

Supporting Information Analytical Methods

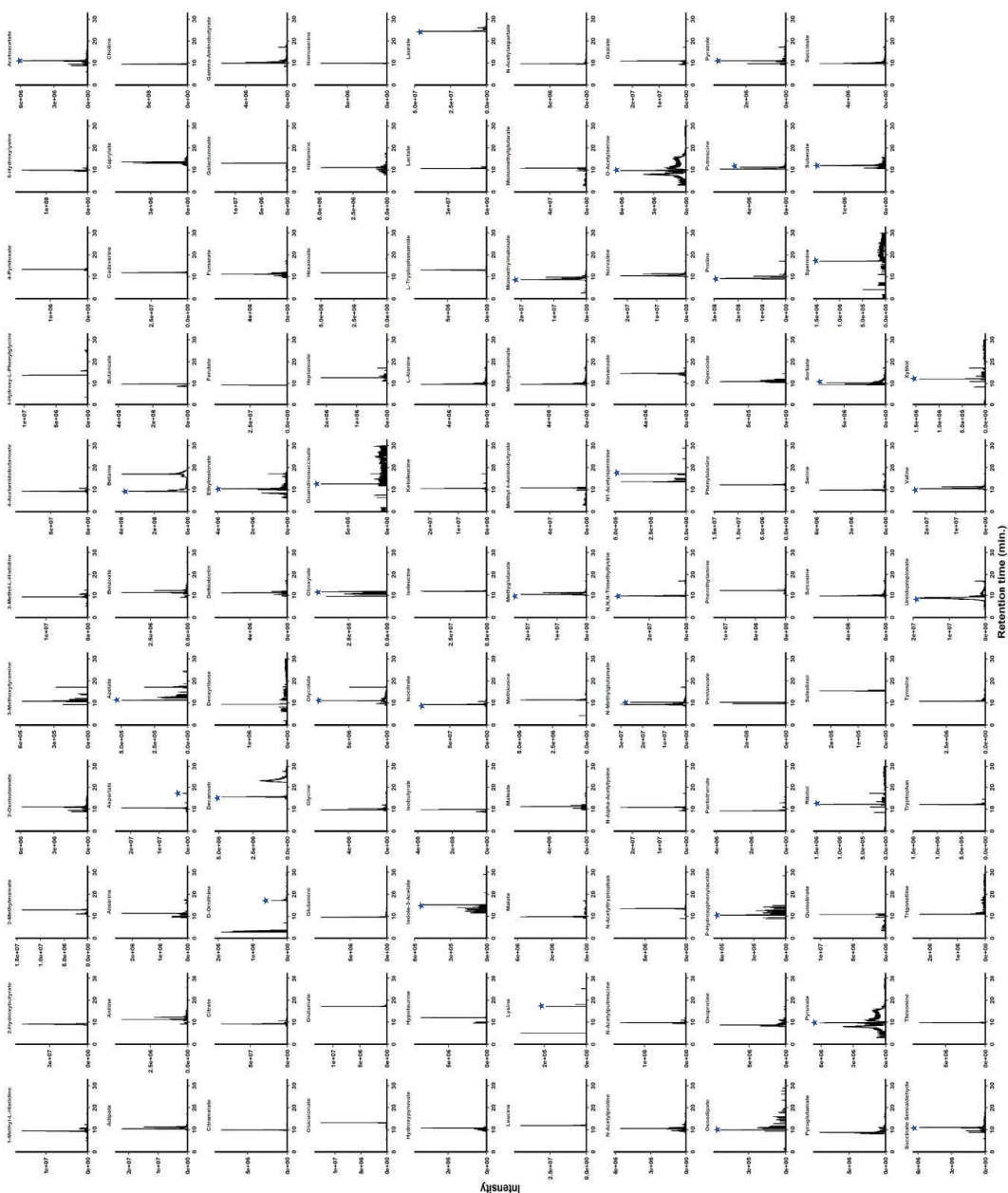
Analysis of Endogenous Metabolites using Multifunctional Derivatization and Capillary RPLC-MS

Julius Agongo,^{*a} Michael Armbruster^b, Christopher Arnatt^c and James Edwards^d

