanedione |
| 359 | HMDB0032629 | 2',5'-Dihydroxyacetophenone |
| 360 | HMDB0032572 | Methylparaben |
| 361 | HMDB0029662 | 3',5'-Dihydroxyacetophenone |
| 362 | HMDB0029661 | 3',4'-Dihydroxyacetophenone |
| 363 | HMDB0032604 | 2-Methoxybenzoic acid |
| 364 | HMDB0034172 | Methyl 2-hydroxybenzoate |
| 365 | HMDB0032606 | 3-Methoxybenzoic acid |
| 366 | HMDB0041283 | NA |
| 367 | HMDB0004815 | 4-Hydroxy-3-methylbenzoic acid |
| 368 | HMDB0012308 | Vanillin |
| 369 | HMDB0032919 | Ethyl 2-furanyl diketone |
| 370 | HMDB0172091 | NA |
| 371 | HMDB0032399 | Methyl furfuracrylate |
| 372 | HMDB0000703 | Mandelic acid |
| 373 | HMDB0000669 | Ortho-Hydroxyphenylacetic acid |
| 374 | HMDB0060390 | NA |
| 375 | HMDB0003791 | 3,4-Dihydroxyphenylacetaldehyde |
| 376 | HMDB0062635 | NA |
| 377 | HMDB0031609 | Phenoxyacetic acid |
| 378 | HMDB0000440 | 3-Hydroxyphenylacetic acid |
| 379 | HMDB0001101 | p-Anisic acid |
| 380 | HMDB0000020 | p-Hydroxyphenylacetic acid |
| 381 | HMDB0002390 | 3-Cresotinic acid |
| 382 | HMDB0000216 | Norepinephrine |
| 383 | HMDB0035178 | 6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone |
| 384 | HMDB0037685 | NA |
| 385 | HMDB0155164 | NA |
| 386 | HMDB0001537 | 6-Hydroxydopamine |
| 387 | HMDB0000239 | Pyridoxine |
| 388 | HMDB0004817 | 5-Hydroxydopamine |
| 389 | HMDB0012150 | 2-Keto-6-acetamidocaproate |
| 390 | HMDB0168723 | NA |
| 391 | HMDB0168724 | NA |
| 392 | HMDB0142963 | NA |
| 393 | HMDB0061157 | NA |
| 394 | HMDB0029449 | (2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid |
| 395 | HMDB0033453 | Fagomine |
| 396 | HMDB0032354 | S-Isopropyl 3-methylbut-2-enethioate |
| 397 | HMDB0162077 | NA |
| 398 | HMDB0162076 | NA |
| 399 | HMDB0162073 | NA |
| 400 | HMDB0031797 | 2-Isopropylphenyl methylcarbamate |
| 401 | HMDB0003892 | (S)-N-Methylsalsolinol |
| 402 | HMDB0003626 | (R)-N-Methylsalsolinol |
| 403 | HMDB0036906 | NA |
| 404 | HMDB0012484 | (R)-1,2-dimethyl-5,6-dihydroxy-tetrahydroisoquinoline |
| 405 | HMDB0012469 | (-)-Salsoline |
| 406 | HMDB0035072 | 2-Methylpropyl 2-aminobenzoate |
| 407 | HMDB0037698 | NA |

| | | |
|-----|-------------|---|
| 408 | HMDB0162075 | NA |
| 409 | HMDB0060303 | (2-Naphthyl)methanol |
| 410 | HMDB0032861 | 2-Methoxynaphthalene |
| 411 | HMDB0060322 | 1-Hydroxymethylnaphthalene |
| 412 | HMDB0061285 | NA |
| 413 | HMDB0040768 | NA |
| 414 | HMDB0000671 | Indolelactic acid |
| 415 | HMDB0032755 | Methyl 1-methoxy-1H-indole-3-carboxylate |
| 416 | HMDB0011621 | Cinnamoylglycine |
| 417 | HMDB0004096 | 5-Methoxyindoleacetate |
| 418 | HMDB0030179 | Edulitine |
| 419 | HMDB0059765 | NA |
| 420 | HMDB0161245 | NA |
| 421 | HMDB0183147 | NA |
| 422 | HMDB0183148 | NA |
| 423 | HMDB0161242 | NA |
| 424 | HMDB0163576 | NA |
| 425 | HMDB0161243 | NA |
| 426 | HMDB0183149 | NA |
| 427 | HMDB0161246 | NA |
| 428 | HMDB0161244 | NA |
| 429 | HMDB0161241 | NA |
| 430 | HMDB0000734 | Indoleacrylic acid |
| 431 | HMDB0154664 | NA |
| 432 | HMDB0033249 | 6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine |
| 433 | HMDB0032234 | 2,5-Dimethyl-3-furanthiol acetate |
| 434 | HMDB0037732 | NA |
| 435 | HMDB0094704 | N-Propionylmethionine |
| 436 | HMDB0151312 | NA |
| 437 | HMDB0163546 | NA |
| 438 | HMDB0240314 | NA |
| 439 | HMDB0240352 | NA |
| 440 | HMDB0240315 | NA |
| 441 | HMDB0041500 | NA |
| 442 | HMDB0240555 | NA |
| 443 | HMDB0032688 | (Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne |
| 444 | HMDB0157323 | NA |
| 445 | HMDB0157320 | NA |
| 446 | HMDB0157322 | NA |
| 447 | HMDB0157321 | NA |
| 448 | HMDB0059767 | NA |
| 449 | HMDB0157324 | NA |
| 450 | HMDB0033584 | Diethyl tartrate |
| 451 | HMDB0031460 | NA |
| 452 | HMDB0038791 | NA |
| 453 | HMDB0038183 | NA |
| 454 | HMDB0029939 | 6-Amino-9H-purine-9-propanoic acid |
| 455 | HMDB0169421 | NA |
| 456 | HMDB0163468 | NA |
| 457 | HMDB0163469 | NA |
| 458 | HMDB0179168 | NA |
| 459 | HMDB0163465 | NA |
| 460 | HMDB0163466 | NA |
| 461 | HMDB0094711 | NA |
| 462 | HMDB0059936 | NA |
| 463 | HMDB0062081 | NA |
| 464 | HMDB0060287 | NA |
| 465 | HMDB0059937 | NA |
| 466 | HMDB0036396 | NA |
| 467 | HMDB0040165 | NA |
| 468 | HMDB0036188 | NA |
| 469 | HMDB0036213 | NA |
| 470 | HMDB0040203 | NA |
| 471 | HMDB0040202 | NA |
| 472 | HMDB0163470 | NA |
| 473 | HMDB0014018 | 4-Hydroxypropofol |
| 474 | HMDB0037389 | NA |
| 475 | HMDB0038292 | NA |
| 476 | HMDB0040439 | NA |
| 477 | HMDB0039685 | NA |
| 478 | HMDB0041497 | NA |
| 479 | HMDB0031840 | (S,Z)-Lyratol acetate |
| 480 | HMDB0035801 | (2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate |
| 481 | HMDB0035375 | Ethyl (2E,4E,7Z)-Decatrienoate |
| 482 | HMDB0035376 | Ethyl (2E,4Z,7Z)-Decatrienoate |
| 483 | HMDB0132986 | NA |
| 484 | HMDB0034450 | Neocnidilide |
| 485 | HMDB0032567 | Hexylresorcinol |
| 486 | HMDB0035126 | (À)-Myrtenyl acetate |
| 487 | HMDB0041610 | NA |
| 488 | HMDB0038046 | NA |
| 489 | HMDB0037018 | NA |
| 490 | HMDB0037231 | NA |
| 491 | HMDB0035085 | Vulgarole |
| 492 | HMDB0041572 | NA |
| 493 | HMDB0029388 | Cucurbitic acid |
| 494 | HMDB0037326 | NA |

| | | |
|-----|-------------|--|
| 495 | HMDB0033601 | Dihydrojasmonic acid |
| 496 | HMDB0040195 | NA |
| 497 | HMDB0035723 | (1R,2S,3S,4R)-p-Menthane-2,3-diol |
| 498 | HMDB0034457 | Propyl heptanoate |
| 499 | HMDB0061987 | NA |
| 500 | HMDB0062146 | NA |
| 501 | HMDB0038038 | NA |
| 502 | HMDB0036228 | 2-Methylpropyl hexanoate |
| 503 | HMDB0040167 | NA |
| 504 | HMDB0036136 | NA |
| 505 | HMDB0187563 | NA |
| 506 | HMDB0037387 | NA |
| 507 | HMDB0000511 | Capric acid |
| 508 | HMDB0031264 | Methyl nonanoate |
| 509 | HMDB0094654 | 1-Methylethyl heptanoic acid |
| 510 | HMDB0171179 | NA |
| 511 | HMDB0171178 | NA |
| 512 | HMDB0171177 | NA |
| 513 | HMDB0171176 | NA |
| 514 | HMDB0179213 | NA |
| 515 | HMDB0179212 | NA |
| 516 | HMDB0179927 | NA |
| 517 | HMDB0180500 | NA |
| 518 | HMDB0180498 | NA |
| 519 | HMDB0180499 | NA |
| 520 | HMDB0180497 | NA |
| 521 | HMDB0180502 | NA |
| 522 | HMDB0180501 | NA |
| 523 | HMDB0180503 | NA |
| 524 | HMDB0180504 | NA |
| 525 | HMDB0171175 | NA |
| 526 | HMDB0061805 | NA |
| 527 | HMDB0180097 | NA |
| 528 | HMDB0032302 | Heptanal propyleneglycol acetal |
| 529 | HMDB0032155 | Acetaldehyde 1,3-octanediol acetal |
| 530 | HMDB0032264 | Ethyl 2-ethylhexanoate |
| 531 | HMDB0032315 | Hexanal butane-2,3-diol acetal |
| 532 | HMDB0032045 | Pentyl 3-methylbutanoate |
| 533 | HMDB0041216 | NA |
| 534 | HMDB0034849 | 4-Methylnonanoic acid |
| 535 | HMDB0037849 | Hexyl 2-methylpropanoate |
| 536 | HMDB0040157 | NA |
| 537 | HMDB0033620 | Hexyl butyrate |
| 538 | HMDB0035595 | trans-p-Menthane-1,8-diol |
| 539 | HMDB0029760 | 1,1-Diethoxy-2-hexene |
| 540 | HMDB0032070 | Isooctyl acetate |
| 541 | HMDB0040211 | NA |
| 542 | HMDB0040529 | NA |
| 543 | HMDB0038783 | NA |
| 544 | HMDB0036145 | NA |
| 545 | HMDB0039218 | NA |
| 546 | HMDB0038602 | Octyl acetate |
| 547 | HMDB0030029 | Isopentyl isopentanoate |
| 548 | HMDB0031739 | 7-Hydroxy-3,7-dimethyloctanal |
| 549 | HMDB0035360 | N-Methyl-1-deoxynojirimycin |
| 550 | HMDB0029741 | 2-Isopropyl-3,5-dimethoxy-6-methylpyrazine |
| 551 | HMDB0040551 | NA |
| 552 | HMDB0240493 | NA |
| 553 | HMDB0029224 | N-methylphenylalanine |
| 554 | HMDB0029223 | alpha-Methylphenylalanine |
| 555 | HMDB0005199 | (R)-Salsolinol |
| 556 | HMDB0031811 | 3,5-Dimethylphenyl methylcarbamate |
| 557 | HMDB0039655 | NA |
| 558 | HMDB0030372 | Maltoxazine |
| 559 | HMDB0040021 | NA |
| 560 | HMDB0033763 | Ethyl N-methylanthranilate |
| 561 | HMDB0042012 | NA |
| 562 | HMDB0001189 | 2(N)-Methyl-norsalsolinol |
| 563 | HMDB0041931 | NA |
| 564 | HMDB0029135 | Valyl-Proline |
| 565 | HMDB0003581 | Dethiobiotin |
| 566 | HMDB0029030 | Prolyl-Valine |
| 567 | HMDB0036683 | NA |
| 568 | HMDB0059826 | NA |
| 569 | HMDB0059696 | NA |
| 570 | HMDB0061824 | NA |
| 571 | HMDB0013287 | Ne,Ne dimethyllysine |
| 572 | HMDB0000904 | Citrulline |
| 573 | HMDB0003148 | Argininic acid |
| 574 | HMDB0003269 | Nicotinuric acid |
| 575 | HMDB0164043 | NA |
| 576 | HMDB0176142 | NA |
| 577 | HMDB0041912 | NA |
| 578 | HMDB0059766 | NA |
| 579 | HMDB0032055 | N-Acetylhistidine |
| 580 | HMDB0033455 | 2-Hydroxy-3-methyl-9H-carbazole |
| 581 | HMDB0033487 | 1-Hydroxy-3-methyl-9H-carbazole |

| | | |
|-----|-------------|---|
| 582 | HMDB0038915 | NA |
| 583 | HMDB0164006 | NA |
| 584 | HMDB0164005 | NA |
| 585 | HMDB0164004 | NA |
| 586 | HMDB0032888 | Acetyl vitamin K5 |
| 587 | HMDB0039455 | NA |
| 588 | HMDB0041830 | NA |
| 589 | HMDB0029430 | Methionine sulfoximine |
| 590 | HMDB0013609 | D-Tryptophan |
| 591 | HMDB0013840 | 3-Hydroxymethylantipyrine |
| 592 | HMDB0060533 | NA |
| 593 | HMDB0060878 | NA |
| 594 | HMDB0030396 | (Ás)-Tryptophan |
| 595 | HMDB0060967 | NA |
| 596 | HMDB0014892 | Ethotoin |
| 597 | HMDB0000929 | L-Tryptophan |
| 598 | HMDB0028848 | Glycyl-Phenylalanine |
| 599 | HMDB0028995 | Phenylalanyl-Glycine |
| 600 | HMDB0036394 | NA |
| 601 | HMDB0240354 | NA |
| 602 | HMDB0040334 | NA |
| 603 | HMDB0040336 | NA |
| 604 | HMDB0040337 | NA |
| 605 | HMDB0040335 | NA |
| 606 | HMDB0040109 | NA |
| 607 | HMDB0040110 | NA |
| 608 | HMDB0040067 | NA |
| 609 | HMDB0040086 | NA |
| 610 | HMDB0040084 | NA |
| 611 | HMDB0040085 | NA |
| 612 | HMDB0040087 | NA |
| 613 | HMDB0040089 | NA |
| 614 | HMDB0040083 | NA |
| 615 | HMDB0040088 | NA |
| 616 | HMDB0041008 | NA |
| 617 | HMDB0166252 | NA |
| 618 | HMDB0030703 | Dhelwangin |
| 619 | HMDB0032663 | Acoramone |
| 620 | HMDB0040629 | NA |
| 621 | HMDB0030680 | Diplosporin |
| 622 | HMDB0040890 | NA |
| 623 | HMDB0036203 | NA |
| 624 | HMDB0032552 | Vanillin 1,2-butylene glycol acetal |
| 625 | HMDB0127765 | NA |
| 626 | HMDB0127761 | NA |
| 627 | HMDB0125801 | NA |
| 628 | HMDB0124917 | NA |
| 629 | HMDB0124919 | NA |
| 630 | HMDB0135709 | NA |
| 631 | HMDB0182833 | NA |
| 632 | HMDB0182835 | NA |
| 633 | HMDB0182837 | NA |
| 634 | HMDB0169500 | NA |
| 635 | HMDB0169499 | NA |
| 636 | HMDB0169498 | NA |
| 637 | HMDB0166269 | NA |
| 638 | HMDB0124920 | NA |
| 639 | HMDB0172372 | NA |
| 640 | HMDB0172373 | NA |
| 641 | HMDB0172374 | NA |
| 642 | HMDB0172375 | NA |
| 643 | HMDB0172376 | NA |
| 644 | HMDB0177973 | NA |
| 645 | HMDB0177972 | NA |
| 646 | HMDB0182836 | NA |
| 647 | HMDB0132987 | NA |
| 648 | HMDB0034135 | Isoeugenol acetate |
| 649 | HMDB0041410 | NA |
| 650 | HMDB0035071 | Verimol I |
| 651 | HMDB0031973 | (2RS,5RS)-(E)-2-(2-Phenylethenyl)-1,3-dioxan-5-ol |
| 652 | HMDB0135898 | NA |
| 653 | HMDB0132972 | NA |
| 654 | HMDB0033594 | Cuelure |
| 655 | HMDB0030762 | Ethyl trans-p-methoxycinnamate |
| 656 | HMDB0032348 | Isoeugenyl acetate |
| 657 | HMDB0034122 | Aceteugenol |
| 658 | HMDB0031729 | Phenylmethylglycidic ester |
| 659 | HMDB0132977 | NA |
| 660 | HMDB0127763 | NA |
| 661 | HMDB0132974 | NA |
| 662 | HMDB0132975 | NA |
| 663 | HMDB0132976 | NA |
| 664 | HMDB0163525 | NA |
| 665 | HMDB0167932 | NA |
| 666 | HMDB0170957 | NA |
| 667 | HMDB0182630 | NA |
| 668 | HMDB0179403 | NA |

| | | |
|-----|-------------|---|
| 669 | HMDB0182629 | NA |
| 670 | HMDB0182627 | NA |
| 671 | HMDB0182628 | NA |
| 672 | HMDB0182631 | NA |
| 673 | HMDB0179404 | NA |
| 674 | HMDB0039710 | NA |
| 675 | HMDB0036998 | NA |
| 676 | HMDB0036117 | NA |
| 677 | HMDB0040883 | NA |
| 678 | HMDB0039052 | NA |
| 679 | HMDB0179402 | NA |
| 680 | HMDB0176286 | NA |
| 681 | HMDB0176282 | NA |
| 682 | HMDB0131084 | NA |
| 683 | HMDB0178771 | NA |
| 684 | HMDB0176285 | NA |
| 685 | HMDB0176283 | NA |
| 686 | HMDB0176284 | NA |
| 687 | HMDB0179401 | NA |
| 688 | HMDB0179400 | NA |
| 689 | HMDB0178775 | NA |
| 690 | HMDB0178773 | NA |
| 691 | HMDB0178774 | NA |
| 692 | HMDB0178772 | NA |
| 693 | HMDB0178770 | NA |
| 694 | HMDB0178769 | NA |
| 695 | HMDB0164284 | NA |
| 696 | HMDB0164282 | NA |
| 697 | HMDB0164283 | NA |
| 698 | HMDB0164280 | NA |
| 699 | HMDB0164279 | NA |
| 700 | HMDB0164281 | NA |
| 701 | HMDB0000933 | Traumatic acid |
| 702 | HMDB0030994 | 5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid |
| 703 | HMDB0037816 | NA |
| 704 | HMDB0037135 | NA |
| 705 | HMDB0032871 | Sedanonic acid |
| 706 | HMDB0032797 | Jasmonic acid |
| 707 | HMDB0037104 | NA |
| 708 | HMDB0041573 | NA |
| 709 | HMDB0037735 | NA |
| 710 | HMDB0033102 | Dihydro-3-(2-octenyl)-2,5-furandione |
| 711 | HMDB0037642 | NA |
| 712 | HMDB0039669 | NA |
| 713 | HMDB0033640 | 7-Methyl-3-methylene-1,6,7-octanetriol |
| 714 | HMDB0038186 | NA |
| 715 | HMDB0010725 | (R)-3-Hydroxydecanoic acid |
| 716 | HMDB0040329 | NA |
| 717 | HMDB0034783 | cis-p-Menthane-1,7,8-triol |
| 718 | HMDB0033574 | (1R,2R,4R,8R)-p-Menthane-2,8,9-triol |
| 719 | HMDB0033201 | 9-Hydroxydecanoic acid |
| 720 | HMDB0039668 | NA |
| 721 | HMDB0039470 | NA |
| 722 | HMDB0039893 | NA |
| 723 | HMDB0180105 | NA |
| 724 | HMDB0180106 | NA |
| 725 | HMDB0180104 | NA |
| 726 | HMDB0179930 | NA |
| 727 | HMDB0179931 | NA |
| 728 | HMDB0179932 | NA |
| 729 | HMDB0179929 | NA |
| 730 | HMDB0180588 | NA |
| 731 | HMDB0180587 | NA |
| 732 | HMDB0180586 | NA |
| 733 | HMDB0041600 | NA |
| 734 | HMDB0179928 | NA |
| 735 | HMDB0002203 | 3-Hydroxycapric acid |
| 736 | HMDB0094656 | 2-Hydroxydecanoate |
| 737 | HMDB0180585 | NA |
| 738 | HMDB0180589 | NA |
| 739 | HMDB0059663 | 5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate |
| 740 | HMDB0062721 | NA |
| 741 | HMDB0168420 | NA |
| 742 | HMDB0062551 | 4-ethylphenylsulfate |
| 743 | HMDB0035593 | Rishitin |
| 744 | HMDB0037605 | NA |
| 745 | HMDB0036790 | NA |
| 746 | HMDB0036791 | NA |
| 747 | HMDB0037820 | NA |
| 748 | HMDB0040178 | NA |
| 749 | HMDB0160293 | NA |
| 750 | HMDB0160295 | NA |
| 751 | HMDB0160291 | NA |
| 752 | HMDB0160290 | NA |
| 753 | HMDB0160289 | NA |
| 754 | HMDB0160292 | NA |
| 755 | HMDB0160296 | NA |

| | | |
|-----|-------------|--|
| 756 | HMDB0160294 | NA |
| 757 | HMDB0160298 | NA |
| 758 | HMDB0160297 | NA |
| 759 | HMDB0032369 | L-Menthyl acetoacetate |
| 760 | HMDB0033619 | Hexyl hexanoate |
| 761 | HMDB0059868 | NA |
| 762 | HMDB0032440 | Nonanal propyleneglycol acetal |
| 763 | HMDB0061988 | NA |
| 764 | HMDB0035410 | (R)-Dihydrocitronellol acetate |
| 765 | HMDB0000638 | Dodecanoic acid |
| 766 | HMDB0040166 | NA |
| 767 | HMDB0030998 | Ethyl decanoate |
| 768 | HMDB0034137 | Octyl 2-methylpropanoate |
| 769 | HMDB0036225 | NA |
| 770 | HMDB0034136 | Octyl butanoate |
| 771 | HMDB0034128 | Isopropyl nonanoate |
| 772 | HMDB0032310 | 2-Heptyl butyrate |
| 773 | HMDB0168119 | NA |
| 774 | HMDB0168120 | NA |
| 775 | HMDB0168121 | NA |
| 776 | HMDB0015050 | Phenformin |
| 777 | HMDB0004231 | Pantothenol |
| 778 | HMDB0061683 | NA |
| 779 | HMDB0031813 | N-Carbamoyl-2-amino-2-(4-hydroxyphenyl)acetic acid |
| 780 | HMDB0000014 | Deoxycytidine |
| 781 | HMDB0028732 | Asparaginy-Hydroxyproline |
| 782 | HMDB0028858 | Hydroxypropyl-Asparagine |
| 783 | HMDB0040046 | NA |
| 784 | HMDB0161863 | NA |
| 785 | HMDB0161860 | NA |
| 786 | HMDB0041444 | NA |
| 787 | HMDB0033452 | Koenoline |
| 788 | HMDB0161862 | NA |
| 789 | HMDB0161861 | NA |
| 790 | HMDB0161859 | NA |
| 791 | HMDB0161858 | NA |
| 792 | HMDB0161857 | NA |
| 793 | HMDB0094651 | PyroGlu-Val |
| 794 | HMDB0029018 | Prolyl-Hydroxyproline |
| 795 | HMDB0028871 | Hydroxypropyl-Proline |
| 796 | HMDB0006695 | Prolylhydroxyproline |
| 797 | HMDB0040573 | NA |
| 798 | HMDB0060747 | NA |
| 799 | HMDB0011754 | Methyldopa |
| 800 | HMDB0001434 | 3-Methoxytyrosine |
| 801 | HMDB0011172 | gamma-Glutamylvaline |
| 802 | HMDB0029162 | NA |
| 803 | HMDB0028756 | Aspartyl-Isoleucine |
| 804 | HMDB0028903 | Isoleucyl-Aspartate |
| 805 | HMDB0028925 | Leucyl-Aspartate |
| 806 | HMDB0028832 | Glutamylvaline |
| 807 | HMDB0059717 | NA |
| 808 | HMDB0029126 | Valyl-Glutamate |
| 809 | HMDB0028757 | Aspartyl-Leucine |
| 810 | HMDB0011166 | L-beta-aspartyl-L-leucine |
| 811 | HMDB0151781 | NA |
| 812 | HMDB0151783 | NA |
| 813 | HMDB0151788 | NA |
| 814 | HMDB0151787 | NA |
| 815 | HMDB0151784 | NA |
| 816 | HMDB0035016 | 2-Phenylethyl pentanoate |
| 817 | HMDB0132932 | NA |
| 818 | HMDB0132940 | NA |
| 819 | HMDB0151780 | NA |
| 820 | HMDB0001925 | Ibuprofen |
| 821 | HMDB0034472 | 3-Phenylpropyl 2-methylpropanoate |
| 822 | HMDB0034470 | 2-Phenylpropyl isobutyrate |
| 823 | HMDB0038605 | NA |
| 824 | HMDB0040431 | NA |
| 825 | HMDB0036391 | NA |
| 826 | HMDB0036025 | 2,4,6-Trimethyl-4-phenyl-1,3-dioxane |
| 827 | HMDB0037194 | NA |
| 828 | HMDB0034469 | 2-Phenylpropyl butyrate |
| 829 | HMDB0037623 | NA |
| 830 | HMDB0036240 | NA |
| 831 | HMDB0035017 | 2-Phenylethyl 3-methylbutanoate |
| 832 | HMDB0037720 | NA |
| 833 | HMDB0035008 | 3-Methylbutyl phenylacetate |
| 834 | HMDB0036386 | NA |
| 835 | HMDB0033196 | (E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one |
| 836 | HMDB0037604 | NA |
| 837 | HMDB0029669 | Eremopetasinorone A |
| 838 | HMDB0035181 | xi-8,9-Dehydrotheaspirone |
| 839 | HMDB0039101 | NA |
| 840 | HMDB0034556 | 3-Acetoxy-3-methyl-1-phenylbutane |
| 841 | HMDB0032176 | Benzyl hexanoate |
| 842 | HMDB0163212 | NA |

