Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information Analytical Methods

Multifunctional Derivatization of Endogenous Metabolites using Capillary RPLC-MS

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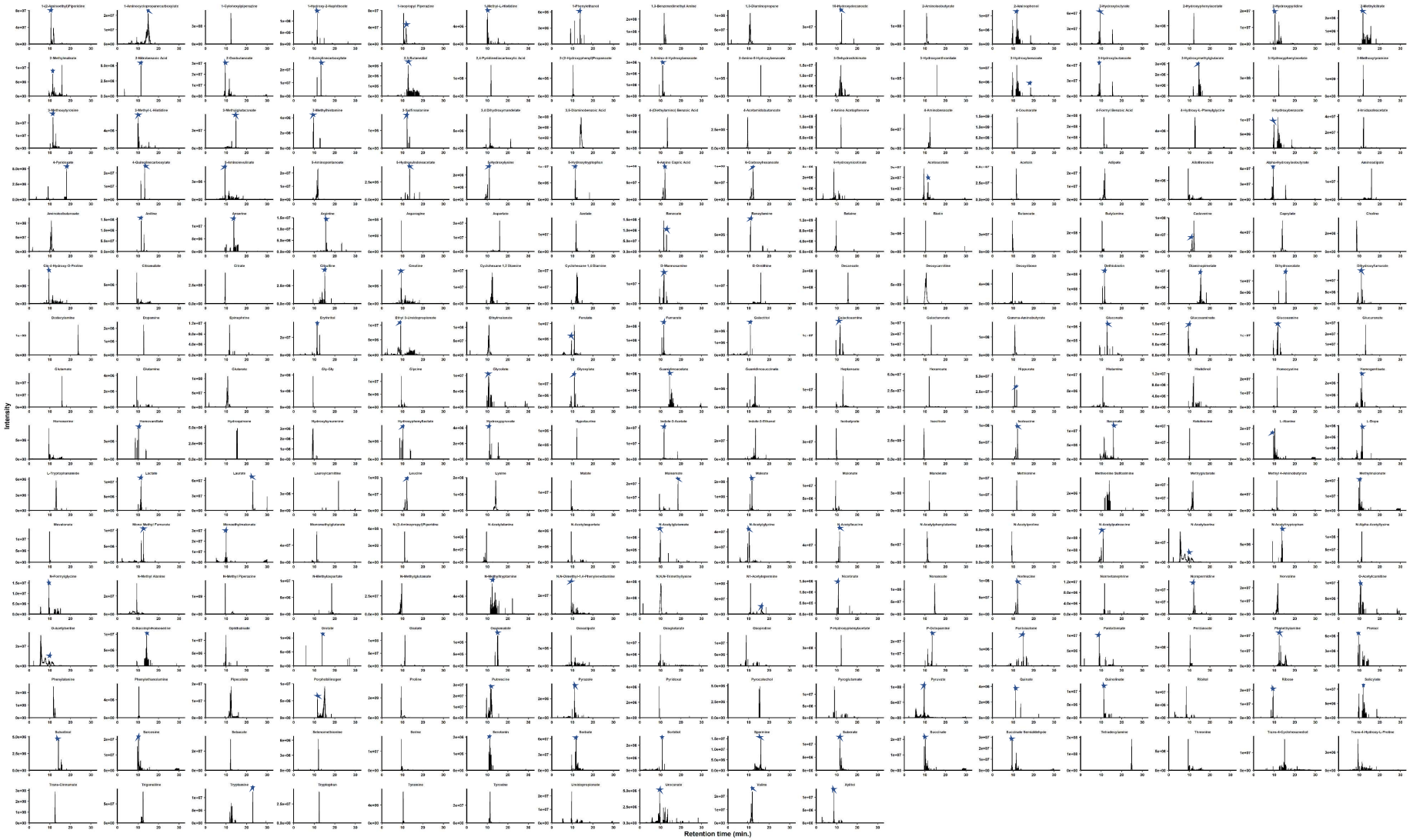
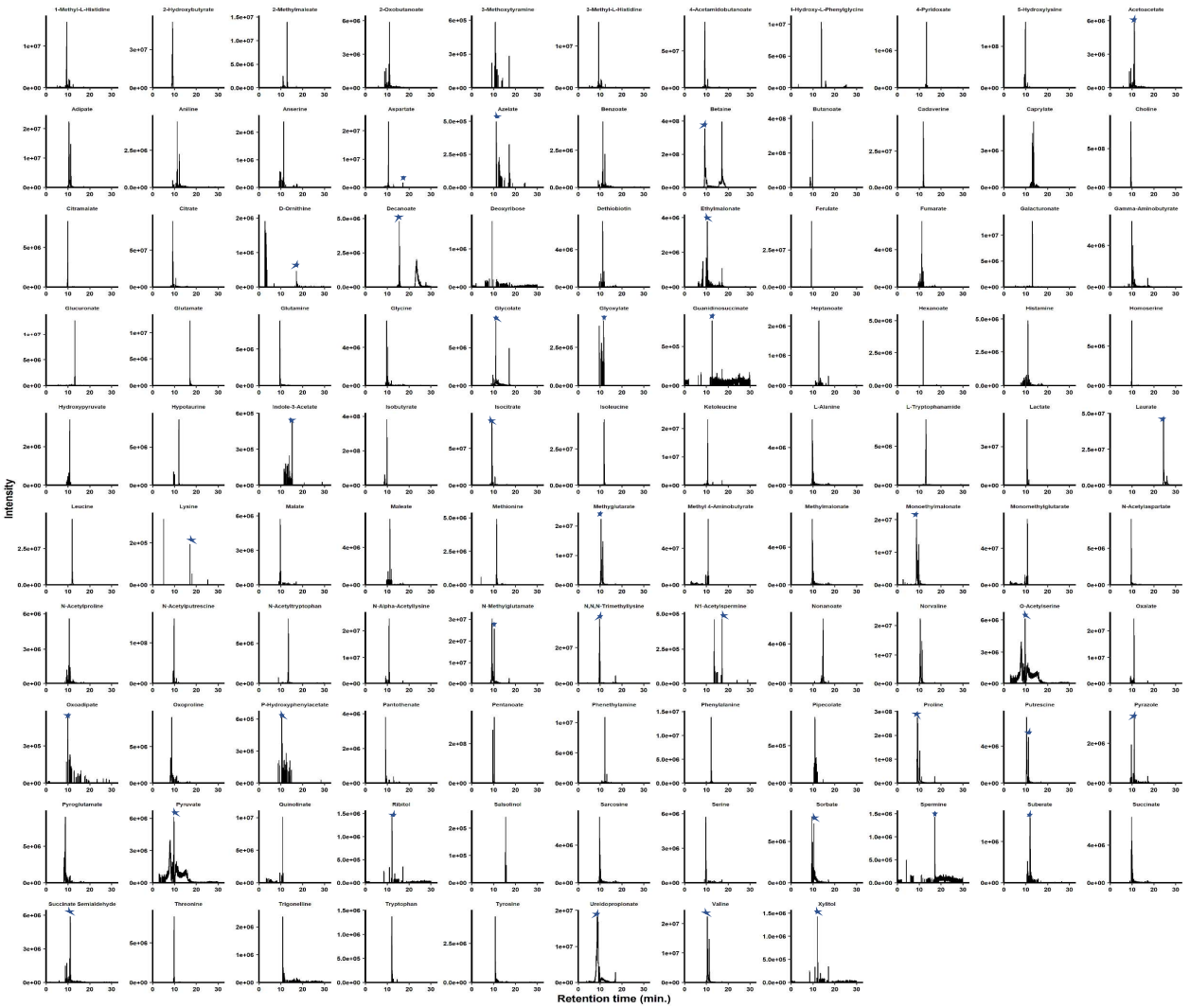
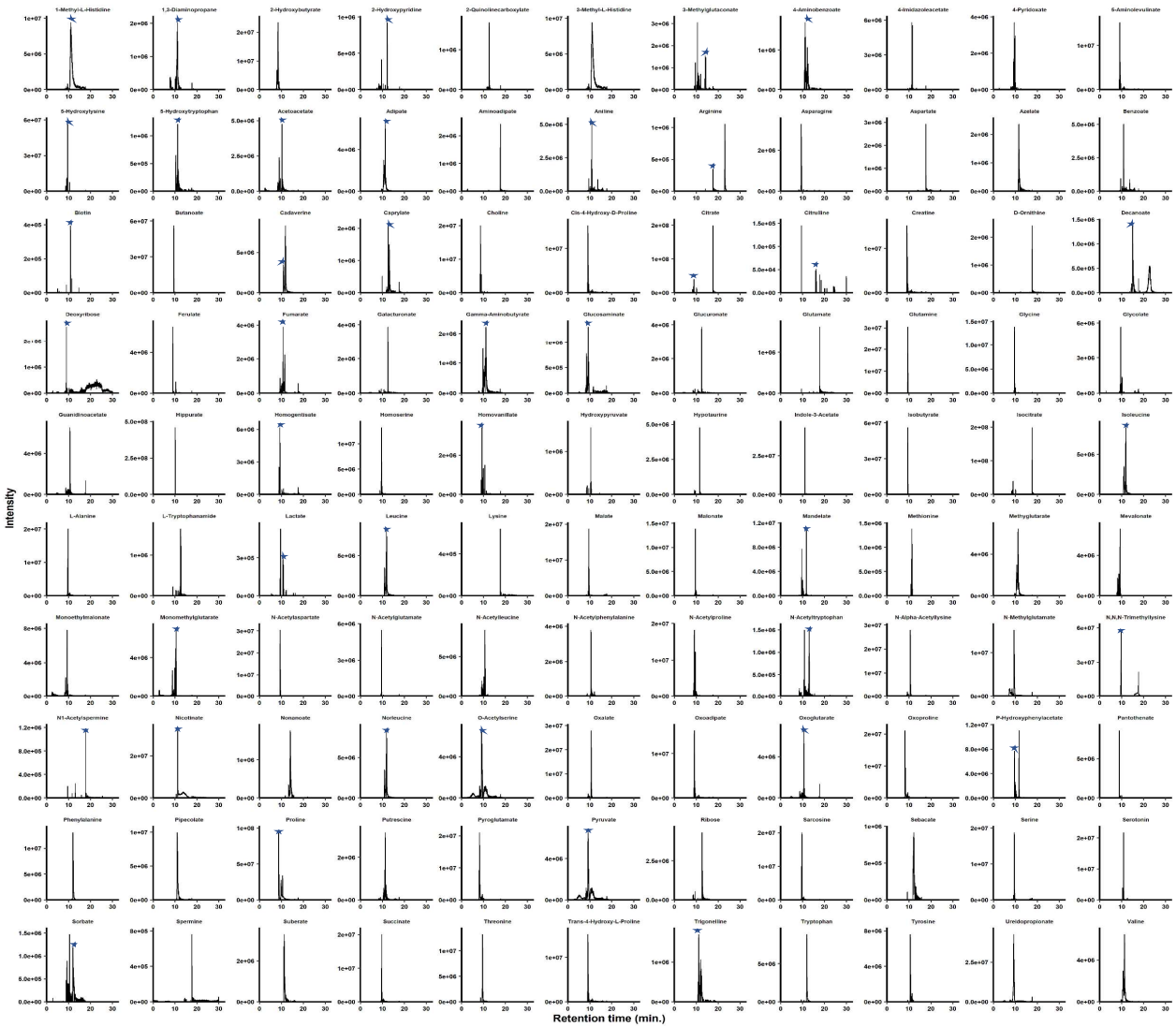


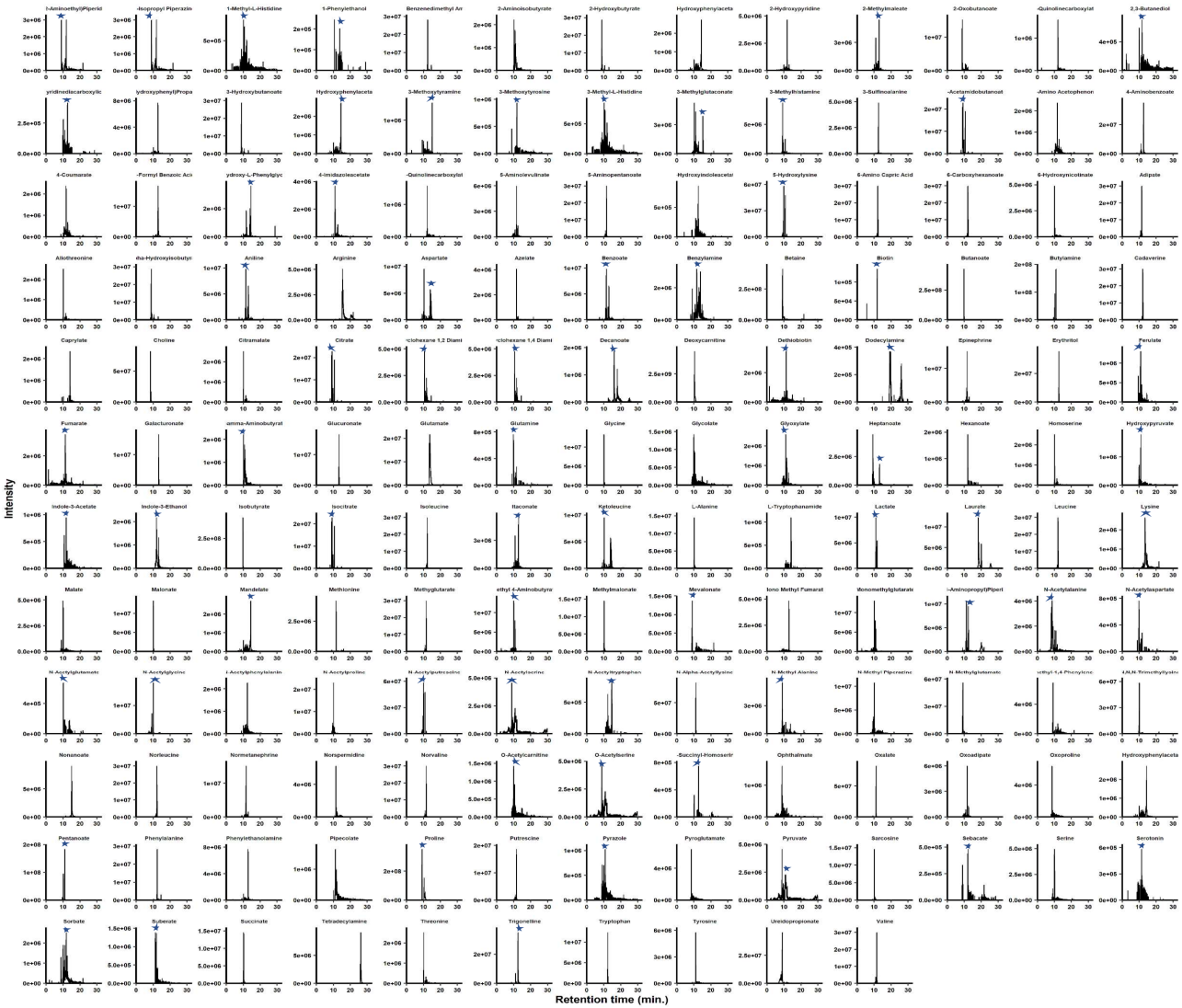
Supplementary Figure 1. Reconstructed Ion Chromatogram for 250 derivatized metabolite standards



Supplementary Figure 2. Reconstructed Ion Chromatogram for 107 derivatized metabolite targeted in Bovine aortic endothelia cells (BAECs).



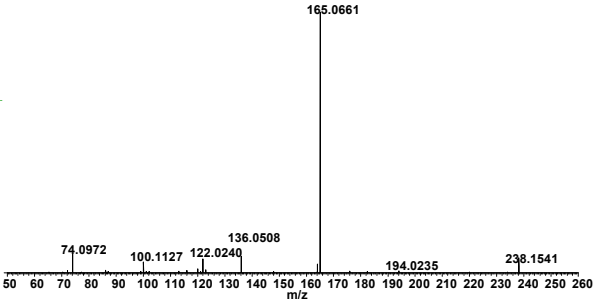
Supplementary Figure 3. Reconstructed Ion Chromatogram for 111 derivatized metabolite targeted in human urine



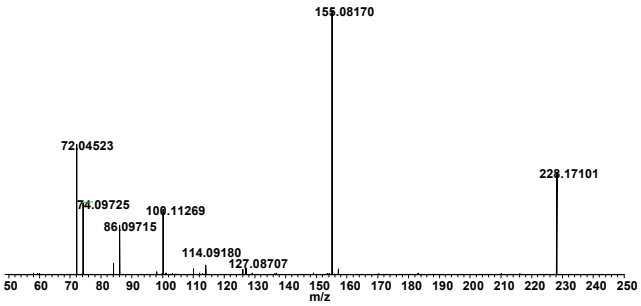
Supplementary Figure 4. Reconstructed Ion Chromatogram for 153 tagged metabolite targeted in human serum .

Supplementary Figure 5. MS/MS spectra for 250 derivatized metabolite standards

1. 6-HYDROXYNICOTINATE



2. PYROGLUTAMATE/OXOPROLINE



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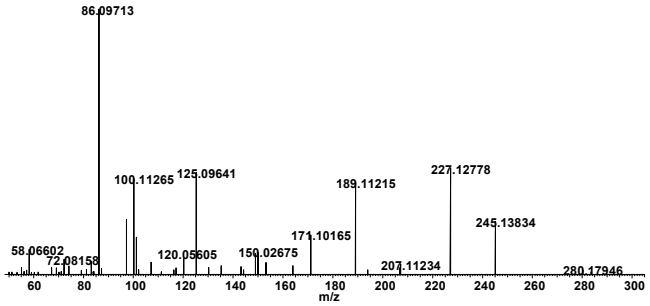

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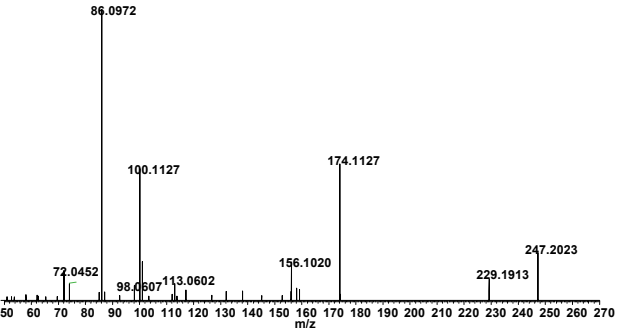

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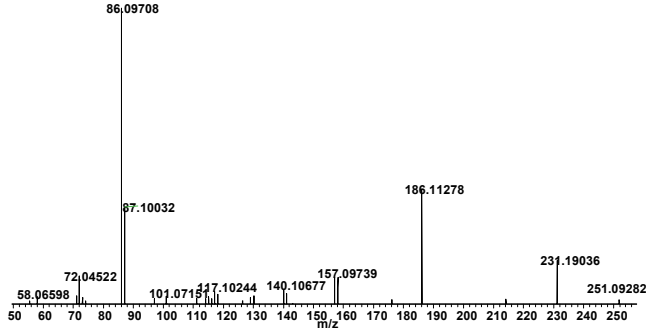

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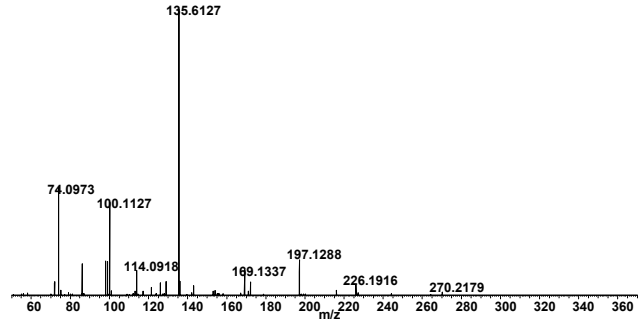

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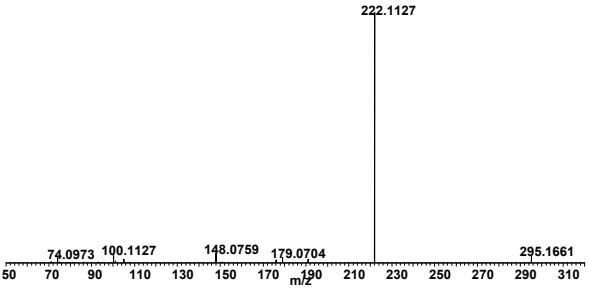