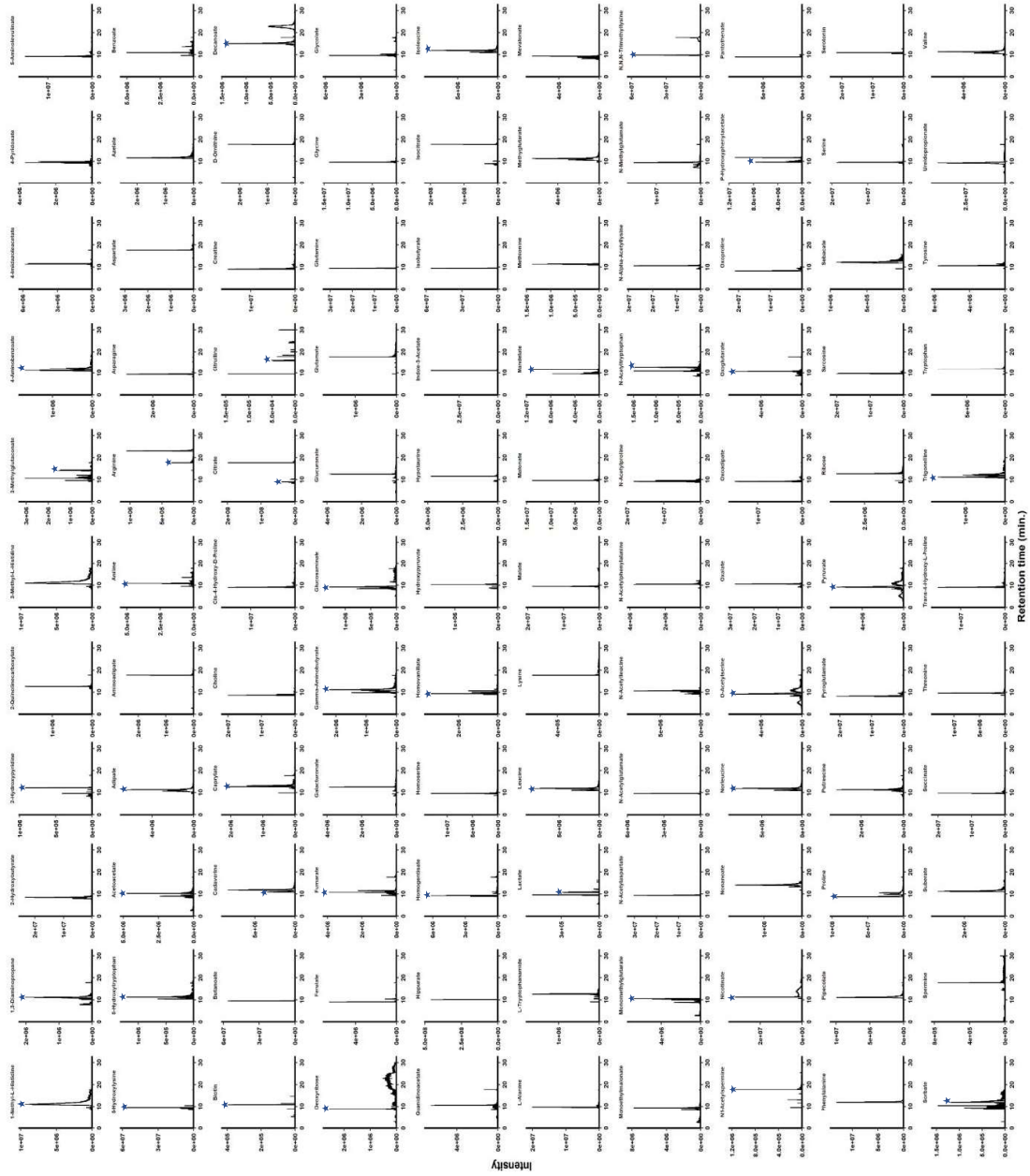
Department of Chemistry and Biochemistry, Saint Louis
University,
3501 Laclede Ave, St Louis, MO, 63103, USA

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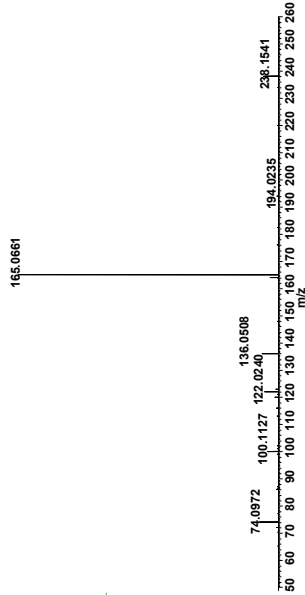
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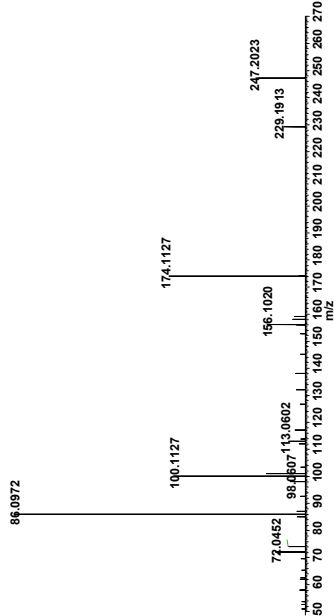
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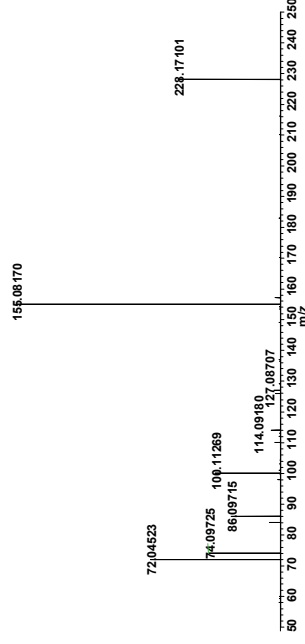
1. 6-HYDROXYNICOTINATE