| | | |
|-----|-------------|---|
| 843 | HMDB0151805 | NA |
| 844 | HMDB0151793 | NA |
| 845 | HMDB0151794 | NA |
| 846 | HMDB0151789 | NA |
| 847 | HMDB0151790 | NA |
| 848 | HMDB0151791 | NA |
| 849 | HMDB0151785 | NA |
| 850 | HMDB0151786 | NA |
| 851 | HMDB0151792 | NA |
| 852 | HMDB0014604 | Nabumetone |
| 853 | HMDB0176774 | NA |
| 854 | HMDB0176773 | NA |
| 855 | HMDB0176775 | NA |
| 856 | HMDB0061836 | NA |
| 857 | HMDB0032133 | Bisphenol A |
| 858 | HMDB0033878 | (S)-Curzeone |
| 859 | HMDB0135597 | NA |
| 860 | HMDB0170855 | NA |
| 861 | HMDB0179330 | NA |
| 862 | HMDB0179331 | NA |
| 863 | HMDB0038202 | NA |
| 864 | HMDB0036767 | NA |
| 865 | HMDB0036455 | NA |
| 866 | HMDB0035902 | Enokipodin B |
| 867 | HMDB0040903 | NA |
| 868 | HMDB0038188 | NA |
| 869 | HMDB0031916 | 5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran |
| 870 | HMDB0037558 | NA |
| 871 | HMDB0036473 | NA |
| 872 | HMDB0037801 | NA |
| 873 | HMDB0030911 | 2-Oxo-5,11(13)-eudesmadien-12,8-olide |
| 874 | HMDB0031900 | Methyl (2E,4Z,6E,8E,10E)-4,8-dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoate |
| 875 | HMDB0036488 | NA |
| 876 | HMDB0038547 | NA |
| 877 | HMDB0041920 | NA |
| 878 | HMDB0179332 | NA |
| 879 | HMDB0059946 | NA |
| 880 | HMDB0041618 | NA |
| 881 | HMDB0176325 | NA |
| 882 | HMDB0059947 | NA |
| 883 | HMDB0176328 | NA |
| 884 | HMDB0000872 | Tetradecanedioic acid |
| 885 | HMDB0176327 | NA |
| 886 | HMDB0040429 | NA |
| 887 | HMDB0176326 | NA |
| 888 | HMDB0040219 | NA |
| 889 | HMDB0029397 | L-Nicotianine |
| 890 | HMDB0000732 | Hydroxykynurenine |
| 891 | HMDB0012819 | 5-Hydroxykynurenine |
| 892 | HMDB0014787 | Stavudine |
| 893 | HMDB0011631 | L-3-Hydroxykynurenine |
| 894 | HMDB0060750 | NA |
| 895 | HMDB0002224 | 5-Methyldeoxycytidine |
| 896 | HMDB0028861 | Hydroxypropyl-Glutamine |
| 897 | HMDB0038516 | NA |
| 898 | HMDB0028798 | Glutaminyhydroxyproline |
| 899 | HMDB0028877 | Hydroxypropyl-Gamma-glutamate |
| 900 | HMDB0178266 | NA |
| 901 | HMDB0037694 | NA |
| 902 | HMDB0040006 | NA |
| 903 | HMDB0037695 | NA |
| 904 | HMDB0042008 | NA |
| 905 | HMDB0033430 | Tanakine |
| 906 | HMDB0033429 | Tanakamine |
| 907 | HMDB0142966 | NA |
| 908 | HMDB0029448 | DL-Ornithino-L-alanine |
| 909 | HMDB0041858 | NA |
| 910 | HMDB0135607 | NA |
| 911 | HMDB0141386 | NA |
| 912 | HMDB0135600 | NA |
| 913 | HMDB0135404 | NA |
| 914 | HMDB0135599 | NA |
| 915 | HMDB0141385 | NA |
| 916 | HMDB0141387 | NA |
| 917 | HMDB0135604 | NA |
| 918 | HMDB0135603 | NA |
| 919 | HMDB0135602 | NA |
| 920 | HMDB0032584 | 4-Hydroxychalcone |
| 921 | HMDB0037696 | NA |
| 922 | HMDB0014922 | Mefenamic acid |
| 923 | HMDB0040380 | NA |
| 924 | HMDB0029366 | N-[2-(4-Hydroxyphenyl)ethyl]benzamide |
| 925 | HMDB0147191 | NA |
| 926 | HMDB0131062 | NA |
| 927 | HMDB0131065 | NA |
| 928 | HMDB0036050 | NA |
| 929 | HMDB0033771 | Cyperine |

| | | |
|------|-------------|---|
| 930 | HMDB0030690 | (E)-Suberenol |
| 931 | HMDB0039592 | NA |
| 932 | HMDB0030788 | Citrusal |
| 933 | HMDB0135759 | NA |
| 934 | HMDB0135760 | NA |
| 935 | HMDB0135761 | NA |
| 936 | HMDB0141827 | NA |
| 937 | HMDB0151855 | NA |
| 938 | HMDB0153660 | NA |
| 939 | HMDB0135757 | NA |
| 940 | HMDB0135758 | NA |
| 941 | HMDB0129916 | NA |
| 942 | HMDB0129917 | NA |
| 943 | HMDB0129919 | NA |
| 944 | HMDB0129920 | NA |
| 945 | HMDB0129922 | NA |
| 946 | HMDB0131064 | NA |
| 947 | HMDB0131066 | NA |
| 948 | HMDB0131067 | NA |
| 949 | HMDB0132269 | NA |
| 950 | HMDB0129918 | NA |
| 951 | HMDB0030854 | (S)-Auraptenol |
| 952 | HMDB0030110 | Celerin |
| 953 | HMDB0030948 | Dihydrowyerone |
| 954 | HMDB0039142 | NA |
| 955 | HMDB0041192 | NA |
| 956 | HMDB0034133 | 3-(1,1-Dimethylallyl)scopoletin |
| 957 | HMDB0030853 | (R)-Meranzin |
| 958 | HMDB0033015 | 5,6-Dihydroyangonin |
| 959 | HMDB0035254 | 7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone |
| 960 | HMDB0033016 | 7,8-Dihydroyangonin |
| 961 | HMDB0030578 | Apigravin |
| 962 | HMDB0032953 | 7-Methoxy-5-prenyloxycoumarin |
| 963 | HMDB0061290 | NA |
| 964 | HMDB0061303 | NA |
| 965 | HMDB0039146 | NA |
| 966 | HMDB0037679 | NA |
| 967 | HMDB0035019 | Phenethyl salicylate |
| 968 | HMDB0029302 | 1-Phenyl-6,7-dihydroxy-isochroman |
| 969 | HMDB0036347 | NA |
| 970 | HMDB0002209 | Equol |
| 971 | HMDB0130495 | NA |
| 972 | HMDB0014713 | Fenoprofen |
| 973 | HMDB0135409 | NA |
| 974 | HMDB0135406 | NA |
| 975 | HMDB0135408 | NA |
| 976 | HMDB0135407 | NA |
| 977 | HMDB0135593 | NA |
| 978 | HMDB0135594 | NA |
| 979 | HMDB0135405 | NA |
| 980 | HMDB0130496 | NA |
| 981 | HMDB0135355 | NA |
| 982 | HMDB0135397 | NA |
| 983 | HMDB0135595 | NA |
| 984 | HMDB0151857 | NA |
| 985 | HMDB0130497 | NA |
| 986 | HMDB0168444 | NA |
| 987 | HMDB0135601 | NA |
| 988 | HMDB0168447 | NA |
| 989 | HMDB0148520 | NA |
| 990 | HMDB0168443 | NA |
| 991 | HMDB0182848 | NA |
| 992 | HMDB0168445 | NA |
| 993 | HMDB0168442 | NA |
| 994 | HMDB0135596 | NA |
| 995 | HMDB0168446 | NA |
| 996 | HMDB0029953 | D-erythro-D-galacto-octitol |
| 997 | HMDB0151802 | NA |
| 998 | HMDB0151796 | NA |
| 999 | HMDB0151800 | NA |
| 1000 | HMDB0151798 | NA |
| 1001 | HMDB0151801 | NA |
| 1002 | HMDB0151797 | NA |
| 1003 | HMDB0151799 | NA |
| 1004 | HMDB0037492 | NA |
| 1005 | HMDB0032589 | 1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone |
| 1006 | HMDB0061823 | NA |
| 1007 | HMDB0061942 | NA |
| 1008 | HMDB0040424 | NA |
| 1009 | HMDB0132933 | NA |
| 1010 | HMDB0132935 | NA |
| 1011 | HMDB0132936 | NA |
| 1012 | HMDB0132937 | NA |
| 1013 | HMDB0132939 | NA |
| 1014 | HMDB0132948 | NA |
| 1015 | HMDB0060478 | gamma-Glutamyl-beta-cyanoalanine |
| 1016 | HMDB0000089 | Cytidine |

| | | |
|------|-------------|--|
| 1017 | HMDB0015122 | Cytarabine |
| 1018 | HMDB0155273 | NA |
| 1019 | HMDB0001904 | 3-Nitrotyrosine |
| 1020 | HMDB0028751 | Aspartyl-Glutamine |
| 1021 | HMDB0028793 | Glutaminylaspartic acid |
| 1022 | HMDB0029144 | gamma-Glutamylasparagine |
| 1023 | HMDB0028814 | Glutamylasparagine |
| 1024 | HMDB0028730 | Asparaginy-Glutamate |
| 1025 | HMDB0028767 | Aspartyl-Gamma-glutamate |
| 1026 | HMDB0033701 | Hydrocotarnine |
| 1027 | HMDB0031770 | Carbofuran |
| 1028 | HMDB0014798 | Metaxalone |
| 1029 | HMDB0139892 | NA |
| 1030 | HMDB0138550 | NA |
| 1031 | HMDB0033925 | Oroselone |
| 1032 | HMDB0032998 | 2-Methoxyxanthone |
| 1033 | HMDB0161779 | NA |
| 1034 | HMDB0161778 | NA |
| 1035 | HMDB0161783 | NA |
| 1036 | HMDB0161782 | NA |
| 1037 | HMDB0161780 | NA |
| 1038 | HMDB0162111 | NA |
| 1039 | HMDB0162103 | NA |
| 1040 | HMDB0162104 | NA |
| 1041 | HMDB0162105 | NA |
| 1042 | HMDB0162108 | NA |
| 1043 | HMDB0162109 | NA |
| 1044 | HMDB0162106 | NA |
| 1045 | HMDB0162107 | NA |
| 1046 | HMDB0162110 | NA |
| 1047 | HMDB0162112 | NA |
| 1048 | HMDB0161832 | NA |
| 1049 | HMDB0161833 | NA |
| 1050 | HMDB0161834 | NA |
| 1051 | HMDB0149051 | NA |
| 1052 | HMDB0149050 | NA |
| 1053 | HMDB0149006 | NA |
| 1054 | HMDB0148541 | NA |
| 1055 | HMDB0148540 | NA |
| 1056 | HMDB0148786 | NA |
| 1057 | HMDB0148785 | NA |
| 1058 | HMDB0148998 | NA |
| 1059 | HMDB0149048 | NA |
| 1060 | HMDB0147226 | NA |
| 1061 | HMDB0148542 | NA |
| 1062 | HMDB0128505 | NA |
| 1063 | HMDB0148539 | NA |
| 1064 | HMDB0145646 | NA |
| 1065 | HMDB0145647 | NA |
| 1066 | HMDB0145645 | NA |
| 1067 | HMDB0135172 | NA |
| 1068 | HMDB0149007 | NA |
| 1069 | HMDB0128506 | NA |
| 1070 | HMDB0128503 | NA |
| 1071 | HMDB0128504 | NA |
| 1072 | HMDB0040876 | NA |
| 1073 | HMDB0030946 | (2E,11Z)-Wyerone acid |
| 1074 | HMDB0041016 | NA |
| 1075 | HMDB0030595 | Suberenone |
| 1076 | HMDB0033735 | Graveolone |
| 1077 | HMDB0039430 | NA |
| 1078 | HMDB0004215 | 3,3',4'5-Tetrahydroxystilbene |
| 1079 | HMDB0170845 | NA |
| 1080 | HMDB0164057 | NA |
| 1081 | HMDB0135900 | NA |
| 1082 | HMDB0135902 | NA |
| 1083 | HMDB0135904 | NA |
| 1084 | HMDB0164055 | NA |
| 1085 | HMDB0164056 | NA |
| 1086 | HMDB0164058 | NA |
| 1087 | HMDB0170846 | NA |
| 1088 | HMDB0170974 | NA |
| 1089 | HMDB0170976 | NA |
| 1090 | HMDB0170979 | NA |
| 1091 | HMDB0170978 | NA |
| 1092 | HMDB0131284 | NA |
| 1093 | HMDB0131285 | NA |
| 1094 | HMDB0127824 | NA |
| 1095 | HMDB0131281 | NA |
| 1096 | HMDB0131283 | NA |
| 1097 | HMDB0170977 | NA |
| 1098 | HMDB0031668 | Dihydrodeoxy-8-epiaustdiol |
| 1099 | HMDB0034056 | 5-(3,4-Methylenedioxyphenyl)pentanoic acid |
| 1100 | HMDB0037681 | NA |
| 1101 | HMDB0029470 | Isodillapiole |
| 1102 | HMDB0041379 | NA |
| 1103 | HMDB0135906 | NA |

| | | |
|------|-------------|--|
| 1104 | HMDB0038563 | NA |
| 1105 | HMDB0037130 | NA |
| 1106 | HMDB0094660 | Diethyl phthalic acid |
| 1107 | HMDB0033776 | Apiole |
| 1108 | HMDB0029226 | 5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone |
| 1109 | HMDB0135689 | NA |
| 1110 | HMDB0013247 | Monobutylphthalate |
| 1111 | HMDB0030725 | Dillapiol |
| 1112 | HMDB0002056 | Monoisobutyl phthalic acid |
| 1113 | HMDB0147179 | NA |
| 1114 | HMDB0140340 | NA |
| 1115 | HMDB0173973 | NA |
| 1116 | HMDB0173971 | NA |
| 1117 | HMDB0173972 | NA |
| 1118 | HMDB0173975 | NA |
| 1119 | HMDB0173976 | NA |
| 1120 | HMDB0177472 | NA |
| 1121 | HMDB0177470 | NA |
| 1122 | HMDB0173974 | NA |
| 1123 | HMDB0128944 | NA |
| 1124 | HMDB0131630 | NA |
| 1125 | HMDB0128958 | NA |
| 1126 | HMDB0039027 | NA |
| 1127 | HMDB0128963 | NA |
| 1128 | HMDB0138052 | NA |
| 1129 | HMDB0128962 | NA |
| 1130 | HMDB0030882 | (S)-Rutaretin |
| 1131 | HMDB0128960 | NA |
| 1132 | HMDB0128961 | NA |
| 1133 | HMDB0032838 | Dorsteniol |
| 1134 | HMDB0131653 | NA |
| 1135 | HMDB0147178 | NA |
| 1136 | HMDB0131691 | NA |
| 1137 | HMDB0131700 | NA |
| 1138 | HMDB0167944 | NA |
| 1139 | HMDB0163475 | NA |
| 1140 | HMDB0171044 | NA |
| 1141 | HMDB0167134 | NA |
| 1142 | HMDB0028752 | Aspartyl-Glutamate |
| 1143 | HMDB0029145 | NA |
| 1144 | HMDB0030419 | gamma-Glutamylaspartic acid |
| 1145 | HMDB0062501 | NA |
| 1146 | HMDB0028815 | Glutamylaspartic acid |
| 1147 | HMDB0030413 | NA |
| 1148 | HMDB0011164 | L-beta-aspartyl-L-glutamic acid |
| 1149 | HMDB0000767 | Pseudouridine |
| 1150 | HMDB0000296 | Uridine |
| 1151 | HMDB0156330 | NA |
| 1152 | HMDB0126635 | NA |
| 1153 | HMDB0130466 | NA |
| 1154 | HMDB0130477 | NA |
| 1155 | HMDB0006794 | 5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate |
| 1156 | HMDB0157260 | NA |
| 1157 | HMDB0157259 | NA |
| 1158 | HMDB0125157 | NA |
| 1159 | HMDB0166885 | NA |
| 1160 | HMDB0155302 | NA |
| 1161 | HMDB0180914 | NA |
| 1162 | HMDB0177249 | NA |
| 1163 | HMDB0163614 | NA |
| 1164 | HMDB0028833 | Glutamyl-Gamma-glutamate |
| 1165 | HMDB0028796 | Glutamylglutamic acid |
| 1166 | HMDB0029147 | N-gamma-Glutamylglutamine |
| 1167 | HMDB0028817 | Glutamylglutamine |
| 1168 | HMDB0011738 | N2-gamma-Glutamylglutamine |
| 1169 | HMDB0005766 | Norophthalmic acid |
| 1170 | HMDB0240577 | NA |
| 1171 | HMDB0000982 | 5-Methylcytidine |
| 1172 | HMDB0039229 | Pyro-L-glutamyl-L-glutamine |
| 1173 | HMDB0032559 | (Åś)-2-(1-Methylpropyl)-4,6-dinitrophenol |
| 1174 | HMDB0033610 | Pandamarilactam 3x |
| 1175 | HMDB0139906 | NA |
| 1176 | HMDB0164387 | NA |
| 1177 | HMDB0000086 | Glycerophosphocholine |
| 1178 | HMDB0142996 | NA |
| 1179 | HMDB0143005 | NA |
| 1180 | HMDB0151865 | NA |
| 1181 | HMDB0137520 | NA |
| 1182 | HMDB0130494 | NA |
| 1183 | HMDB0135588 | NA |
| 1184 | HMDB0135591 | NA |
| 1185 | HMDB0135592 | NA |
| 1186 | HMDB0137534 | NA |
| 1187 | HMDB0135587 | NA |
| 1188 | HMDB0135590 | NA |
| 1189 | HMDB0151856 | NA |
| 1190 | HMDB0032130 | 3',4'-Dihydroxychalcone |

| | | |
|------|-------------|---|
| 1191 | HMDB0135586 | NA |
| 1192 | HMDB0153774 | NA |
| 1193 | HMDB0036738 | NA |
| 1194 | HMDB0039612 | NA |
| 1195 | HMDB0032129 | 2',5'-Dihydroxychalcone |
| 1196 | HMDB0014643 | Tolmetin |
| 1197 | HMDB0033345 | (\hat{A} \hat{s})-Ribaline |
| 1198 | HMDB0041329 | NA |
| 1199 | HMDB0032924 | 3-Furanmethanol glucoside |
| 1200 | HMDB0130798 | NA |
| 1201 | HMDB0130839 | NA |
| 1202 | HMDB0126546 | NA |
| 1203 | HMDB0167013 | NA |
| 1204 | HMDB0175219 | NA |
| 1205 | HMDB0167016 | NA |
| 1206 | HMDB0002091 | Isovalerylglucuronide |
| 1207 | HMDB0167014 | NA |
| 1208 | HMDB0175223 | NA |
| 1209 | HMDB0143217 | NA |
| 1210 | HMDB0175224 | NA |
| 1211 | HMDB0175227 | NA |
| 1212 | HMDB0175220 | NA |
| 1213 | HMDB0033065 | (x)-1,2-Propanediol 1-O-b-D-glucopyranoside |
| 1214 | HMDB0060917 | NA |
| 1215 | HMDB0144816 | NA |
| 1216 | HMDB0184077 | NA |
| 1217 | HMDB0029155 | NA |
| 1218 | HMDB0034367 | gamma-Glutamylmethionine |
| 1219 | HMDB0028972 | Methionyl-Glutamate |
| 1220 | HMDB0028825 | Glutamylmethionine |
| 1221 | HMDB0060663 | NA |
| 1222 | HMDB0177722 | NA |
| 1223 | HMDB0040790 | NA |
| 1224 | HMDB0033351 | Methoxybrassinin |
| 1225 | HMDB0155171 | NA |
| 1226 | HMDB0002062 | Norepinephrine sulfate |
| 1227 | HMDB0156032 | NA |
| 1228 | HMDB0155175 | NA |
| 1229 | HMDB0155133 | NA |
| 1230 | HMDB0156031 | NA |
| 1231 | HMDB0155132 | NA |
| 1232 | HMDB0240695 | NA |
| 1233 | HMDB0168085 | NA |
| 1234 | HMDB0167573 | NA |
| 1235 | HMDB0153240 | NA |
| 1236 | HMDB0148680 | NA |
| 1237 | HMDB0130908 | NA |
| 1238 | HMDB0150257 | NA |
| 1239 | HMDB0150666 | NA |
| 1240 | HMDB0150667 | NA |
| 1241 | HMDB0151413 | NA |
| 1242 | HMDB0151710 | NA |
| 1243 | HMDB0151717 | NA |
| 1244 | HMDB0151989 | NA |
| 1245 | HMDB0152004 | NA |
| 1246 | HMDB0152130 | NA |
| 1247 | HMDB0153396 | NA |
| 1248 | HMDB0147592 | NA |
| 1249 | HMDB0128588 | NA |
| 1250 | HMDB0130320 | NA |
| 1251 | HMDB0130374 | NA |
| 1252 | HMDB0130909 | NA |
| 1253 | HMDB0130905 | NA |
| 1254 | HMDB0130928 | NA |
| 1255 | HMDB0130926 | NA |
| 1256 | HMDB0132873 | NA |
| 1257 | HMDB0140458 | NA |
| 1258 | HMDB0140466 | NA |
| 1259 | HMDB0140465 | NA |
| 1260 | HMDB0140471 | NA |
| 1261 | HMDB0140478 | NA |
| 1262 | HMDB0141217 | NA |
| 1263 | HMDB0128584 | NA |
| 1264 | HMDB0146278 | NA |
| 1265 | HMDB0132455 | NA |
| 1266 | HMDB0130379 | NA |
| 1267 | HMDB0036629 | NA |
| 1268 | HMDB0029522 | 5,7-Dihydroxy-3-methoxyflavone |
| 1269 | HMDB0133330 | NA |
| 1270 | HMDB0132457 | NA |
| 1271 | HMDB0031428 | Farnisin |
| 1272 | HMDB0039166 | NA |
| 1273 | HMDB0039578 | NA |
| 1274 | HMDB0005781 | Glycitein |
| 1275 | HMDB0002338 | Biochanin A |
| 1276 | HMDB0034127 | Prunetin |
| 1277 | HMDB0180733 | NA |

| | | |
|------|-------------|--|
| 1278 | HMDB0147591 | NA |
| 1279 | HMDB0041758 | NA |
| 1280 | HMDB0041776 | NA |
| 1281 | HMDB0031720 | Xenognosin B |
| 1282 | HMDB0030768 | 2-(6-Hydroxy-2-methoxy-3,4-methylenedioxyphenyl)benzofuran |
| 1283 | HMDB0141945 | NA |
| 1284 | HMDB0132850 | NA |
| 1285 | HMDB0147530 | NA |
| 1286 | HMDB0150245 | NA |
| 1287 | HMDB0132886 | NA |
| 1288 | HMDB0130929 | NA |
| 1289 | HMDB0134889 | NA |
| 1290 | HMDB0137557 | NA |
| 1291 | HMDB0125118 | NA |
| 1292 | HMDB0145984 | NA |
| 1293 | HMDB0175189 | NA |
| 1294 | HMDB0175187 | NA |
| 1295 | HMDB0175188 | NA |
| 1296 | HMDB0162484 | NA |
| 1297 | HMDB0033197 | 2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione |
| 1298 | HMDB0036047 | NA |
| 1299 | HMDB0059661 | NA |
| 1300 | HMDB0015088 | Rizatriptan |
| 1301 | HMDB0014873 | Naftifine |
| 1302 | HMDB0014578 | Cyproheptadine |
| 1303 | HMDB0186509 | NA |
| 1304 | HMDB0184957 | NA |
| 1305 | HMDB0184936 | NA |
| 1306 | HMDB0062677 | NA |
| 1307 | HMDB0004590 | 19-Nor-5-androstenediol |
| 1308 | HMDB0032464 | Phenethyl decanoate |
| 1309 | HMDB0002697 | 19-Norandrosterone |
| 1310 | HMDB0032672 | 4,8,12,15-Octadecatetraenoic acid |
| 1311 | HMDB0005886 | 19-Noretiocholanolone |
| 1312 | HMDB0034382 | (E,E)-11,13-Octadecadien-9-ynoic acid |
| 1313 | HMDB0006547 | Stearidonic acid |
| 1314 | HMDB0186501 | NA |
| 1315 | HMDB0186507 | NA |
| 1316 | HMDB0186508 | NA |
| 1317 | HMDB0062288 | NA |
| 1318 | HMDB0186510 | NA |
| 1319 | HMDB0186500 | NA |
| 1320 | HMDB0186506 | NA |
| 1321 | HMDB0186505 | NA |
| 1322 | HMDB0186504 | NA |
| 1323 | HMDB0186502 | NA |
| 1324 | HMDB0186497 | NA |
| 1325 | HMDB0186499 | NA |
| 1326 | HMDB0186498 | NA |
| 1327 | HMDB0112093 | NA |
| 1328 | HMDB0112099 | NA |
| 1329 | HMDB0112102 | NA |
| 1330 | HMDB0112103 | NA |
| 1331 | HMDB0186503 | NA |
| 1332 | HMDB0034586 | (9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid |
| 1333 | HMDB0031088 | 12,13-Epoxy-9,15-octadecadienoic acid |
| 1334 | HMDB0029969 | Squamostanal A |
| 1335 | HMDB0031103 | 2-Hydroxylinolenic acid |
| 1336 | HMDB0036832 | NA |
| 1337 | HMDB0030950 | 15,16-Epoxy-9,12-octadecadienoic acid |
| 1338 | HMDB0029786 | 10-Oxo-11-octadecen-13-olide |
| 1339 | HMDB0011108 | 17-Hydroxylinolenic acid |
| 1340 | HMDB0010224 | 9-HOTE |
| 1341 | HMDB0010220 | 9(10)-EpODE |
| 1342 | HMDB0010206 | 15(16)-EpODE |
| 1343 | HMDB0010200 | A-12(13)-EpODE |
| 1344 | HMDB0010203 | 13-HOTE |
| 1345 | HMDB0004669 | 9-OxoODE |
| 1346 | HMDB0004668 | 13-OxoODE |
| 1347 | HMDB0031934 | (9S,10E,12Z,15Z)-9-Hydroxy-10,12,15-octadecatrienoic acid |
| 1348 | HMDB0030995 | (2'E,4'Z,8E)-Colneleic acid |
| 1349 | HMDB0061644 | NA |
| 1350 | HMDB0039603 | NA |
| 1351 | HMDB0061979 | NA |
| 1352 | HMDB0033791 | (E)-3-Hexadecenoic acid |
| 1353 | HMDB0038958 | NA |
| 1354 | HMDB0031711 | 15-Hexadecanolide |
| 1355 | HMDB0003229 | Palmitoleic acid |
| 1356 | HMDB0010735 | Trans-Hexa-dec-2-enoic acid |
| 1357 | HMDB0037647 | NA |
| 1358 | HMDB0041422 | NA |
| 1359 | HMDB0032638 | (Z)-5-Hexadecenoic acid |
| 1360 | HMDB0031053 | (E)-6-Hexadecenoic acid |
| 1361 | HMDB0035877 | (Z)-13-Hexadecenoic acid |
| 1362 | HMDB0031145 | 5-Dodecyldihydro-2(3H)-furanone |
| 1363 | HMDB0002186 | Hypogeic acid |
| 1364 | HMDB0171478 | NA |

| | | |
|------|-------------|--|
| 1365 | HMDB0171479 | NA |
| 1366 | HMDB0171477 | NA |
| 1367 | HMDB0012328 | Palmitelaidic acid |
| 1368 | HMDB0171476 | NA |
| 1369 | HMDB0000756 | L-Hexanoylcarnitine |
| 1370 | HMDB0000705 | Hexanoylcarnitine |
| 1371 | HMDB0014413 | Ropinirole |
| 1372 | HMDB0015070 | Oxymetazoline |
| 1373 | HMDB0061189 | NA |
| 1374 | HMDB0062555 | hydroxyisovaleroyl carnitine |
| 1375 | HMDB0240421 | NA |
| 1376 | HMDB0040904 | NA |
| 1377 | HMDB0168550 | NA |
| 1378 | HMDB0168551 | NA |
| 1379 | HMDB0168552 | NA |
| 1380 | HMDB0168553 | NA |
| 1381 | HMDB0168554 | NA |
| 1382 | HMDB0168549 | NA |
| 1383 | HMDB0137260 | NA |
| 1384 | HMDB0137271 | NA |
| 1385 | HMDB0030974 | 8-Acetoxy-4-acoren-3-one |
| 1386 | HMDB0031928 | Panaxytriol |
| 1387 | HMDB0030801 | 1-(4-Hydroxy-3-methoxyphenyl)-3-decanone |
| 1388 | HMDB0039251 | NA |
| 1389 | HMDB0134775 | NA |
| 1390 | HMDB0038798 | NA |
| 1391 | HMDB0035075 | Tanacetol B |
| 1392 | HMDB0060952 | NA |
| 1393 | HMDB0014521 | Palonosetron |
| 1394 | HMDB0030283 | Hydrocinchonine |
| 1395 | HMDB0175409 | NA |
| 1396 | HMDB0175412 | NA |
| 1397 | HMDB0175413 | NA |
| 1398 | HMDB0175414 | NA |
| 1399 | HMDB0175415 | NA |
| 1400 | HMDB0175408 | NA |
| 1401 | HMDB0175410 | NA |
| 1402 | HMDB0175411 | NA |
| 1403 | HMDB0160594 | NA |
| 1404 | HMDB0173892 | NA |
| 1405 | HMDB0175402 | NA |
| 1406 | HMDB0175403 | NA |
| 1407 | HMDB0175404 | NA |
| 1408 | HMDB0175405 | NA |
| 1409 | HMDB0175406 | NA |
| 1410 | HMDB0175407 | NA |
| 1411 | HMDB0030964 | Linolenelaidic acid |
| 1412 | HMDB0001388 | Alpha-Linolenic acid |
| 1413 | HMDB0003073 | Gamma-Linolenic acid |
| 1414 | HMDB0030962 | Calendic acid |
| 1415 | HMDB0030963 | Punicic acid |
| 1416 | HMDB0160589 | NA |
| 1417 | HMDB0160588 | NA |
| 1418 | HMDB0112194 | NA |
| 1419 | HMDB0062652 | NA |
| 1420 | HMDB0173890 | NA |
| 1421 | HMDB0160590 | NA |
| 1422 | HMDB0160592 | NA |
| 1423 | HMDB0160591 | NA |
| 1424 | HMDB0160593 | NA |
| 1425 | HMDB0160595 | NA |
| 1426 | HMDB0173886 | NA |
| 1427 | HMDB0173885 | NA |
| 1428 | HMDB0173887 | NA |
| 1429 | HMDB0173889 | NA |
| 1430 | HMDB0173891 | NA |
| 1431 | HMDB0173888 | NA |
| 1432 | HMDB0173893 | NA |
| 1433 | HMDB0004667 | 13S-hydroxyoctadecadienoic acid |
| 1434 | HMDB0061708 | NA |
| 1435 | HMDB0029796 | (Z)-13-Oxo-9-octadecenoic acid |
| 1436 | HMDB0029998 | 12-Hydroxy-8,10-octadecadienoic acid |
| 1437 | HMDB0029978 | Avenoleic acid |
| 1438 | HMDB0010223 | 9-HODE |
| 1439 | HMDB0004701 | 9,10-Epoxyoctadecenoic acid |
| 1440 | HMDB0004702 | 12,13-EpOME |
| 1441 | HMDB0004670 | Alpha-dimorphecolic acid |
| 1442 | HMDB0000220 | Palmitic acid |
| 1443 | HMDB0060083 | NA |
| 1444 | HMDB0061373 | NA |
| 1445 | HMDB0032324 | Hexyl decanoate |
| 1446 | HMDB0032249 | Dodecyl butyrate |
| 1447 | HMDB0033166 | Octyl octanoate |
| 1448 | HMDB0032065 | Butyl dodecanoate |
| 1449 | HMDB0036210 | NA |
| 1450 | HMDB0034153 | Ethyl tetradecanoate |
| 1451 | HMDB0031068 | Isopalmitic acid |