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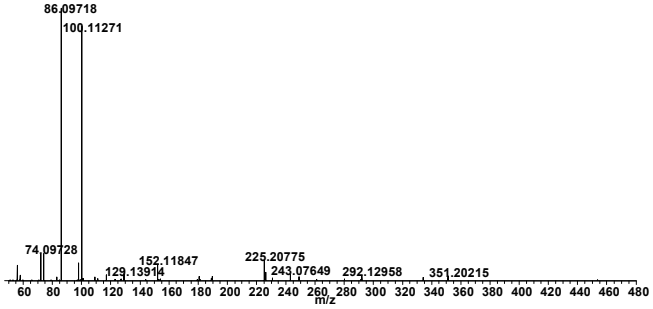

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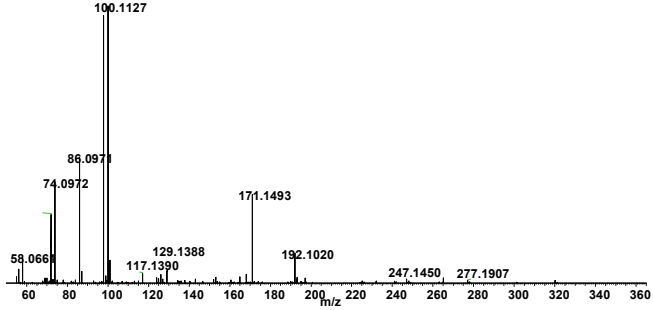
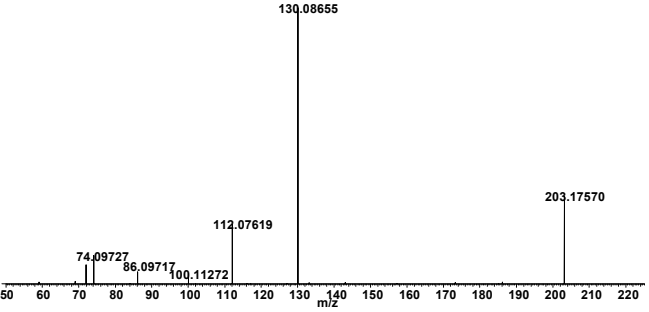


Supplementary Figure 6. MS/MS spectra for 250 derivatized metabolite standards

12. 2/3/ALPHA-HYDROXYISOBUTYRATE



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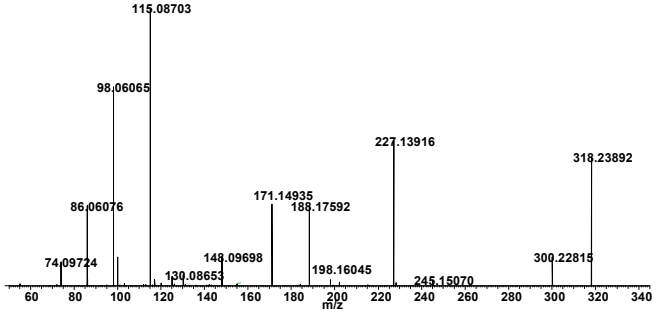

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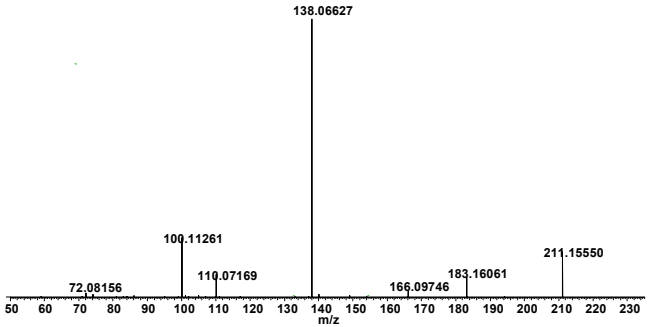

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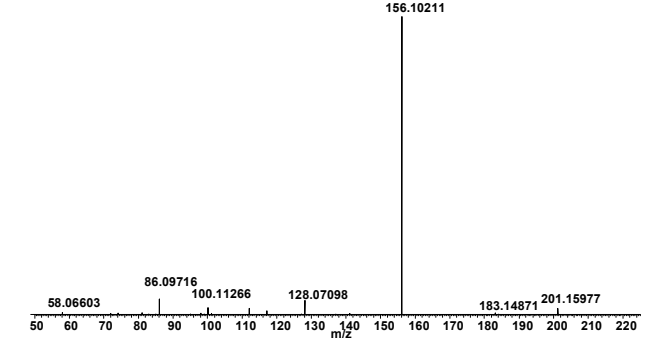

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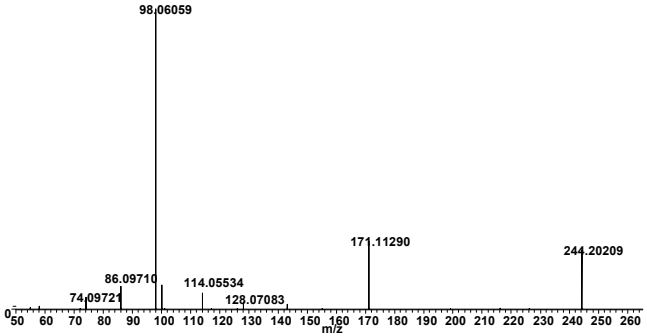

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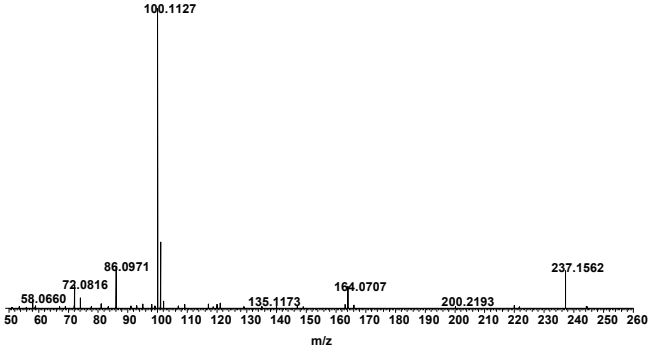

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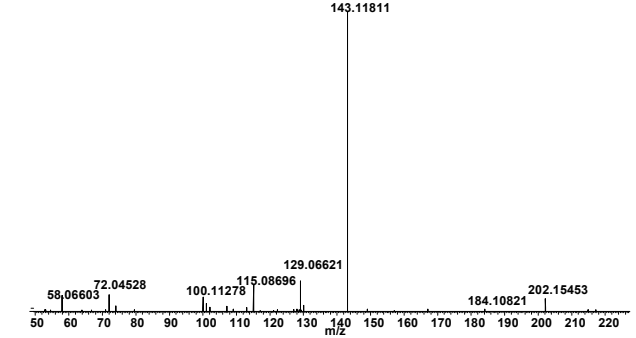
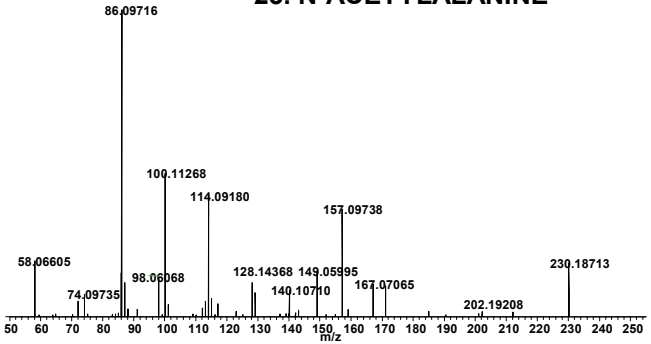


23. N-ACETYLALANINE



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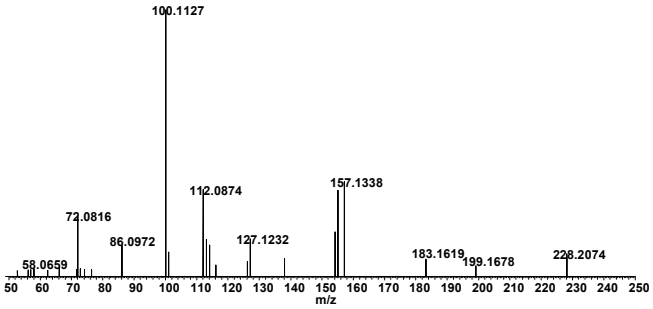

Supplementary Figure 7. MS/MS spectra for 250 derivatized metabolite standards

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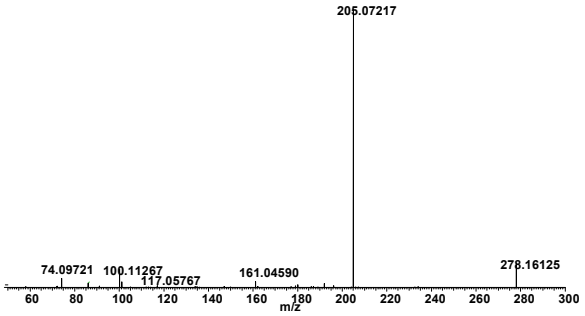

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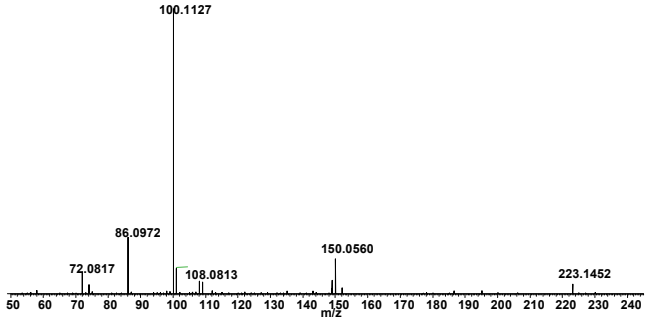

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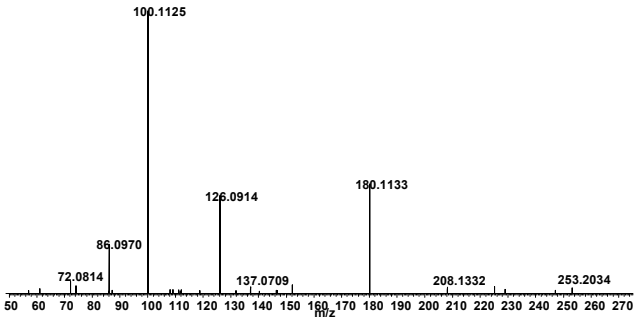

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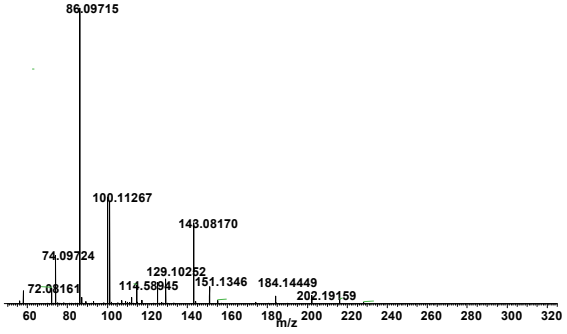

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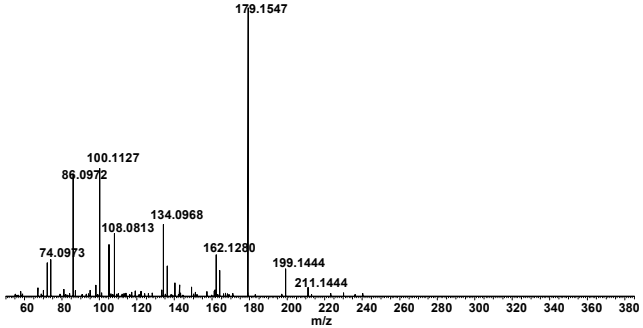

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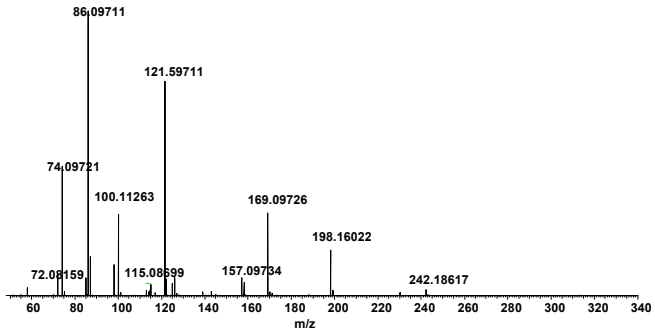

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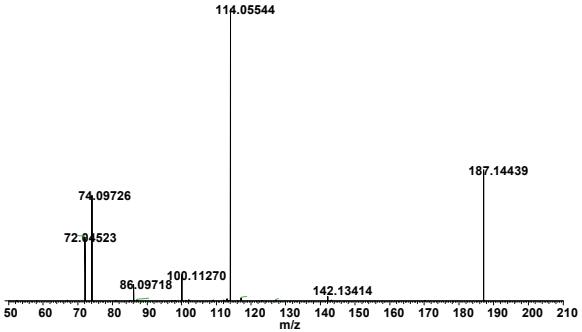

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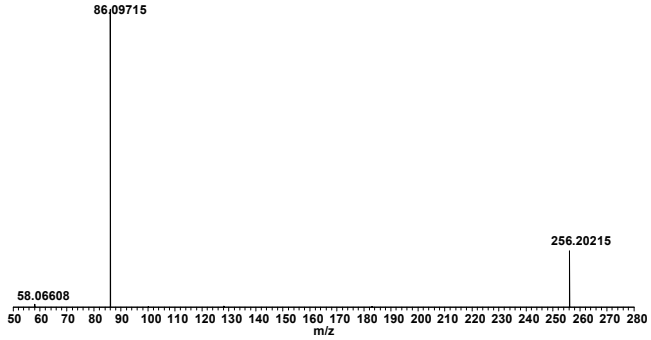

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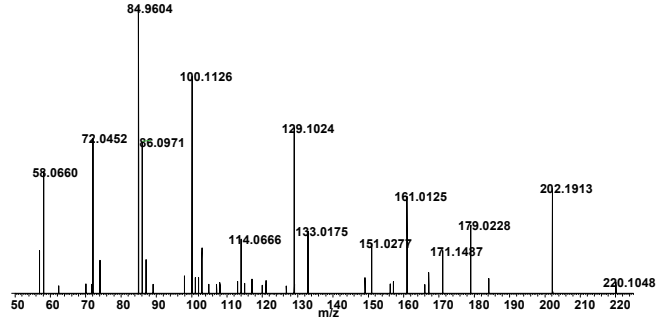
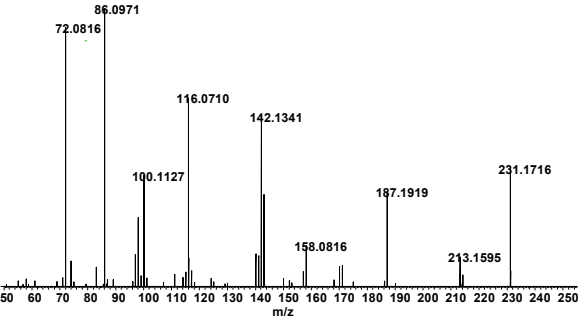
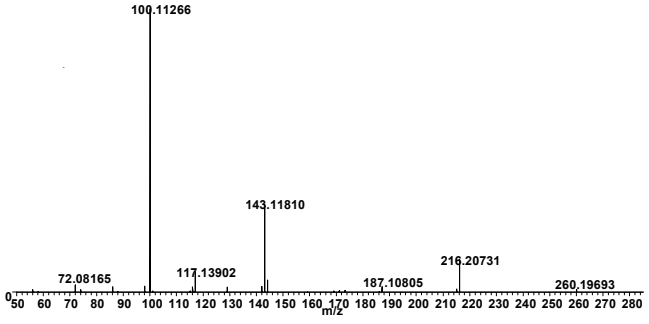


Supplementary Figure 8. MS/MS spectra for 250 derivatized metabolite standards

36. UREIDOPROPIONATE



37. N-METHYLGLUTAMATE



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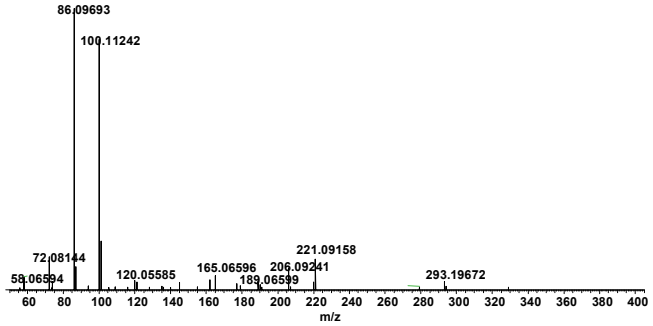

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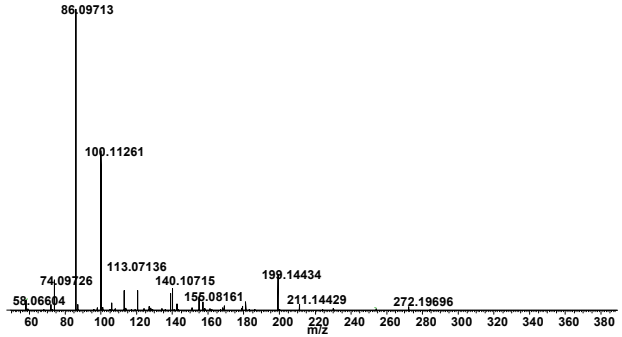

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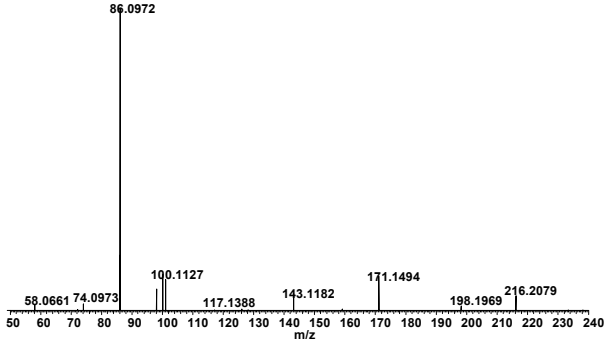

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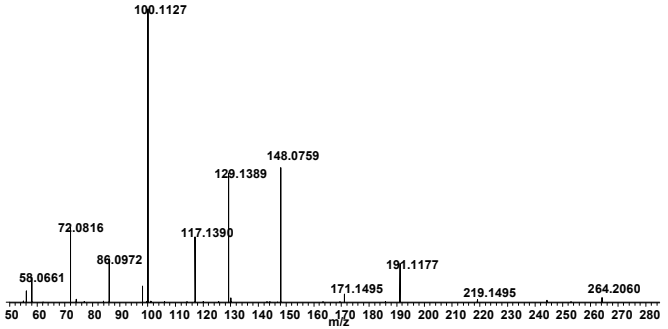

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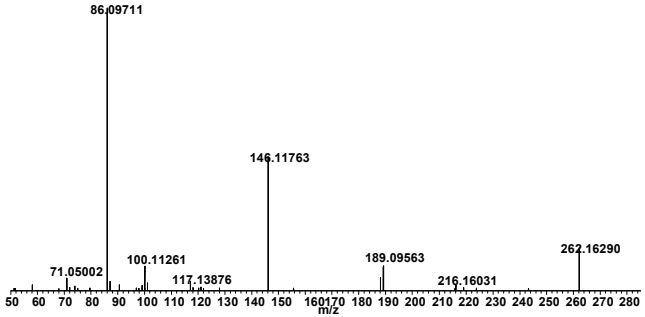

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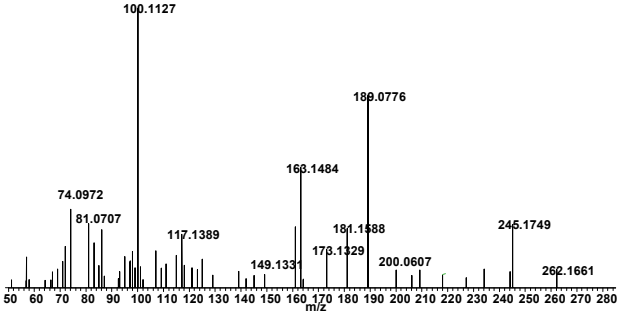