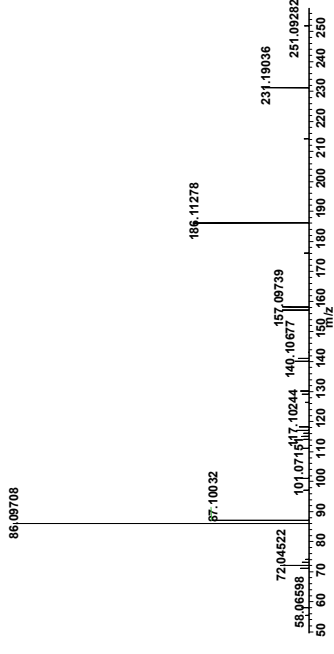
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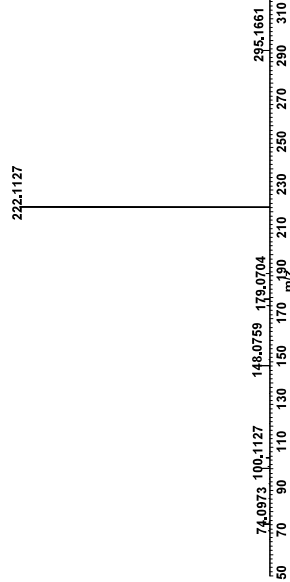
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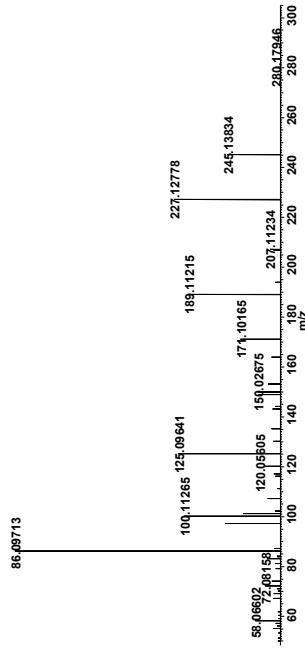
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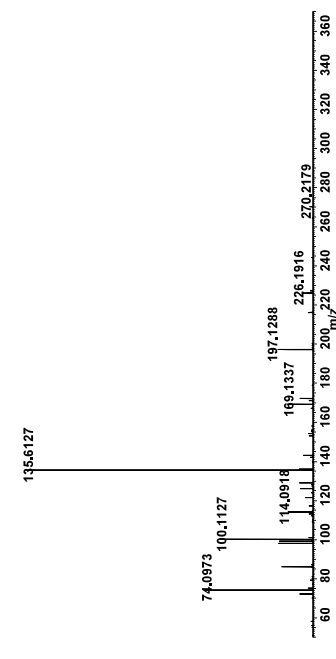
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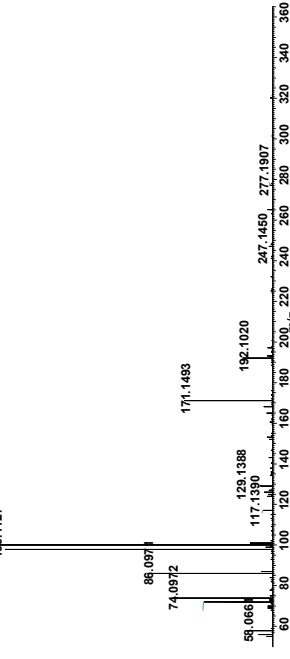
4. RIBITOL/XYLITOL