| | | |
|------|-------------|-------------------------------|
| 1452 | HMDB0002396 | Trimethyltridecanoic acid |
| 1453 | HMDB0240660 | NA |
| 1454 | HMDB0166396 | NA |
| 1455 | HMDB0155323 | NA |
| 1456 | HMDB0125616 | NA |
| 1457 | HMDB0157443 | NA |
| 1458 | HMDB0125615 | NA |
| 1459 | HMDB0155324 | NA |
| 1460 | HMDB0155326 | NA |
| 1461 | HMDB0155327 | NA |
| 1462 | HMDB0157445 | NA |
| 1463 | HMDB0157442 | NA |
| 1464 | HMDB0166395 | NA |
| 1465 | HMDB0156225 | NA |
| 1466 | HMDB0156223 | NA |
| 1467 | HMDB0156224 | NA |
| 1468 | HMDB0156222 | NA |
| 1469 | HMDB0155825 | NA |
| 1470 | HMDB0166394 | NA |
| 1471 | HMDB0125614 | NA |
| 1472 | HMDB0125613 | NA |
| 1473 | HMDB0157444 | NA |
| 1474 | HMDB0155325 | NA |
| 1475 | HMDB0164008 | NA |
| 1476 | HMDB0062577 | NA |
| 1477 | HMDB0003950 | 7-Methylinosine |
| 1478 | HMDB0002721 | 1-Methylinosine |
| 1479 | HMDB0033060 | Piperolactam A |
| 1480 | HMDB0034319 | Furofoline |
| 1481 | HMDB0038882 | NA |
| 1482 | HMDB0038880 | NA |
| 1483 | HMDB0029918 | Arabinofuranobiose |
| 1484 | HMDB0029894 | Xylobiose |
| 1485 | HMDB0038855 | NA |
| 1486 | HMDB0029619 | Arabinopyranobiose |
| 1487 | HMDB0038881 | NA |
| 1488 | HMDB0179982 | NA |
| 1489 | HMDB0179983 | NA |
| 1490 | HMDB0179984 | NA |
| 1491 | HMDB0028745 | Asparaginylnl-Gamma-glutamate |
| 1492 | HMDB0028792 | Glutaminylnlasparagine |
| 1493 | HMDB0028729 | Asparaginylnl-Glutamine |
| 1494 | HMDB0126535 | NA |
| 1495 | HMDB0126543 | NA |
| 1496 | HMDB0126529 | NA |
| 1497 | HMDB0126544 | NA |
| 1498 | HMDB0126525 | NA |
| 1499 | HMDB0126540 | NA |
| 1500 | HMDB0126536 | NA |
| 1501 | HMDB0126532 | NA |
| 1502 | HMDB0126531 | NA |
| 1503 | HMDB0126528 | NA |
| 1504 | HMDB0126526 | NA |
| 1505 | HMDB0140895 | NA |
| 1506 | HMDB0140584 | NA |
| 1507 | HMDB0140434 | NA |
| 1508 | HMDB0240404 | NA |
| 1509 | HMDB0132291 | NA |
| 1510 | HMDB0140896 | NA |
| 1511 | HMDB0140901 | NA |
| 1512 | HMDB0140900 | NA |
| 1513 | HMDB0172131 | NA |
| 1514 | HMDB0171705 | NA |
| 1515 | HMDB0168714 | NA |
| 1516 | HMDB0168707 | NA |
| 1517 | HMDB0159585 | NA |
| 1518 | HMDB0157245 | NA |
| 1519 | HMDB0152783 | NA |
| 1520 | HMDB0145741 | NA |
| 1521 | HMDB0145740 | NA |
| 1522 | HMDB0172133 | NA |
| 1523 | HMDB0134099 | NA |
| 1524 | HMDB0159586 | NA |
| 1525 | HMDB0132292 | NA |
| 1526 | HMDB0041648 | NA |
| 1527 | HMDB0041721 | NA |
| 1528 | HMDB0059967 | NA |
| 1529 | HMDB0061117 | NA |
| 1530 | HMDB0011719 | Homovanillic acid sulfate |
| 1531 | HMDB0002899 | Ellagic acid |
| 1532 | HMDB0015039 | Ethacrynic acid |
| 1533 | HMDB0060626 | NA |
| 1534 | HMDB0039096 | NA |
| 1535 | HMDB0173636 | NA |
| 1536 | HMDB0041314 | NA |
| 1537 | HMDB0130350 | NA |
| 1538 | HMDB0130347 | NA |

| | | |
|------|-------------|---|
| 1539 | HMDB0175079 | NA |
| 1540 | HMDB0178312 | NA |
| 1541 | HMDB0141160 | NA |
| 1542 | HMDB0141105 | NA |
| 1543 | HMDB0141099 | NA |
| 1544 | HMDB0141080 | NA |
| 1545 | HMDB0141122 | NA |
| 1546 | HMDB0141079 | NA |
| 1547 | HMDB0141126 | NA |
| 1548 | HMDB0141149 | NA |
| 1549 | HMDB0141119 | NA |
| 1550 | HMDB0040889 | NA |
| 1551 | HMDB0129039 | NA |
| 1552 | HMDB0138953 | NA |
| 1553 | HMDB0141045 | NA |
| 1554 | HMDB0138954 | NA |
| 1555 | HMDB0138952 | NA |
| 1556 | HMDB0138951 | NA |
| 1557 | HMDB0138956 | NA |
| 1558 | HMDB0140994 | NA |
| 1559 | HMDB0138959 | NA |
| 1560 | HMDB0138955 | NA |
| 1561 | HMDB0138957 | NA |
| 1562 | HMDB0138958 | NA |
| 1563 | HMDB0141056 | NA |
| 1564 | HMDB0141150 | NA |
| 1565 | HMDB0141152 | NA |
| 1566 | HMDB0141153 | NA |
| 1567 | HMDB0141164 | NA |
| 1568 | HMDB0146848 | NA |
| 1569 | HMDB0146849 | NA |
| 1570 | HMDB0141181 | NA |
| 1571 | HMDB0141151 | NA |
| 1572 | HMDB0141180 | NA |
| 1573 | HMDB0141162 | NA |
| 1574 | HMDB0141161 | NA |
| 1575 | HMDB0141169 | NA |
| 1576 | HMDB0141163 | NA |
| 1577 | HMDB0141145 | NA |
| 1578 | HMDB0141146 | NA |
| 1579 | HMDB0141057 | NA |
| 1580 | HMDB0141101 | NA |
| 1581 | HMDB0141102 | NA |
| 1582 | HMDB0141100 | NA |
| 1583 | HMDB0141103 | NA |
| 1584 | HMDB0141106 | NA |
| 1585 | HMDB0141107 | NA |
| 1586 | HMDB0141120 | NA |
| 1587 | HMDB0141121 | NA |
| 1588 | HMDB0141130 | NA |
| 1589 | HMDB0141129 | NA |
| 1590 | HMDB0141128 | NA |
| 1591 | HMDB0141127 | NA |
| 1592 | HMDB0141139 | NA |
| 1593 | HMDB0141140 | NA |
| 1594 | HMDB0141170 | NA |
| 1595 | HMDB0036635 | NA |
| 1596 | HMDB0041298 | NA |
| 1597 | HMDB0033310 | Moracin C |
| 1598 | HMDB0031744 | Artocarbene |
| 1599 | HMDB0141044 | NA |
| 1600 | HMDB0138682 | NA |
| 1601 | HMDB0011741 | gamma-Glutamyltyrosine |
| 1602 | HMDB0029161 | NA |
| 1603 | HMDB0029104 | Tyrosyl-Glutamate |
| 1604 | HMDB0028831 | Glutamyltyrosine |
| 1605 | HMDB0062553 | NA |
| 1606 | HMDB0041309 | NA |
| 1607 | HMDB0000839 | Pentaporphyrin I |
| 1608 | HMDB0029428 | Hypoglycin B |
| 1609 | HMDB0061318 | NA |
| 1610 | HMDB0015102 | Desloratadine |
| 1611 | HMDB0170226 | NA |
| 1612 | HMDB0170229 | NA |
| 1613 | HMDB0170227 | NA |
| 1614 | HMDB0170230 | NA |
| 1615 | HMDB0170228 | NA |
| 1616 | HMDB0004704 | 9,10-DHOME |
| 1617 | HMDB0061650 | 9,10-Epoxystearic acid |
| 1618 | HMDB0004705 | 12,13-DHOME |
| 1619 | HMDB0041220 | NA |
| 1620 | HMDB0031679 | (9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid |
| 1621 | HMDB0000782 | Octadecanedioic acid |
| 1622 | HMDB0015401 | Nelarabine |
| 1623 | HMDB0005862 | 2-Methylguanosine |
| 1624 | HMDB0006038 | 3'-O-Methylguanosine |
| 1625 | HMDB0001563 | 1-Methylguanosine |

| | | |
|------|-------------|-------------------------|
| 1626 | HMDB0001107 | 7-Methylguanosine |
| 1627 | HMDB0029076 | Tryptophyl-Alanine |
| 1628 | HMDB0028698 | Alanyl-Tryptophan |
| 1629 | HMDB0142223 | NA |
| 1630 | HMDB0013209 | Alanyltryptophan |
| 1631 | HMDB0165476 | NA |
| 1632 | HMDB0165475 | NA |
| 1633 | HMDB0165471 | NA |
| 1634 | HMDB0165472 | NA |
| 1635 | HMDB0126113 | NA |
| 1636 | HMDB0130135 | NA |
| 1637 | HMDB0130132 | NA |
| 1638 | HMDB0130129 | NA |
| 1639 | HMDB0145822 | NA |
| 1640 | HMDB0130130 | NA |
| 1641 | HMDB0164665 | NA |
| 1642 | HMDB0130133 | NA |
| 1643 | HMDB0130019 | NA |
| 1644 | HMDB0126116 | NA |
| 1645 | HMDB0126115 | NA |
| 1646 | HMDB0130136 | NA |
| 1647 | HMDB0126114 | NA |
| 1648 | HMDB0178290 | NA |
| 1649 | HMDB0178289 | NA |
| 1650 | HMDB0181208 | NA |
| 1651 | HMDB0060994 | NA |
| 1652 | HMDB0183805 | NA |
| 1653 | HMDB0156418 | NA |
| 1654 | HMDB0156413 | NA |
| 1655 | HMDB0156410 | NA |
| 1656 | HMDB0156411 | NA |
| 1657 | HMDB0156408 | NA |
| 1658 | HMDB0156409 | NA |
| 1659 | HMDB0156404 | NA |
| 1660 | HMDB0156405 | NA |
| 1661 | HMDB0061925 | NA |
| 1662 | HMDB0156406 | NA |
| 1663 | HMDB0156407 | NA |
| 1664 | HMDB0156401 | NA |
| 1665 | HMDB0156403 | NA |
| 1666 | HMDB0156402 | NA |
| 1667 | HMDB0001852 | All-trans-retinoic acid |
| 1668 | HMDB0156412 | NA |
| 1669 | HMDB0179600 | NA |
| 1670 | HMDB0012874 | 9,13-cis-Retinoate |
| 1671 | HMDB0012788 | 4-OH-Retinal |
| 1672 | HMDB0036710 | NA |
| 1673 | HMDB0036564 | NA |
| 1674 | HMDB0036697 | NA |
| 1675 | HMDB0036711 | NA |
| 1676 | HMDB0038702 | NA |
| 1677 | HMDB0012329 | 4-Oxoretinol |
| 1678 | HMDB0006219 | 13-cis-Retinoic acid |
| 1679 | HMDB0041925 | NA |
| 1680 | HMDB0002369 | 9-cis-Retinoic acid |
| 1681 | HMDB0179597 | NA |
| 1682 | HMDB0179596 | NA |
| 1683 | HMDB0179598 | NA |
| 1684 | HMDB0183803 | NA |
| 1685 | HMDB0183804 | NA |
| 1686 | HMDB0183807 | NA |
| 1687 | HMDB0183806 | NA |
| 1688 | HMDB0183808 | NA |
| 1689 | HMDB0183810 | NA |
| 1690 | HMDB0183811 | NA |
| 1691 | HMDB0183813 | NA |
| 1692 | HMDB0179593 | NA |
| 1693 | HMDB0179594 | NA |
| 1694 | HMDB0183809 | NA |
| 1695 | HMDB0062222 | NA |
| 1696 | HMDB0062293 | NA |
| 1697 | HMDB0062296 | NA |
| 1698 | HMDB0062408 | NA |
| 1699 | HMDB0137419 | NA |
| 1700 | HMDB0137428 | NA |
| 1701 | HMDB0183812 | NA |
| 1702 | HMDB0183814 | NA |
| 1703 | HMDB0183815 | NA |
| 1704 | HMDB0183816 | NA |
| 1705 | HMDB0001337 | Leukotriene A4 |
| 1706 | HMDB0036776 | NA |
| 1707 | HMDB0036839 | NA |
| 1708 | HMDB0030101 | Methyl [8]-Shogaol |
| 1709 | HMDB0036930 | NA |
| 1710 | HMDB0036724 | NA |
| 1711 | HMDB0035311 | Galanal A |
| 1712 | HMDB0039012 | NA |

| | | |
|------|-------------|--|
| 1713 | HMDB0036698 | NA |
| 1714 | HMDB0036706 | NA |
| 1715 | HMDB0037523 | NA |
| 1716 | HMDB0036806 | NA |
| 1717 | HMDB0035116 | (ent-7alpha)-7-Hydroxy-8(14),15-pimaradien-19-oic acid |
| 1718 | HMDB0039716 | NA |
| 1719 | HMDB0005081 | 5-HEPE |
| 1720 | HMDB0006027 | Oxymesterone |
| 1721 | HMDB0010202 | 12-HEPE |
| 1722 | HMDB0010205 | 14,15-EpETE |
| 1723 | HMDB0010210 | 15-KETE |
| 1724 | HMDB0010209 | 15-HEPE |
| 1725 | HMDB0010212 | 17,18-EpETE |
| 1726 | HMDB0010217 | 5-KETE |
| 1727 | HMDB0041058 | NA |
| 1728 | HMDB0036712 | NA |
| 1729 | HMDB0038521 | NA |
| 1730 | HMDB0036752 | NA |
| 1731 | HMDB0036713 | NA |
| 1732 | HMDB0012534 | 11R-HEPE |
| 1733 | HMDB0012611 | 18R-HEPE |
| 1734 | HMDB0013633 | 12-KETE |
| 1735 | HMDB0060053 | NA |
| 1736 | HMDB0061114 | NA |
| 1737 | HMDB0179595 | NA |
| 1738 | HMDB0155274 | NA |
| 1739 | HMDB0037844 | NA |
| 1740 | HMDB0141976 | NA |
| 1741 | HMDB0171302 | NA |
| 1742 | HMDB0171300 | NA |
| 1743 | HMDB0171299 | NA |
| 1744 | HMDB0171301 | NA |
| 1745 | HMDB0034618 | 2-O-Benzoyl-D-glucose |
| 1746 | HMDB0038492 | NA |
| 1747 | HMDB0011686 | p-Cresol glucuronide |
| 1748 | HMDB0062439 | 9-Hydroxybenzo[a]pyrene-4,5-oxide |
| 1749 | HMDB0029102 | Tyrosyl-Cysteine |
| 1750 | HMDB0028787 | Cysteinyl-Tyrosine |
| 1751 | HMDB0168641 | NA |
| 1752 | HMDB0168639 | NA |
| 1753 | HMDB0164918 | NA |
| 1754 | HMDB0164919 | NA |
| 1755 | HMDB0164920 | NA |
| 1756 | HMDB0005764 | Melanostatin |
| 1757 | HMDB0036329 | NA |
| 1758 | HMDB0060578 | NA |
| 1759 | HMDB0061098 | NA |
| 1760 | HMDB0161587 | NA |
| 1761 | HMDB0138221 | NA |
| 1762 | HMDB0030432 | Linalyl cinnamate |
| 1763 | HMDB0038050 | NA |
| 1764 | HMDB0003422 | Boldione |
| 1765 | HMDB0029913 | Gynocardin |
| 1766 | HMDB0240490 | NA |
| 1767 | HMDB0059998 | NA |
| 1768 | HMDB0041272 | NA |
| 1769 | HMDB0124997 | NA |
| 1770 | HMDB0029498 | 3'-Methoxyfukiic acid |
| 1771 | HMDB0135181 | NA |
| 1772 | HMDB0125471 | NA |
| 1773 | HMDB0004326 | 2'-O-Methyladenosine |
| 1774 | HMDB0004044 | N6-Methyladenosine |
| 1775 | HMDB0006023 | 3'-O-Methyladenosine |
| 1776 | HMDB0003331 | 1-Methyladenosine |
| 1777 | HMDB0006832 | S-Glutaryl dihydro lipamide |
| 1778 | HMDB0037843 | NA |
| 1779 | HMDB0030266 | Berberrubine |
| 1780 | HMDB0187656 | NA |
| 1781 | HMDB0030391 | Cepharadione B |
| 1782 | HMDB0061366 | NA |
| 1783 | HMDB0029395 | L-L-Homoglutathione |
| 1784 | HMDB0135641 | NA |
| 1785 | HMDB0179385 | NA |
| 1786 | HMDB0179388 | NA |
| 1787 | HMDB0179383 | NA |
| 1788 | HMDB0179382 | NA |
| 1789 | HMDB0163720 | NA |
| 1790 | HMDB0173550 | NA |
| 1791 | HMDB0135574 | NA |
| 1792 | HMDB0135576 | NA |
| 1793 | HMDB0135572 | NA |
| 1794 | HMDB0135564 | NA |
| 1795 | HMDB0135568 | NA |
| 1796 | HMDB0134573 | NA |
| 1797 | HMDB0134571 | NA |
| 1798 | HMDB0135570 | NA |
| 1799 | HMDB0158752 | NA |

| | | |
|------|-------------|---|
| 1800 | HMDB0158753 | NA |
| 1801 | HMDB0155927 | NA |
| 1802 | HMDB0155928 | NA |
| 1803 | HMDB0161130 | NA |
| 1804 | HMDB0041096 | NA |
| 1805 | HMDB0158750 | NA |
| 1806 | HMDB0158751 | NA |
| 1807 | HMDB0159487 | NA |
| 1808 | HMDB0159488 | NA |
| 1809 | HMDB0159490 | NA |
| 1810 | HMDB0159830 | NA |
| 1811 | HMDB0161128 | NA |
| 1812 | HMDB0161127 | NA |
| 1813 | HMDB0161129 | NA |
| 1814 | HMDB0161132 | NA |
| 1815 | HMDB0161133 | NA |
| 1816 | HMDB0166865 | NA |
| 1817 | HMDB0159483 | NA |
| 1818 | HMDB0159484 | NA |
| 1819 | HMDB0159482 | NA |
| 1820 | HMDB0158755 | NA |
| 1821 | HMDB0158759 | NA |
| 1822 | HMDB0158758 | NA |
| 1823 | HMDB0159491 | NA |
| 1824 | HMDB0158756 | NA |
| 1825 | HMDB0158876 | NA |
| 1826 | HMDB0158877 | NA |
| 1827 | HMDB0159485 | NA |
| 1828 | HMDB0061135 | NA |
| 1829 | HMDB0015176 | Melphalan |
| 1830 | HMDB0127928 | NA |
| 1831 | HMDB0037110 | NA |
| 1832 | HMDB0145098 | NA |
| 1833 | HMDB0175072 | NA |
| 1834 | HMDB0041450 | NA |
| 1835 | HMDB0038322 | NA |
| 1836 | HMDB0032909 | 2-(4-Methoxyphenyl)naphthalic anhydride |
| 1837 | HMDB0175074 | NA |
| 1838 | HMDB0175080 | NA |
| 1839 | HMDB0175081 | NA |
| 1840 | HMDB0175083 | NA |
| 1841 | HMDB0175073 | NA |
| 1842 | HMDB0175082 | NA |
| 1843 | HMDB0163581 | NA |
| 1844 | HMDB0163582 | NA |
| 1845 | HMDB0163584 | NA |
| 1846 | HMDB0038580 | NA |
| 1847 | HMDB0033631 | Lactapiperanol D |
| 1848 | HMDB0180021 | NA |
| 1849 | HMDB0180098 | NA |
| 1850 | HMDB0180100 | NA |
| 1851 | HMDB0180099 | NA |
| 1852 | HMDB0180102 | NA |
| 1853 | HMDB0034780 | Capsiate |
| 1854 | HMDB0180103 | NA |
| 1855 | HMDB0184951 | NA |
| 1856 | HMDB0184949 | NA |
| 1857 | HMDB0184953 | NA |
| 1858 | HMDB0012799 | 5'-Carboxy-gamma-chromanol |
| 1859 | HMDB0184954 | NA |
| 1860 | HMDB0184950 | NA |
| 1861 | HMDB0061677 | NA |
| 1862 | HMDB0000552 | 3-Methylglutaryl carnitine |
| 1863 | HMDB0039044 | NA |
| 1864 | HMDB0131544 | NA |
| 1865 | HMDB0153683 | NA |
| 1866 | HMDB0134716 | NA |
| 1867 | HMDB0131577 | NA |
| 1868 | HMDB0140842 | NA |
| 1869 | HMDB0039858 | NA |
| 1870 | HMDB0150310 | NA |
| 1871 | HMDB0150311 | NA |
| 1872 | HMDB0030019 | 4'-Methoxymucidin |
| 1873 | HMDB0125543 | NA |
| 1874 | HMDB0125544 | NA |
| 1875 | HMDB0125545 | NA |
| 1876 | HMDB0125547 | NA |
| 1877 | HMDB0125546 | NA |
| 1878 | HMDB0125548 | NA |
| 1879 | HMDB0129031 | NA |
| 1880 | HMDB0129032 | NA |
| 1881 | HMDB0141104 | NA |
| 1882 | HMDB0141131 | NA |
| 1883 | HMDB0141141 | NA |
| 1884 | HMDB0141165 | NA |
| 1885 | HMDB0141171 | NA |
| 1886 | HMDB0129034 | NA |

| | | |
|------|-------------|--------------------------------|
| 1887 | HMDB0149106 | NA |
| 1888 | HMDB0140204 | NA |
| 1889 | HMDB0140116 | NA |
| 1890 | HMDB0129033 | NA |
| 1891 | HMDB0129035 | NA |
| 1892 | HMDB0129037 | NA |
| 1893 | HMDB0129036 | NA |
| 1894 | HMDB0129038 | NA |
| 1895 | HMDB0140114 | NA |
| 1896 | HMDB0140118 | NA |
| 1897 | HMDB0140117 | NA |
| 1898 | HMDB0140115 | NA |
| 1899 | HMDB0146850 | NA |
| 1900 | HMDB0040670 | NA |
| 1901 | HMDB0176556 | NA |
| 1902 | HMDB0000495 | Androstanediol |
| 1903 | HMDB0159493 | NA |
| 1904 | HMDB0158029 | NA |
| 1905 | HMDB0000554 | Dihydroandrosterone |
| 1906 | HMDB0000551 | Etiocholanediol |
| 1907 | HMDB0000458 | 5a-Androstane-3a,17a-diol |
| 1908 | HMDB0000383 | 3a,17a-Dihydroxy-5b-androstane |
| 1909 | HMDB0000493 | 5a-Androstane-3b,17b-diol |
| 1910 | HMDB0000369 | 3b,17b-Dihydroxyetiocholane |
| 1911 | HMDB0000412 | 3b,17a-Dihydroxy-5a-androstane |
| 1912 | HMDB0060437 | Androstan-3alpha,17beta-diol |
| 1913 | HMDB0167160 | NA |
| 1914 | HMDB0167157 | NA |
| 1915 | HMDB0156083 | NA |
| 1916 | HMDB0167154 | NA |
| 1917 | HMDB0167155 | NA |
| 1918 | HMDB0167156 | NA |
| 1919 | HMDB0062521 | NA |
| 1920 | HMDB0167161 | NA |
| 1921 | HMDB0167158 | NA |
| 1922 | HMDB0173640 | NA |
| 1923 | HMDB0186461 | NA |
| 1924 | HMDB0167171 | NA |
| 1925 | HMDB0167170 | NA |
| 1926 | HMDB0186443 | NA |
| 1927 | HMDB0167159 | NA |
| 1928 | HMDB0167165 | NA |
| 1929 | HMDB0167163 | NA |
| 1930 | HMDB0167162 | NA |
| 1931 | HMDB0167164 | NA |
| 1932 | HMDB0167169 | NA |
| 1933 | HMDB0167168 | NA |
| 1934 | HMDB0167167 | NA |
| 1935 | HMDB0167166 | NA |
| 1936 | HMDB0014613 | Dronabinol |
| 1937 | HMDB0038533 | NA |
| 1938 | HMDB0013121 | 7-Dehydropregnenolone |
| 1939 | HMDB0031924 | 4-Nerolidylcatechol |
| 1940 | HMDB0041865 | NA |
| 1941 | HMDB0001830 | Progesterone |
| 1942 | HMDB0156085 | NA |
| 1943 | HMDB0137415 | NA |
| 1944 | HMDB0137402 | NA |
| 1945 | HMDB0156084 | NA |
| 1946 | HMDB0156089 | NA |
| 1947 | HMDB0186441 | NA |
| 1948 | HMDB0186440 | NA |
| 1949 | HMDB0186438 | NA |
| 1950 | HMDB0186439 | NA |
| 1951 | HMDB0186444 | NA |
| 1952 | HMDB0186457 | NA |
| 1953 | HMDB0186462 | NA |
| 1954 | HMDB0186435 | NA |
| 1955 | HMDB0186437 | NA |
| 1956 | HMDB0156091 | NA |
| 1957 | HMDB0156092 | NA |
| 1958 | HMDB0156093 | NA |
| 1959 | HMDB0156090 | NA |
| 1960 | HMDB0156094 | NA |
| 1961 | HMDB0156095 | NA |
| 1962 | HMDB0156840 | NA |
| 1963 | HMDB0158166 | NA |
| 1964 | HMDB0173643 | NA |
| 1965 | HMDB0173642 | NA |
| 1966 | HMDB0173641 | NA |
| 1967 | HMDB0173645 | NA |
| 1968 | HMDB0173644 | NA |
| 1969 | HMDB0173646 | NA |
| 1970 | HMDB0173647 | NA |
| 1971 | HMDB0173648 | NA |
| 1972 | HMDB0186436 | NA |
| 1973 | HMDB0062609 | NA |