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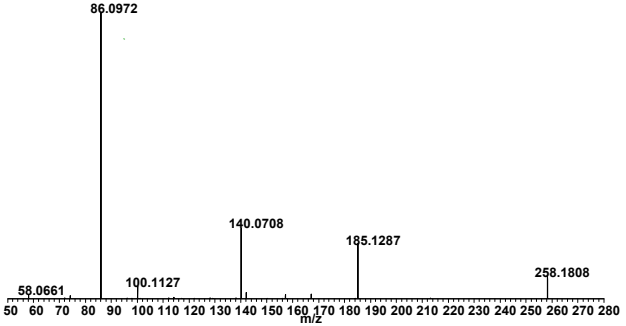
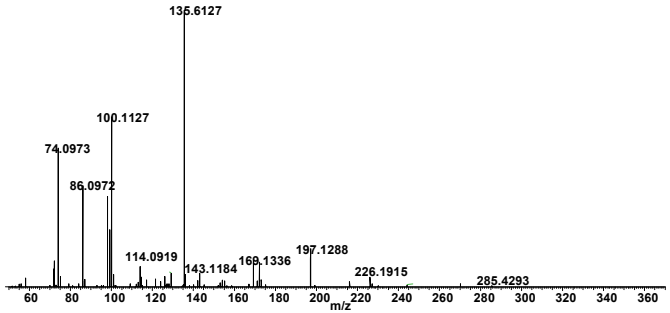
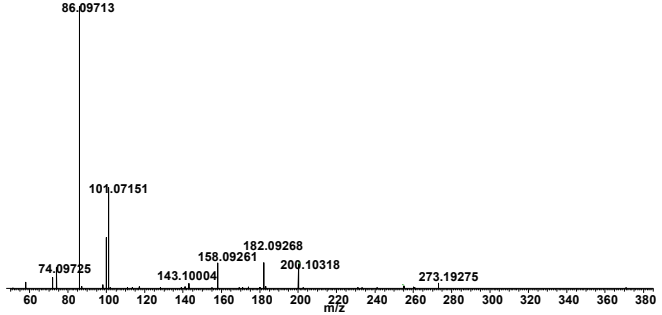


Supplementary Figure 9. MS/MS spectra for 250 derivatized metabolite standards

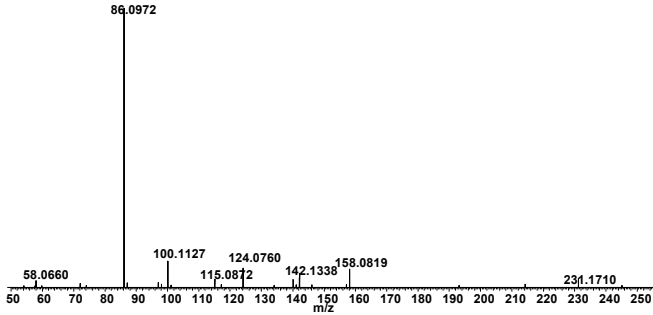
46. OXOGLUTARATE



47. ASPARAGINE/GLY-GLY



49. MONOETHYLMALONATE



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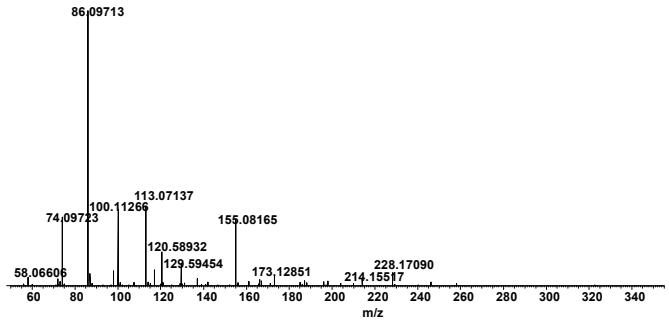

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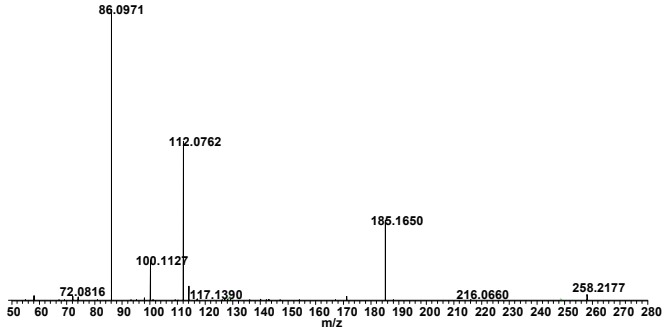

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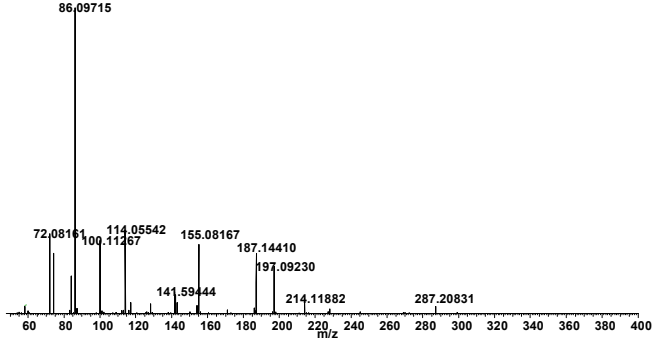
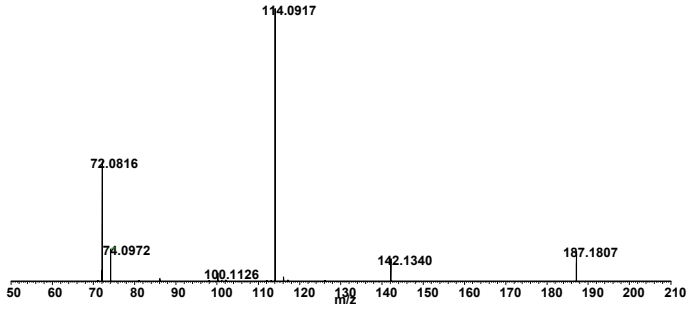
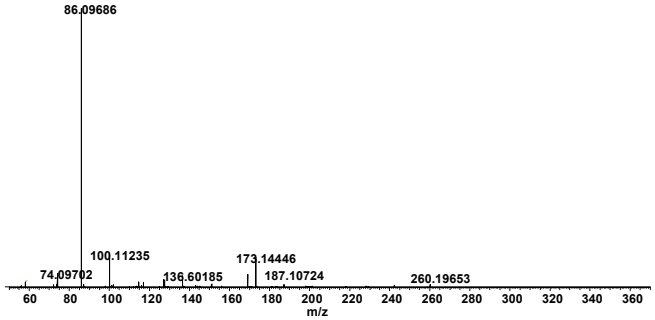


56. ISOBUTYRATE/BUTANOATE



58. THREONINE/ALLOTHREONINE/HOMOSERINE



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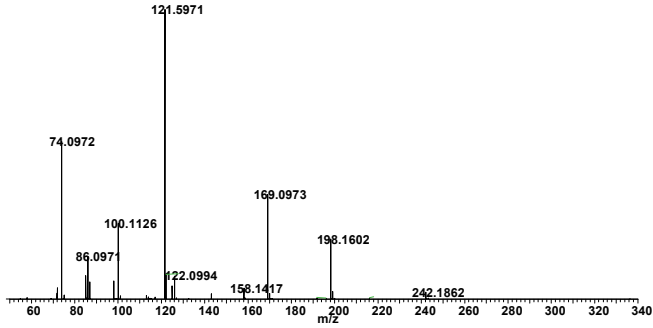
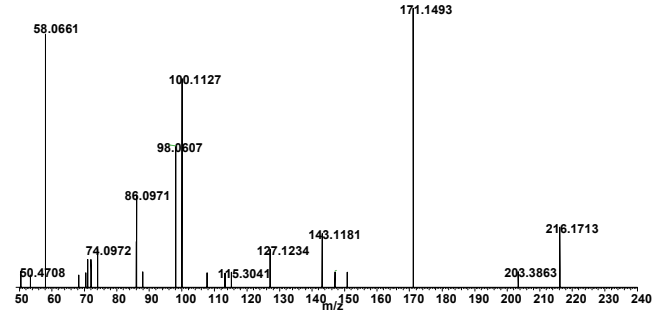
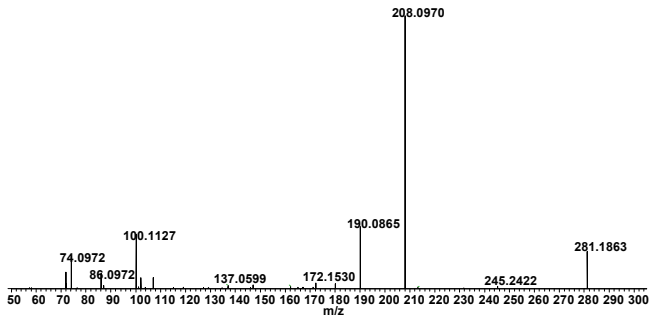


Supplementary Figure 10. MS/MS spectra for 250 derivatized metabolite standards

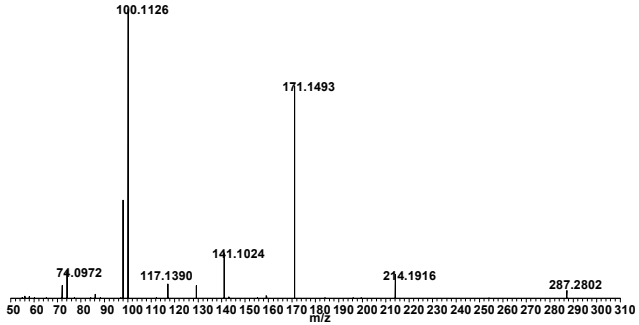
62. N-ACETYLGLYCINE



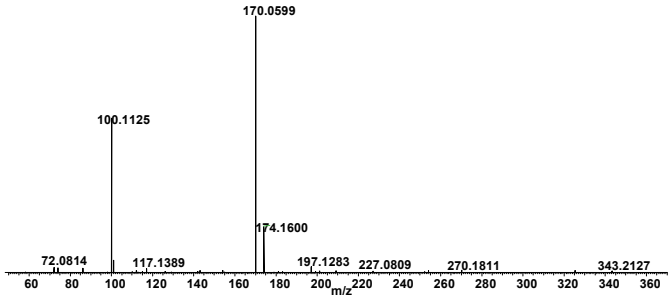
63. HOMOVANILLATE/ HYDROXYPHENYLLACTATE



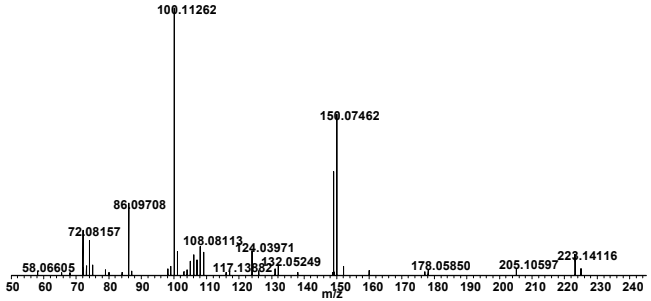
65. N,N,N-TRIMETHYLLYSINE



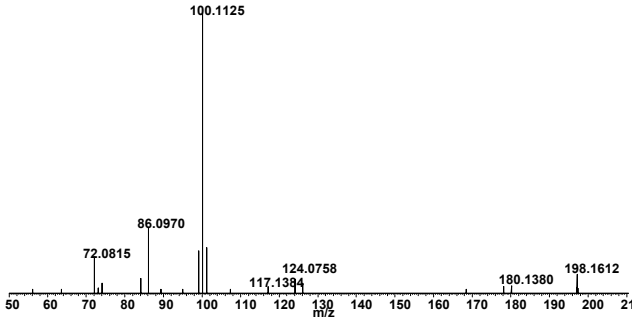
66. BIOTIN



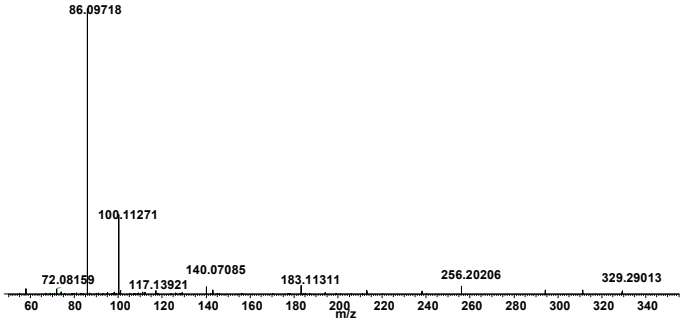
67. 2-HYDROXYPYRIDINE



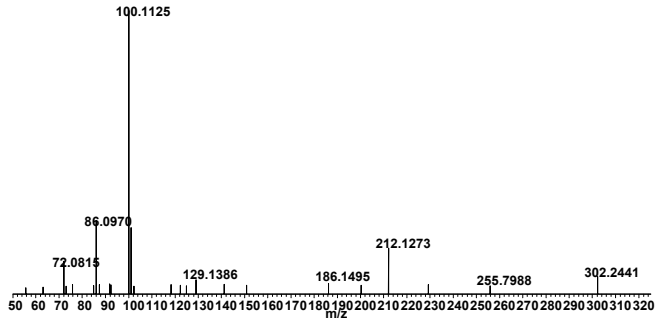
68. 1/3-METHYL-L-HISTIDINE



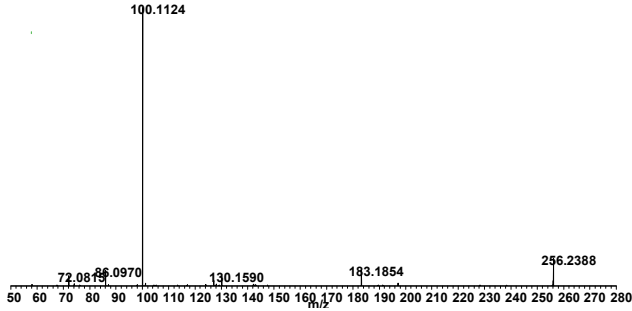
70. GLUTARATE/ETHYLMALONATE



72. GLYCOLATE

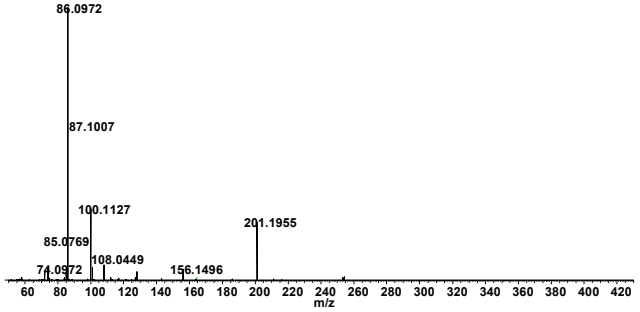


73. 1-ISOPROPYL PIPERAZINE

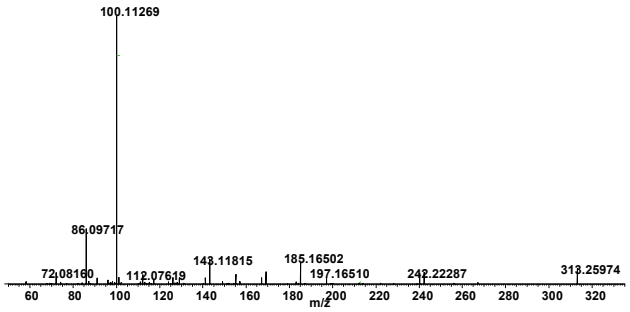


Supplementary Figure 11. MS/MS spectra for 250 derivatized metabolite standards

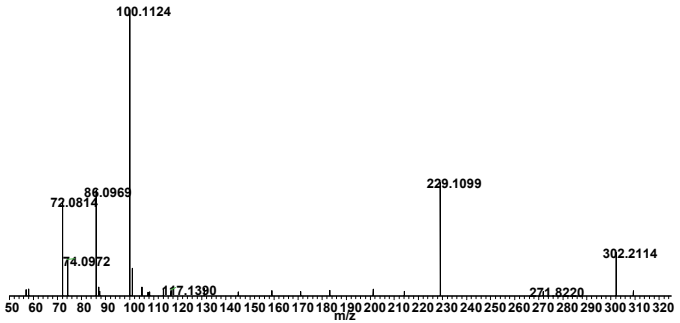
74. BUTYLAMINE/ PENTANOATE



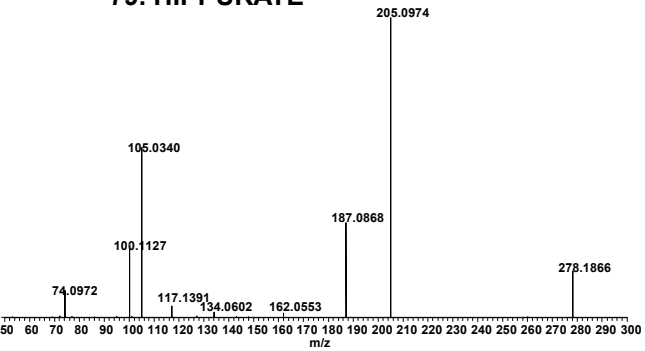
76. DETHIOBIOTIN/MALEATE



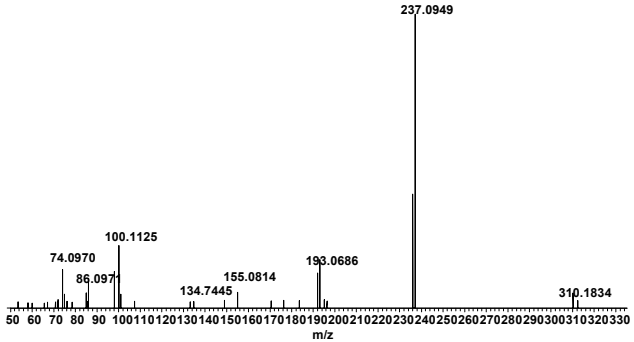
78. O-ACETYLCARNITINE



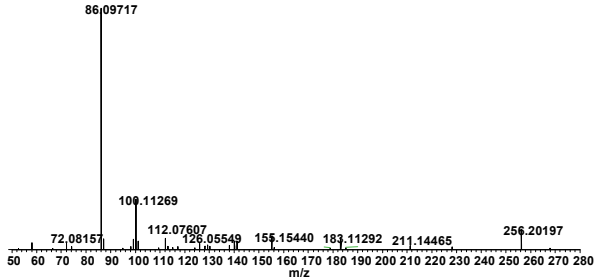
79. HIPPURATE



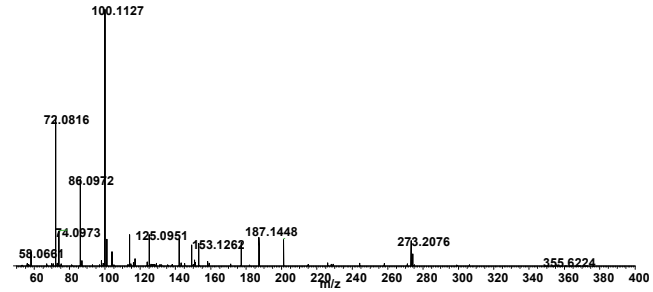
80. SORBITOL/ GALACTITOL



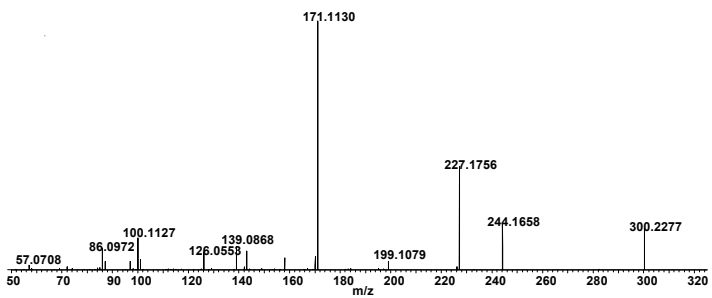
82. 1,3-DIAMINOPROPANE/AMINOISOBUTANOATE



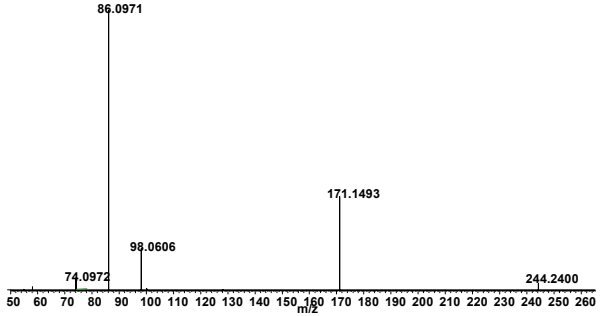
84. N-ACETYLSERINE/ O-ACETYLSERINE



86. GLYOXYLATE

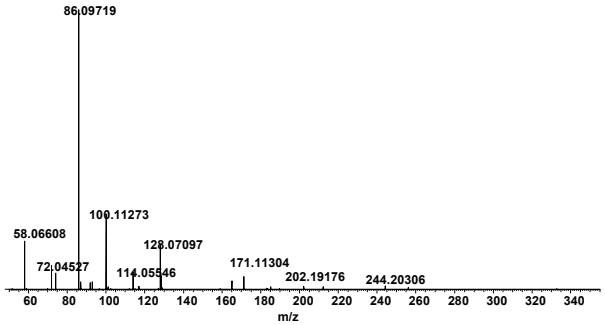


87. DEOXYCARNITINE

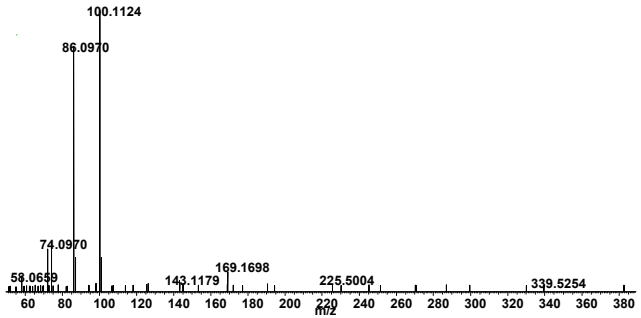


Supplementary Figure 12. MS/MS spectra for 250 derivatized metabolite standards

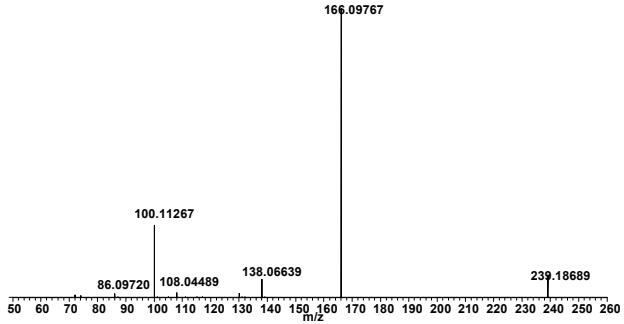
88. GAMMA-AMINOBUTYRATE/2-AMINOISOBUTYRATE