| | | |
|------|-------------|--|
| 1974 | HMDB0060424 | 7alpha-Hydroxypregnenolone |
| 1975 | HMDB0060407 | 5alpha-Dihydrodeoxycorticosterone |
| 1976 | HMDB0031462 | [10]-Shogaol |
| 1977 | HMDB0033918 | (15alpha,20R)-15,20-Dihydroxypregn-4-en-3-one |
| 1978 | HMDB0011653 | 17-alpha,20-alpha-Dihydroxypregn-4-en-3-one |
| 1979 | HMDB0004026 | 21-Hydroxypregnenolone |
| 1980 | HMDB0003851 | 3a,7a-Dihydroxy-5b-cholestanate |
| 1981 | HMDB0000363 | 17a-Hydroxypregnenolone |
| 1982 | HMDB0000315 | 16-a-Hydroxypregnenolone |
| 1983 | HMDB0173549 | NA |
| 1984 | HMDB0125510 | NA |
| 1985 | HMDB0125509 | NA |
| 1986 | HMDB0060017 | NA |
| 1987 | HMDB0125511 | NA |
| 1988 | HMDB0125508 | NA |
| 1989 | HMDB0125512 | NA |
| 1990 | HMDB0187598 | NA |
| 1991 | HMDB0015513 | Fludiazepam |
| 1992 | HMDB0162772 | NA |
| 1993 | HMDB0162714 | NA |
| 1994 | HMDB0162760 | NA |
| 1995 | HMDB0162710 | NA |
| 1996 | HMDB0162708 | NA |
| 1997 | HMDB0162758 | NA |
| 1998 | HMDB0033374 | Benzyl glycinate 4-methylbenzenesulfonate salt |
| 1999 | HMDB0161228 | NA |
| 2000 | HMDB0161229 | NA |
| 2001 | HMDB0159742 | NA |
| 2002 | HMDB0185385 | NA |
| 2003 | HMDB0181751 | NA |
| 2004 | HMDB0181741 | NA |
| 2005 | HMDB0039733 | NA |
| 2006 | HMDB0004662 | S-(Hydroxymethyl)glutathione |
| 2007 | HMDB0014848 | Ibandronate |
| 2008 | HMDB0029391 | N-Jasmonoylisoleucine |
| 2009 | HMDB0006320 | 2,6 Dimethylheptanoyl carnitine |
| 2010 | HMDB0013288 | Nonanoylcarnitine |
| 2011 | HMDB0032549 | N-Undecylbenzenesulfonic acid |
| 2012 | HMDB0171053 | NA |
| 2013 | HMDB0171052 | NA |
| 2014 | HMDB0180006 | NA |
| 2015 | HMDB0179178 | NA |
| 2016 | HMDB0179822 | NA |
| 2017 | HMDB0179824 | NA |
| 2018 | HMDB0163506 | NA |
| 2019 | HMDB0179826 | NA |
| 2020 | HMDB0179828 | NA |
| 2021 | HMDB0171049 | NA |
| 2022 | HMDB0171046 | NA |
| 2023 | HMDB0040461 | NA |
| 2024 | HMDB0163490 | NA |
| 2025 | HMDB0163491 | NA |
| 2026 | HMDB0163494 | NA |
| 2027 | HMDB0163498 | NA |
| 2028 | HMDB0163499 | NA |
| 2029 | HMDB0163495 | NA |
| 2030 | HMDB0170942 | NA |
| 2031 | HMDB0163526 | NA |
| 2032 | HMDB0163505 | NA |
| 2033 | HMDB0163502 | NA |
| 2034 | HMDB0171045 | NA |
| 2035 | HMDB0029084 | Tryptophyl-Hydroxyproline |
| 2036 | HMDB0181182 | NA |
| 2037 | HMDB0028874 | Hydroxyprolyl-Tryptophan |
| 2038 | HMDB0138126 | NA |
| 2039 | HMDB0138125 | NA |
| 2040 | HMDB0138129 | NA |
| 2041 | HMDB0138130 | NA |
| 2042 | HMDB0138127 | NA |
| 2043 | HMDB0179081 | NA |
| 2044 | HMDB0138131 | NA |
| 2045 | HMDB0138132 | NA |
| 2046 | HMDB0138128 | NA |
| 2047 | HMDB0138133 | NA |
| 2048 | HMDB0138134 | NA |
| 2049 | HMDB0138276 | NA |
| 2050 | HMDB0171363 | NA |
| 2051 | HMDB0186298 | NA |
| 2052 | HMDB0031976 | Methyl (9Z)-10'-oxo-6,10'-diapo-6-carotenoate |
| 2053 | HMDB0033294 | 5-Methoxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone |
| 2054 | HMDB0040761 | NA |
| 2055 | HMDB0061027 | NA |
| 2056 | HMDB0015191 | Praziquantel |
| 2057 | HMDB0154672 | NA |
| 2058 | HMDB0154674 | NA |
| 2059 | HMDB0154675 | NA |
| 2060 | HMDB0154673 | NA |

| | | |
|------|-------------|--------------------------------|
| 2061 | HMDB0154671 | NA |
| 2062 | HMDB0154670 | NA |
| 2063 | HMDB0029566 | Isopulegone caffeate |
| 2064 | HMDB0154668 | NA |
| 2065 | HMDB0134704 | NA |
| 2066 | HMDB0147915 | NA |
| 2067 | HMDB0154665 | NA |
| 2068 | HMDB0154669 | NA |
| 2069 | HMDB0154666 | NA |
| 2070 | HMDB0154667 | NA |
| 2071 | HMDB0148183 | NA |
| 2072 | HMDB0153649 | NA |
| 2073 | HMDB0125854 | NA |
| 2074 | HMDB0141256 | NA |
| 2075 | HMDB0124819 | NA |
| 2076 | HMDB0125836 | NA |
| 2077 | HMDB0125842 | NA |
| 2078 | HMDB0133467 | NA |
| 2079 | HMDB0041386 | NA |
| 2080 | HMDB0034412 | 2'-O-Methylphaseollinisoflavan |
| 2081 | HMDB0039439 | NA |
| 2082 | HMDB0033672 | 4'-O-Methylglabridin |
| 2083 | HMDB0029514 | Licochalcone A |
| 2084 | HMDB0033782 | Bergamottin |
| 2085 | HMDB0039309 | NA |
| 2086 | HMDB0030846 | Archangelin |
| 2087 | HMDB0039438 | NA |
| 2088 | HMDB0033671 | 2'-O-Methylglabridin |
| 2089 | HMDB0032665 | Licoagrocarpin |
| 2090 | HMDB0031633 | Orientanol B |
| 2091 | HMDB0001272 | Nicotine glucuronide |
| 2092 | HMDB0032808 | Niazirinin |
| 2093 | HMDB0131864 | NA |
| 2094 | HMDB0124924 | NA |
| 2095 | HMDB0131867 | NA |
| 2096 | HMDB0133539 | NA |
| 2097 | HMDB0124927 | NA |
| 2098 | HMDB0125807 | NA |
| 2099 | HMDB0131075 | NA |
| 2100 | HMDB0133516 | NA |
| 2101 | HMDB0133495 | NA |
| 2102 | HMDB0133485 | NA |
| 2103 | HMDB0133468 | NA |
| 2104 | HMDB0131866 | NA |
| 2105 | HMDB0131865 | NA |
| 2106 | HMDB0124928 | NA |
| 2107 | HMDB0124929 | NA |
| 2108 | HMDB0124838 | NA |
| 2109 | HMDB0124800 | NA |
| 2110 | HMDB0124826 | NA |
| 2111 | HMDB0124829 | NA |
| 2112 | HMDB0124835 | NA |
| 2113 | HMDB0124837 | NA |
| 2114 | HMDB0124922 | NA |
| 2115 | HMDB0130876 | NA |
| 2116 | HMDB0138809 | NA |
| 2117 | HMDB0150217 | NA |
| 2118 | HMDB0150219 | NA |
| 2119 | HMDB0124822 | NA |
| 2120 | HMDB0150216 | NA |
| 2121 | HMDB0150218 | NA |
| 2122 | HMDB0150215 | NA |
| 2123 | HMDB0147761 | NA |
| 2124 | HMDB0147762 | NA |
| 2125 | HMDB0147765 | NA |
| 2126 | HMDB0147767 | NA |
| 2127 | HMDB0147766 | NA |
| 2128 | HMDB0147764 | NA |
| 2129 | HMDB0147768 | NA |
| 2130 | HMDB0147769 | NA |
| 2131 | HMDB0149836 | NA |
| 2132 | HMDB0150181 | NA |
| 2133 | HMDB0150186 | NA |
| 2134 | HMDB0150185 | NA |
| 2135 | HMDB0150182 | NA |
| 2136 | HMDB0150184 | NA |
| 2137 | HMDB0150187 | NA |
| 2138 | HMDB0150214 | NA |
| 2139 | HMDB0035440 | alpha,beta-Dihydroxanthohumol |
| 2140 | HMDB0030666 | Chalepin acetate |
| 2141 | HMDB0035403 | Gingerenone A |
| 2142 | HMDB0030798 | Myricanone |
| 2143 | HMDB0033880 | Mammea B/AC cyclo D |
| 2144 | HMDB0033879 | Mammea B/AD cyclo D |
| 2145 | HMDB0030333 | Fragransol C |
| 2146 | HMDB0041401 | NA |
| 2147 | HMDB0138808 | NA |

| | | |
|------|-------------|---|
| 2148 | HMDB0184970 | NA |
| 2149 | HMDB0184809 | NA |
| 2150 | HMDB0033108 | Semilepidinoside B |
| 2151 | HMDB0240296 | NA |
| 2152 | HMDB0166033 | NA |
| 2153 | HMDB0012492 | 1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylate |
| 2154 | HMDB0029992 | Tetrahydropentoxylone |
| 2155 | HMDB0166038 | NA |
| 2156 | HMDB0166035 | NA |
| 2157 | HMDB0166036 | NA |
| 2158 | HMDB0014720 | Voriconazole |
| 2159 | HMDB0014258 | R-138727 |
| 2160 | HMDB0131015 | NA |
| 2161 | HMDB0131014 | NA |
| 2162 | HMDB0131011 | NA |
| 2163 | HMDB0131013 | NA |
| 2164 | HMDB0136701 | NA |
| 2165 | HMDB0140161 | NA |
| 2166 | HMDB0171360 | NA |
| 2167 | HMDB0171359 | NA |
| 2168 | HMDB0171362 | NA |
| 2169 | HMDB0171358 | NA |
| 2170 | HMDB0171355 | NA |
| 2171 | HMDB0171354 | NA |
| 2172 | HMDB0032955 | 5-(6-Hydroxy-3,7-dimethyl-2,7-octadienyloxy)-7-methoxycoumarin |
| 2173 | HMDB0038690 | NA |
| 2174 | HMDB0171361 | NA |
| 2175 | HMDB0034179 | Malabaricano |
| 2176 | HMDB0031889 | (1(10)E,4E,6a,8b)-8-Angeloyloxy-14-oxo-1(10),4,11(13)-germacatrien-12,6-olide |
| 2177 | HMDB0031753 | 2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol |
| 2178 | HMDB0038219 | NA |
| 2179 | HMDB0040388 | NA |
| 2180 | HMDB0040421 | NA |
| 2181 | HMDB0036691 | NA |
| 2182 | HMDB0039610 | NA |
| 2183 | HMDB0125864 | NA |
| 2184 | HMDB0172929 | NA |
| 2185 | HMDB0148194 | NA |
| 2186 | HMDB0040834 | NA |
| 2187 | HMDB0040809 | NA |
| 2188 | HMDB0041100 | NA |
| 2189 | HMDB0041417 | NA |
| 2190 | HMDB0035427 | Glicoisoflavanone |
| 2191 | HMDB0014559 | Ampicillin |
| 2192 | HMDB0015428 | Cefradine |
| 2193 | HMDB0062731 | Dodecamethylpentasiloxane |
| 2194 | HMDB0182884 | NA |
| 2195 | HMDB0004239 | 13,14-Dihydro PGF2a |
| 2196 | HMDB0002689 | 13,14-Dihydro PGE1 |
| 2197 | HMDB0002685 | Prostaglandin F1a |
| 2198 | HMDB0165171 | NA |
| 2199 | HMDB0035508 | Annoglabasin F |
| 2200 | HMDB0014701 | Doxapram |
| 2201 | HMDB0175496 | NA |
| 2202 | HMDB0175499 | NA |
| 2203 | HMDB0175502 | NA |
| 2204 | HMDB0175506 | NA |
| 2205 | HMDB0175509 | NA |
| 2206 | HMDB0175505 | NA |
| 2207 | HMDB0175517 | NA |
| 2208 | HMDB0175521 | NA |
| 2209 | HMDB0175520 | NA |
| 2210 | HMDB0175516 | NA |
| 2211 | HMDB0175513 | NA |
| 2212 | HMDB0175512 | NA |
| 2213 | HMDB0012280 | Phytosphingosine-1-P |
| 2214 | HMDB0062531 | NA |
| 2215 | HMDB0000277 | Sphingosine 1-phosphate |
| 2216 | HMDB0059630 | NA |
| 2217 | HMDB0094648 | Leu-Leu-Leu |
| 2218 | HMDB0005076 | 13,14-Dihydro PGF-1a |
| 2219 | HMDB0164534 | NA |
| 2220 | HMDB0002082 | Bisnorcholic acid |
| 2221 | HMDB0040698 | NA |
| 2222 | HMDB0184271 | NA |
| 2223 | HMDB0183492 | NA |
| 2224 | HMDB0156837 | NA |
| 2225 | HMDB0156831 | NA |
| 2226 | HMDB0156835 | NA |
| 2227 | HMDB0156889 | NA |
| 2228 | HMDB0156836 | NA |
| 2229 | HMDB0157597 | NA |
| 2230 | HMDB0157601 | NA |
| 2231 | HMDB0157602 | NA |
| 2232 | HMDB0157742 | NA |
| 2233 | HMDB0157743 | NA |
| 2234 | HMDB0157738 | NA |

| | | |
|------|-------------|---|
| 2235 | HMDB0157739 | NA |
| 2236 | HMDB0157603 | NA |
| 2237 | HMDB0157604 | NA |
| 2238 | HMDB0157599 | NA |
| 2239 | HMDB0157600 | NA |
| 2240 | HMDB0156838 | NA |
| 2241 | HMDB0156832 | NA |
| 2242 | HMDB0155046 | NA |
| 2243 | HMDB0156806 | NA |
| 2244 | HMDB0156826 | NA |
| 2245 | HMDB0156827 | NA |
| 2246 | HMDB0156829 | NA |
| 2247 | HMDB0156830 | NA |
| 2248 | HMDB0156828 | NA |
| 2249 | HMDB0156834 | NA |
| 2250 | HMDB0156833 | NA |
| 2251 | HMDB0157740 | NA |
| 2252 | HMDB0157741 | NA |
| 2253 | HMDB0158276 | NA |
| 2254 | HMDB0167960 | NA |
| 2255 | HMDB0167961 | NA |
| 2256 | HMDB0167962 | NA |
| 2257 | HMDB0167964 | NA |
| 2258 | HMDB0167963 | NA |
| 2259 | HMDB0167966 | NA |
| 2260 | HMDB0167965 | NA |
| 2261 | HMDB0167968 | NA |
| 2262 | HMDB0167967 | NA |
| 2263 | HMDB0170452 | NA |
| 2264 | HMDB0170451 | NA |
| 2265 | HMDB0186750 | NA |
| 2266 | HMDB0000903 | Tetrahydrocortisone |
| 2267 | HMDB0003259 | Dihydrocortisol |
| 2268 | HMDB0006753 | 3a,11b,21-Trihydroxy-20-oxo-5b-pregnan-18-al |
| 2269 | HMDB0006754 | 11b,21-Dihydroxy-3,20-oxo-5b-pregnan-18-al |
| 2270 | HMDB0006760 | 11b,17a,21-Trihydroxypreg-nenolone |
| 2271 | HMDB0032553 | Vanillin 3-(L-menthoxy)propane-1,2-diol acetal |
| 2272 | HMDB0013157 | 18-Hydroxy-11-dehydrotetrahydrocorticosterone |
| 2273 | HMDB0013164 | 2-Hydroxy-lauroylcarnitine |
| 2274 | HMDB0061638 | NA |
| 2275 | HMDB0185679 | NA |
| 2276 | HMDB0185658 | NA |
| 2277 | HMDB0185694 | NA |
| 2278 | HMDB0185682 | NA |
| 2279 | HMDB0185676 | NA |
| 2280 | HMDB0185661 | NA |
| 2281 | HMDB0185673 | NA |
| 2282 | HMDB0185698 | NA |
| 2283 | HMDB0185670 | NA |
| 2284 | HMDB0185667 | NA |
| 2285 | HMDB0185664 | NA |
| 2286 | HMDB0179611 | NA |
| 2287 | HMDB0179614 | NA |
| 2288 | HMDB0179608 | NA |
| 2289 | HMDB0179615 | NA |
| 2290 | HMDB0179605 | NA |
| 2291 | HMDB0179606 | NA |
| 2292 | HMDB0179618 | NA |
| 2293 | HMDB0179619 | NA |
| 2294 | HMDB0179623 | NA |
| 2295 | HMDB0179626 | NA |
| 2296 | HMDB0182175 | NA |
| 2297 | HMDB0179627 | NA |
| 2298 | HMDB0182176 | NA |
| 2299 | HMDB0014334 | Bortezomib |
| 2300 | HMDB0061005 | NA |
| 2301 | HMDB0060583 | NA |
| 2302 | HMDB0030868 | Citreoviridin A |
| 2303 | HMDB0030523 | Citreoviridin C |
| 2304 | HMDB0036462 | NA |
| 2305 | HMDB0035027 | Melleolide F |
| 2306 | HMDB0035774 | Armillyl orsellinate |
| 2307 | HMDB0015459 | Cortisone acetate |
| 2308 | HMDB0038917 | NA |
| 2309 | HMDB0031380 | (6beta,7alpha,12beta,13beta)-7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide |
| 2310 | HMDB0179899 | NA |
| 2311 | HMDB0179900 | NA |
| 2312 | HMDB0179898 | NA |
| 2313 | HMDB0179897 | NA |
| 2314 | HMDB0179895 | NA |
| 2315 | HMDB0179894 | NA |
| 2316 | HMDB0179893 | NA |
| 2317 | HMDB0179896 | NA |
| 2318 | HMDB0060833 | NA |
| 2319 | HMDB0185381 | NA |
| 2320 | HMDB0002873 | Deacetyldiltiazem |
| 2321 | HMDB0124912 | NA |

| | | |
|------|-------------|--|
| 2322 | HMDB0124915 | NA |
| 2323 | HMDB0124828 | NA |
| 2324 | HMDB0124911 | NA |
| 2325 | HMDB0124914 | NA |
| 2326 | HMDB0124913 | NA |
| 2327 | HMDB0125800 | NA |
| 2328 | HMDB0131078 | NA |
| 2329 | HMDB0131080 | NA |
| 2330 | HMDB0131077 | NA |
| 2331 | HMDB0130292 | NA |
| 2332 | HMDB0130291 | NA |
| 2333 | HMDB0130288 | NA |
| 2334 | HMDB0130290 | NA |
| 2335 | HMDB0130289 | NA |
| 2336 | HMDB0130100 | NA |
| 2337 | HMDB0130099 | NA |
| 2338 | HMDB0124817 | NA |
| 2339 | HMDB0124816 | NA |
| 2340 | HMDB0124815 | NA |
| 2341 | HMDB0124810 | NA |
| 2342 | HMDB0124811 | NA |
| 2343 | HMDB0124813 | NA |
| 2344 | HMDB0124812 | NA |
| 2345 | HMDB0133480 | NA |
| 2346 | HMDB0149865 | NA |
| 2347 | HMDB0149860 | NA |
| 2348 | HMDB0149855 | NA |
| 2349 | HMDB0149846 | NA |
| 2350 | HMDB0149841 | NA |
| 2351 | HMDB0149835 | NA |
| 2352 | HMDB0149834 | NA |
| 2353 | HMDB0146994 | NA |
| 2354 | HMDB0146992 | NA |
| 2355 | HMDB0146993 | NA |
| 2356 | HMDB0146989 | NA |
| 2357 | HMDB0133520 | NA |
| 2358 | HMDB0133514 | NA |
| 2359 | HMDB0133513 | NA |
| 2360 | HMDB0133493 | NA |
| 2361 | HMDB0133492 | NA |
| 2362 | HMDB0133481 | NA |
| 2363 | HMDB0146939 | NA |
| 2364 | HMDB0131836 | NA |
| 2365 | HMDB0131837 | NA |
| 2366 | HMDB0131838 | NA |
| 2367 | HMDB0133527 | NA |
| 2368 | HMDB0133537 | NA |
| 2369 | HMDB0137511 | NA |
| 2370 | HMDB0146987 | NA |
| 2371 | HMDB0146988 | NA |
| 2372 | HMDB0146986 | NA |
| 2373 | HMDB0146947 | NA |
| 2374 | HMDB0146945 | NA |
| 2375 | HMDB0146944 | NA |
| 2376 | HMDB0146941 | NA |
| 2377 | HMDB0146940 | NA |
| 2378 | HMDB0146938 | NA |
| 2379 | HMDB0138813 | NA |
| 2380 | HMDB0131079 | NA |
| 2381 | HMDB0039066 | NA |
| 2382 | HMDB0041416 | NA |
| 2383 | HMDB0030826 | 2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-methylenedioxyphenyl)-1-propanol |
| 2384 | HMDB0035182 | Licoriphenone |
| 2385 | HMDB0032733 | (8R,8'R,9S)-9-Hydroxy-3,4-dimethoxy-3',4'-methylenoxy-9,9'-epoxylignan |
| 2386 | HMDB0005789 | Tetrahydrocurcumin |
| 2387 | HMDB0030087 | (-)-Arctigenin |
| 2388 | HMDB0032734 | 9-Hydroxy-3',4'-dimethoxy-3,4-methylenedioxy-9,9'-epoxylignan |
| 2389 | HMDB0164958 | NA |
| 2390 | HMDB0029510 | Garcinone B |
| 2391 | HMDB0034436 | Rotenone |
| 2392 | HMDB0036984 | NA |
| 2393 | HMDB0148796 | NA |
| 2394 | HMDB0146129 | NA |
| 2395 | HMDB0173953 | NA |
| 2396 | HMDB0184813 | NA |
| 2397 | HMDB0184985 | NA |
| 2398 | HMDB0184812 | NA |
| 2399 | HMDB0184811 | NA |
| 2400 | HMDB0184810 | NA |
| 2401 | HMDB0173968 | NA |
| 2402 | HMDB0173965 | NA |
| 2403 | HMDB0173956 | NA |
| 2404 | HMDB0172273 | NA |
| 2405 | HMDB0172275 | NA |
| 2406 | HMDB0172274 | NA |
| 2407 | HMDB0174261 | NA |
| 2408 | HMDB0174260 | NA |

| | | |
|------|-------------|--|
| 2409 | HMDB0174265 | NA |
| 2410 | HMDB0174262 | NA |
| 2411 | HMDB0174263 | NA |
| 2412 | HMDB0174264 | NA |
| 2413 | HMDB0174266 | NA |
| 2414 | HMDB0155085 | NA |
| 2415 | HMDB0155087 | NA |
| 2416 | HMDB0154867 | NA |
| 2417 | HMDB0154866 | NA |
| 2418 | HMDB0155080 | NA |
| 2419 | HMDB0155083 | NA |
| 2420 | HMDB0155082 | NA |
| 2421 | HMDB0155081 | NA |
| 2422 | HMDB0155084 | NA |
| 2423 | HMDB0155086 | NA |
| 2424 | HMDB0174267 | NA |
| 2425 | HMDB0174268 | NA |
| 2426 | HMDB0184842 | NA |
| 2427 | HMDB0184845 | NA |
| 2428 | HMDB0184846 | NA |
| 2429 | HMDB0184848 | NA |
| 2430 | HMDB0184847 | NA |
| 2431 | HMDB0184849 | NA |
| 2432 | HMDB0184851 | NA |
| 2433 | HMDB0184850 | NA |
| 2434 | HMDB0185576 | NA |
| 2435 | HMDB0185577 | NA |
| 2436 | HMDB0184843 | NA |
| 2437 | HMDB0184841 | NA |
| 2438 | HMDB0184144 | NA |
| 2439 | HMDB0184143 | NA |
| 2440 | HMDB0184146 | NA |
| 2441 | HMDB0184145 | NA |
| 2442 | HMDB0184147 | NA |
| 2443 | HMDB0184148 | NA |
| 2444 | HMDB0184150 | NA |
| 2445 | HMDB0184149 | NA |
| 2446 | HMDB0184168 | NA |
| 2447 | HMDB0184844 | NA |
| 2448 | HMDB0185578 | NA |
| 2449 | HMDB0003550 | Calcidiol |
| 2450 | HMDB0060132 | NA |
| 2451 | HMDB0060131 | NA |
| 2452 | HMDB0015504 | Alfacalcidol |
| 2453 | HMDB0000501 | 7-Ketocholesterol |
| 2454 | HMDB0001993 | 7a-Hydroxy-cholestene-3-one |
| 2455 | HMDB0006722 | 25-Hydroxytachysterol3 |
| 2456 | HMDB0006721 | 5,6-trans-25-Hydroxyvitamin D3 |
| 2457 | HMDB0035585 | 1-Phenyl-1,3-heneicosanedione |
| 2458 | HMDB0034328 | (3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol |
| 2459 | HMDB0036012 | 5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone |
| 2460 | HMDB0039871 | NA |
| 2461 | HMDB0159655 | NA |
| 2462 | HMDB0159658 | NA |
| 2463 | HMDB0159656 | NA |
| 2464 | HMDB0159657 | NA |
| 2465 | HMDB0159654 | NA |
| 2466 | HMDB0159653 | NA |
| 2467 | HMDB0159651 | NA |
| 2468 | HMDB0159652 | NA |
| 2469 | HMDB0062675 | NA |
| 2470 | HMDB0062664 | NA |
| 2471 | HMDB0062419 | NA |
| 2472 | HMDB0062420 | NA |
| 2473 | HMDB0062607 | NA |
| 2474 | HMDB0172263 | NA |
| 2475 | HMDB0172264 | NA |
| 2476 | HMDB0185568 | NA |
| 2477 | HMDB0185570 | NA |
| 2478 | HMDB0185567 | NA |
| 2479 | HMDB0185569 | NA |
| 2480 | HMDB0185572 | NA |
| 2481 | HMDB0185575 | NA |
| 2482 | HMDB0185571 | NA |
| 2483 | HMDB0185574 | NA |
| 2484 | HMDB0185566 | NA |
| 2485 | HMDB0172272 | NA |
| 2486 | HMDB0172262 | NA |
| 2487 | HMDB0172266 | NA |
| 2488 | HMDB0172268 | NA |
| 2489 | HMDB0172265 | NA |
| 2490 | HMDB0172267 | NA |
| 2491 | HMDB0172270 | NA |
| 2492 | HMDB0172269 | NA |
| 2493 | HMDB0172271 | NA |
| 2494 | HMDB0185573 | NA |
| 2495 | HMDB0006280 | 7-a,25-Dihydroxycholesterol |

| | | |
|------|-------------|---|
| 2496 | HMDB0060136 | 7alpha,24S-Dihydroxycholesterol |
| 2497 | HMDB0011644 | (24R)-Cholest-5-ene-3-beta,7-alpha,24-triol |
| 2498 | HMDB0006894 | 3a,7a-Dihydroxy-5b-cholestan-26-al |
| 2499 | HMDB0006887 | 7a,12a-Dihydroxy-5b-cholestan-3-one |
| 2500 | HMDB0006886 | 7a,12a-Dihydroxy-5a-cholestan-3-one |
| 2501 | HMDB0006764 | 17a,20a-Dihydroxycholesterol |
| 2502 | HMDB0006763 | 20a,22b-Dihydroxycholesterol |
| 2503 | HMDB0006281 | 7-a,27-Dihydroxycholesterol |
| 2504 | HMDB0035951 | Erucylacetone |
| 2505 | HMDB0037260 | NA |
| 2506 | HMDB0158333 | NA |
| 2507 | HMDB0150478 | NA |
| 2508 | HMDB0150475 | NA |
| 2509 | HMDB0162509 | NA |
| 2510 | HMDB0150477 | NA |
| 2511 | HMDB0038347 | NA |
| 2512 | HMDB0150474 | NA |
| 2513 | HMDB0150463 | NA |
| 2514 | HMDB0150458 | NA |
| 2515 | HMDB0150468 | NA |
| 2516 | HMDB0150470 | NA |
| 2517 | HMDB0150457 | NA |
| 2518 | HMDB0150453 | NA |
| 2519 | HMDB0150469 | NA |
| 2520 | HMDB0150452 | NA |
| 2521 | HMDB0149868 | NA |
| 2522 | HMDB0150462 | NA |
| 2523 | HMDB0140070 | NA |
| 2524 | HMDB0153459 | NA |
| 2525 | HMDB0153444 | NA |
| 2526 | HMDB0153474 | NA |
| 2527 | HMDB0153627 | NA |
| 2528 | HMDB0153466 | NA |
| 2529 | HMDB0139521 | NA |
| 2530 | HMDB0139520 | NA |
| 2531 | HMDB0139517 | NA |
| 2532 | HMDB0139504 | NA |
| 2533 | HMDB0139507 | NA |
| 2534 | HMDB0139514 | NA |
| 2535 | HMDB0149502 | NA |
| 2536 | HMDB0153458 | NA |
| 2537 | HMDB0153451 | NA |
| 2538 | HMDB0153443 | NA |
| 2539 | HMDB0139516 | NA |
| 2540 | HMDB0139508 | NA |
| 2541 | HMDB0139513 | NA |
| 2542 | HMDB0035876 | Mesuagin |
| 2543 | HMDB0180147 | NA |
| 2544 | HMDB0013842 | O-Deethylated candesartan |
| 2545 | HMDB0144444 | NA |
| 2546 | HMDB0144965 | NA |
| 2547 | HMDB0144871 | NA |
| 2548 | HMDB0142647 | NA |
| 2549 | HMDB0144859 | NA |
| 2550 | HMDB0144408 | NA |
| 2551 | HMDB0144379 | NA |
| 2552 | HMDB0142761 | NA |
| 2553 | HMDB0142694 | NA |
| 2554 | HMDB0144418 | NA |
| 2555 | HMDB0144964 | NA |
| 2556 | HMDB0142682 | NA |
| 2557 | HMDB0144733 | NA |
| 2558 | HMDB0038793 | NA |
| 2559 | HMDB0038787 | NA |
| 2560 | HMDB0175541 | NA |
| 2561 | HMDB0175530 | NA |
| 2562 | HMDB0175535 | NA |
| 2563 | HMDB0175538 | NA |
| 2564 | HMDB0147025 | NA |
| 2565 | HMDB0147021 | NA |
| 2566 | HMDB0147020 | NA |
| 2567 | HMDB0147022 | NA |
| 2568 | HMDB0147019 | NA |
| 2569 | HMDB0147018 | NA |
| 2570 | HMDB0147024 | NA |
| 2571 | HMDB0147026 | NA |
| 2572 | HMDB0147023 | NA |
| 2573 | HMDB0168741 | NA |
| 2574 | HMDB0148765 | NA |
| 2575 | HMDB0148764 | NA |
| 2576 | HMDB0148762 | NA |
| 2577 | HMDB0148763 | NA |
| 2578 | HMDB0148761 | NA |
| 2579 | HMDB0148760 | NA |
| 2580 | HMDB0148759 | NA |
| 2581 | HMDB0168739 | NA |
| 2582 | HMDB0168747 | NA |

| | | |
|------|-------------|-------------------------------|
| 2583 | HMDB0168748 | NA |
| 2584 | HMDB0168750 | NA |
| 2585 | HMDB0168749 | NA |
| 2586 | HMDB0168740 | NA |
| 2587 | HMDB0168742 | NA |
| 2588 | HMDB0168743 | NA |
| 2589 | HMDB0168745 | NA |
| 2590 | HMDB0168744 | NA |
| 2591 | HMDB0168746 | NA |
| 2592 | HMDB0037039 | NA |
| 2593 | HMDB0014838 | Eplerenone |
| 2594 | HMDB0030404 | Armillaripin |
| 2595 | HMDB0041407 | NA |
| 2596 | HMDB0039380 | NA |
| 2597 | HMDB0173683 | NA |
| 2598 | HMDB0173687 | NA |
| 2599 | HMDB0173691 | NA |
| 2600 | HMDB0173689 | NA |
| 2601 | HMDB0173685 | NA |
| 2602 | HMDB0062292 | NA |
| 2603 | HMDB0062282 | NA |
| 2604 | HMDB0062274 | NA |
| 2605 | HMDB0034662 | Dihydrofukinolide |
| 2606 | HMDB0164538 | NA |
| 2607 | HMDB0164536 | NA |
| 2608 | HMDB0164537 | NA |
| 2609 | HMDB0240233 | NA |
| 2610 | HMDB0139759 | NA |
| 2611 | HMDB0139773 | NA |
| 2612 | HMDB0139772 | NA |
| 2613 | HMDB0139774 | NA |
| 2614 | HMDB0139775 | NA |
| 2615 | HMDB0139761 | NA |
| 2616 | HMDB0139764 | NA |
| 2617 | HMDB0139762 | NA |
| 2618 | HMDB0139760 | NA |
| 2619 | HMDB0139763 | NA |
| 2620 | HMDB0139766 | NA |
| 2621 | HMDB0139767 | NA |
| 2622 | HMDB0139765 | NA |
| 2623 | HMDB0139768 | NA |
| 2624 | HMDB0139769 | NA |
| 2625 | HMDB0139771 | NA |
| 2626 | HMDB0139770 | NA |
| 2627 | HMDB0139778 | NA |
| 2628 | HMDB0139776 | NA |
| 2629 | HMDB0139777 | NA |
| 2630 | HMDB0038618 | NA |
| 2631 | HMDB0183867 | NA |
| 2632 | HMDB0183864 | NA |
| 2633 | HMDB0183876 | NA |
| 2634 | HMDB0183860 | NA |
| 2635 | HMDB0183873 | NA |
| 2636 | HMDB0183891 | NA |
| 2637 | HMDB0183870 | NA |
| 2638 | HMDB0183894 | NA |
| 2639 | HMDB0036548 | NA |
| 2640 | HMDB0012560 | 13'-Hydroxy-alpha-tocotrienol |
| 2641 | HMDB0035730 | Camellectediol |
| 2642 | HMDB0041212 | NA |
| 2643 | HMDB0033806 | 2'-O-Methylcajanone |
| 2644 | HMDB0030849 | Artocarpin |
| 2645 | HMDB0140394 | NA |
| 2646 | HMDB0129645 | NA |
| 2647 | HMDB0134743 | NA |
| 2648 | HMDB0162013 | NA |
| 2649 | HMDB0162016 | NA |
| 2650 | HMDB0162004 | NA |
| 2651 | HMDB0142798 | NA |
| 2652 | HMDB0142979 | NA |
| 2653 | HMDB0142983 | NA |
| 2654 | HMDB0142989 | NA |
| 2655 | HMDB0142992 | NA |
| 2656 | HMDB0142993 | NA |
| 2657 | HMDB0143013 | NA |
| 2658 | HMDB0143016 | NA |
| 2659 | HMDB0142982 | NA |
| 2660 | HMDB0142838 | NA |
| 2661 | HMDB0142799 | NA |
| 2662 | HMDB0142805 | NA |
| 2663 | HMDB0142795 | NA |
| 2664 | HMDB0142808 | NA |
| 2665 | HMDB0142824 | NA |
| 2666 | HMDB0142822 | NA |
| 2667 | HMDB0142828 | NA |
| 2668 | HMDB0142834 | NA |
| 2669 | HMDB0142809 | NA |

| | | |
|------|-------------|----------------|
| 2670 | HMDB0143017 | NA |
| 2671 | HMDB0143090 | NA |
| 2672 | HMDB0143094 | NA |
| 2673 | HMDB0143096 | NA |
| 2674 | HMDB0143100 | NA |
| 2675 | HMDB0143110 | NA |
| 2676 | HMDB0143964 | NA |
| 2677 | HMDB0143966 | NA |
| 2678 | HMDB0143091 | NA |
| 2679 | HMDB0143087 | NA |
| 2680 | HMDB0143080 | NA |
| 2681 | HMDB0143023 | NA |
| 2682 | HMDB0143026 | NA |
| 2683 | HMDB0143027 | NA |
| 2684 | HMDB0143067 | NA |
| 2685 | HMDB0143070 | NA |
| 2686 | HMDB0143071 | NA |
| 2687 | HMDB0143106 | NA |
| 2688 | HMDB0143081 | NA |
| 2689 | HMDB0142788 | NA |
| 2690 | HMDB0142729 | NA |
| 2691 | HMDB0142725 | NA |
| 2692 | HMDB0142719 | NA |
| 2693 | HMDB0142718 | NA |
| 2694 | HMDB0142715 | NA |
| 2695 | HMDB0142739 | NA |
| 2696 | HMDB0143077 | NA |
| 2697 | HMDB0142728 | NA |
| 2698 | HMDB0142735 | NA |
| 2699 | HMDB0142738 | NA |
| 2700 | HMDB0142789 | NA |
| 2701 | HMDB0142785 | NA |
| 2702 | HMDB0142758 | NA |
| 2703 | HMDB0142759 | NA |
| 2704 | HMDB0142755 | NA |
| 2705 | HMDB0142748 | NA |
| 2706 | HMDB0142749 | NA |
| 2707 | HMDB0142745 | NA |
| 2708 | HMDB0035858 | Obacunone |
| 2709 | HMDB0035031 | Desoxylimonin |
| 2710 | HMDB0039920 | NA |
| 2711 | HMDB0039918 | NA |
| 2712 | HMDB0039919 | NA |
| 2713 | HMDB0015013 | Flupenthixol |
| 2714 | HMDB0184201 | NA |
| 2715 | HMDB0183261 | NA |
| 2716 | HMDB0183260 | NA |
| 2717 | HMDB0183262 | NA |
| 2718 | HMDB0183264 | NA |
| 2719 | HMDB0183267 | NA |
| 2720 | HMDB0183269 | NA |
| 2721 | HMDB0184206 | NA |
| 2722 | HMDB0184207 | NA |
| 2723 | HMDB0183254 | NA |
| 2724 | HMDB0183258 | NA |
| 2725 | HMDB0183250 | NA |
| 2726 | HMDB0183251 | NA |
| 2727 | HMDB0039214 | NA |
| 2728 | HMDB0036631 | NA |
| 2729 | HMDB0030688 | Cyclomulberrin |
| 2730 | HMDB0040480 | NA |
| 2731 | HMDB0029506 | Kuwanon B |
| 2732 | HMDB0029505 | Kuwanon A |
| 2733 | HMDB0131612 | NA |
| 2734 | HMDB0131610 | NA |
| 2735 | HMDB0131607 | NA |
| 2736 | HMDB0131606 | NA |
| 2737 | HMDB0131608 | NA |
| 2738 | HMDB0131609 | NA |
| 2739 | HMDB0131611 | NA |
| 2740 | HMDB0166772 | NA |
| 2741 | HMDB0166773 | NA |
| 2742 | HMDB0185408 | NA |
| 2743 | HMDB0185426 | NA |
| 2744 | HMDB0160312 | NA |
| 2745 | HMDB0160311 | NA |
| 2746 | HMDB0160309 | NA |
| 2747 | HMDB0160306 | NA |
| 2748 | HMDB0160305 | NA |
| 2749 | HMDB0160308 | NA |
| 2750 | HMDB0160314 | NA |
| 2751 | HMDB0160317 | NA |
| 2752 | HMDB0160320 | NA |
| 2753 | HMDB0036340 | NA |
| 2754 | HMDB0160333 | NA |
| 2755 | HMDB0160330 | NA |
| 2756 | HMDB0160332 | NA |

| | | |
|------|-------------|--|
| 2757 | HMDB0160329 | NA |
| 2758 | HMDB0160327 | NA |
| 2759 | HMDB0160326 | NA |
| 2760 | HMDB0160324 | NA |
| 2761 | HMDB0160323 | NA |
| 2762 | HMDB0160321 | NA |
| 2763 | HMDB0165007 | NA |
| 2764 | HMDB0165008 | NA |
| 2765 | HMDB0175389 | NA |
| 2766 | HMDB0175386 | NA |
| 2767 | HMDB0038562 | NA |
| 2768 | HMDB0014843 | Delavirdine |
| 2769 | HMDB0014565 | Spironolactone |
| 2770 | HMDB0180016 | NA |
| 2771 | HMDB0180015 | NA |
| 2772 | HMDB0015164 | Topotecan |
| 2773 | HMDB0145175 | NA |
| 2774 | HMDB0139832 | NA |
| 2775 | HMDB0139824 | NA |
| 2776 | HMDB0139838 | NA |
| 2777 | HMDB0139829 | NA |
| 2778 | HMDB0139833 | NA |
| 2779 | HMDB0139834 | NA |
| 2780 | HMDB0139836 | NA |
| 2781 | HMDB0139835 | NA |
| 2782 | HMDB0139837 | NA |
| 2783 | HMDB0139830 | NA |
| 2784 | HMDB0139831 | NA |
| 2785 | HMDB0139826 | NA |
| 2786 | HMDB0139825 | NA |
| 2787 | HMDB0139823 | NA |
| 2788 | HMDB0042019 | NA |
| 2789 | HMDB0165600 | NA |
| 2790 | HMDB0165605 | NA |
| 2791 | HMDB0163371 | NA |
| 2792 | HMDB0165603 | NA |
| 2793 | HMDB0165607 | NA |
| 2794 | HMDB0179376 | NA |
| 2795 | HMDB0179375 | NA |
| 2796 | HMDB0179380 | NA |
| 2797 | HMDB0179379 | NA |
| 2798 | HMDB0163370 | NA |
| 2799 | HMDB0041991 | NA |
| 2800 | HMDB0035142 | (3beta,17alpha,23S)-17,23-Epoxy-3,29-dihydroxy-27-norlanost-8-en-24-one |
| 2801 | HMDB0035995 | 2-(Methoxycarbonyl)-5-methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone |
| 2802 | HMDB0164769 | NA |
| 2803 | HMDB0032669 | (3beta,5alpha,9alpha,22E,24R)-3,5,9-Trihydroxy-23-methylergosta-7,22-dien-6-one |
| 2804 | HMDB0014780 | Pemetrexed |
| 2805 | HMDB0181044 | NA |
| 2806 | HMDB0181045 | NA |
| 2807 | HMDB0139597 | NA |
| 2808 | HMDB0139606 | NA |
| 2809 | HMDB0139601 | NA |
| 2810 | HMDB0139602 | NA |
| 2811 | HMDB0029900 | Lucuminoside |
| 2812 | HMDB0164389 | NA |
| 2813 | HMDB0164395 | NA |
| 2814 | HMDB0164391 | NA |
| 2815 | HMDB0036334 | NA |
| 2816 | HMDB0142846 | NA |
| 2817 | HMDB0132661 | NA |
| 2818 | HMDB0155455 | NA |
| 2819 | HMDB0155391 | NA |
| 2820 | HMDB0155394 | NA |
| 2821 | HMDB0155396 | NA |
| 2822 | HMDB0155406 | NA |
| 2823 | HMDB0158123 | NA |
| 2824 | HMDB0155403 | NA |
| 2825 | HMDB0155401 | NA |
| 2826 | HMDB0155400 | NA |
| 2827 | HMDB0155388 | NA |
| 2828 | HMDB0155385 | NA |
| 2829 | HMDB0155412 | NA |
| 2830 | HMDB0154709 | NA |
| 2831 | HMDB0154708 | NA |
| 2832 | HMDB0155409 | NA |
| 2833 | HMDB0155398 | NA |
| 2834 | HMDB0035864 | 13-Hydroxy-5'-O-methylmelledonal |
| 2835 | HMDB0038159 | NA |
| 2836 | HMDB0035690 | 6-O-Methylarmillaridin |
| 2837 | HMDB0157763 | NA |
| 2838 | HMDB0157761 | NA |
| 2839 | HMDB0157764 | NA |
| 2840 | HMDB0157766 | NA |
| 2841 | HMDB0157765 | NA |
| 2842 | HMDB0158281 | NA |
| 2843 | HMDB0170458 | NA |

| | | |
|------|-------------|---|
| 2844 | HMDB0170461 | NA |
| 2845 | HMDB0157760 | NA |
| 2846 | HMDB0157759 | NA |
| 2847 | HMDB0157609 | NA |
| 2848 | HMDB0157611 | NA |
| 2849 | HMDB0157614 | NA |
| 2850 | HMDB0156809 | NA |
| 2851 | HMDB0157607 | NA |
| 2852 | HMDB0157758 | NA |
| 2853 | HMDB0157613 | NA |
| 2854 | HMDB0157610 | NA |
| 2855 | HMDB0157612 | NA |
| 2856 | HMDB0014818 | Moricizine |
| 2857 | HMDB0172090 | NA |
| 2858 | HMDB0030452 | Blasticidin S |
| 2859 | HMDB0035973 | Lucidenic acid M |
| 2860 | HMDB0164014 | NA |
| 2861 | HMDB0171518 | NA |
| 2862 | HMDB0174361 | NA |
| 2863 | HMDB0174360 | NA |
| 2864 | HMDB0174359 | NA |
| 2865 | HMDB0174715 | NA |
| 2866 | HMDB0174374 | NA |
| 2867 | HMDB0174370 | NA |
| 2868 | HMDB0174371 | NA |
| 2869 | HMDB0174372 | NA |
| 2870 | HMDB0174373 | NA |
| 2871 | HMDB0174367 | NA |
| 2872 | HMDB0174363 | NA |
| 2873 | HMDB0174364 | NA |
| 2874 | HMDB0174362 | NA |
| 2875 | HMDB0174365 | NA |
| 2876 | HMDB0174366 | NA |
| 2877 | HMDB0174369 | NA |
| 2878 | HMDB0174368 | NA |
| 2879 | HMDB0183788 | NA |
| 2880 | HMDB0183785 | NA |
| 2881 | HMDB0183779 | NA |
| 2882 | HMDB0183773 | NA |
| 2883 | HMDB0183776 | NA |
| 2884 | HMDB0174714 | NA |
| 2885 | HMDB0174358 | NA |
| 2886 | HMDB0174356 | NA |
| 2887 | HMDB0174357 | NA |
| 2888 | HMDB0174355 | NA |
| 2889 | HMDB0000969 | 1,25-Dihydroxyvitamin D3-26,23-lactone |
| 2890 | HMDB0164012 | NA |
| 2891 | HMDB0174354 | NA |
| 2892 | HMDB0174353 | NA |
| 2893 | HMDB0174352 | NA |
| 2894 | HMDB0171517 | NA |
| 2895 | HMDB0012936 | Dynorphin B (10-13) |
| 2896 | HMDB0240599 | NA |
| 2897 | HMDB0155347 | NA |
| 2898 | HMDB0155348 | NA |
| 2899 | HMDB0034064 | 2-Angeloyl-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one |
| 2900 | HMDB0036571 | NA |
| 2901 | HMDB0035489 | Linalool 3,6-oxide primeveroside |
| 2902 | HMDB0031367 | Linalool oxide D 3-[apiosyl-(1->6)-glucoside] |
| 2903 | HMDB0182246 | NA |
| 2904 | HMDB0182247 | NA |
| 2905 | HMDB0182263 | NA |
| 2906 | HMDB0015631 | Alvimopan |
| 2907 | HMDB0061149 | NA |
| 2908 | HMDB0029989 | Dulciol B |
| 2909 | HMDB0033316 | Garcinone E |
| 2910 | HMDB0029990 | Dulciol A |
| 2911 | HMDB0156274 | NA |
| 2912 | HMDB0162419 | NA |
| 2913 | HMDB0177052 | NA |
| 2914 | HMDB0040747 | NA |
| 2915 | HMDB0148895 | NA |
| 2916 | HMDB0040607 | NA |
| 2917 | HMDB0034183 | Licoricidin |
| 2918 | HMDB0014420 | Olmesartan |
| 2919 | HMDB0060584 | NA |
| 2920 | HMDB0035068 | Melleolide M |
| 2921 | HMDB0179387 | NA |
| 2922 | HMDB0179386 | NA |
| 2923 | HMDB0179390 | NA |
| 2924 | HMDB0179389 | NA |
| 2925 | HMDB0061104 | NA |
| 2926 | HMDB0139815 | NA |
| 2927 | HMDB0144973 | NA |
| 2928 | HMDB0144948 | NA |
| 2929 | HMDB0144943 | NA |
| 2930 | HMDB0144938 | NA |

| | | |
|------|-------------|---|
| 2931 | HMDB0139798 | NA |
| 2932 | HMDB0139801 | NA |
| 2933 | HMDB0139799 | NA |
| 2934 | HMDB0139800 | NA |
| 2935 | HMDB0139797 | NA |
| 2936 | HMDB0144978 | NA |
| 2937 | HMDB0139796 | NA |
| 2938 | HMDB0139795 | NA |
| 2939 | HMDB0144983 | NA |
| 2940 | HMDB0144998 | NA |
| 2941 | HMDB0144988 | NA |
| 2942 | HMDB0144933 | NA |
| 2943 | HMDB0144918 | NA |
| 2944 | HMDB0139811 | NA |
| 2945 | HMDB0139813 | NA |
| 2946 | HMDB0139809 | NA |
| 2947 | HMDB0139806 | NA |
| 2948 | HMDB0139807 | NA |
| 2949 | HMDB0139808 | NA |
| 2950 | HMDB0139814 | NA |
| 2951 | HMDB0139816 | NA |
| 2952 | HMDB0139805 | NA |
| 2953 | HMDB0139817 | NA |
| 2954 | HMDB0139812 | NA |
| 2955 | HMDB0139818 | NA |
| 2956 | HMDB0139804 | NA |
| 2957 | HMDB0139820 | NA |
| 2958 | HMDB0139819 | NA |
| 2959 | HMDB0139803 | NA |
| 2960 | HMDB0144913 | NA |
| 2961 | HMDB0139802 | NA |
| 2962 | HMDB0145003 | NA |
| 2963 | HMDB0144993 | NA |
| 2964 | HMDB0145038 | NA |
| 2965 | HMDB0145034 | NA |
| 2966 | HMDB0145032 | NA |
| 2967 | HMDB0139810 | NA |
| 2968 | HMDB0145018 | NA |
| 2969 | HMDB0145013 | NA |
| 2970 | HMDB0145008 | NA |
| 2971 | HMDB0032622 | Phenethyl rutinoid |
| 2972 | HMDB0094682 | 5alpha-Androstan-3alpha,17beta-diol disulfate |
| 2973 | HMDB0240625 | NA |
| 2974 | HMDB0172330 | NA |
| 2975 | HMDB0159770 | NA |
| 2976 | HMDB0159769 | NA |
| 2977 | HMDB0159767 | NA |
| 2978 | HMDB0159766 | NA |
| 2979 | HMDB0159765 | NA |
| 2980 | HMDB0159768 | NA |
| 2981 | HMDB0062421 | NA |
| 2982 | HMDB0062416 | NA |
| 2983 | HMDB0159772 | NA |
| 2984 | HMDB0159774 | NA |
| 2985 | HMDB0159773 | NA |
| 2986 | HMDB0159897 | NA |
| 2987 | HMDB0159894 | NA |
| 2988 | HMDB0159896 | NA |
| 2989 | HMDB0159893 | NA |
| 2990 | HMDB0159889 | NA |
| 2991 | HMDB0159890 | NA |
| 2992 | HMDB0159892 | NA |
| 2993 | HMDB0159891 | NA |
| 2994 | HMDB0000558 | 5a-Cholestane-3a,7a,12a,23,25-pentol |
| 2995 | HMDB0002208 | Cholestane-3,7,12,24,25-pentol |
| 2996 | HMDB0000483 | 5b-Cholestane-3a,7a,12a,23S,25-pentol |
| 2997 | HMDB0000556 | 5b-Cholestane-3a,7a,12a,24,25-pentol |
| 2998 | HMDB0000513 | 5b-Cholestane-3a,7a,12a,23R,25-pentol |
| 2999 | HMDB0002180 | 5b-Cholestane-3a,7a,12a,25,26-pentol |
| 3000 | HMDB0011187 | TG(8:0/8:0/8:0) |
| 3001 | HMDB0059930 | NA |
| 3002 | HMDB0035144 | (3beta,17alpha,23S,24S)-17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-15-one |
| 3003 | HMDB0170385 | NA |
| 3004 | HMDB0035221 | (3beta,17alpha,23S)-17,23-Epoxy-3,28,29-trihydroxy-27-norlanost-8-en-24-one |
| 3005 | HMDB0170384 | NA |
| 3006 | HMDB0167563 | NA |
| 3007 | HMDB0167569 | NA |
| 3008 | HMDB0167571 | NA |
| 3009 | HMDB0167565 | NA |
| 3010 | HMDB0172392 | NA |
| 3011 | HMDB0172390 | NA |
| 3012 | HMDB0167567 | NA |
| 3013 | HMDB0062208 | NA |
| 3014 | HMDB0159763 | NA |
| 3015 | HMDB0159762 | NA |
| 3016 | HMDB0000359 | 3a,7a-Dihydroxycoprostanic acid |
| 3017 | HMDB0159775 | NA |

| | | |
|------|-------------|---|
| 3018 | HMDB0159887 | NA |
| 3019 | HMDB0003533 | 3a,7a,12a-Trihydroxy-5b-cholestan-26-al |
| 3020 | HMDB0159898 | NA |
| 3021 | HMDB0159886 | NA |
| 3022 | HMDB0034065 | 2,9-Bis(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oplopadien-3-one |
| 3023 | HMDB0032601 | Muzanzagenin |
| 3024 | HMDB0014936 | Gentamicin |
| 3025 | HMDB0160543 | NA |
| 3026 | HMDB0160539 | NA |
| 3027 | HMDB0160541 | NA |
| 3028 | HMDB0160540 | NA |
| 3029 | HMDB0160542 | NA |
| 3030 | HMDB0160544 | NA |
| 3031 | HMDB0160545 | NA |
| 3032 | HMDB0160516 | NA |
| 3033 | HMDB0160517 | NA |
| 3034 | HMDB0160518 | NA |
| 3035 | HMDB0160515 | NA |
| 3036 | HMDB0160519 | NA |
| 3037 | HMDB0160522 | NA |
| 3038 | HMDB0160521 | NA |
| 3039 | HMDB0160520 | NA |
| 3040 | HMDB0160523 | NA |
| 3041 | HMDB0160526 | NA |
| 3042 | HMDB0160524 | NA |
| 3043 | HMDB0160525 | NA |
| 3044 | HMDB0160528 | NA |
| 3045 | HMDB0160529 | NA |
| 3046 | HMDB0160527 | NA |
| 3047 | HMDB0160530 | NA |
| 3048 | HMDB0172528 | NA |
| 3049 | HMDB0170464 | NA |
| 3050 | HMDB0059931 | NA |
| 3051 | HMDB0040118 | NA |
| 3052 | HMDB0240598 | NA |
| 3053 | HMDB0160534 | NA |
| 3054 | HMDB0160531 | NA |
| 3055 | HMDB0160532 | NA |
| 3056 | HMDB0160533 | NA |
| 3057 | HMDB0160538 | NA |
| 3058 | HMDB0160535 | NA |
| 3059 | HMDB0160536 | NA |
| 3060 | HMDB0160537 | NA |
| 3061 | HMDB0039079 | NA |
| 3062 | HMDB0039024 | NA |
| 3063 | HMDB0184086 | NA |
| 3064 | HMDB0002385 | Celastrol |
| 3065 | HMDB0015057 | Buprenorphine |
| 3066 | HMDB0062331 | NA |
| 3067 | HMDB0010379 | LysoPC(14:0) |
| 3068 | HMDB0061691 | NA |
| 3069 | HMDB0161447 | NA |
| 3070 | HMDB0179451 | NA |
| 3071 | HMDB0062337 | NA |
| 3072 | HMDB0010381 | LysoPC(15:0) |
| 3073 | HMDB0011130 | LysoPE(18:0/0:0) |
| 3074 | HMDB0011129 | LysoPE(0:0/18:0) |
| 3075 | HMDB0062305 | NA |
| 3076 | HMDB0172584 | NA |
| 3077 | HMDB0172583 | NA |
| 3078 | HMDB0154880 | NA |
| 3079 | HMDB0184865 | NA |
| 3080 | HMDB0172431 | NA |
| 3081 | HMDB0175550 | NA |
| 3082 | HMDB0172429 | NA |
| 3083 | HMDB0175542 | NA |
| 3084 | HMDB0175548 | NA |
| 3085 | HMDB0175549 | NA |
| 3086 | HMDB0034216 | Adouetine X |
| 3087 | HMDB0030199 | Frangulanine |
| 3088 | HMDB0032879 | all-trans-Carophyll yellow |
| 3089 | HMDB0010380 | LysoPC(14:1(9Z)) |
| 3090 | HMDB0170639 | NA |
| 3091 | HMDB0170632 | NA |
| 3092 | HMDB0170638 | NA |
| 3093 | HMDB0170641 | NA |
| 3094 | HMDB0170637 | NA |
| 3095 | HMDB0170661 | NA |
| 3096 | HMDB0170640 | NA |
| 3097 | HMDB0170634 | NA |
| 3098 | HMDB0170636 | NA |
| 3099 | HMDB0170633 | NA |
| 3100 | HMDB0170635 | NA |
| 3101 | HMDB0170642 | NA |
| 3102 | HMDB0041532 | NA |
| 3103 | HMDB0030901 | Eremopetasitenin B2 |
| 3104 | HMDB0039930 | NA |