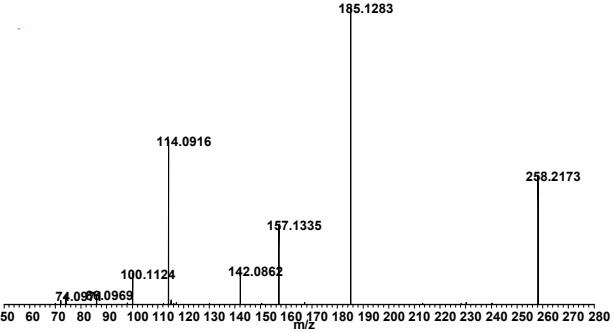
90. CADAVERINE



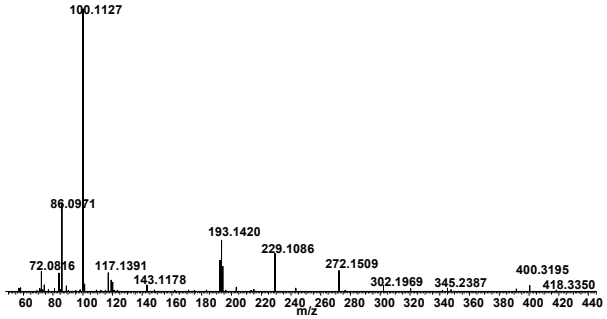
91. HISTAMINE



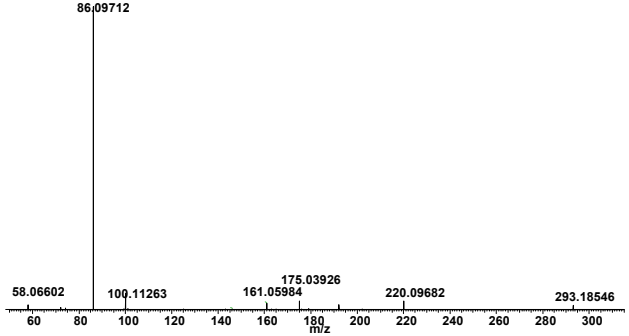
N-ACETYLPUTRESCINE



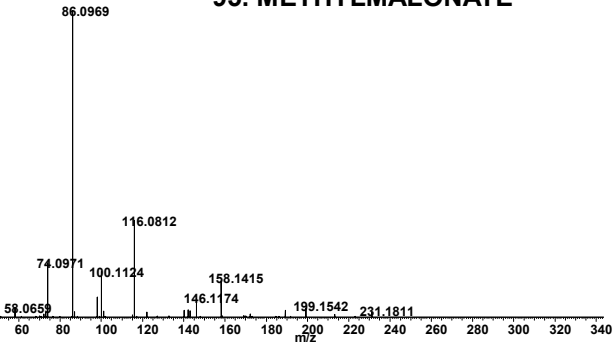
93. QUINATE



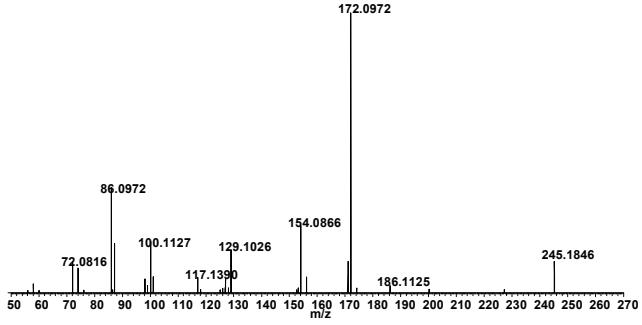
94. FERULATE



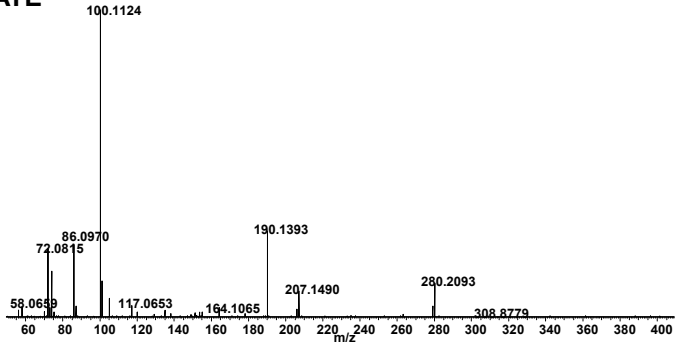
95. METHYLMALONATE



96. METHYL 4-AMINOBUTYRATE/ MONOMETHYLGLUTARATE

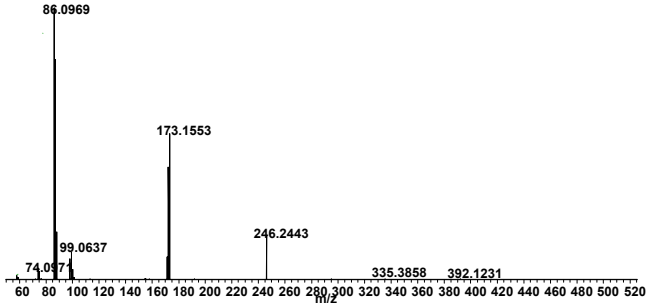


98. 3-AMINO-4-HYDROXYBENZOATE

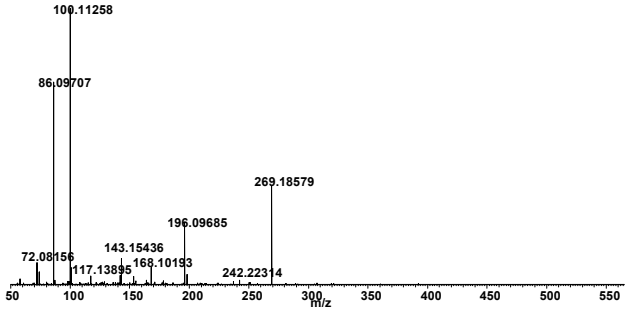


Supplementary Figure 13. MS/MS spectra for 250 derivatized metabolite standards

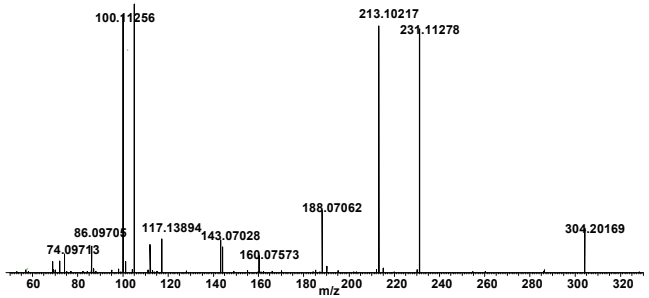
99. QUINOLINATE



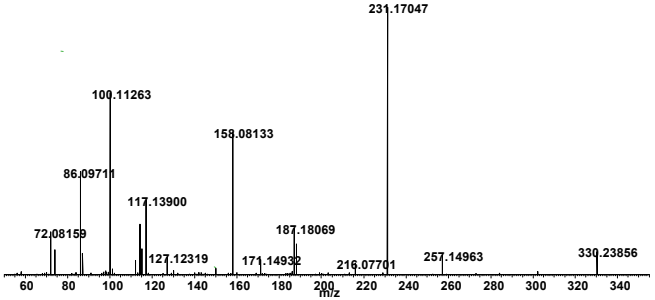
100. 3,4 DIHYDROXYMANDELATE



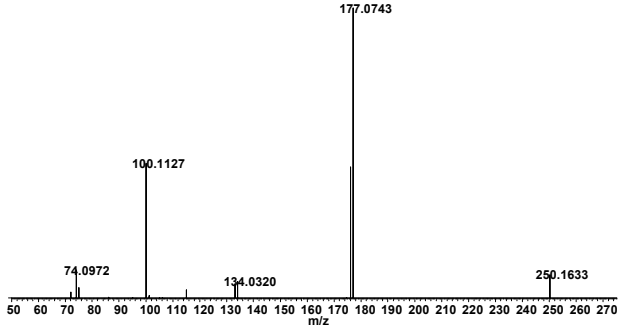
101. SEROTONIN



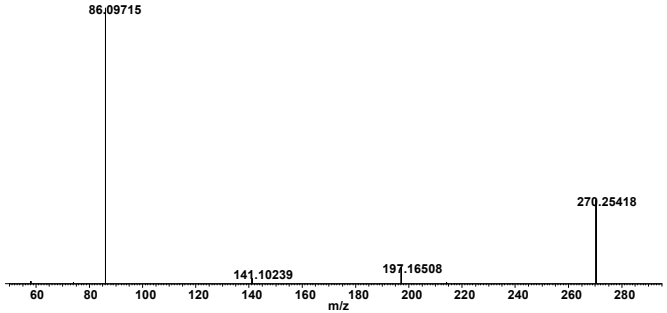
101. HYDROXYPYRUVATE



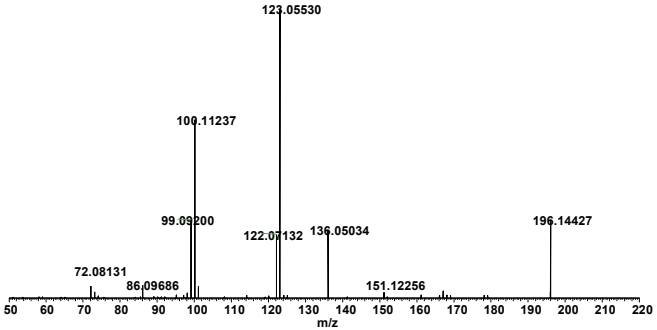
102. ERYTHRITOL



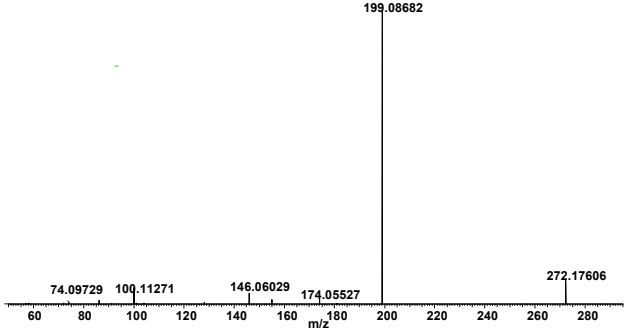
103. N-(3-AMINOPROPYL)PIPERIDNE



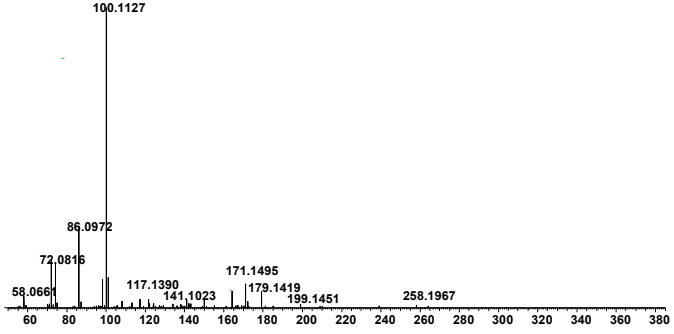
104. PYRAZOLE



105. 2-QUINOLINECARBOXYLATE

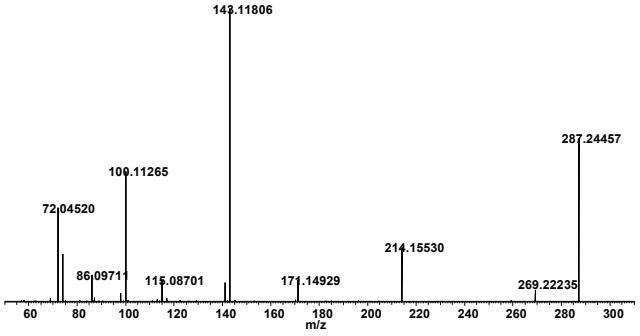


106. 5-AMINOLEVULINATE

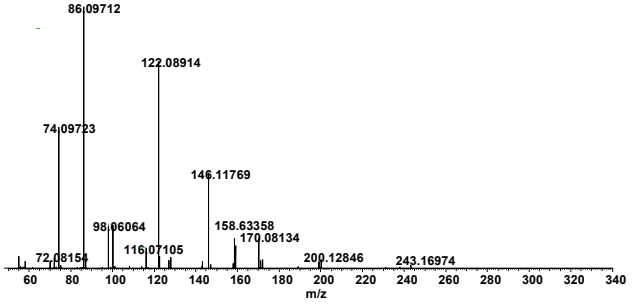


Supplementary Figure 14. MS/MS spectra for 250 derivatized metabolite standards

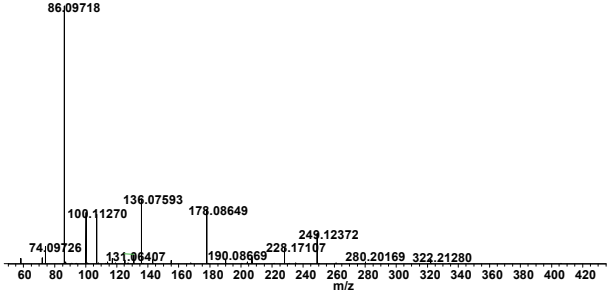
107. OXALATE/N-ALPHA-ACETYLLYSINE



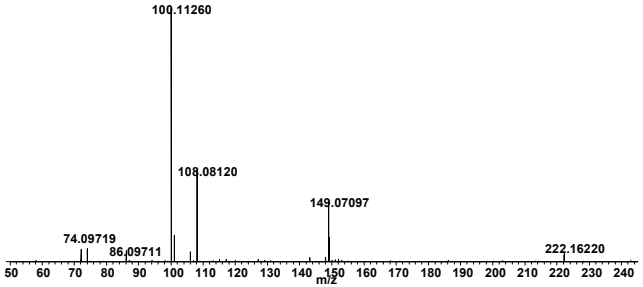
109. LACTATE



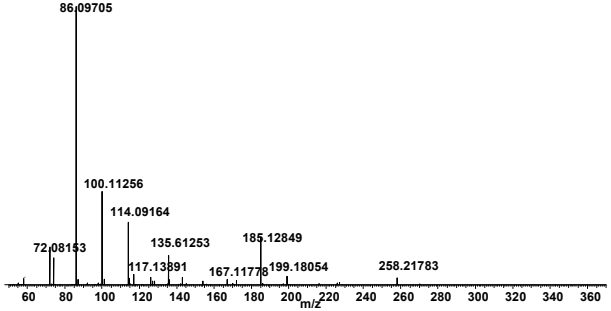
110. TYROSINE



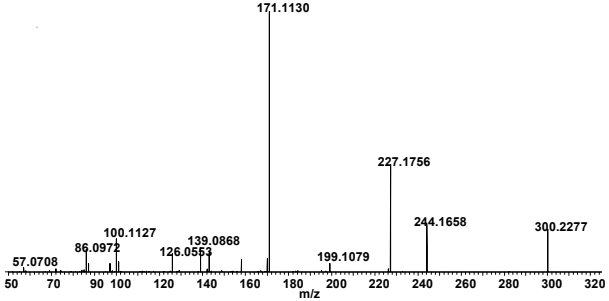
111. NICOTINATE



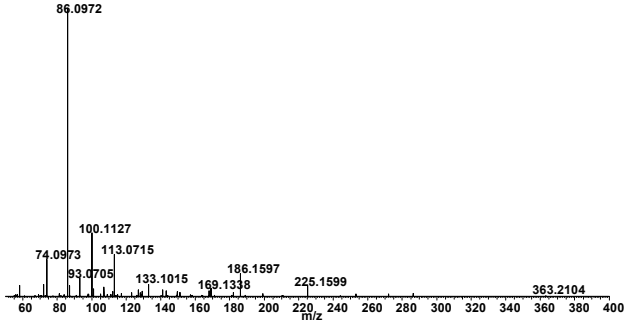
112. VALINE/NORVALINE



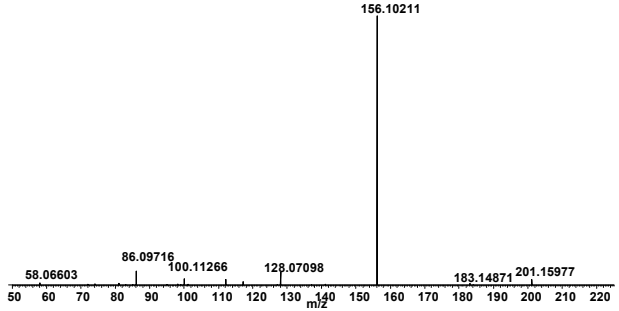
114. DIHYDROXYFUMARATE



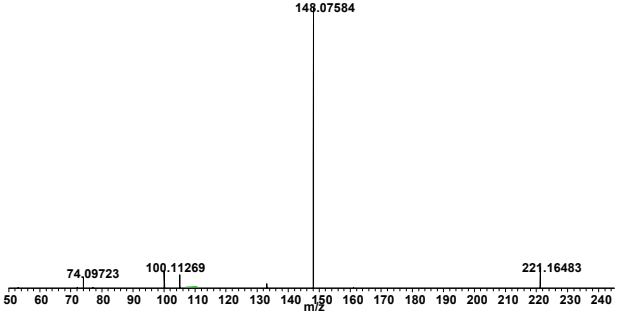
116. SUBERATE



117. ACETOACETATE/SUCCINATE SEMIALDEHYDE

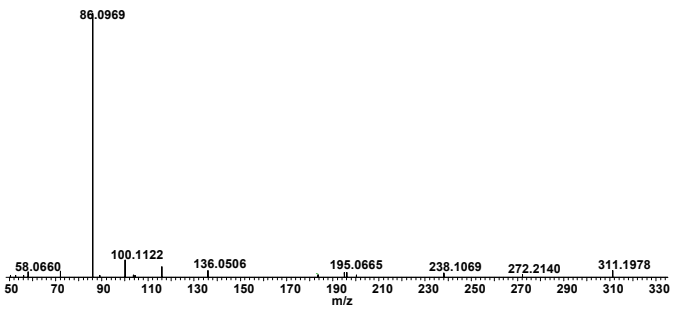


119. 3-METHOXYTYROSINE

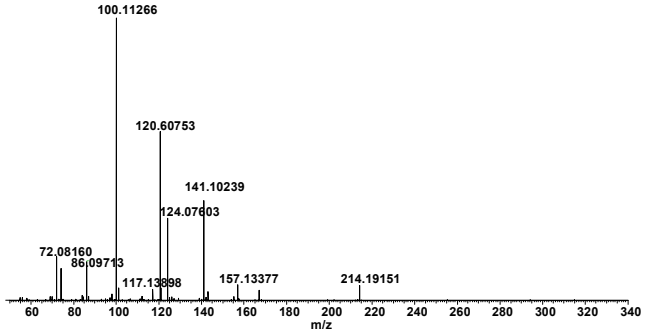


Supplementary Figure 15. MS/MS spectra for 250 derivatized metabolite standards

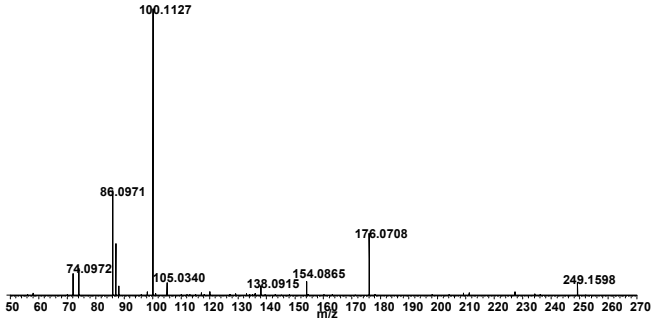
120. HOMOCYSTINE



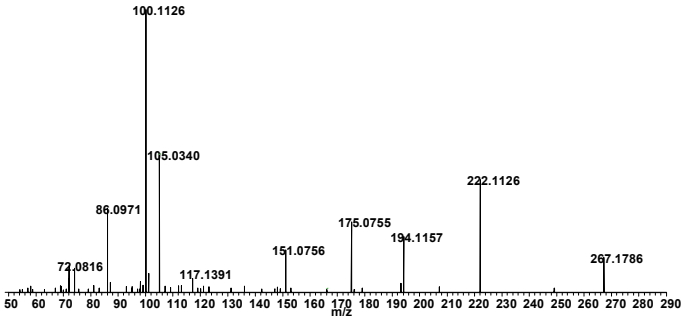
121. FUMARATE



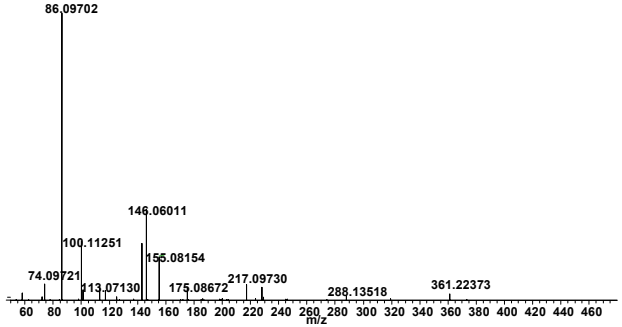
122. 4-FORMYL BENZOIC ACID



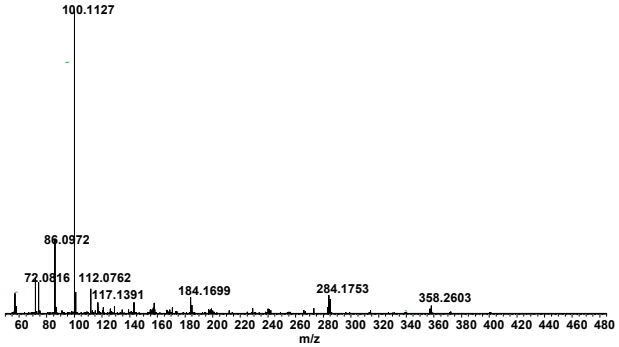
123. HOMOGENTISATE



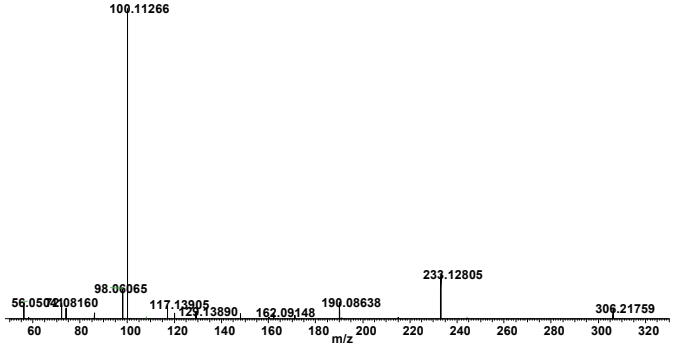
124. 5-HYDROXYTRYPTOPHAN



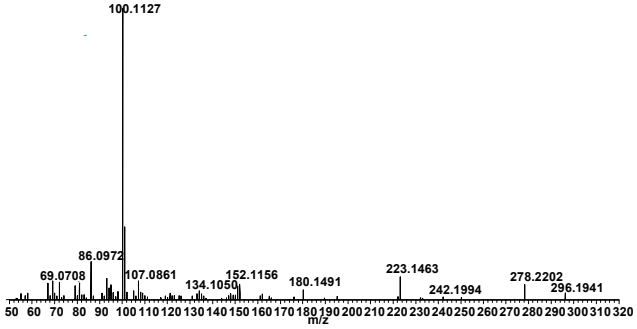
125. KETOLEUCINE



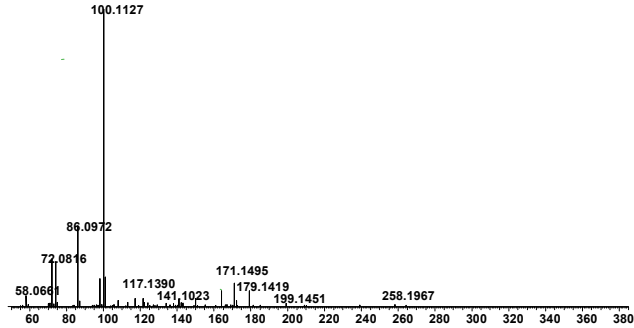
126. N-ACETYLPHENYLALANINE



127. L-DOPA

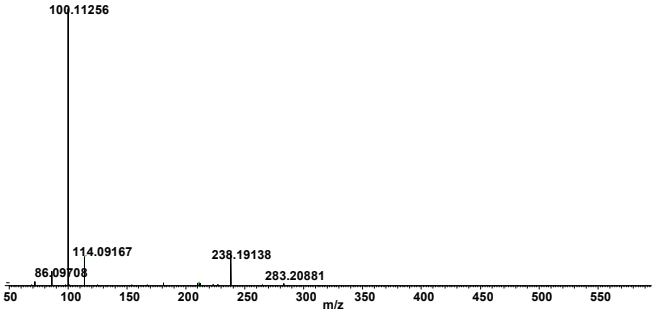


128. OXOADIPATE

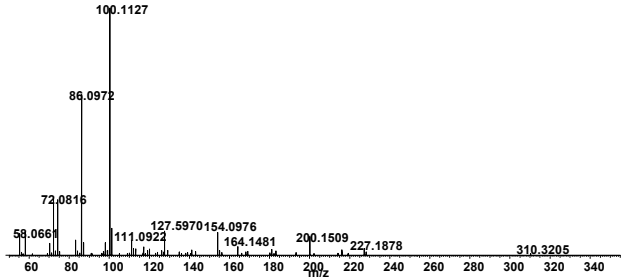


Supplementary Figure 16. MS/MS spectra for 250 derivatized metabolite standards

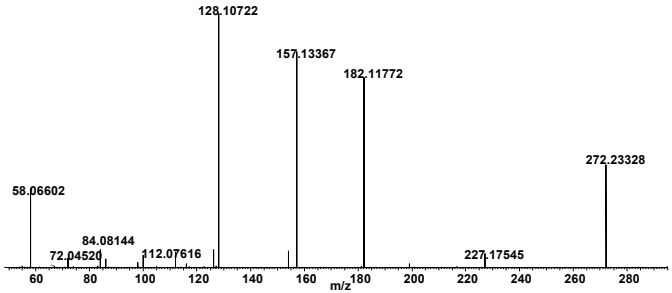
129. EPINEPHRINE/NORMETANEPHRINE



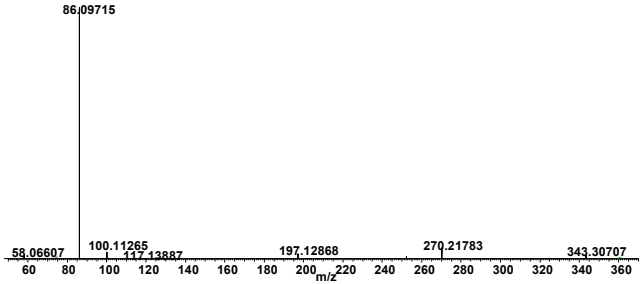
131. 2-METHYLMALEATE



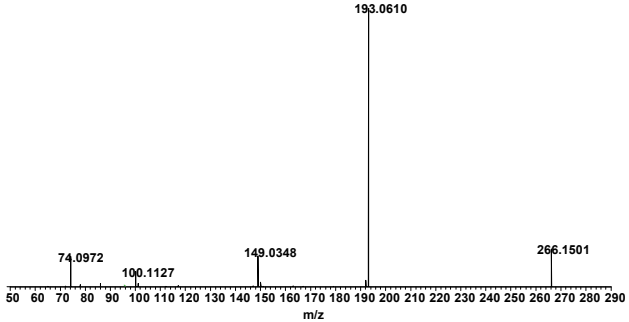
132. N-ACETYLLEUCINE