| | | |
|------|-------------|--|
| 3105 | HMDB0164234 | NA |
| 3106 | HMDB0135504 | NA |
| 3107 | HMDB0135508 | NA |
| 3108 | HMDB0135506 | NA |
| 3109 | HMDB0031943 | (Z)-N-[(4-hydroxyphenyl)methyl]ethoxycarbothioamide 4'-(tri-acetylramnoside) |
| 3110 | HMDB0133632 | NA |
| 3111 | HMDB0133629 | NA |
| 3112 | HMDB0133763 | NA |
| 3113 | HMDB0133762 | NA |
| 3114 | HMDB0135654 | NA |
| 3115 | HMDB0179487 | NA |
| 3116 | HMDB0179486 | NA |
| 3117 | HMDB0133631 | NA |
| 3118 | HMDB0133626 | NA |
| 3119 | HMDB0133623 | NA |
| 3120 | HMDB0133634 | NA |
| 3121 | HMDB0170798 | NA |
| 3122 | HMDB0170797 | NA |
| 3123 | HMDB0170793 | NA |
| 3124 | HMDB0170796 | NA |
| 3125 | HMDB0170791 | NA |
| 3126 | HMDB0170792 | NA |
| 3127 | HMDB0184654 | NA |
| 3128 | HMDB0184468 | NA |
| 3129 | HMDB0139941 | NA |
| 3130 | HMDB0139958 | NA |
| 3131 | HMDB0035635 | Kanokoside A |
| 3132 | HMDB0004482 | 2-Methoxyestrone 3-glucuronide |
| 3133 | HMDB0154676 | NA |
| 3134 | HMDB0169584 | NA |
| 3135 | HMDB0146115 | NA |
| 3136 | HMDB0161563 | NA |
| 3137 | HMDB0161564 | NA |
| 3138 | HMDB0161602 | NA |
| 3139 | HMDB0161603 | NA |
| 3140 | HMDB0061034 | NA |
| 3141 | HMDB0033709 | Desglucocoroloside |
| 3142 | HMDB0015110 | Dipyridamole |
| 3143 | HMDB0011481 | LysoPE(0:0/20:0) |
| 3144 | HMDB0012108 | LysoPC(17:0) |
| 3145 | HMDB0011511 | LysoPE(20:0/0:0) |
| 3146 | HMDB0114750 | NA |
| 3147 | HMDB0062304 | NA |
| 3148 | HMDB0030291 | Daphniphylline |
| 3149 | HMDB0183973 | NA |
| 3150 | HMDB0174607 | NA |
| 3151 | HMDB0174422 | NA |
| 3152 | HMDB0171595 | NA |
| 3153 | HMDB0167550 | NA |
| 3154 | HMDB0167544 | NA |
| 3155 | HMDB0167357 | NA |
| 3156 | HMDB0166718 | NA |
| 3157 | HMDB0166240 | NA |
| 3158 | HMDB0162256 | NA |
| 3159 | HMDB0145366 | NA |
| 3160 | HMDB0145272 | NA |
| 3161 | HMDB0145271 | NA |
| 3162 | HMDB0145352 | NA |
| 3163 | HMDB0145351 | NA |
| 3164 | HMDB0029429 | Malformin |
| 3165 | HMDB0015181 | Fluocinonide |
| 3166 | HMDB0158654 | NA |
| 3167 | HMDB0169107 | NA |
| 3168 | HMDB0169101 | NA |
| 3169 | HMDB0169097 | NA |
| 3170 | HMDB0169099 | NA |
| 3171 | HMDB0169095 | NA |
| 3172 | HMDB0158636 | NA |
| 3173 | HMDB0158660 | NA |
| 3174 | HMDB0158646 | NA |
| 3175 | HMDB0158642 | NA |
| 3176 | HMDB0158643 | NA |
| 3177 | HMDB0158650 | NA |
| 3178 | HMDB0158656 | NA |
| 3179 | HMDB0158639 | NA |
| 3180 | HMDB0169105 | NA |
| 3181 | HMDB0169110 | NA |
| 3182 | HMDB0171268 | NA |
| 3183 | HMDB0171269 | NA |
| 3184 | HMDB0169108 | NA |
| 3185 | HMDB0171261 | NA |
| 3186 | HMDB0033412 | Gibberellin A20 13-glucoside |
| 3187 | HMDB0171272 | NA |
| 3188 | HMDB0171264 | NA |
| 3189 | HMDB0171258 | NA |
| 3190 | HMDB0171257 | NA |
| 3191 | HMDB0171253 | NA |

| | | |
|------|-------------|--------------------------|
| 3192 | HMDB0171254 | NA |
| 3193 | HMDB0169103 | NA |
| 3194 | HMDB0169111 | NA |
| 3195 | HMDB0171273 | NA |
| 3196 | HMDB0158225 | NA |
| 3197 | HMDB0158226 | NA |
| 3198 | HMDB0158228 | NA |
| 3199 | HMDB0158231 | NA |
| 3200 | HMDB0158234 | NA |
| 3201 | HMDB0158235 | NA |
| 3202 | HMDB0158238 | NA |
| 3203 | HMDB0158621 | NA |
| 3204 | HMDB0158625 | NA |
| 3205 | HMDB0158629 | NA |
| 3206 | HMDB0158223 | NA |
| 3207 | HMDB0158633 | NA |
| 3208 | HMDB0038610 | NA |
| 3209 | HMDB0037084 | NA |
| 3210 | HMDB0157580 | NA |
| 3211 | HMDB0158210 | NA |
| 3212 | HMDB0158213 | NA |
| 3213 | HMDB0158219 | NA |
| 3214 | HMDB0158216 | NA |
| 3215 | HMDB0158221 | NA |
| 3216 | HMDB0062314 | NA |
| 3217 | HMDB0114749 | NA |
| 3218 | HMDB0114769 | NA |
| 3219 | HMDB0140042 | NA |
| 3220 | HMDB0167203 | NA |
| 3221 | HMDB0167209 | NA |
| 3222 | HMDB0167206 | NA |
| 3223 | HMDB0167200 | NA |
| 3224 | HMDB0167195 | NA |
| 3225 | HMDB0167174 | NA |
| 3226 | HMDB0167177 | NA |
| 3227 | HMDB0167180 | NA |
| 3228 | HMDB0167183 | NA |
| 3229 | HMDB0167189 | NA |
| 3230 | HMDB0167186 | NA |
| 3231 | HMDB0167192 | NA |
| 3232 | HMDB0167196 | NA |
| 3233 | HMDB0167197 | NA |
| 3234 | HMDB0167227 | NA |
| 3235 | HMDB0167213 | NA |
| 3236 | HMDB0167212 | NA |
| 3237 | HMDB0167216 | NA |
| 3238 | HMDB0167217 | NA |
| 3239 | HMDB0167220 | NA |
| 3240 | HMDB0167223 | NA |
| 3241 | HMDB0035700 | Lucidenic acid J |
| 3242 | HMDB0157584 | NA |
| 3243 | HMDB0157593 | NA |
| 3244 | HMDB0157590 | NA |
| 3245 | HMDB0157587 | NA |
| 3246 | HMDB0174900 | NA |
| 3247 | HMDB0034362 | Desglucocheirotxin |
| 3248 | HMDB0166971 | NA |
| 3249 | HMDB0166972 | NA |
| 3250 | HMDB0166970 | NA |
| 3251 | HMDB0173681 | NA |
| 3252 | HMDB0173690 | NA |
| 3253 | HMDB0173684 | NA |
| 3254 | HMDB0186464 | NA |
| 3255 | HMDB0177528 | NA |
| 3256 | HMDB0173682 | NA |
| 3257 | HMDB0173688 | NA |
| 3258 | HMDB0173686 | NA |
| 3259 | HMDB0240602 | NA |
| 3260 | HMDB0031388 | 23-Hydroxyphysalolactone |
| 3261 | HMDB0173080 | NA |
| 3262 | HMDB0015101 | Telmisartan |
| 3263 | HMDB0164474 | NA |
| 3264 | HMDB0164482 | NA |
| 3265 | HMDB0164483 | NA |
| 3266 | HMDB0164491 | NA |
| 3267 | HMDB0164495 | NA |
| 3268 | HMDB0164506 | NA |
| 3269 | HMDB0164502 | NA |
| 3270 | HMDB0140666 | NA |
| 3271 | HMDB0140667 | NA |
| 3272 | HMDB0140668 | NA |
| 3273 | HMDB0032648 | Muridienin 1 |
| 3274 | HMDB0032850 | Muricadienin |
| 3275 | HMDB0182791 | NA |
| 3276 | HMDB0182792 | NA |
| 3277 | HMDB0178155 | NA |
| 3278 | HMDB0178154 | NA |

| | | |
|------|-------------|---------------------|
| 3279 | HMDB0178156 | NA |
| 3280 | HMDB0178157 | NA |
| 3281 | HMDB0176412 | NA |
| 3282 | HMDB0176411 | NA |
| 3283 | HMDB0145377 | NA |
| 3284 | HMDB0143804 | NA |
| 3285 | HMDB0143801 | NA |
| 3286 | HMDB0143805 | NA |
| 3287 | HMDB0145376 | NA |
| 3288 | HMDB0145294 | NA |
| 3289 | HMDB0145309 | NA |
| 3290 | HMDB0039235 | NA |
| 3291 | HMDB0171416 | NA |
| 3292 | HMDB0171414 | NA |
| 3293 | HMDB0171413 | NA |
| 3294 | HMDB0171410 | NA |
| 3295 | HMDB0171409 | NA |
| 3296 | HMDB0171405 | NA |
| 3297 | HMDB0171393 | NA |
| 3298 | HMDB0171406 | NA |
| 3299 | HMDB0171402 | NA |
| 3300 | HMDB0171401 | NA |
| 3301 | HMDB0171391 | NA |
| 3302 | HMDB0171392 | NA |
| 3303 | HMDB0171417 | NA |
| 3304 | HMDB0171442 | NA |
| 3305 | HMDB0040636 | NA |
| 3306 | HMDB0171388 | NA |
| 3307 | HMDB0171387 | NA |
| 3308 | HMDB0171386 | NA |
| 3309 | HMDB0140195 | NA |
| 3310 | HMDB0136702 | NA |
| 3311 | HMDB0131022 | NA |
| 3312 | HMDB0131017 | NA |
| 3313 | HMDB0131021 | NA |
| 3314 | HMDB0131023 | NA |
| 3315 | HMDB0006595 | Alpha-Trisaccharide |
| 3316 | HMDB0160574 | NA |
| 3317 | HMDB0170548 | NA |
| 3318 | HMDB0160573 | NA |
| 3319 | HMDB0129853 | NA |
| 3320 | HMDB0149574 | NA |
| 3321 | HMDB0157964 | NA |
| 3322 | HMDB0157968 | NA |
| 3323 | HMDB0157967 | NA |
| 3324 | HMDB0157963 | NA |
| 3325 | HMDB0159724 | NA |
| 3326 | HMDB0158391 | NA |
| 3327 | HMDB0157971 | NA |
| 3328 | HMDB0158388 | NA |
| 3329 | HMDB0158398 | NA |
| 3330 | HMDB0158392 | NA |
| 3331 | HMDB0157976 | NA |
| 3332 | HMDB0158389 | NA |
| 3333 | HMDB0159722 | NA |
| 3334 | HMDB0158397 | NA |
| 3335 | HMDB0157972 | NA |
| 3336 | HMDB0158395 | NA |
| 3337 | HMDB0157980 | NA |
| 3338 | HMDB0157979 | NA |
| 3339 | HMDB0157975 | NA |
| 3340 | HMDB0158400 | NA |
| 3341 | HMDB0158401 | NA |
| 3342 | HMDB0159005 | NA |
| 3343 | HMDB0159006 | NA |
| 3344 | HMDB0159011 | NA |
| 3345 | HMDB0159008 | NA |
| 3346 | HMDB0159009 | NA |
| 3347 | HMDB0159015 | NA |
| 3348 | HMDB0159014 | NA |
| 3349 | HMDB0159012 | NA |
| 3350 | HMDB0159713 | NA |
| 3351 | HMDB0159725 | NA |
| 3352 | HMDB0159712 | NA |
| 3353 | HMDB0159716 | NA |
| 3354 | HMDB0159715 | NA |
| 3355 | HMDB0159718 | NA |
| 3356 | HMDB0159721 | NA |
| 3357 | HMDB0159002 | NA |
| 3358 | HMDB0159000 | NA |
| 3359 | HMDB0158404 | NA |
| 3360 | HMDB0158403 | NA |
| 3361 | HMDB0158981 | NA |
| 3362 | HMDB0158983 | NA |
| 3363 | HMDB0158980 | NA |
| 3364 | HMDB0158984 | NA |
| 3365 | HMDB0158986 | NA |

| | | |
|------|-------------|--|
| 3366 | HMDB0158987 | NA |
| 3367 | HMDB0158989 | NA |
| 3368 | HMDB0158990 | NA |
| 3369 | HMDB0158995 | NA |
| 3370 | HMDB0158992 | NA |
| 3371 | HMDB0158993 | NA |
| 3372 | HMDB0158996 | NA |
| 3373 | HMDB0159003 | NA |
| 3374 | HMDB0159719 | NA |
| 3375 | HMDB0158999 | NA |
| 3376 | HMDB0158394 | NA |
| 3377 | HMDB0034402 | Physalin I |
| 3378 | HMDB0060499 | NPC |
| 3379 | HMDB0186322 | NA |
| 3380 | HMDB0186334 | NA |
| 3381 | HMDB0186323 | NA |
| 3382 | HMDB0186328 | NA |
| 3383 | HMDB0186335 | NA |
| 3384 | HMDB0186340 | NA |
| 3385 | HMDB0186341 | NA |
| 3386 | HMDB0186338 | NA |
| 3387 | HMDB0186342 | NA |
| 3388 | HMDB0186345 | NA |
| 3389 | HMDB0186337 | NA |
| 3390 | HMDB0186332 | NA |
| 3391 | HMDB0186331 | NA |
| 3392 | HMDB0186351 | NA |
| 3393 | HMDB0186326 | NA |
| 3394 | HMDB0186348 | NA |
| 3395 | HMDB0131873 | NA |
| 3396 | HMDB0186325 | NA |
| 3397 | HMDB0035520 | Vomifoliol 9-[xylosyl-(1->6)-glucoside] |
| 3398 | HMDB0185602 | NA |
| 3399 | HMDB0185601 | NA |
| 3400 | HMDB0185603 | NA |
| 3401 | HMDB0029773 | 6S,9R-Dihydroxy-4,7E-megastigmadien-3-one 9-[apiosyl-(1->6)-glucoside] |
| 3402 | HMDB0038923 | NA |
| 3403 | HMDB0015129 | Neomycin |
| 3404 | HMDB0002160 | Harderoporphyrinogen |
| 3405 | HMDB0039454 | NA |
| 3406 | HMDB0173693 | NA |
| 3407 | HMDB0173692 | NA |
| 3408 | HMDB0173699 | NA |
| 3409 | HMDB0173698 | NA |
| 3410 | HMDB0142988 | NA |
| 3411 | HMDB0142998 | NA |
| 3412 | HMDB0142997 | NA |
| 3413 | HMDB0143001 | NA |
| 3414 | HMDB0142987 | NA |
| 3415 | HMDB0142978 | NA |
| 3416 | HMDB0142977 | NA |
| 3417 | HMDB0142917 | NA |
| 3418 | HMDB0142918 | NA |
| 3419 | HMDB0142919 | NA |
| 3420 | HMDB0142921 | NA |
| 3421 | HMDB0142920 | NA |
| 3422 | HMDB0142926 | NA |
| 3423 | HMDB0142929 | NA |
| 3424 | HMDB0142928 | NA |
| 3425 | HMDB0142927 | NA |
| 3426 | HMDB0143002 | NA |
| 3427 | HMDB0143007 | NA |
| 3428 | HMDB0143006 | NA |
| 3429 | HMDB0143108 | NA |
| 3430 | HMDB0143104 | NA |
| 3431 | HMDB0143098 | NA |
| 3432 | HMDB0143093 | NA |
| 3433 | HMDB0143086 | NA |
| 3434 | HMDB0143085 | NA |
| 3435 | HMDB0143076 | NA |
| 3436 | HMDB0143075 | NA |
| 3437 | HMDB0143066 | NA |
| 3438 | HMDB0143065 | NA |
| 3439 | HMDB0143061 | NA |
| 3440 | HMDB0143060 | NA |
| 3441 | HMDB0143022 | NA |
| 3442 | HMDB0143012 | NA |
| 3443 | HMDB0143011 | NA |
| 3444 | HMDB0143021 | NA |
| 3445 | HMDB0142916 | NA |
| 3446 | HMDB0142915 | NA |
| 3447 | HMDB0142901 | NA |
| 3448 | HMDB0142899 | NA |
| 3449 | HMDB0142902 | NA |
| 3450 | HMDB0142900 | NA |
| 3451 | HMDB0142905 | NA |
| 3452 | HMDB0142904 | NA |

| | | |
|------|-------------|--|
| 3453 | HMDB0142903 | NA |
| 3454 | HMDB0142908 | NA |
| 3455 | HMDB0142911 | NA |
| 3456 | HMDB0142913 | NA |
| 3457 | HMDB0142914 | NA |
| 3458 | HMDB0142912 | NA |
| 3459 | HMDB0142930 | NA |
| 3460 | HMDB0165936 | NA |
| 3461 | HMDB0165918 | NA |
| 3462 | HMDB0173230 | NA |
| 3463 | HMDB0173229 | NA |
| 3464 | HMDB0165966 | NA |
| 3465 | HMDB0164809 | NA |
| 3466 | HMDB0034433 | Riboflavine 2',3',4',5'-tetrabutanoate |
| 3467 | HMDB0157944 | NA |
| 3468 | HMDB0157945 | NA |
| 3469 | HMDB0157949 | NA |
| 3470 | HMDB0157950 | NA |
| 3471 | HMDB0157951 | NA |
| 3472 | HMDB0157955 | NA |
| 3473 | HMDB0157956 | NA |
| 3474 | HMDB0157943 | NA |
| 3475 | HMDB0157938 | NA |
| 3476 | HMDB0157939 | NA |
| 3477 | HMDB0157937 | NA |
| 3478 | HMDB0157933 | NA |
| 3479 | HMDB0157932 | NA |
| 3480 | HMDB0157931 | NA |
| 3481 | HMDB0157898 | NA |
| 3482 | HMDB0157896 | NA |
| 3483 | HMDB0157957 | NA |
| 3484 | HMDB0158932 | NA |
| 3485 | HMDB0158968 | NA |
| 3486 | HMDB0158964 | NA |
| 3487 | HMDB0158963 | NA |
| 3488 | HMDB0158958 | NA |
| 3489 | HMDB0158959 | NA |
| 3490 | HMDB0158953 | NA |
| 3491 | HMDB0158954 | NA |
| 3492 | HMDB0158949 | NA |
| 3493 | HMDB0158948 | NA |
| 3494 | HMDB0158944 | NA |
| 3495 | HMDB0158943 | NA |
| 3496 | HMDB0158937 | NA |
| 3497 | HMDB0158938 | NA |
| 3498 | HMDB0158939 | NA |
| 3499 | HMDB0158933 | NA |
| 3500 | HMDB0158969 | NA |
| 3501 | HMDB0157897 | NA |
| 3502 | HMDB0157050 | NA |
| 3503 | HMDB0157221 | NA |
| 3504 | HMDB0157842 | NA |
| 3505 | HMDB0157841 | NA |
| 3506 | HMDB0157843 | NA |
| 3507 | HMDB0157847 | NA |
| 3508 | HMDB0157846 | NA |
| 3509 | HMDB0157851 | NA |
| 3510 | HMDB0157848 | NA |
| 3511 | HMDB0157853 | NA |
| 3512 | HMDB0157215 | NA |
| 3513 | HMDB0157218 | NA |
| 3514 | HMDB0157212 | NA |
| 3515 | HMDB0157051 | NA |
| 3516 | HMDB0157054 | NA |
| 3517 | HMDB0157057 | NA |
| 3518 | HMDB0157060 | NA |
| 3519 | HMDB0157066 | NA |
| 3520 | HMDB0157063 | NA |
| 3521 | HMDB0157206 | NA |
| 3522 | HMDB0157205 | NA |
| 3523 | HMDB0157209 | NA |
| 3524 | HMDB0157852 | NA |
| 3525 | HMDB0157856 | NA |
| 3526 | HMDB0157857 | NA |
| 3527 | HMDB0157876 | NA |
| 3528 | HMDB0157881 | NA |
| 3529 | HMDB0157882 | NA |
| 3530 | HMDB0157883 | NA |
| 3531 | HMDB0157886 | NA |
| 3532 | HMDB0157887 | NA |
| 3533 | HMDB0157888 | NA |
| 3534 | HMDB0157891 | NA |
| 3535 | HMDB0157892 | NA |
| 3536 | HMDB0157893 | NA |
| 3537 | HMDB0157878 | NA |
| 3538 | HMDB0157877 | NA |
| 3539 | HMDB0157858 | NA |

| | | |
|------|-------------|--|
| 3540 | HMDB0157861 | NA |
| 3541 | HMDB0157862 | NA |
| 3542 | HMDB0157863 | NA |
| 3543 | HMDB0157866 | NA |
| 3544 | HMDB0157867 | NA |
| 3545 | HMDB0157868 | NA |
| 3546 | HMDB0157871 | NA |
| 3547 | HMDB0157873 | NA |
| 3548 | HMDB0157872 | NA |
| 3549 | HMDB0030115 | Kuwanon V |
| 3550 | HMDB0036105 | NA |
| 3551 | HMDB0036400 | NA |
| 3552 | HMDB0129844 | NA |
| 3553 | HMDB0129842 | NA |
| 3554 | HMDB0129843 | NA |
| 3555 | HMDB0007094 | DG(15:0/24:1(15Z)/0:0) |
| 3556 | HMDB0055994 | NA |
| 3557 | HMDB0007822 | DG(24:1(15Z)/15:0/0:0) |
| 3558 | HMDB0165986 | NA |
| 3559 | HMDB0165987 | NA |
| 3560 | HMDB0166012 | NA |
| 3561 | HMDB0166013 | NA |
| 3562 | HMDB0166011 | NA |
| 3563 | HMDB0166007 | NA |
| 3564 | HMDB0170721 | NA |
| 3565 | HMDB0166009 | NA |
| 3566 | HMDB0166010 | NA |
| 3567 | HMDB0166004 | NA |
| 3568 | HMDB0166005 | NA |
| 3569 | HMDB0166003 | NA |
| 3570 | HMDB0166006 | NA |
| 3571 | HMDB0167988 | NA |
| 3572 | HMDB0167989 | NA |
| 3573 | HMDB0168064 | NA |
| 3574 | HMDB0170719 | NA |
| 3575 | HMDB0170718 | NA |
| 3576 | HMDB0168079 | NA |
| 3577 | HMDB0168080 | NA |
| 3578 | HMDB0168077 | NA |
| 3579 | HMDB0168076 | NA |
| 3580 | HMDB0168068 | NA |
| 3581 | HMDB0168067 | NA |
| 3582 | HMDB0168065 | NA |
| 3583 | HMDB0166001 | NA |
| 3584 | HMDB0166002 | NA |
| 3585 | HMDB0170734 | NA |
| 3586 | HMDB0165975 | NA |
| 3587 | HMDB0165973 | NA |
| 3588 | HMDB0165879 | NA |
| 3589 | HMDB0165880 | NA |
| 3590 | HMDB0170735 | NA |
| 3591 | HMDB0170737 | NA |
| 3592 | HMDB0166008 | NA |
| 3593 | HMDB0165977 | NA |
| 3594 | HMDB0165978 | NA |
| 3595 | HMDB0165999 | NA |
| 3596 | HMDB0165985 | NA |
| 3597 | HMDB0165984 | NA |
| 3598 | HMDB0165976 | NA |
| 3599 | HMDB0165983 | NA |
| 3600 | HMDB0165980 | NA |
| 3601 | HMDB0165981 | NA |
| 3602 | HMDB0165982 | NA |
| 3603 | HMDB0165979 | NA |
| 3604 | HMDB0177535 | NA |
| 3605 | HMDB0177543 | NA |
| 3606 | HMDB0177537 | NA |
| 3607 | HMDB0177545 | NA |
| 3608 | HMDB0177544 | NA |
| 3609 | HMDB0177546 | NA |
| 3610 | HMDB0177536 | NA |
| 3611 | HMDB0166014 | NA |
| 3612 | HMDB0165988 | NA |
| 3613 | HMDB0184229 | NA |
| 3614 | HMDB0186286 | NA |
| 3615 | HMDB0033242 | Glycylserylprolylmethionylphenylalanylvalinamide |
| 3616 | HMDB0143644 | NA |
| 3617 | HMDB0041431 | NA |
| 3618 | HMDB0175656 | NA |
| 3619 | HMDB0175651 | NA |
| 3620 | HMDB0175661 | NA |
| 3621 | HMDB0175662 | NA |
| 3622 | HMDB0175652 | NA |
| 3623 | HMDB0175657 | NA |
| 3624 | HMDB0186380 | NA |
| 3625 | HMDB0186379 | NA |
| 3626 | HMDB0186374 | NA |

| | | |
|------|-------------|--|
| 3627 | HMDB0186377 | NA |
| 3628 | HMDB0186373 | NA |
| 3629 | HMDB0186376 | NA |
| 3630 | HMDB0168025 | NA |
| 3631 | HMDB0168023 | NA |
| 3632 | HMDB0165935 | NA |
| 3633 | HMDB0168024 | NA |
| 3634 | HMDB0168022 | NA |
| 3635 | HMDB0168019 | NA |
| 3636 | HMDB0168021 | NA |
| 3637 | HMDB0168018 | NA |
| 3638 | HMDB0168020 | NA |
| 3639 | HMDB0168017 | NA |
| 3640 | HMDB0168016 | NA |
| 3641 | HMDB0168015 | NA |
| 3642 | HMDB0168014 | NA |
| 3643 | HMDB0168012 | NA |
| 3644 | HMDB0168026 | NA |
| 3645 | HMDB0168027 | NA |
| 3646 | HMDB0168033 | NA |
| 3647 | HMDB0168045 | NA |
| 3648 | HMDB0168044 | NA |
| 3649 | HMDB0168042 | NA |
| 3650 | HMDB0168043 | NA |
| 3651 | HMDB0168041 | NA |
| 3652 | HMDB0168040 | NA |
| 3653 | HMDB0168039 | NA |
| 3654 | HMDB0168038 | NA |
| 3655 | HMDB0168037 | NA |
| 3656 | HMDB0168035 | NA |
| 3657 | HMDB0168036 | NA |
| 3658 | HMDB0168034 | NA |
| 3659 | HMDB0168032 | NA |
| 3660 | HMDB0168030 | NA |
| 3661 | HMDB0165933 | NA |
| 3662 | HMDB0165934 | NA |
| 3663 | HMDB0165912 | NA |
| 3664 | HMDB0165911 | NA |
| 3665 | HMDB0165913 | NA |
| 3666 | HMDB0165914 | NA |
| 3667 | HMDB0165910 | NA |
| 3668 | HMDB0165909 | NA |
| 3669 | HMDB0165907 | NA |
| 3670 | HMDB0165904 | NA |
| 3671 | HMDB0165906 | NA |
| 3672 | HMDB0165908 | NA |
| 3673 | HMDB0165917 | NA |
| 3674 | HMDB0165916 | NA |
| 3675 | HMDB0165915 | NA |
| 3676 | HMDB0165932 | NA |
| 3677 | HMDB0165931 | NA |
| 3678 | HMDB0165928 | NA |
| 3679 | HMDB0165930 | NA |
| 3680 | HMDB0165929 | NA |
| 3681 | HMDB0165927 | NA |
| 3682 | HMDB0165924 | NA |
| 3683 | HMDB0165926 | NA |
| 3684 | HMDB0165925 | NA |
| 3685 | HMDB0165922 | NA |
| 3686 | HMDB0164570 | NA |
| 3687 | HMDB0161716 | NA |
| 3688 | HMDB0161714 | NA |
| 3689 | HMDB0161713 | NA |
| 3690 | HMDB0161715 | NA |
| 3691 | HMDB0161718 | NA |
| 3692 | HMDB0161746 | NA |
| 3693 | HMDB0161717 | NA |
| 3694 | HMDB0184567 | NA |
| 3695 | HMDB0184569 | NA |
| 3696 | HMDB0184661 | NA |
| 3697 | HMDB0184244 | NA |
| 3698 | HMDB0184594 | NA |
| 3699 | HMDB0184660 | NA |
| 3700 | HMDB0166018 | NA |
| 3701 | HMDB0165992 | NA |
| 3702 | HMDB0002429 | (3a,5b)-24-oxo-24-[(2-sulfoethyl)amino]cholan-3-yl-b-D-Glucopyranosiduronic acid |
| 3703 | HMDB0161194 | NA |
| 3704 | HMDB0036288 | NA |
| 3705 | HMDB0036660 | NA |
| 3706 | HMDB0156311 | NA |
| 3707 | HMDB0156310 | NA |
| 3708 | HMDB0127537 | NA |
| 3709 | HMDB0127536 | NA |
| 3710 | HMDB0127543 | NA |
| 3711 | HMDB0127542 | NA |
| 3712 | HMDB0127544 | NA |
| 3713 | HMDB0002318 | Capsianoside I |

| | | |
|------|-------------|------------------------|
| 3714 | HMDB0015392 | Posaconazole |
| 3715 | HMDB0174236 | NA |
| 3716 | HMDB0174233 | NA |
| 3717 | HMDB0174234 | NA |
| 3718 | HMDB0174235 | NA |
| 3719 | HMDB0001261 | Coproporphyrinogen III |
| 3720 | HMDB0002158 | Coproporphyrinogen I |
| 3721 | HMDB0037590 | NA |
| 3722 | HMDB0036527 | NA |
| 3723 | HMDB0039365 | NA |
| 3724 | HMDB0036529 | NA |
| 3725 | HMDB0036528 | NA |
| 3726 | HMDB0061667 | NA |
| 3727 | HMDB0061671 | NA |
| 3728 | HMDB0112234 | NA |
| 3729 | HMDB0112220 | NA |
| 3730 | HMDB0177552 | NA |
| 3731 | HMDB0177551 | NA |
| 3732 | HMDB0177553 | NA |
| 3733 | HMDB0177554 | NA |
| 3734 | HMDB0040155 | NA |
| 3735 | HMDB0039887 | NA |
| 3736 | HMDB0166973 | NA |
| 3737 | HMDB0099701 | NA |
| 3738 | HMDB0100257 | NA |
| 3739 | HMDB0100256 | NA |
| 3740 | HMDB0100259 | NA |
| 3741 | HMDB0100936 | NA |
| 3742 | HMDB0100935 | NA |
| 3743 | HMDB0100937 | NA |
| 3744 | HMDB0100938 | NA |
| 3745 | HMDB0100939 | NA |
| 3746 | HMDB0100940 | NA |
| 3747 | HMDB0101013 | NA |
| 3748 | HMDB0101011 | NA |
| 3749 | HMDB0101012 | NA |
| 3750 | HMDB0101010 | NA |
| 3751 | HMDB0101014 | NA |
| 3752 | HMDB0101015 | NA |
| 3753 | HMDB0101107 | NA |
| 3754 | HMDB0100258 | NA |
| 3755 | HMDB0071838 | NA |
| 3756 | HMDB0099980 | NA |
| 3757 | HMDB0099703 | NA |
| 3758 | HMDB0099702 | NA |
| 3759 | HMDB0099704 | NA |
| 3760 | HMDB0099707 | NA |
| 3761 | HMDB0099705 | NA |
| 3762 | HMDB0099706 | NA |
| 3763 | HMDB0099710 | NA |
| 3764 | HMDB0099711 | NA |
| 3765 | HMDB0099708 | NA |
| 3766 | HMDB0099709 | NA |
| 3767 | HMDB0099712 | NA |
| 3768 | HMDB0099975 | NA |
| 3769 | HMDB0099976 | NA |
| 3770 | HMDB0099978 | NA |
| 3771 | HMDB0099977 | NA |
| 3772 | HMDB0099979 | NA |
| 3773 | HMDB0101106 | NA |
| 3774 | HMDB0101108 | NA |
| 3775 | HMDB0101293 | NA |
| 3776 | HMDB0101290 | NA |
| 3777 | HMDB0101292 | NA |
| 3778 | HMDB0101291 | NA |
| 3779 | HMDB0101294 | NA |
| 3780 | HMDB0101297 | NA |
| 3781 | HMDB0101295 | NA |
| 3782 | HMDB0101296 | NA |
| 3783 | HMDB0101298 | NA |
| 3784 | HMDB0101300 | NA |
| 3785 | HMDB0101301 | NA |
| 3786 | HMDB0101299 | NA |
| 3787 | HMDB0101302 | NA |
| 3788 | HMDB0101304 | NA |
| 3789 | HMDB0101303 | NA |
| 3790 | HMDB0101305 | NA |
| 3791 | HMDB0101289 | NA |
| 3792 | HMDB0101288 | NA |
| 3793 | HMDB0101287 | NA |
| 3794 | HMDB0101110 | NA |
| 3795 | HMDB0101109 | NA |
| 3796 | HMDB0101111 | NA |
| 3797 | HMDB0101114 | NA |
| 3798 | HMDB0101112 | NA |
| 3799 | HMDB0101113 | NA |
| 3800 | HMDB0101115 | NA |

| | | |
|------|-------------|----|
| 3801 | HMDB0101116 | NA |
| 3802 | HMDB0101117 | NA |
| 3803 | HMDB0101281 | NA |
| 3804 | HMDB0101280 | NA |
| 3805 | HMDB0101282 | NA |
| 3806 | HMDB0101285 | NA |
| 3807 | HMDB0101284 | NA |
| 3808 | HMDB0101283 | NA |
| 3809 | HMDB0101286 | NA |
| 3810 | HMDB0101306 | NA |
| 3811 | HMDB0097388 | NA |
| 3812 | HMDB0097627 | NA |
| 3813 | HMDB0097628 | NA |
| 3814 | HMDB0098047 | NA |
| 3815 | HMDB0098046 | NA |
| 3816 | HMDB0098051 | NA |
| 3817 | HMDB0098048 | NA |
| 3818 | HMDB0098050 | NA |
| 3819 | HMDB0098049 | NA |
| 3820 | HMDB0098388 | NA |
| 3821 | HMDB0098391 | NA |
| 3822 | HMDB0098389 | NA |
| 3823 | HMDB0098390 | NA |
| 3824 | HMDB0098392 | NA |
| 3825 | HMDB0098393 | NA |
| 3826 | HMDB0099211 | NA |
| 3827 | HMDB0099209 | NA |
| 3828 | HMDB0097626 | NA |
| 3829 | HMDB0097624 | NA |
| 3830 | HMDB0097625 | NA |
| 3831 | HMDB0097389 | NA |
| 3832 | HMDB0097390 | NA |
| 3833 | HMDB0097391 | NA |
| 3834 | HMDB0097392 | NA |
| 3835 | HMDB0097395 | NA |
| 3836 | HMDB0097394 | NA |
| 3837 | HMDB0097393 | NA |
| 3838 | HMDB0097396 | NA |
| 3839 | HMDB0097397 | NA |
| 3840 | HMDB0097619 | NA |
| 3841 | HMDB0097617 | NA |
| 3842 | HMDB0097618 | NA |
| 3843 | HMDB0097620 | NA |
| 3844 | HMDB0097621 | NA |
| 3845 | HMDB0097622 | NA |
| 3846 | HMDB0097623 | NA |
| 3847 | HMDB0099210 | NA |
| 3848 | HMDB0099212 | NA |
| 3849 | HMDB0099454 | NA |
| 3850 | HMDB0099455 | NA |
| 3851 | HMDB0099456 | NA |
| 3852 | HMDB0099457 | NA |
| 3853 | HMDB0099459 | NA |
| 3854 | HMDB0099458 | NA |
| 3855 | HMDB0099463 | NA |
| 3856 | HMDB0099460 | NA |
| 3857 | HMDB0099461 | NA |
| 3858 | HMDB0099462 | NA |
| 3859 | HMDB0099464 | NA |
| 3860 | HMDB0099599 | NA |
| 3861 | HMDB0099600 | NA |
| 3862 | HMDB0099602 | NA |
| 3863 | HMDB0099603 | NA |
| 3864 | HMDB0099601 | NA |
| 3865 | HMDB0099453 | NA |
| 3866 | HMDB0099337 | NA |
| 3867 | HMDB0099338 | NA |
| 3868 | HMDB0099259 | NA |
| 3869 | HMDB0099261 | NA |
| 3870 | HMDB0099260 | NA |
| 3871 | HMDB0099263 | NA |
| 3872 | HMDB0099262 | NA |
| 3873 | HMDB0099264 | NA |
| 3874 | HMDB0099327 | NA |
| 3875 | HMDB0099328 | NA |
| 3876 | HMDB0099329 | NA |
| 3877 | HMDB0099331 | NA |
| 3878 | HMDB0099330 | NA |
| 3879 | HMDB0099332 | NA |
| 3880 | HMDB0099333 | NA |
| 3881 | HMDB0099335 | NA |
| 3882 | HMDB0099334 | NA |
| 3883 | HMDB0099336 | NA |
| 3884 | HMDB0099604 | NA |
| 3885 | HMDB0105231 | NA |
| 3886 | HMDB0105396 | NA |
| 3887 | HMDB0105395 | NA |

| | | |
|------|-------------|----|
| 3888 | HMDB0105830 | NA |
| 3889 | HMDB0105832 | NA |
| 3890 | HMDB0105831 | NA |
| 3891 | HMDB0105834 | NA |
| 3892 | HMDB0105833 | NA |
| 3893 | HMDB0105835 | NA |
| 3894 | HMDB0106274 | NA |
| 3895 | HMDB0106275 | NA |
| 3896 | HMDB0106276 | NA |
| 3897 | HMDB0106278 | NA |
| 3898 | HMDB0106277 | NA |
| 3899 | HMDB0106279 | NA |
| 3900 | HMDB0107824 | NA |
| 3901 | HMDB0107825 | NA |
| 3902 | HMDB0105397 | NA |
| 3903 | HMDB0105393 | NA |
| 3904 | HMDB0105394 | NA |
| 3905 | HMDB0105232 | NA |
| 3906 | HMDB0105233 | NA |
| 3907 | HMDB0105235 | NA |
| 3908 | HMDB0105306 | NA |
| 3909 | HMDB0105305 | NA |
| 3910 | HMDB0105309 | NA |
| 3911 | HMDB0105308 | NA |
| 3912 | HMDB0105307 | NA |
| 3913 | HMDB0105310 | NA |
| 3914 | HMDB0105386 | NA |
| 3915 | HMDB0105387 | NA |
| 3916 | HMDB0105390 | NA |
| 3917 | HMDB0105389 | NA |
| 3918 | HMDB0105388 | NA |
| 3919 | HMDB0105391 | NA |
| 3920 | HMDB0105392 | NA |
| 3921 | HMDB0107826 | NA |
| 3922 | HMDB0107827 | NA |
| 3923 | HMDB0108348 | NA |
| 3924 | HMDB0109549 | NA |
| 3925 | HMDB0109550 | NA |
| 3926 | HMDB0109551 | NA |
| 3927 | HMDB0109552 | NA |
| 3928 | HMDB0109602 | NA |
| 3929 | HMDB0109599 | NA |
| 3930 | HMDB0109601 | NA |
| 3931 | HMDB0109600 | NA |
| 3932 | HMDB0109659 | NA |
| 3933 | HMDB0109662 | NA |
| 3934 | HMDB0109660 | NA |
| 3935 | HMDB0109661 | NA |
| 3936 | HMDB0109955 | NA |
| 3937 | HMDB0109956 | NA |
| 3938 | HMDB0109958 | NA |
| 3939 | HMDB0108347 | NA |
| 3940 | HMDB0108346 | NA |
| 3941 | HMDB0108349 | NA |
| 3942 | HMDB0107829 | NA |
| 3943 | HMDB0107828 | NA |
| 3944 | HMDB0107874 | NA |
| 3945 | HMDB0107876 | NA |
| 3946 | HMDB0107878 | NA |
| 3947 | HMDB0107875 | NA |
| 3948 | HMDB0107877 | NA |
| 3949 | HMDB0107879 | NA |
| 3950 | HMDB0108054 | NA |
| 3951 | HMDB0108052 | NA |
| 3952 | HMDB0108053 | NA |
| 3953 | HMDB0108055 | NA |
| 3954 | HMDB0108057 | NA |
| 3955 | HMDB0108056 | NA |
| 3956 | HMDB0108344 | NA |
| 3957 | HMDB0108345 | NA |
| 3958 | HMDB0109957 | NA |
| 3959 | HMDB0101527 | NA |
| 3960 | HMDB0102355 | NA |
| 3961 | HMDB0102357 | NA |
| 3962 | HMDB0102356 | NA |
| 3963 | HMDB0102358 | NA |
| 3964 | HMDB0103501 | NA |
| 3965 | HMDB0103500 | NA |
| 3966 | HMDB0103504 | NA |
| 3967 | HMDB0103502 | NA |
| 3968 | HMDB0103503 | NA |
| 3969 | HMDB0103505 | NA |
| 3970 | HMDB0103550 | NA |
| 3971 | HMDB0103551 | NA |
| 3972 | HMDB0103552 | NA |
| 3973 | HMDB0103553 | NA |
| 3974 | HMDB0103554 | NA |

| | | |
|------|-------------|----|
| 3975 | HMDB0103555 | NA |
| 3976 | HMDB0102354 | NA |
| 3977 | HMDB0102353 | NA |
| 3978 | HMDB0101932 | NA |
| 3979 | HMDB0101526 | NA |
| 3980 | HMDB0101528 | NA |
| 3981 | HMDB0101529 | NA |
| 3982 | HMDB0101530 | NA |
| 3983 | HMDB0101531 | NA |
| 3984 | HMDB0101534 | NA |
| 3985 | HMDB0101533 | NA |
| 3986 | HMDB0101532 | NA |
| 3987 | HMDB0101536 | NA |
| 3988 | HMDB0101535 | NA |
| 3989 | HMDB0101537 | NA |
| 3990 | HMDB0101930 | NA |
| 3991 | HMDB0101929 | NA |
| 3992 | HMDB0101928 | NA |
| 3993 | HMDB0101933 | NA |
| 3994 | HMDB0101931 | NA |
| 3995 | HMDB0103608 | NA |
| 3996 | HMDB0103612 | NA |
| 3997 | HMDB0103732 | NA |
| 3998 | HMDB0103734 | NA |
| 3999 | HMDB0103735 | NA |
| 4000 | HMDB0104014 | NA |
| 4001 | HMDB0104015 | NA |
| 4002 | HMDB0104016 | NA |
| 4003 | HMDB0104018 | NA |
| 4004 | HMDB0104017 | NA |
| 4005 | HMDB0104019 | NA |
| 4006 | HMDB0104275 | NA |
| 4007 | HMDB0104278 | NA |
| 4008 | HMDB0104276 | NA |
| 4009 | HMDB0104277 | NA |
| 4010 | HMDB0104279 | NA |
| 4011 | HMDB0104280 | NA |
| 4012 | HMDB0105230 | NA |
| 4013 | HMDB0103733 | NA |
| 4014 | HMDB0103731 | NA |
| 4015 | HMDB0103730 | NA |
| 4016 | HMDB0103609 | NA |
| 4017 | HMDB0103610 | NA |
| 4018 | HMDB0103611 | NA |
| 4019 | HMDB0103613 | NA |
| 4020 | HMDB0103616 | NA |
| 4021 | HMDB0103615 | NA |
| 4022 | HMDB0103614 | NA |
| 4023 | HMDB0103617 | NA |
| 4024 | HMDB0103618 | NA |
| 4025 | HMDB0103619 | NA |
| 4026 | HMDB0103724 | NA |
| 4027 | HMDB0103725 | NA |
| 4028 | HMDB0103727 | NA |
| 4029 | HMDB0103726 | NA |
| 4030 | HMDB0103728 | NA |
| 4031 | HMDB0103729 | NA |
| 4032 | HMDB0105234 | NA |
| 4033 | HMDB0071940 | NA |
| 4034 | HMDB0072157 | NA |
| 4035 | HMDB0072188 | NA |
| 4036 | HMDB0072197 | NA |
| 4037 | HMDB0072209 | NA |
| 4038 | HMDB0072238 | NA |
| 4039 | HMDB0072246 | NA |
| 4040 | HMDB0072249 | NA |
| 4041 | HMDB0072265 | NA |
| 4042 | HMDB0072286 | NA |
| 4043 | HMDB0072287 | NA |
| 4044 | HMDB0072293 | NA |
| 4045 | HMDB0072316 | NA |
| 4046 | HMDB0072320 | NA |
| 4047 | HMDB0072336 | NA |
| 4048 | HMDB0072364 | NA |
| 4049 | HMDB0072368 | NA |
| 4050 | HMDB0072153 | NA |
| 4051 | HMDB0072143 | NA |
| 4052 | HMDB0071965 | NA |
| 4053 | HMDB0071966 | NA |
| 4054 | HMDB0071983 | NA |
| 4055 | HMDB0071989 | NA |
| 4056 | HMDB0071990 | NA |
| 4057 | HMDB0071997 | NA |
| 4058 | HMDB0072012 | NA |
| 4059 | HMDB0072022 | NA |
| 4060 | HMDB0072035 | NA |
| 4061 | HMDB0072064 | NA |

| | | |
|------|-------------|----|
| 4062 | HMDB0072076 | NA |
| 4063 | HMDB0072090 | NA |
| 4064 | HMDB0072117 | NA |
| 4065 | HMDB0072124 | NA |
| 4066 | HMDB0072141 | NA |
| 4067 | HMDB0072142 | NA |
| 4068 | HMDB0072385 | NA |
| 4069 | HMDB0072408 | NA |
| 4070 | HMDB0072718 | NA |
| 4071 | HMDB0072747 | NA |
| 4072 | HMDB0072804 | NA |
| 4073 | HMDB0072825 | NA |
| 4074 | HMDB0072832 | NA |
| 4075 | HMDB0094865 | NA |
| 4076 | HMDB0094866 | NA |
| 4077 | HMDB0094870 | NA |
| 4078 | HMDB0094867 | NA |
| 4079 | HMDB0094868 | NA |
| 4080 | HMDB0094869 | NA |
| 4081 | HMDB0094918 | NA |
| 4082 | HMDB0094917 | NA |
| 4083 | HMDB0094919 | NA |
| 4084 | HMDB0094988 | NA |
| 4085 | HMDB0094992 | NA |
| 4086 | HMDB0072644 | NA |
| 4087 | HMDB0072642 | NA |
| 4088 | HMDB0072410 | NA |
| 4089 | HMDB0072422 | NA |
| 4090 | HMDB0072438 | NA |
| 4091 | HMDB0072442 | NA |
| 4092 | HMDB0072451 | NA |
| 4093 | HMDB0072470 | NA |
| 4094 | HMDB0072496 | NA |
| 4095 | HMDB0072501 | NA |
| 4096 | HMDB0072532 | NA |
| 4097 | HMDB0072534 | NA |
| 4098 | HMDB0072536 | NA |
| 4099 | HMDB0072549 | NA |
| 4100 | HMDB0072563 | NA |
| 4101 | HMDB0072597 | NA |
| 4102 | HMDB0072609 | NA |
| 4103 | HMDB0072607 | NA |
| 4104 | HMDB0094990 | NA |
| 4105 | HMDB0094920 | NA |
| 4106 | HMDB0065069 | NA |
| 4107 | HMDB0065114 | NA |
| 4108 | HMDB0065342 | NA |
| 4109 | HMDB0065682 | NA |
| 4110 | HMDB0065826 | NA |
| 4111 | HMDB0065952 | NA |
| 4112 | HMDB0065955 | NA |
| 4113 | HMDB0066219 | NA |
| 4114 | HMDB0066300 | NA |
| 4115 | HMDB0069739 | NA |
| 4116 | HMDB0071120 | NA |
| 4117 | HMDB0071134 | NA |
| 4118 | HMDB0071167 | NA |
| 4119 | HMDB0071170 | NA |
| 4120 | HMDB0071171 | NA |
| 4121 | HMDB0071183 | NA |
| 4122 | HMDB0065009 | NA |
| 4123 | HMDB0064992 | NA |
| 4124 | HMDB0062962 | NA |
| 4125 | HMDB0063275 | NA |
| 4126 | HMDB0063341 | NA |
| 4127 | HMDB0063426 | NA |
| 4128 | HMDB0063610 | NA |
| 4129 | HMDB0063687 | NA |
| 4130 | HMDB0064065 | NA |
| 4131 | HMDB0064153 | NA |
| 4132 | HMDB0064175 | NA |
| 4133 | HMDB0064236 | NA |
| 4134 | HMDB0064416 | NA |
| 4135 | HMDB0064499 | NA |
| 4136 | HMDB0064579 | NA |
| 4137 | HMDB0064593 | NA |
| 4138 | HMDB0064788 | NA |
| 4139 | HMDB0064975 | NA |
| 4140 | HMDB0071229 | NA |
| 4141 | HMDB0071265 | NA |
| 4142 | HMDB0071627 | NA |
| 4143 | HMDB0071675 | NA |
| 4144 | HMDB0071692 | NA |
| 4145 | HMDB0071701 | NA |
| 4146 | HMDB0071717 | NA |
| 4147 | HMDB0071721 | NA |
| 4148 | HMDB0071749 | NA |

| | | |
|------|-------------|----|
| 4149 | HMDB0071787 | NA |
| 4150 | HMDB0071811 | NA |
| 4151 | HMDB0071862 | NA |
| 4152 | HMDB0071865 | NA |
| 4153 | HMDB0071863 | NA |
| 4154 | HMDB0071878 | NA |
| 4155 | HMDB0071881 | NA |
| 4156 | HMDB0071912 | NA |
| 4157 | HMDB0071920 | NA |
| 4158 | HMDB0071620 | NA |
| 4159 | HMDB0071549 | NA |
| 4160 | HMDB0071266 | NA |
| 4161 | HMDB0071267 | NA |
| 4162 | HMDB0071289 | NA |
| 4163 | HMDB0071349 | NA |
| 4164 | HMDB0071348 | NA |
| 4165 | HMDB0071394 | NA |
| 4166 | HMDB0071405 | NA |
| 4167 | HMDB0071435 | NA |
| 4168 | HMDB0071446 | NA |
| 4169 | HMDB0071468 | NA |
| 4170 | HMDB0071478 | NA |
| 4171 | HMDB0071486 | NA |
| 4172 | HMDB0071495 | NA |
| 4173 | HMDB0071504 | NA |
| 4174 | HMDB0071528 | NA |
| 4175 | HMDB0071539 | NA |
| 4176 | HMDB0071924 | NA |
| 4177 | HMDB0096157 | NA |
| 4178 | HMDB0096818 | NA |
| 4179 | HMDB0096819 | NA |
| 4180 | HMDB0096816 | NA |
| 4181 | HMDB0096820 | NA |
| 4182 | HMDB0096821 | NA |
| 4183 | HMDB0096822 | NA |
| 4184 | HMDB0096981 | NA |
| 4185 | HMDB0096982 | NA |
| 4186 | HMDB0096983 | NA |
| 4187 | HMDB0096987 | NA |
| 4188 | HMDB0096985 | NA |
| 4189 | HMDB0096984 | NA |
| 4190 | HMDB0096986 | NA |
| 4191 | HMDB0096991 | NA |
| 4192 | HMDB0096990 | NA |
| 4193 | HMDB0096988 | NA |
| 4194 | HMDB0096817 | NA |
| 4195 | HMDB0096814 | NA |
| 4196 | HMDB0096623 | NA |
| 4197 | HMDB0096622 | NA |
| 4198 | HMDB0096624 | NA |
| 4199 | HMDB0096625 | NA |
| 4200 | HMDB0096627 | NA |
| 4201 | HMDB0096626 | NA |
| 4202 | HMDB0096703 | NA |
| 4203 | HMDB0096700 | NA |
| 4204 | HMDB0096701 | NA |
| 4205 | HMDB0096702 | NA |
| 4206 | HMDB0096705 | NA |
| 4207 | HMDB0096704 | NA |
| 4208 | HMDB0096811 | NA |
| 4209 | HMDB0096813 | NA |
| 4210 | HMDB0096812 | NA |
| 4211 | HMDB0096815 | NA |
| 4212 | HMDB0096989 | NA |
| 4213 | HMDB0096992 | NA |
| 4214 | HMDB0097208 | NA |
| 4215 | HMDB0097210 | NA |
| 4216 | HMDB0097209 | NA |
| 4217 | HMDB0097212 | NA |
| 4218 | HMDB0097213 | NA |
| 4219 | HMDB0097215 | NA |
| 4220 | HMDB0097214 | NA |
| 4221 | HMDB0097216 | NA |
| 4222 | HMDB0097217 | NA |
| 4223 | HMDB0097380 | NA |
| 4224 | HMDB0097382 | NA |
| 4225 | HMDB0097383 | NA |
| 4226 | HMDB0097381 | NA |
| 4227 | HMDB0097384 | NA |
| 4228 | HMDB0097386 | NA |
| 4229 | HMDB0097387 | NA |
| 4230 | HMDB0097211 | NA |
| 4231 | HMDB0097207 | NA |
| 4232 | HMDB0096995 | NA |
| 4233 | HMDB0096993 | NA |
| 4234 | HMDB0096994 | NA |
| 4235 | HMDB0096996 | NA |