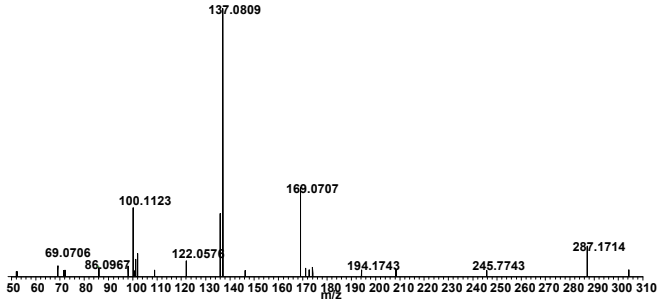
133. PUTRESCINE



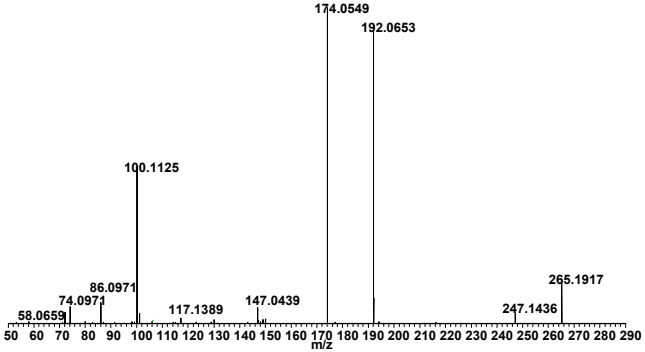
134. 2-NITROBENZOIC ACID



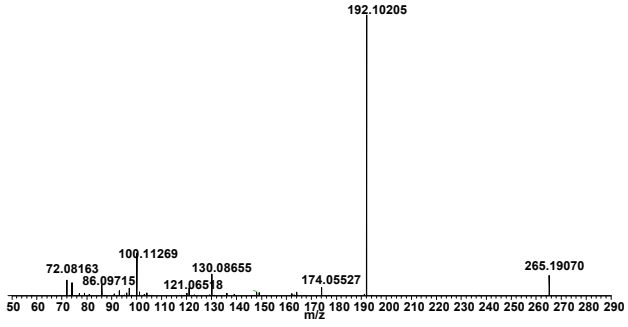
135. 1-HYDROXY-2-NAPHTHOATE



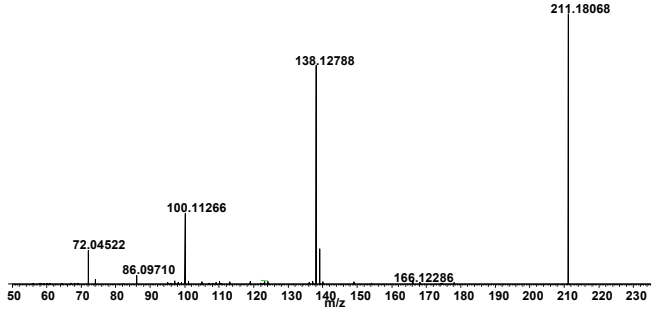
136. PHENYLETHANOLAMINE



137. 3-(2-HYDROXYPHENYL)PROPANOATE

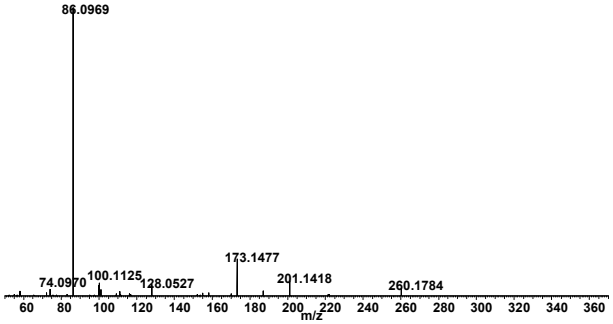


138. SORBATE

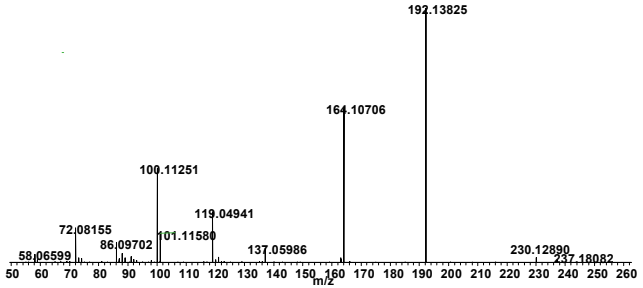


Supplementary Figure 17. MS/MS spectra for 250 derivatized metabolite standards

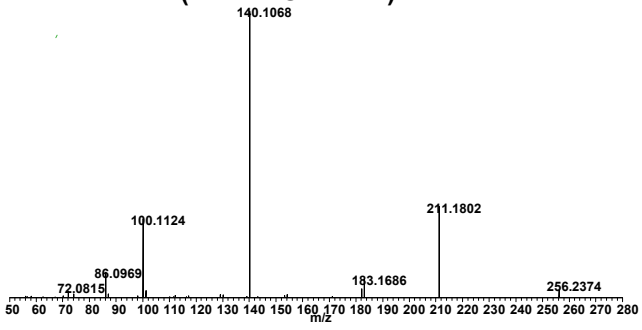
139. CITRAMALATE



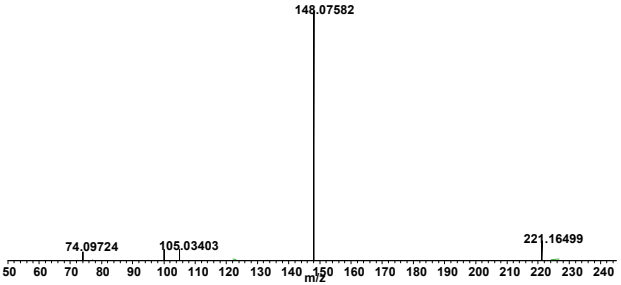
140. 2-AMINOPHENOL



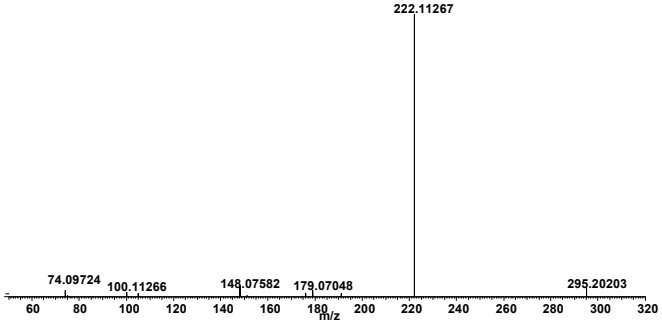
141. 1-(2-AMINOETHYL)PIPERIDINE



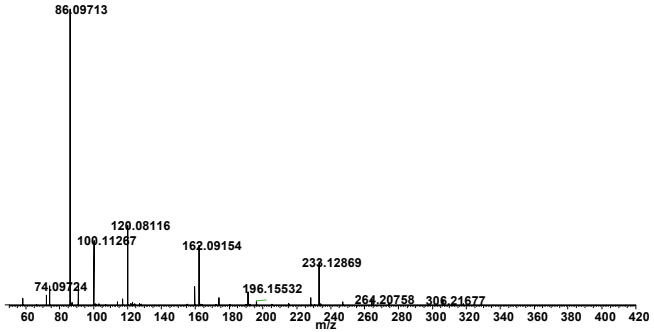
142. BENZOATE/ANILINE



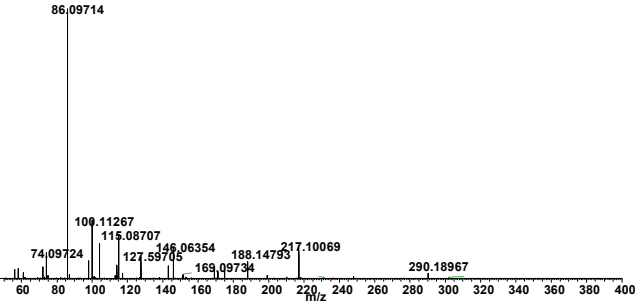
144. 3-METHOXYTYRAMINE



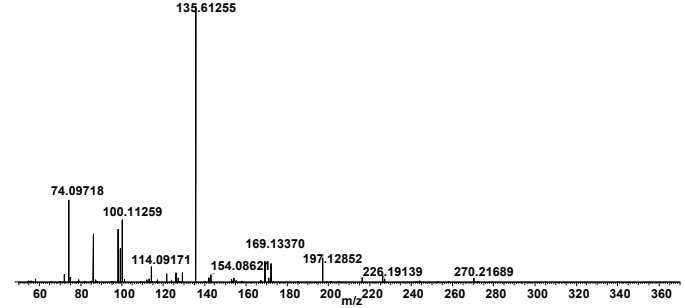
145. PHENYLALANINE



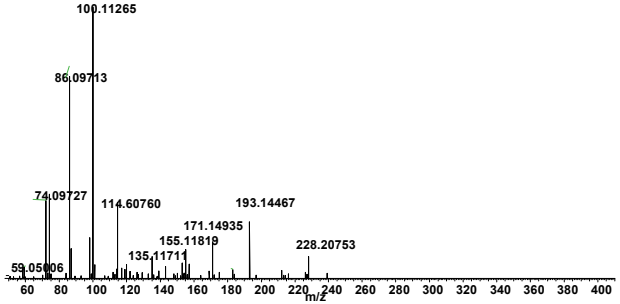
146. METHIONINE



147. 5-AMINOPENTANOATE/2-METHYGLUTARATE/ADIPATE

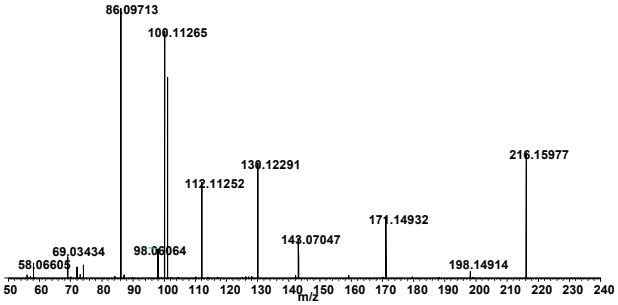


150. AZELATE

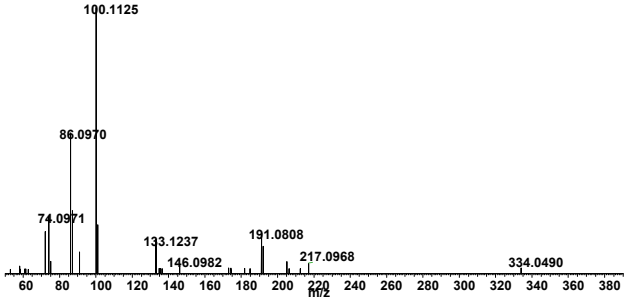


Supplementary Figure 18. MS/MS spectra for 250 derivatized metabolite standards

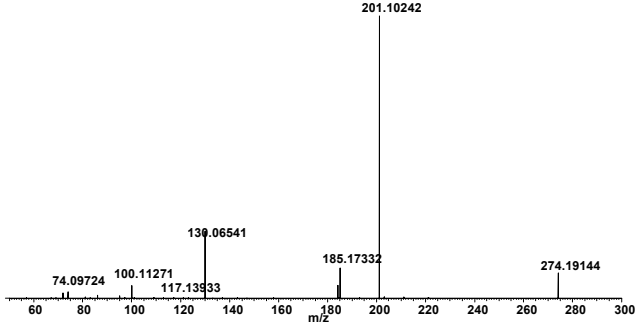
151. ACETOIN



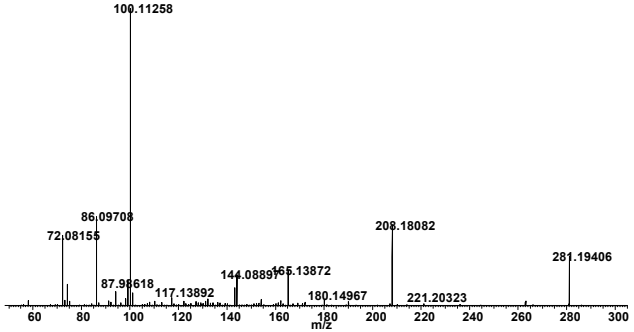
152. 2,4-PYRIDINEDIACARBOXYLIC ACID



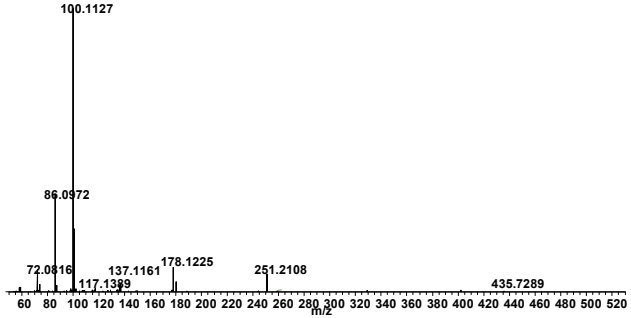
153. INDOLE-3-ACETATE



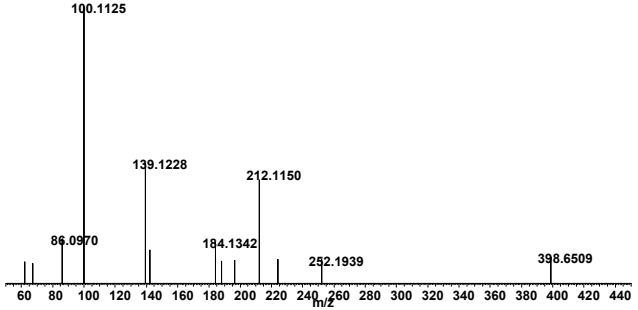
154. D-MANNOSAMINE/GLUCOSAMINE/GALACTOSAMINE



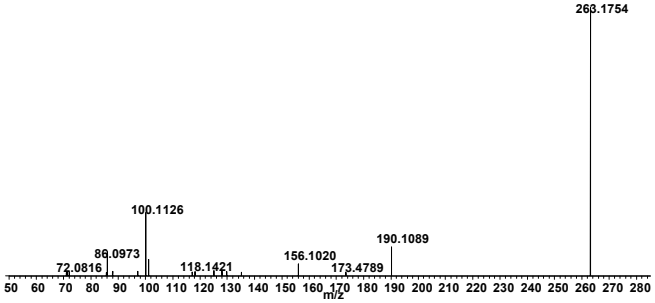
157. 2-METHYLCITRATE



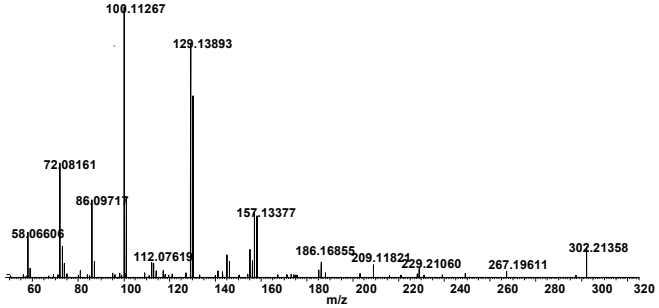
158. SELENOMETHIONINE



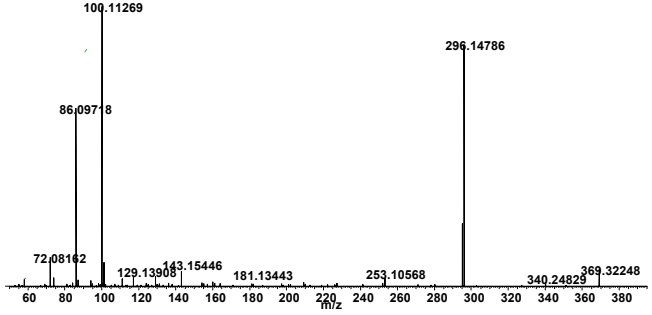
159. 4-AMINO ACETOPHENONE/ 4-COUMARATE



161. N-METHYLTRYPTAMINE

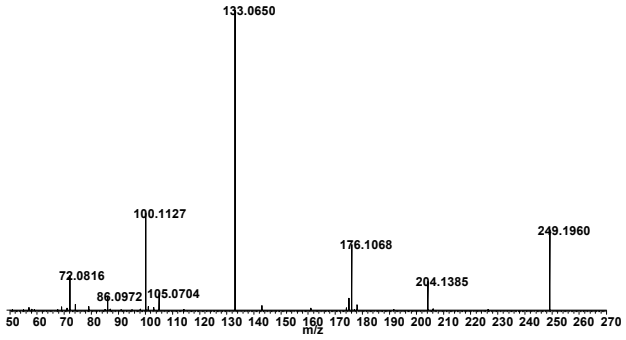


162. CYCLOHEXANE 1,2 DIAMINE

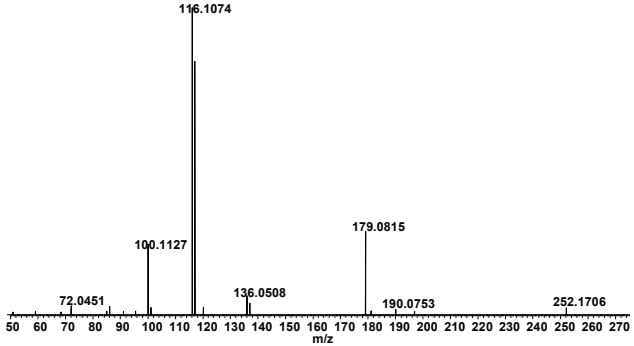


Supplementary Figure 19. MS/MS spectra for 250 derivatized metabolite standards

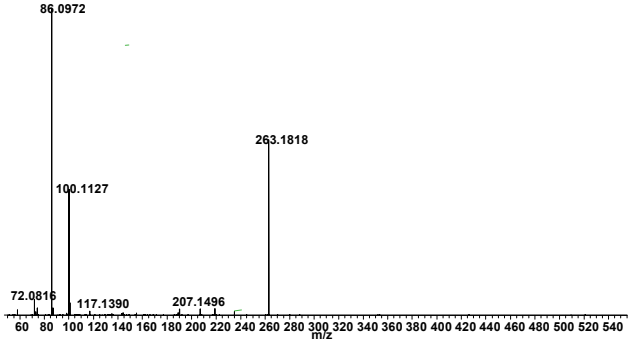
163. PHENETHYLAMINE



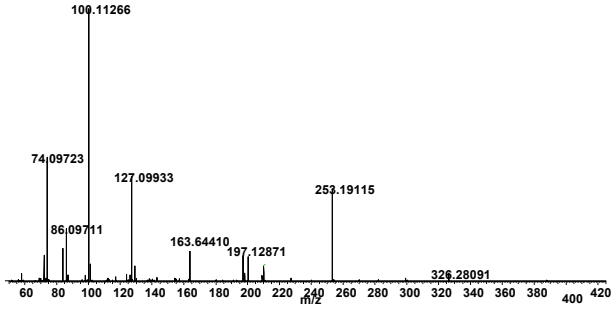
164. 3-HYDROXYANTHRANILATE



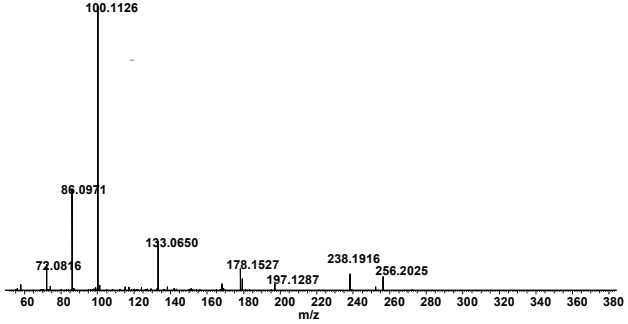
165. 3-DEHYDROSHIKIMATE



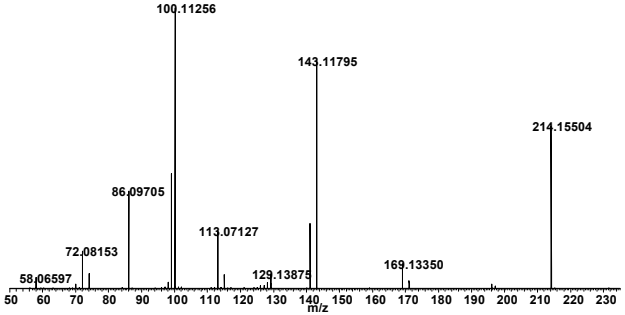
166. SEBACATE



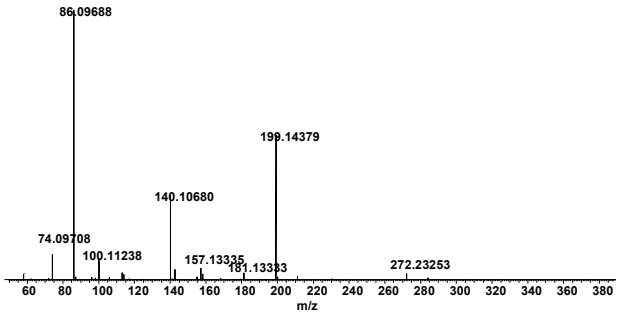
167. PIPECOLATE



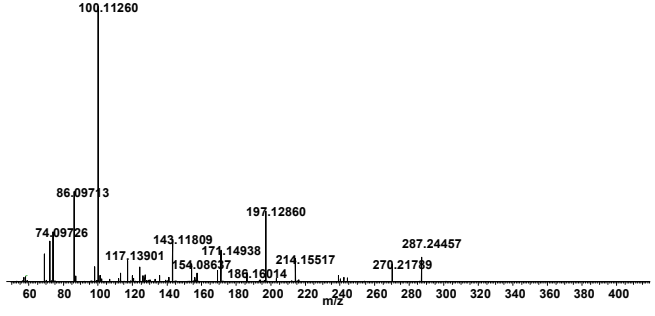
168. HEXANOATE



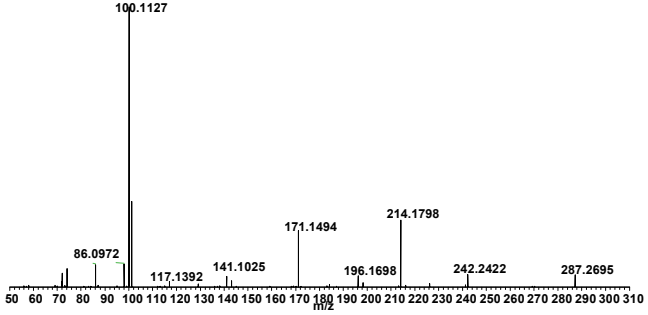
169. LEUCINE/ISOLEUCINE/NORLEUCINE



172. NORSPERMIDINE

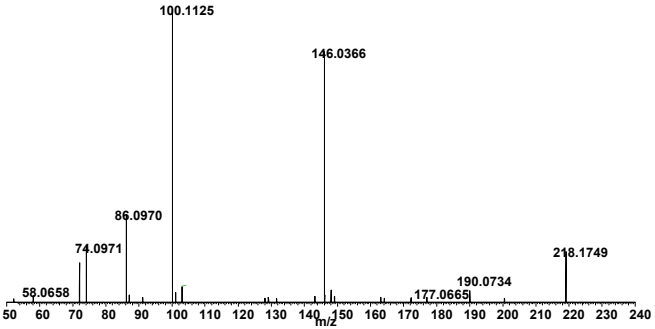


173. 10-HYDROXYDECANOATE

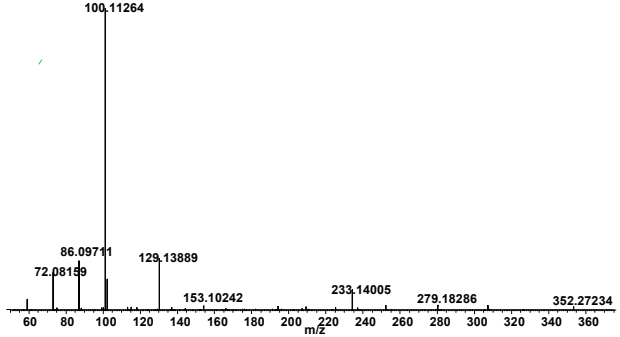


Supplementary Figure 20. MS/MS spectra for 250 derivatized metabolite standards

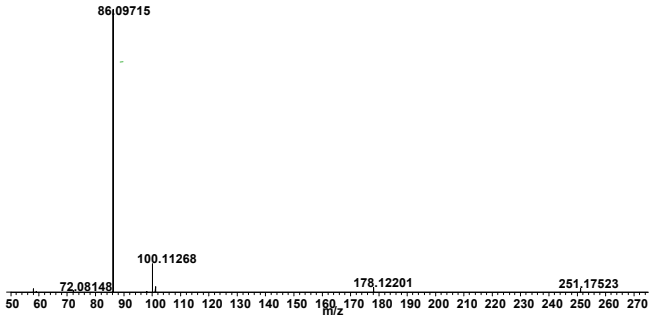
174. 2,3-BUTANEDIOL



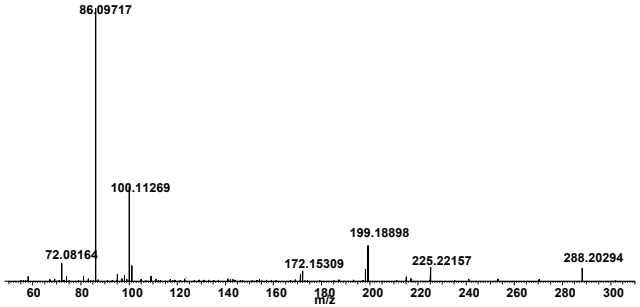
175. 4-IMIDAZOLEACETATE



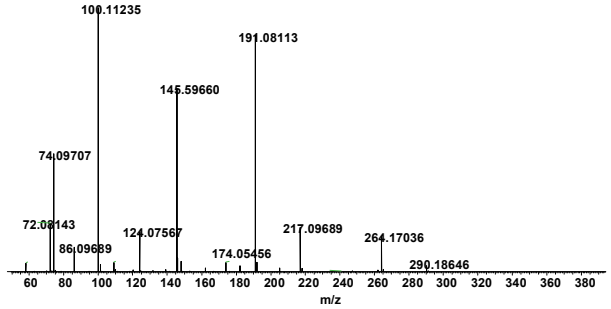
176. 2/3/P-HYDROXYPHENYLACETATE/MANDELATE