| | | |
|------|-------------|----|
| 4236 | HMDB0096997 | NA |
| 4237 | HMDB0096999 | NA |
| 4238 | HMDB0096998 | NA |
| 4239 | HMDB0097000 | NA |
| 4240 | HMDB0097002 | NA |
| 4241 | HMDB0097003 | NA |
| 4242 | HMDB0097001 | NA |
| 4243 | HMDB0097004 | NA |
| 4244 | HMDB0097007 | NA |
| 4245 | HMDB0097005 | NA |
| 4246 | HMDB0097006 | NA |
| 4247 | HMDB0097206 | NA |
| 4248 | HMDB0097385 | NA |
| 4249 | HMDB0096156 | NA |
| 4250 | HMDB0094991 | NA |
| 4251 | HMDB0095128 | NA |
| 4252 | HMDB0095129 | NA |
| 4253 | HMDB0095258 | NA |
| 4254 | HMDB0095260 | NA |
| 4255 | HMDB0095259 | NA |
| 4256 | HMDB0095264 | NA |
| 4257 | HMDB0095261 | NA |
| 4258 | HMDB0095262 | NA |
| 4259 | HMDB0095263 | NA |
| 4260 | HMDB0095268 | NA |
| 4261 | HMDB0095265 | NA |
| 4262 | HMDB0095266 | NA |
| 4263 | HMDB0095267 | NA |
| 4264 | HMDB0095269 | NA |
| 4265 | HMDB0095379 | NA |
| 4266 | HMDB0095124 | NA |
| 4267 | HMDB0095126 | NA |
| 4268 | HMDB0095127 | NA |
| 4269 | HMDB0094989 | NA |
| 4270 | HMDB0094993 | NA |
| 4271 | HMDB0094994 | NA |
| 4272 | HMDB0094995 | NA |
| 4273 | HMDB0094996 | NA |
| 4274 | HMDB0094997 | NA |
| 4275 | HMDB0094999 | NA |
| 4276 | HMDB0094998 | NA |
| 4277 | HMDB0095119 | NA |
| 4278 | HMDB0095118 | NA |
| 4279 | HMDB0095122 | NA |
| 4280 | HMDB0095121 | NA |
| 4281 | HMDB0095123 | NA |
| 4282 | HMDB0095120 | NA |
| 4283 | HMDB0095125 | NA |
| 4284 | HMDB0095378 | NA |
| 4285 | HMDB0095380 | NA |
| 4286 | HMDB0096155 | NA |
| 4287 | HMDB0095538 | NA |
| 4288 | HMDB0095539 | NA |
| 4289 | HMDB0095644 | NA |
| 4290 | HMDB0095645 | NA |
| 4291 | HMDB0095649 | NA |
| 4292 | HMDB0095648 | NA |
| 4293 | HMDB0095647 | NA |
| 4294 | HMDB0095646 | NA |
| 4295 | HMDB0095928 | NA |
| 4296 | HMDB0095926 | NA |
| 4297 | HMDB0095925 | NA |
| 4298 | HMDB0095927 | NA |
| 4299 | HMDB0096153 | NA |
| 4300 | HMDB0096154 | NA |
| 4301 | HMDB0096158 | NA |
| 4302 | HMDB0095537 | NA |
| 4303 | HMDB0095536 | NA |
| 4304 | HMDB0095534 | NA |
| 4305 | HMDB0095382 | NA |
| 4306 | HMDB0095384 | NA |
| 4307 | HMDB0095381 | NA |
| 4308 | HMDB0095383 | NA |
| 4309 | HMDB0095385 | NA |
| 4310 | HMDB0095386 | NA |
| 4311 | HMDB0095387 | NA |
| 4312 | HMDB0095388 | NA |
| 4313 | HMDB0095389 | NA |
| 4314 | HMDB0095535 | NA |
| 4315 | HMDB0095531 | NA |
| 4316 | HMDB0095532 | NA |
| 4317 | HMDB0095533 | NA |
| 4318 | HMDB0095530 | NA |
| 4319 | HMDB0095529 | NA |
| 4320 | HMDB0095528 | NA |
| 4321 | HMDB0182265 | NA |
| 4322 | HMDB0182264 | NA |

| | | |
|------|-------------|--|
| 4323 | HMDB0182266 | NA |
| 4324 | HMDB0164217 | NA |
| 4325 | HMDB0164215 | NA |
| 4326 | HMDB0038059 | NA |
| 4327 | HMDB0000789 | Pentacarboxylporphyrin I |
| 4328 | HMDB0164605 | NA |
| 4329 | HMDB0164603 | NA |
| 4330 | HMDB0164601 | NA |
| 4331 | HMDB0010374 | CE(22:5(4Z,7Z,10Z,13Z,16Z)) |
| 4332 | HMDB0010375 | CE(22:5(7Z,10Z,13Z,16Z,19Z)) |
| 4333 | HMDB0062457 | NA |
| 4334 | HMDB0056323 | NA |
| 4335 | HMDB0056277 | NA |
| 4336 | HMDB0056263 | NA |
| 4337 | HMDB0056257 | NA |
| 4338 | HMDB0056242 | NA |
| 4339 | HMDB0056226 | NA |
| 4340 | HMDB0056108 | NA |
| 4341 | HMDB0056085 | NA |
| 4342 | HMDB0056080 | NA |
| 4343 | HMDB0007355 | DG(18:4(6Z,9Z,12Z,15Z)/24:1(15Z)/0:0) |
| 4344 | HMDB0007635 | DG(22:1(13Z)/20:4(8Z,11Z,14Z,17Z)/0:0) |
| 4345 | HMDB0007661 | DG(22:2(13Z,16Z)/20:3(5Z,8Z,11Z)/0:0) |
| 4346 | HMDB0007662 | DG(22:2(13Z,16Z)/20:3(8Z,11Z,14Z)/0:0) |
| 4347 | HMDB0007688 | DG(22:4(7Z,10Z,13Z,16Z)/20:1(11Z)/0:0) |
| 4348 | HMDB0007716 | DG(22:5(4Z,7Z,10Z,13Z,16Z)/20:0/0:0) |
| 4349 | HMDB0007745 | DG(22:5(7Z,10Z,13Z,16Z,19Z)/20:0/0:0) |
| 4350 | HMDB0007831 | DG(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)/0:0) |
| 4351 | HMDB0007634 | DG(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)/0:0) |
| 4352 | HMDB0007607 | DG(22:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:0) |
| 4353 | HMDB0007381 | DG(20:0/22:5(7Z,10Z,13Z,16Z,19Z)/0:0) |
| 4354 | HMDB0007380 | DG(20:0/22:5(4Z,7Z,10Z,13Z,16Z)/0:0) |
| 4355 | HMDB0007408 | DG(20:1(11Z)/22:4(7Z,10Z,13Z,16Z)/0:0) |
| 4356 | HMDB0007465 | DG(20:3(5Z,8Z,11Z)/22:2(13Z,16Z)/0:0) |
| 4357 | HMDB0007494 | DG(20:3(8Z,11Z,14Z)/22:2(13Z,16Z)/0:0) |
| 4358 | HMDB0007522 | DG(20:4(5Z,8Z,11Z,14Z)/22:1(13Z)/0:0) |
| 4359 | HMDB0007551 | DG(20:4(8Z,11Z,14Z,17Z)/22:1(13Z)/0:0) |
| 4360 | HMDB0007579 | DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:0/0:0) |
| 4361 | HMDB0144337 | NA |
| 4362 | HMDB0144336 | NA |
| 4363 | HMDB0035940 | Mulberrofuran T |
| 4364 | HMDB0006826 | Tetrahydrofolyl-[Glu](n) |
| 4365 | HMDB0012290 | Tetrahydropteroyltri-L-glutamate |
| 4366 | HMDB0165036 | NA |
| 4367 | HMDB0165033 | NA |
| 4368 | HMDB0184675 | NA |
| 4369 | HMDB0127557 | NA |
| 4370 | HMDB0127589 | NA |
| 4371 | HMDB0127593 | NA |
| 4372 | HMDB0127594 | NA |
| 4373 | HMDB0127595 | NA |
| 4374 | HMDB0127608 | NA |
| 4375 | HMDB0127607 | NA |
| 4376 | HMDB0127609 | NA |
| 4377 | HMDB0127556 | NA |
| 4378 | HMDB0127550 | NA |
| 4379 | HMDB0127551 | NA |
| 4380 | HMDB0127549 | NA |
| 4381 | HMDB0127588 | NA |
| 4382 | HMDB0127587 | NA |
| 4383 | HMDB0127583 | NA |
| 4384 | HMDB0127563 | NA |
| 4385 | HMDB0127562 | NA |
| 4386 | HMDB0127564 | NA |
| 4387 | HMDB0127570 | NA |
| 4388 | HMDB0127571 | NA |
| 4389 | HMDB0127569 | NA |
| 4390 | HMDB0127576 | NA |
| 4391 | HMDB0127575 | NA |
| 4392 | HMDB0127577 | NA |
| 4393 | HMDB0127555 | NA |
| 4394 | HMDB0127581 | NA |
| 4395 | HMDB0127582 | NA |
| 4396 | HMDB0031938 | Arachisprenol 10 |
| 4397 | HMDB0030261 | NA |
| 4398 | HMDB0163756 | NA |
| 4399 | HMDB0040745 | NA |
| 4400 | HMDB0164979 | NA |
| 4401 | HMDB0164980 | NA |
| 4402 | HMDB0164978 | NA |
| 4403 | HMDB0164977 | NA |
| 4404 | HMDB0061054 | NA |
| 4405 | HMDB0061057 | NA |
| 4406 | HMDB0012092 | SM(d18:0/22:1(13Z)) |
| 4407 | HMDB0012103 | SM(d18:1/22:0) |
| 4408 | HMDB0061669 | NA |
| 4409 | HMDB0112209 | NA |

| | | |
|------|-------------|---|
| 4410 | HMDB0042752 | NA |
| 4411 | HMDB0043401 | NA |
| 4412 | HMDB0042975 | NA |
| 4413 | HMDB0042982 | NA |
| 4414 | HMDB0043177 | NA |
| 4415 | HMDB0047755 | NA |
| 4416 | HMDB0042542 | NA |
| 4417 | HMDB0042114 | NA |
| 4418 | HMDB0042107 | NA |
| 4419 | HMDB0144075 | NA |
| 4420 | HMDB0182203 | NA |
| 4421 | HMDB0036708 | NA |
| 4422 | HMDB0164984 | NA |
| 4423 | HMDB0164986 | NA |
| 4424 | HMDB0164987 | NA |
| 4425 | HMDB0164985 | NA |
| 4426 | HMDB0055799 | NA |
| 4427 | HMDB0010560 | TG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) |
| 4428 | HMDB0046646 | NA |
| 4429 | HMDB0038431 | NA |
| 4430 | HMDB0047508 | NA |
| 4431 | HMDB0051662 | NA |
| 4432 | HMDB0052140 | NA |
| 4433 | HMDB0051902 | NA |
| 4434 | HMDB0047715 | NA |
| 4435 | HMDB0054410 | NA |
| 4436 | HMDB0004879 | Trihexosylceramide (d18:1/16:0) |
| 4437 | HMDB0051659 | NA |
| 4438 | HMDB0054167 | NA |
| 4439 | HMDB0047434 | NA |
| 4440 | HMDB0054486 | NA |
| 4441 | HMDB0051643 | NA |
| 4442 | HMDB0047682 | NA |
| 4443 | HMDB0047505 | NA |
| 4444 | HMDB0046964 | NA |
| 4445 | HMDB0051851 | NA |
| 4446 | HMDB0047664 | NA |
| 4447 | HMDB0047452 | NA |
| 4448 | HMDB0052106 | NA |
| 4449 | HMDB0047643 | NA |
| 4450 | HMDB0052227 | NA |
| 4451 | HMDB0052101 | NA |
| 4452 | HMDB0052196 | NA |
| 4453 | HMDB0051508 | NA |
| 4454 | HMDB0051995 | NA |
| 4455 | HMDB0053728 | NA |
| 4456 | HMDB0052137 | NA |
| 4457 | HMDB0047429 | NA |
| 4458 | HMDB0051638 | NA |
| 4459 | HMDB0052242 | NA |
| 4460 | HMDB0046946 | NA |
| 4461 | HMDB0047515 | NA |
| 4462 | HMDB0046821 | NA |
| 4463 | HMDB0046773 | NA |
| 4464 | HMDB0046604 | NA |
| 4465 | HMDB0046215 | NA |
| 4466 | HMDB0045865 | NA |
| 4467 | HMDB0050816 | NA |
| 4468 | HMDB0050577 | NA |
| 4469 | HMDB0050431 | NA |
| 4470 | HMDB0047291 | NA |
| 4471 | HMDB0052248 | NA |
| 4472 | HMDB0046778 | NA |
| 4473 | HMDB0051756 | NA |
| 4474 | HMDB0054393 | NA |
| 4475 | HMDB0050721 | NA |
| 4476 | HMDB0050582 | NA |
| 4477 | HMDB0050986 | NA |
| 4478 | HMDB0053352 | NA |
| 4479 | HMDB0053450 | NA |
| 4480 | HMDB0053347 | NA |
| 4481 | HMDB0054407 | NA |
| 4482 | HMDB0051772 | NA |
| 4483 | HMDB0047521 | NA |
| 4484 | HMDB0047544 | NA |
| 4485 | HMDB0054472 | NA |
| 4486 | HMDB0047308 | NA |
| 4487 | HMDB0052256 | NA |
| 4488 | HMDB0054398 | NA |
| 4489 | HMDB0051782 | NA |
| 4490 | HMDB0051867 | NA |
| 4491 | HMDB0052323 | NA |
| 4492 | HMDB0039422 | NA |
| 4493 | HMDB0047520 | NA |
| 4494 | HMDB0052115 | NA |
| 4495 | HMDB0047636 | NA |
| 4496 | HMDB0051989 | NA |

| | | |
|------|-------------|----|
| 4497 | HMDB0047290 | NA |
| 4498 | HMDB0052211 | NA |
| 4499 | HMDB0047619 | NA |
| 4500 | HMDB0047475 | NA |
| 4501 | HMDB0046598 | NA |
| 4502 | HMDB0046939 | NA |
| 4503 | HMDB0051658 | NA |
| 4504 | HMDB0046915 | NA |
| 4505 | HMDB0046772 | NA |
| 4506 | HMDB0047123 | NA |
| 4507 | HMDB0052151 | NA |
| 4508 | HMDB0051523 | NA |
| 4509 | HMDB0051834 | NA |
| 4510 | HMDB0051994 | NA |
| 4511 | HMDB0047504 | NA |
| 4512 | HMDB0054079 | NA |
| 4513 | HMDB0047285 | NA |
| 4514 | HMDB0052136 | NA |
| 4515 | HMDB0051502 | NA |
| 4516 | HMDB0046404 | NA |
| 4517 | HMDB0052009 | NA |
| 4518 | HMDB0051732 | NA |
| 4519 | HMDB0052241 | NA |
| 4520 | HMDB0052100 | NA |
| 4521 | HMDB0054406 | NA |
| 4522 | HMDB0046814 | NA |
| 4523 | HMDB0047538 | NA |
| 4524 | HMDB0046603 | NA |
| 4525 | HMDB0047428 | NA |
| 4526 | HMDB0046059 | NA |
| 4527 | HMDB0045859 | NA |
| 4528 | HMDB0045864 | NA |
| 4529 | HMDB0046189 | NA |
| 4530 | HMDB0045657 | NA |
| 4531 | HMDB0046207 | NA |
| 4532 | HMDB0054392 | NA |
| 4533 | HMDB0051507 | NA |
| 4534 | HMDB0047498 | NA |
| 4535 | HMDB0046796 | NA |
| 4536 | HMDB0052130 | NA |
| 4537 | HMDB0051637 | NA |
| 4538 | HMDB0051231 | NA |
| 4539 | HMDB0050430 | NA |
| 4540 | HMDB0051129 | NA |
| 4541 | HMDB0050576 | NA |
| 4542 | HMDB0050702 | NA |
| 4543 | HMDB0053346 | NA |
| 4544 | HMDB0050425 | NA |
| 4545 | HMDB0046956 | NA |
| 4546 | HMDB0052301 | NA |
| 4547 | HMDB0054541 | NA |
| 4548 | HMDB0046627 | NA |
| 4549 | HMDB0047658 | NA |
| 4550 | HMDB0053823 | NA |
| 4551 | HMDB0047337 | NA |
| 4552 | HMDB0051765 | NA |
| 4553 | HMDB0051652 | NA |
| 4554 | HMDB0054391 | NA |
| 4555 | HMDB0046732 | NA |
| 4556 | HMDB0047300 | NA |
| 4557 | HMDB0046771 | NA |
| 4558 | HMDB0046397 | NA |
| 4559 | HMDB0047496 | NA |
| 4560 | HMDB0052128 | NA |
| 4561 | HMDB0046420 | NA |
| 4562 | HMDB0052157 | NA |
| 4563 | HMDB0046619 | NA |
| 4564 | HMDB0047323 | NA |
| 4565 | HMDB0051636 | NA |
| 4566 | HMDB0046715 | NA |
| 4567 | HMDB0047144 | NA |
| 4568 | HMDB0045650 | NA |
| 4569 | HMDB0047138 | NA |
| 4570 | HMDB0047358 | NA |
| 4571 | HMDB0047565 | NA |
| 4572 | HMDB0046882 | NA |
| 4573 | HMDB0047397 | NA |
| 4574 | HMDB0047444 | NA |
| 4575 | HMDB0052015 | NA |
| 4576 | HMDB0052022 | NA |
| 4577 | HMDB0051650 | NA |
| 4578 | HMDB0047116 | NA |
| 4579 | HMDB0047427 | NA |
| 4580 | HMDB0052099 | NA |
| 4581 | HMDB0046426 | NA |
| 4582 | HMDB0046025 | NA |
| 4583 | HMDB0053345 | NA |

| | | |
|------|-------------|---|
| 4584 | HMDB0050961 | NA |
| 4585 | HMDB0047167 | NA |
| 4586 | HMDB0046565 | NA |
| 4587 | HMDB0046613 | NA |
| 4588 | HMDB0051515 | NA |
| 4589 | HMDB0047351 | NA |
| 4590 | HMDB0047329 | NA |
| 4591 | HMDB0051698 | NA |
| 4592 | HMDB0052142 | NA |
| 4593 | HMDB0050683 | NA |
| 4594 | HMDB0050978 | NA |
| 4595 | HMDB0050575 | NA |
| 4596 | HMDB0052001 | NA |
| 4597 | HMDB0047581 | NA |
| 4598 | HMDB0051748 | NA |
| 4599 | HMDB0046781 | NA |
| 4600 | HMDB0047667 | NA |
| 4601 | HMDB0051660 | NA |
| 4602 | HMDB0052259 | NA |
| 4603 | HMDB0052133 | NA |
| 4604 | HMDB0047501 | NA |
| 4605 | HMDB0051525 | NA |
| 4606 | HMDB0052011 | NA |
| 4607 | HMDB0051783 | NA |
| 4608 | HMDB0051868 | NA |
| 4609 | HMDB0046965 | NA |
| 4610 | HMDB0047684 | NA |
| 4611 | HMDB0052333 | NA |
| 4612 | HMDB0047547 | NA |
| 4613 | HMDB0051655 | NA |
| 4614 | HMDB0052153 | NA |
| 4615 | HMDB0047339 | NA |
| 4616 | HMDB0052138 | NA |
| 4617 | HMDB0054408 | NA |
| 4618 | HMDB0047506 | NA |
| 4619 | HMDB0046629 | NA |
| 4620 | HMDB0054482 | NA |
| 4621 | HMDB0052244 | NA |
| 4622 | HMDB0054403 | NA |
| 4623 | HMDB0002071 | O-2-(acetylamino)-2-deoxy-a-D-Gal-(1->3)-O-[6-deoxy-a-L-Gal-(1->2)]-O-b-D-Gal-(1->3)-O-2-(acetylamino)-2-deoxy-b-D- |
| 4624 | HMDB0015601 | Vapreotide |
| 4625 | HMDB0112241 | NA |

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

5 Selection of Metabolite Set Library

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

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

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

6 Enrichment Analysis

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

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

Enrichment Overview (top 25)

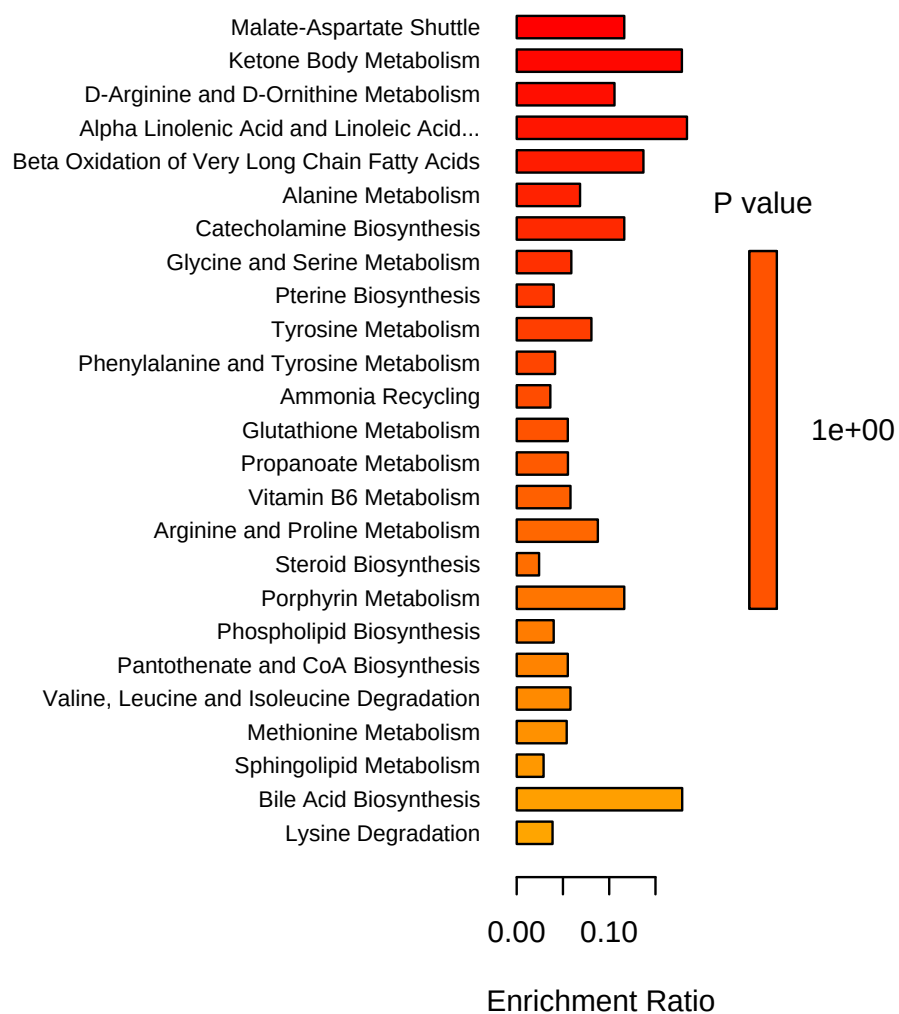


Figure 1: Summary Plot for Over Representation Analysis (ORA)

Table 2: Result from Over Representation Analysis

| | total | expected | hits | Raw p | Holm p | FDR |
|--|-------|----------|------|----------|----------|----------|
| Malate-Aspartate Shuttle | 10 | 8.60 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Ketone Body Metabolism | 13 | 11.20 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| D-Arginine and D-Ornithine Metabolism | 11 | 9.46 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Alpha Linolenic Acid and Linoleic Acid Metabolism | 19 | 16.30 | 3 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Beta Oxidation of Very Long Chain Fatty Acids | 17 | 14.60 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Alanine Metabolism | 17 | 14.60 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Catecholamine Biosynthesis | 20 | 17.20 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Glycine and Serine Metabolism | 59 | 50.80 | 3 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Pterine Biosynthesis | 29 | 25.00 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Tyrosine Metabolism | 72 | 61.90 | 5 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Phenylalanine and Tyrosine Metabolism | 28 | 24.10 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Ammonia Recycling | 32 | 27.50 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Glutathione Metabolism | 21 | 18.10 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Propanoate Metabolism | 42 | 36.10 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Vitamin B6 Metabolism | 20 | 17.20 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Arginine and Proline Metabolism | 53 | 45.60 | 4 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Steroid Biosynthesis | 48 | 41.30 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Porphyrin Metabolism | 40 | 34.40 | 4 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Phospholipid Biosynthesis | 29 | 25.00 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Pantothenate and CoA Biosynthesis | 21 | 18.10 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Valine, Leucine and Isoleucine Degradation | 60 | 51.60 | 3 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Methionine Metabolism | 43 | 37.00 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Sphingolipid Metabolism | 40 | 34.40 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Bile Acid Biosynthesis | 65 | 55.90 | 10 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Lysine Degradation | 30 | 25.80 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Glycerolipid Metabolism | 25 | 21.50 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Pyrimidine Metabolism | 59 | 50.80 | 3 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Nicotinate and Nicotinamide Metabolism | 37 | 31.80 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Purine Metabolism | 74 | 63.70 | 3 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Fatty acid Metabolism | 43 | 37.00 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Folate Metabolism | 29 | 25.00 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Fatty Acid Elongation In Mitochondria | 35 | 30.10 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Citric Acid Cycle | 32 | 27.50 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Starch and Sucrose Metabolism | 31 | 26.70 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Urea Cycle | 29 | 25.00 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Pyruvate Metabolism | 48 | 41.30 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Tryptophan Metabolism | 60 | 51.60 | 9 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Aspartate Metabolism | 35 | 30.10 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Androgen and Estrogen Metabolism | 33 | 28.40 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Glutamate Metabolism | 49 | 42.20 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Retinol Metabolism | 37 | 31.80 | 5 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Arachidonic Acid Metabolism | 69 | 59.40 | 4 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Betaine Metabolism | 21 | 18.10 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Gluconeogenesis | 35 | 30.10 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Steroidogenesis | 43 | 37.00 | 10 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Fatty Acid Biosynthesis | 35 | 30.10 | 7 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Carnitine Synthesis | 22 | 18.90 | 2 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Transfer of Acetyl Groups into Mitochondria | 22 | 18.90 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Mitochondrial Beta-Oxidation of Medium Chain Saturated Fatty Acids | 27 | 23.20 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Warburg Effect | 58 | 49.90 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| Estrone Metabolism | 24 | 20.60 | 1 | 1.00E+00 | 1.00E+00 | 1.00E+00 |

7 Appendix: R Command History

```
[1] "mSet<-InitDataObjects(\"conc\", \"pathora\", FALSE)"
[2] "cmpd.vec<-c(\"HMDB0000123\", \"HMDB0014691\", \"HMDB0031239\", \"HMDB0161401\", \"HMDB0000925\", \"I
[3] "mSet<-Setup.MapData(mSet, cmpd.vec);"
[4] "mSet<-CrossReferencing(mSet, \"hmdb\");"
[5] "mSet<-CreateMappingResultTable(mSet)"
[6] "mSet<-SetKEGG.PathLib(mSet, \"hsa\", \"current\")"
[7] "mSet<-SetMetabolomeFilter(mSet, F);"
[8] "mSet<-CalculateOraScore(mSet, \"rbc\", \"hyperg\")"
[9] "mSet<-PlotPathSummary(mSet, F, \"path_view_0_\", \"png\", 72, width=NA)"
[10] "mSet<-SaveTransformedData(mSet)"
[11] "UpdateDataObjects(\"conc\", \"msetora\", FALSE)"
[12] "mSet<-SetMetabolomeFilter(mSet, F);"
[13] "mSet<-SetCurrentMsetLib(mSet, \"smpdb_pathway\", 2);"
[14] "mSet<-CalculateHyperScore(mSet)"
[15] "mSet<-PlotORA(mSet, \"ora_0_\", \"net\", \"png\", 72, width=NA)"
[16] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_0_\", \"png\", 72, width=NA)"
[17] "mSet<-CalculateHyperScore(mSet)"
[18] "mSet<-PlotORA(mSet, \"ora_1_\", \"net\", \"png\", 72, width=NA)"
[19] "mSet<-PlotEnrichDotPlot(mSet, \"ora\", \"ora_dot_1_\", \"png\", 72, width=NA)"
[20] "mSet<-SaveTransformedData(mSet)"
[21] "mSet<-PreparePDFReport(mSet, \"guest17850890059438804150\")\n"
```

The report was generated on Mon May 24 12:54:45 2021 with R version 4.0.2 (2020-06-22).