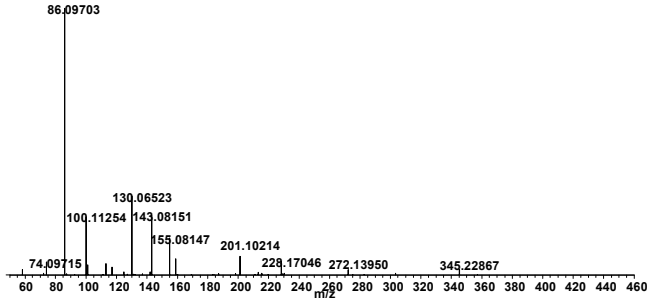
180. TRYPTAMINE



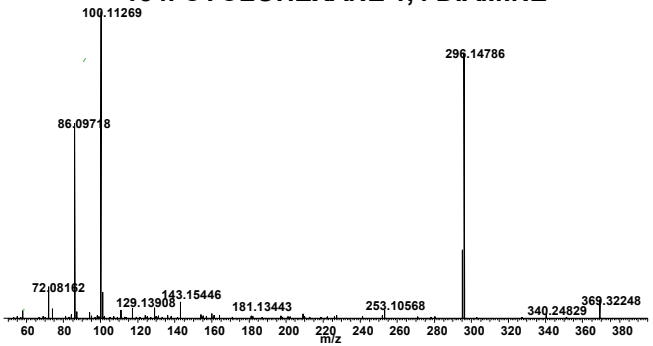
181. 4-AMINOBENZOATE/TRIGONELLINE



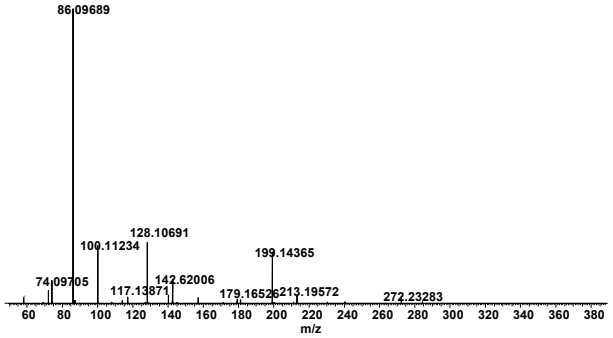
183. TRYPTOPHAN



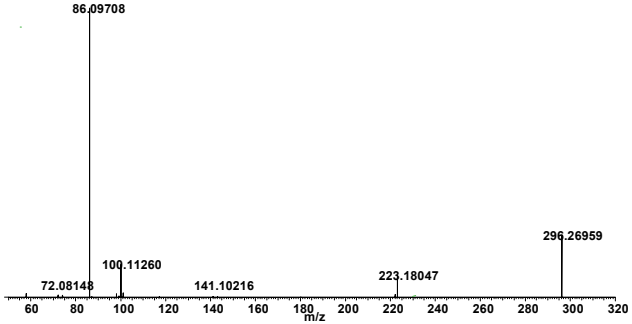
184. CYCLOHEXANE 1,4 DIAMINE



185. 6-AMINO CAPRIC ACID/6-CARBOXYHEXANOATE

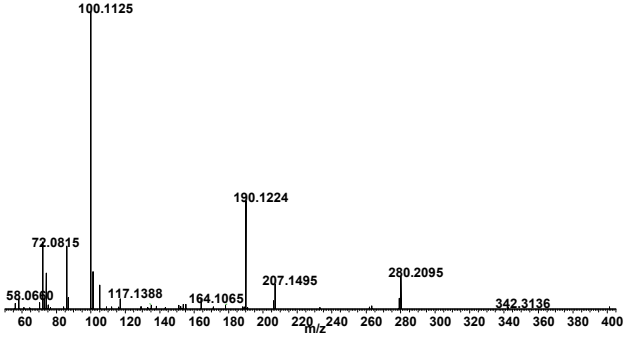


187. 1-CYCLOHEXYLPIPERAZINE

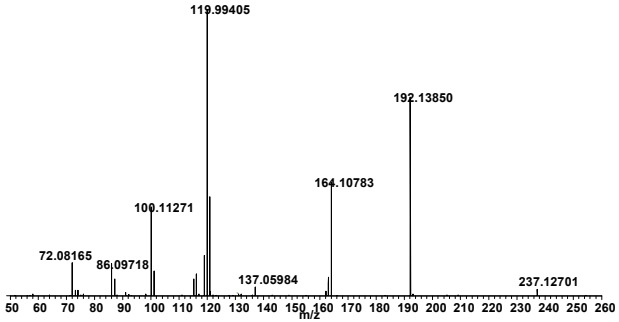


Supplementary Figure 21. MS/MS spectra for 250 derivatized metabolite standards

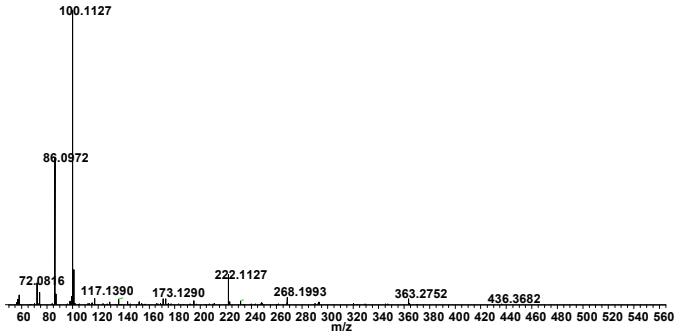
188. 3-SULFINOALANINE



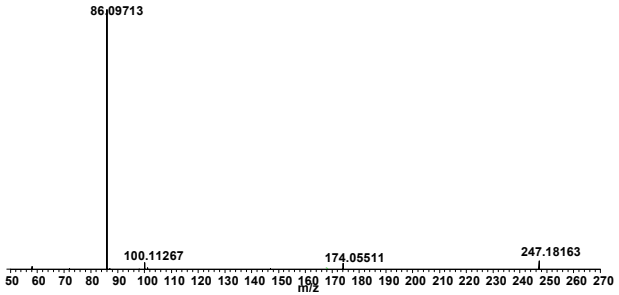
189. HYPOTAURINE



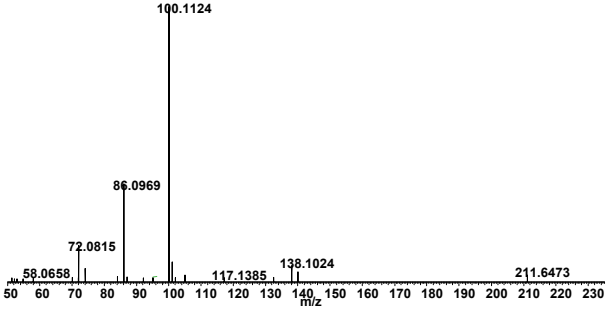
190. DOPAMINE



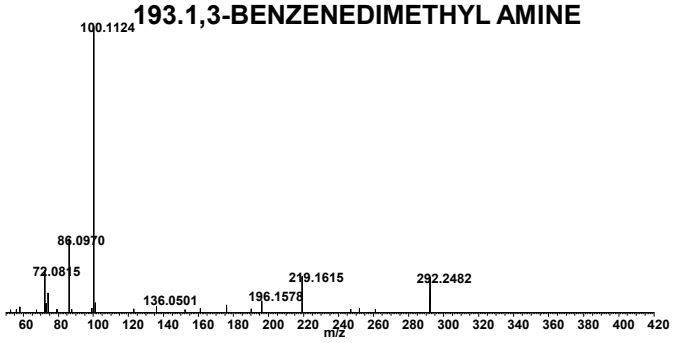
191. TRANS-CINNAMATE



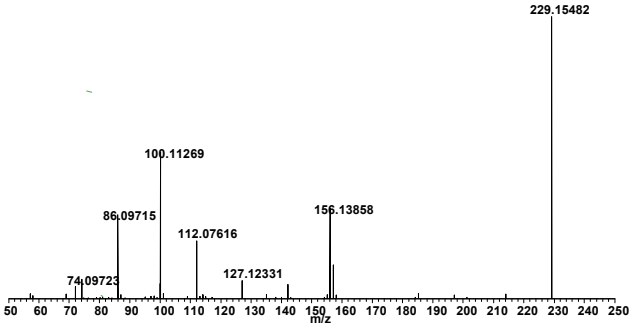
192. GLUCONATE



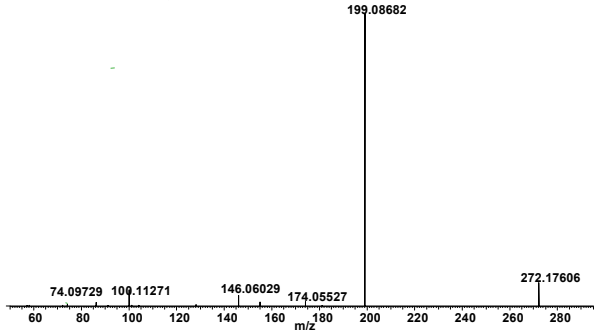
193.1,3-BENZENEDIMETHYL AMINE



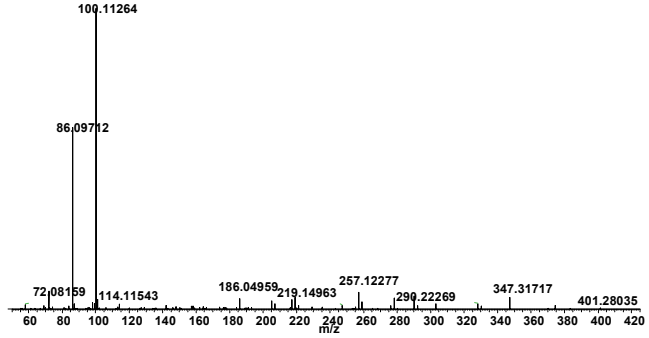
194. MONO METHYL FUMARATE



195. 4-QUINOLINECARBOXYLATE

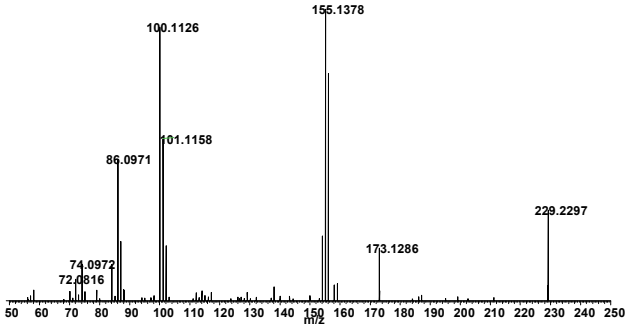


196. GUANIDINOSUCCINATE

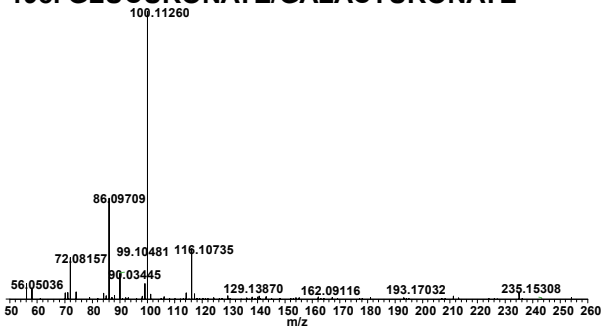


Supplementary Figure 22. MS/MS spectra for 250 derivatized metabolite standards

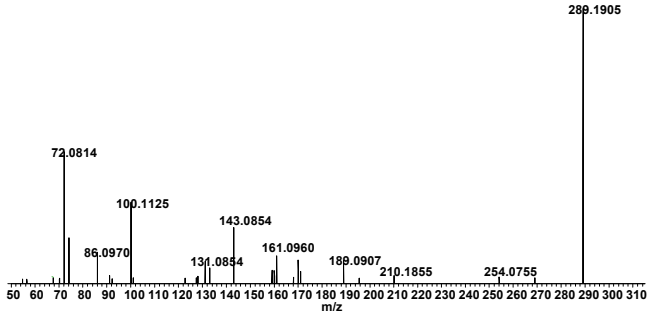
197. HEPTANOATE



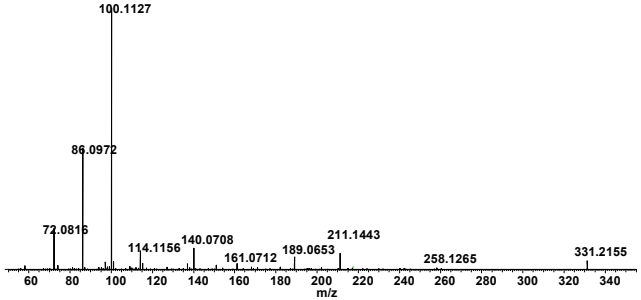
198. GLUCURONATE/GALACTURONATE



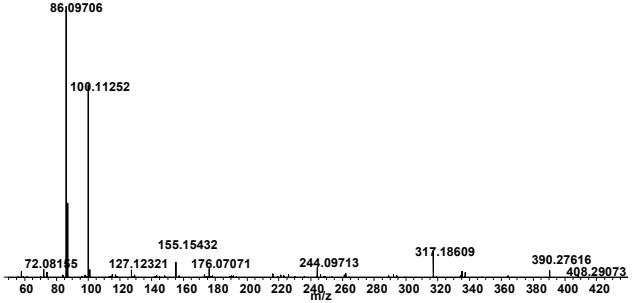
200. INDOLE-3-ETHANOL



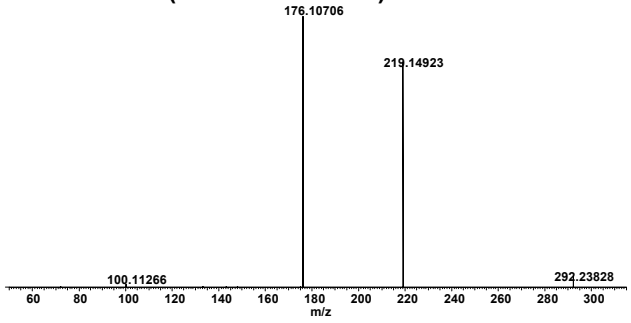
201. L-TRYPTOPHANAMIDE



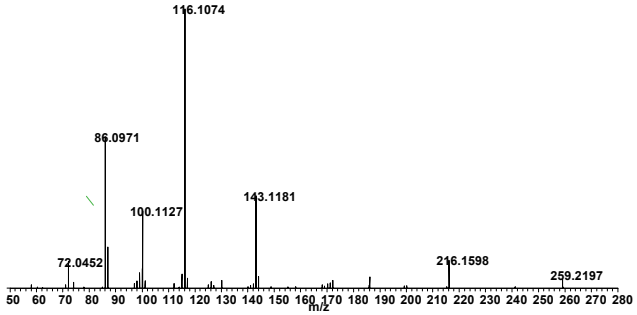
202. P-OCTOPAMINE



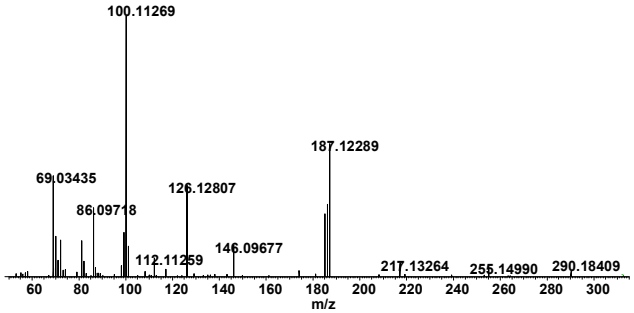
203. 4-(DIETHYLAMINO) BENZOIC ACID



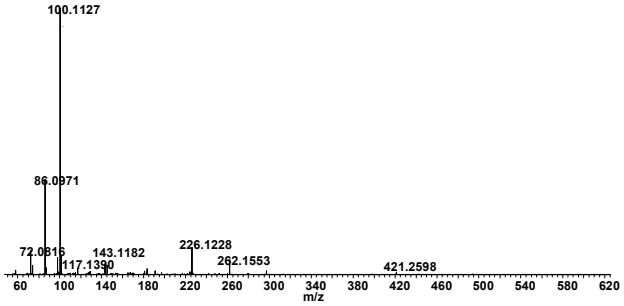
204. ETHYL 3-UREIDOPROPIONATE



205. 5-HYDROXYINDOLEACETATE

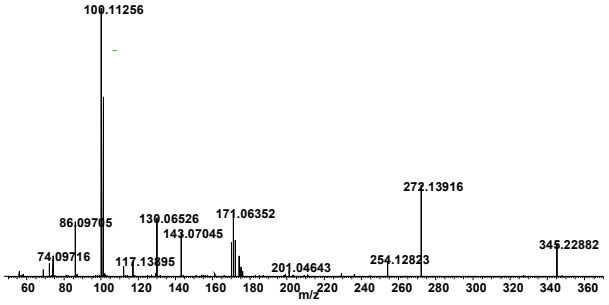


206. ANSERINE

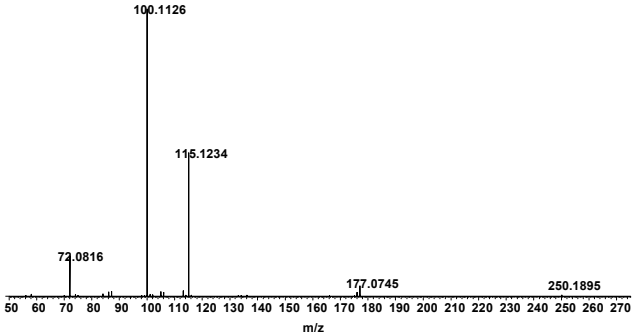


Supplementary Figure 23. MS/MS spectra for 250 derivatized metabolite standards

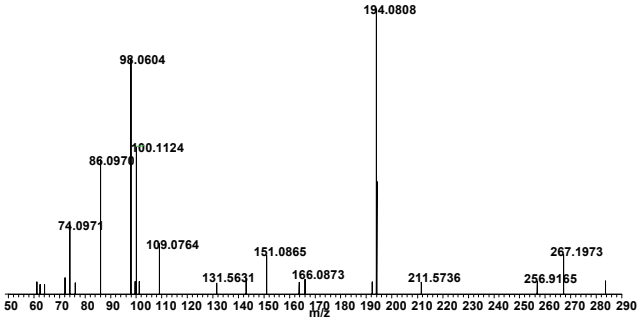
207. N-ACETYLTRYPTOPHAN



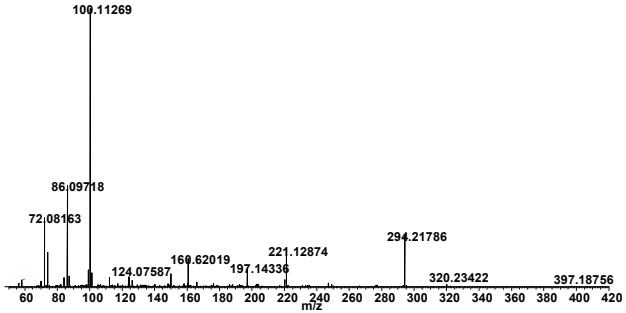
208. 1-PHENYLETHANOL



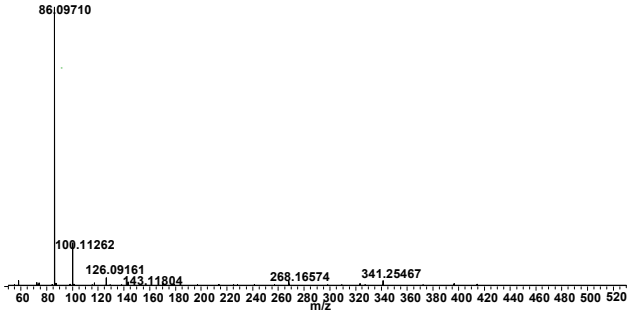
209. METHIONINE SULFOXIMINE



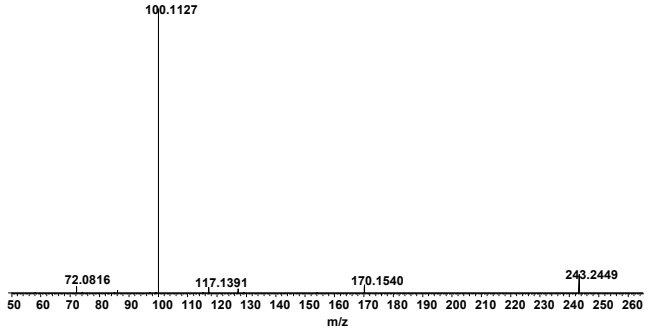
210. 4-HYDROXY-L-PHENYLGLYCINE



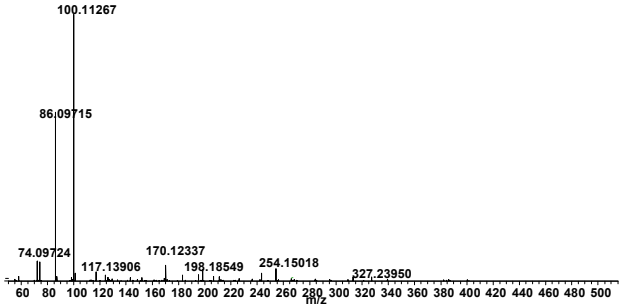
211. LYSINE



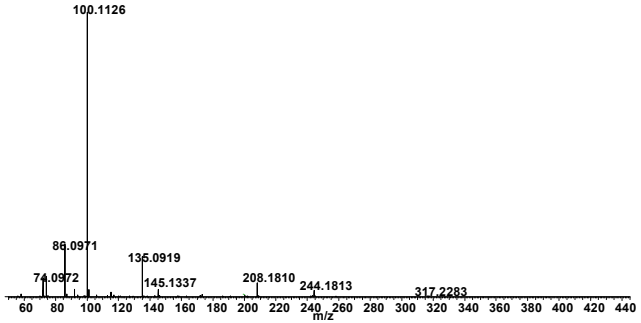
212. CAPRYLATE



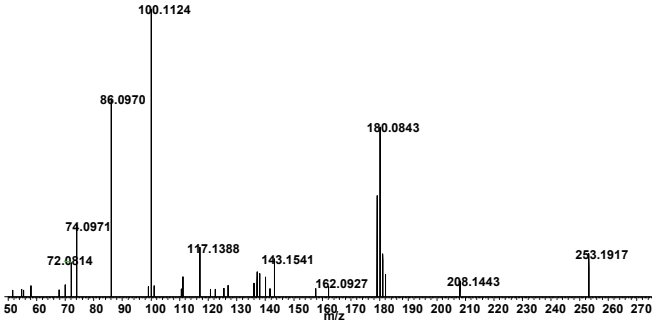
213. AMINOADIPATE



214. O-SUCCINYL-HOMOSERINE

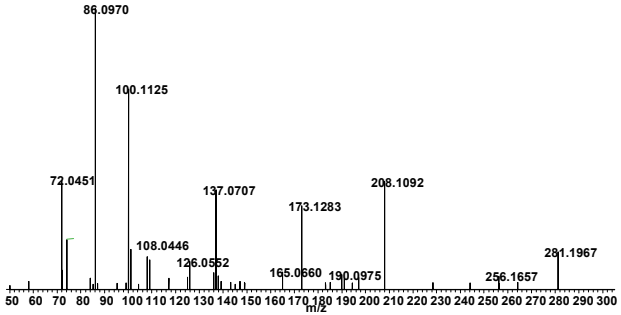


215. 3,5-DIAMINOBENZOIC ACID

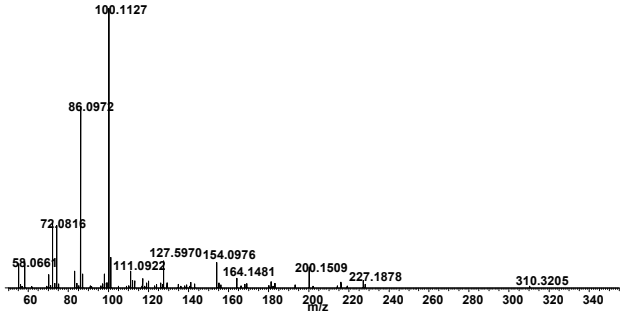


Supplementary Figure 24. MS/MS spectra for 250 derivatized metabolite standards

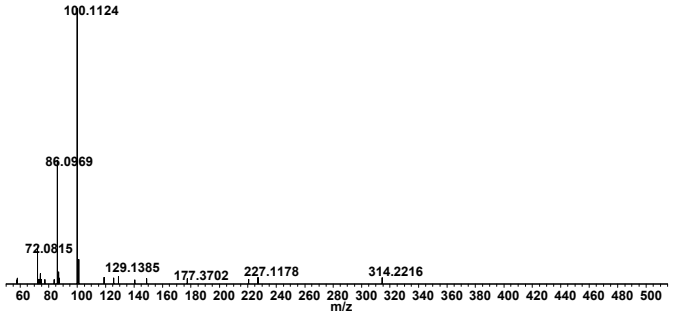
216. SALSOLINOL



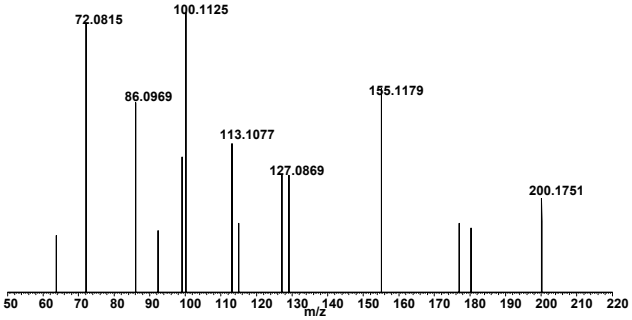
217. ITACONATE



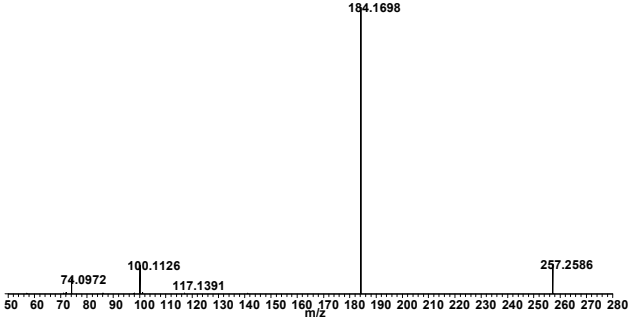
218. 3-HYDROXYMETHYLGLUTARATE



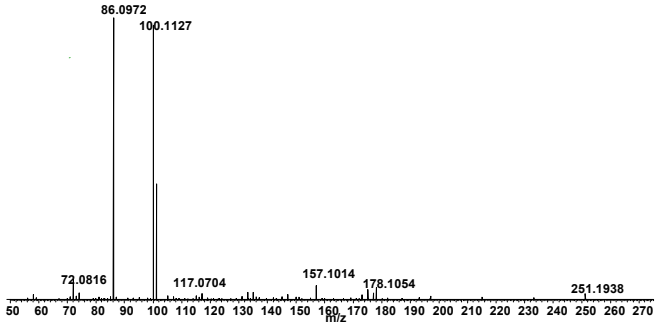
219. 1-AMINOCYCLOPROPANECARBOXYLATE



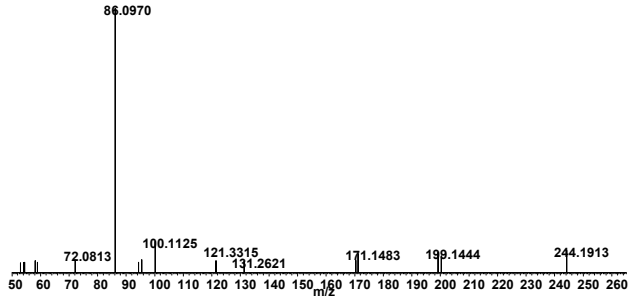
220. NONANOATE



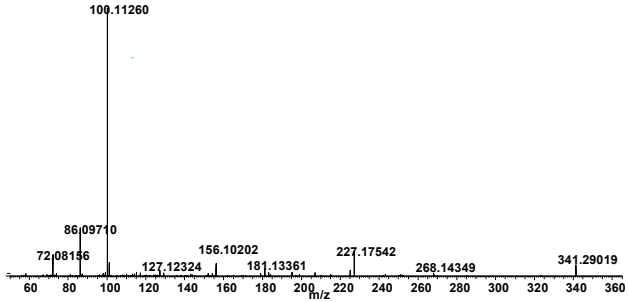
221. OXALOMALATE



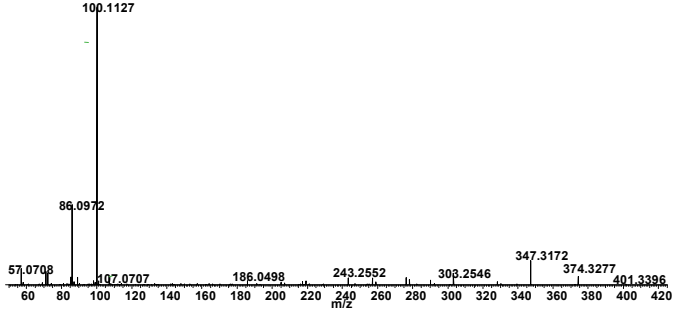
222. TRANS-4-CYCLOHEXANEDIOL



223. 3-METHYLGLUTACONATE

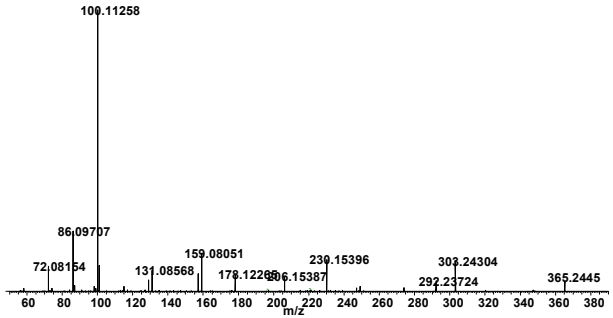


224. CITRULLINE

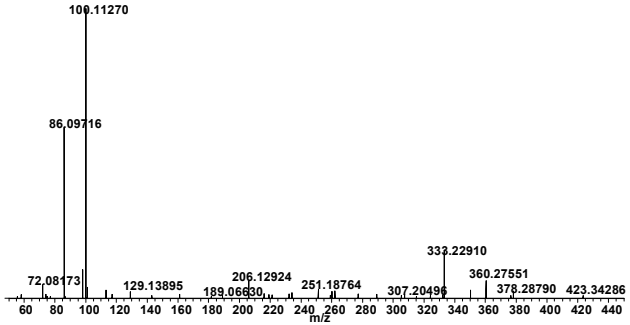


Supplementary Figure 25. MS/MS spectra for 250 derivatized metabolite standards

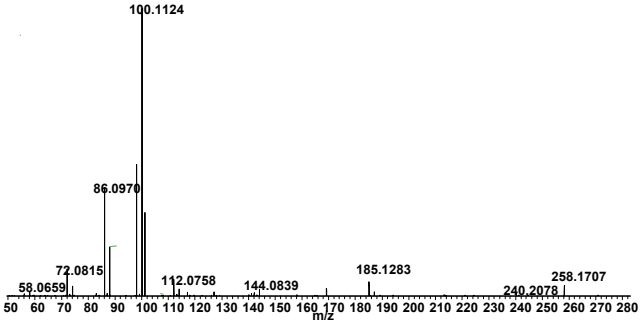
225. PYROCATECHOL/HYDROQUINONE



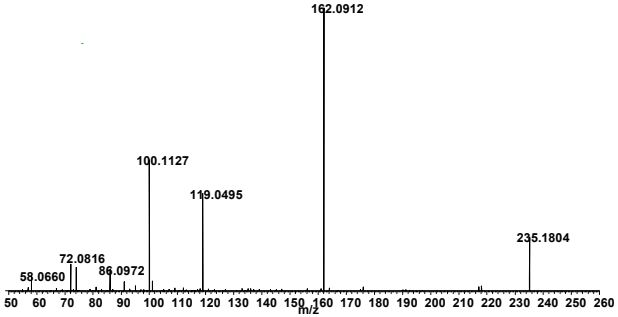
227. PORPHOBILINOGEN



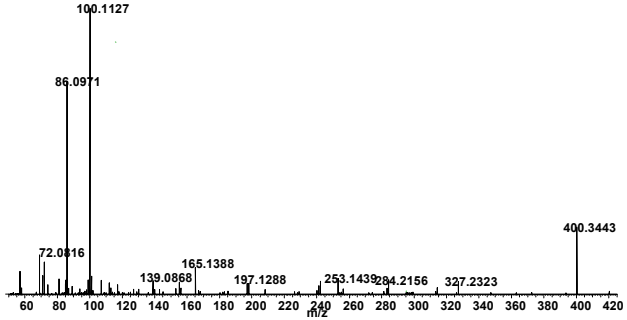
228. PANTOLACTONE



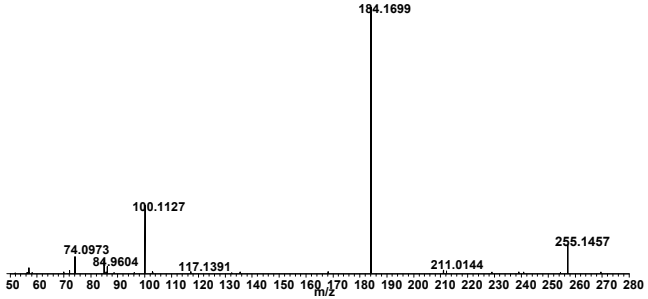
229. BENZYLAMINE



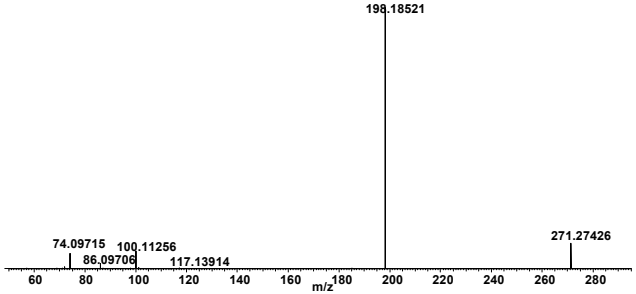
230. ARGININE



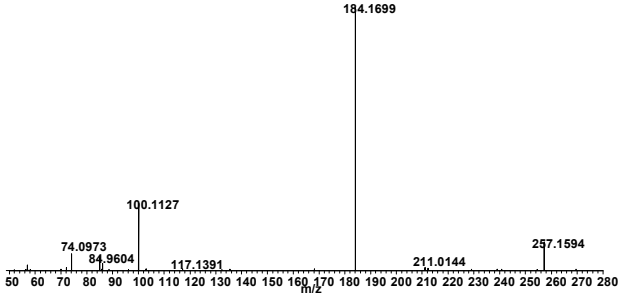
231. OROTATE



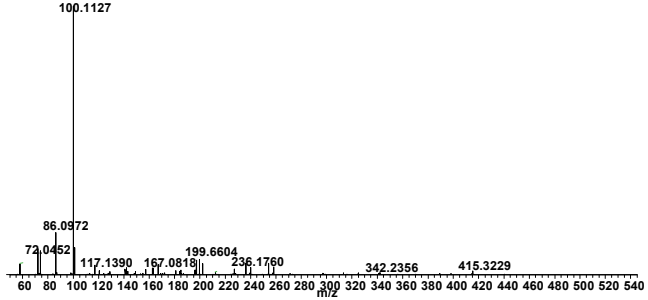
232. DECANOATE



233. DIHYDROOROTATE

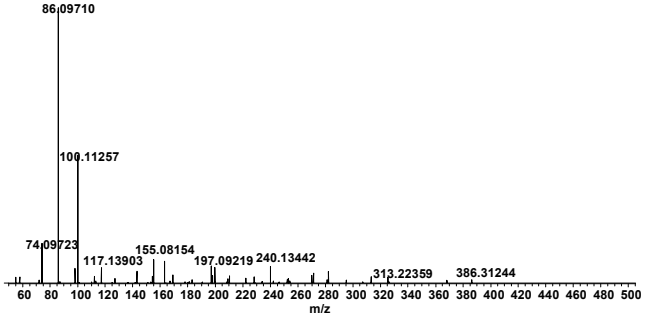


234. DIAMINOPIMELATE

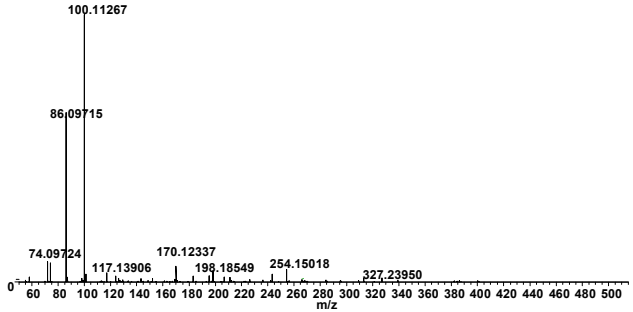


Supplementary Figure 26. MS/MS spectra for 250 derivatized metabolite standards

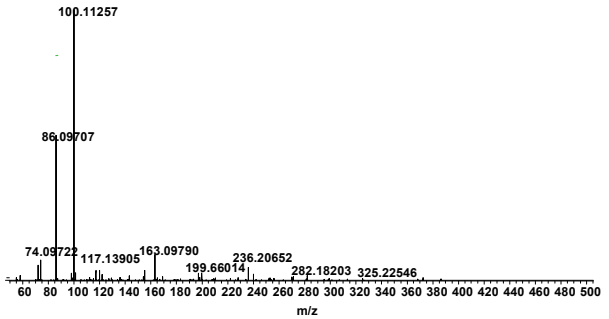
235. ASPARTATE



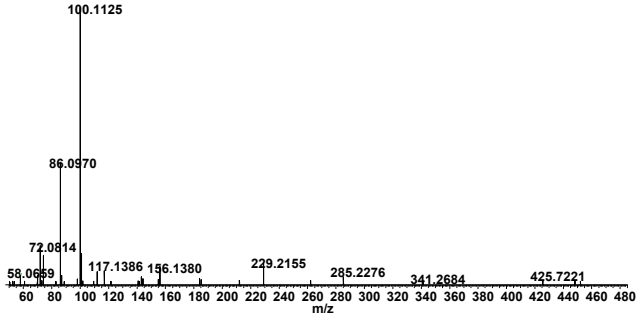
236. D-ORNITHINE



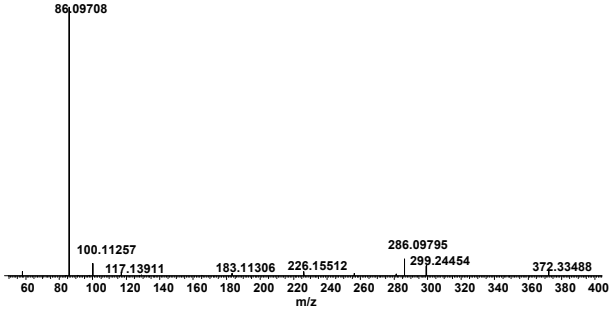
237. GLUTAMATE



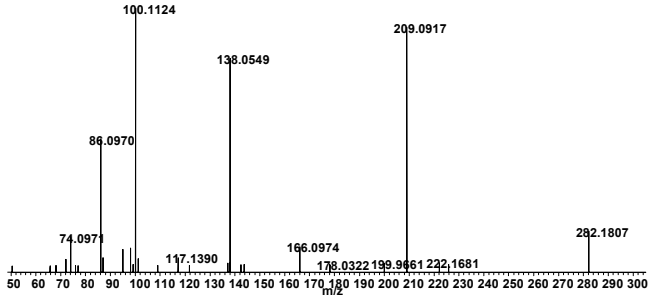
238. SPERMINE



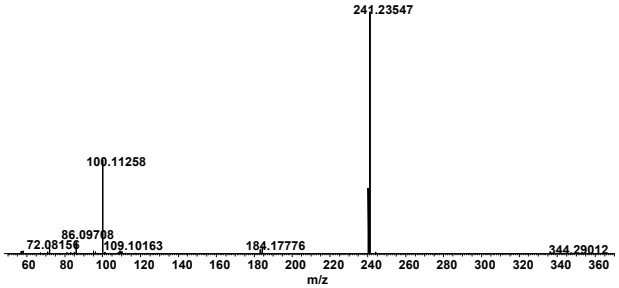
239. N1-ACETYLSPERMINE



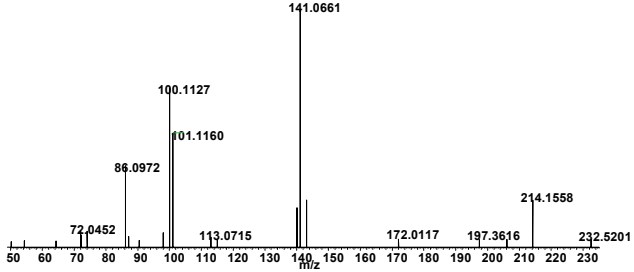
240. 4-PYRIDOXATE



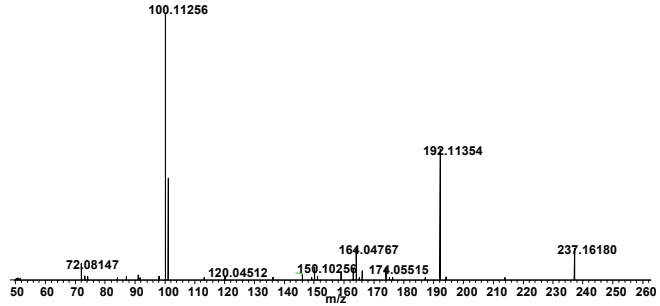
241. N-METHYLASPARTATE



242. MALEAMATE

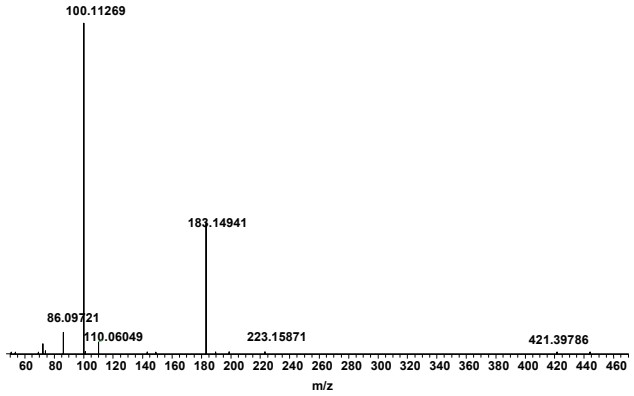


243. 4/3-HYDROXYBENZOATE/ SALICYLATE

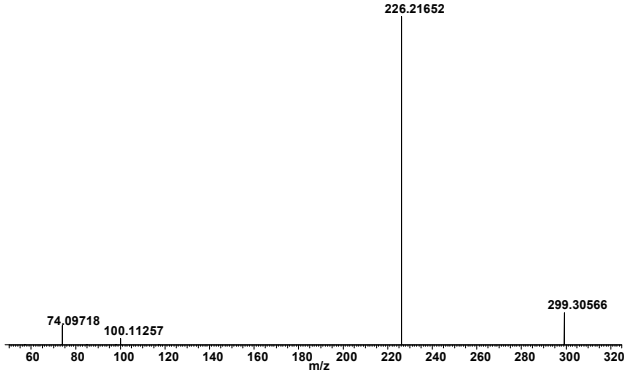


Supplementary Figure 27. MS/MS spectra for 250 derivatized metabolite standards

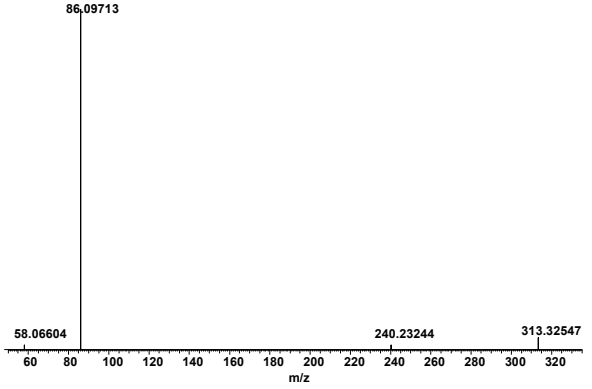
246. LAUROYLCARNITINE



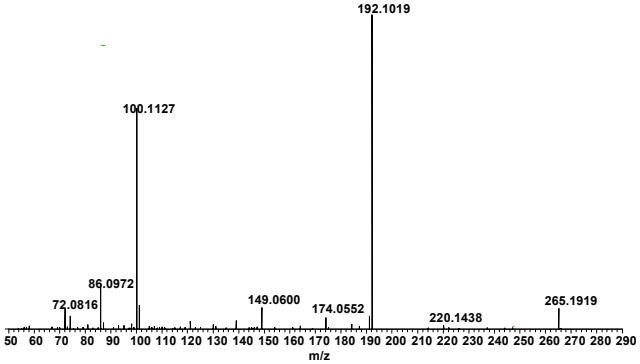
247. LAURATE



248. DODECYLAMINE



249. TYRAMINE



250. TETRADECYLAMINE