8. GUANIDINOACETATE



11. PROLINE

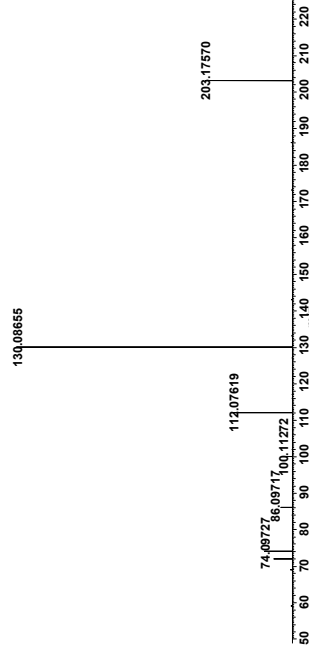


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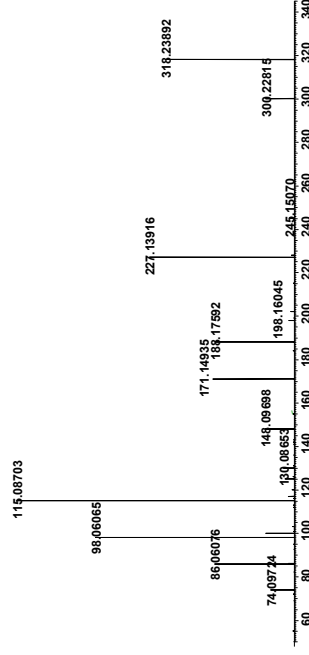


Supplementary Figure 6. MS/MS spectra for 250 derivatized metabolite standards

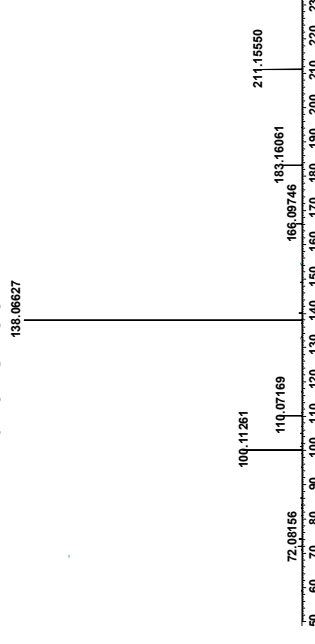
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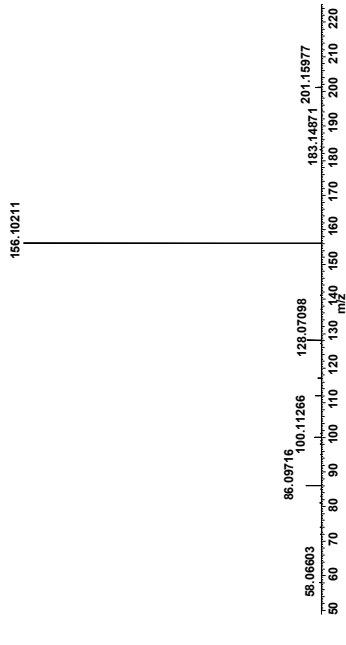
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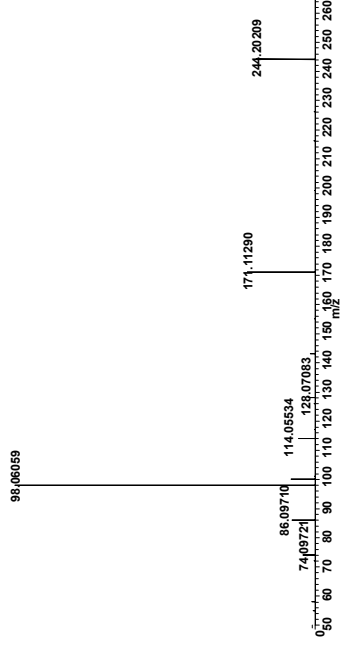
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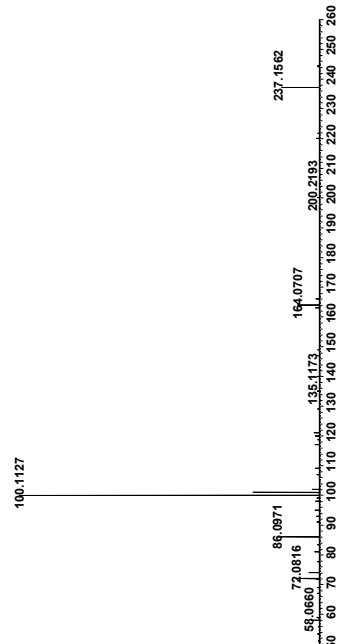
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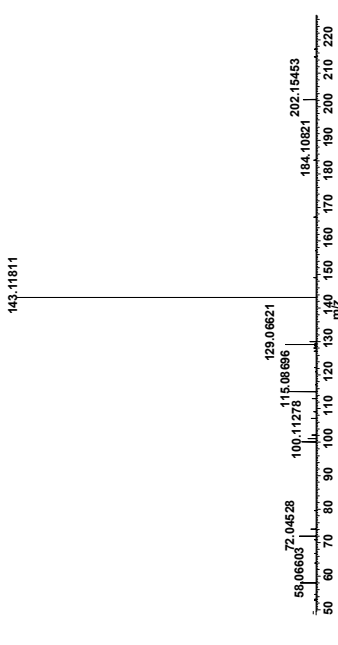
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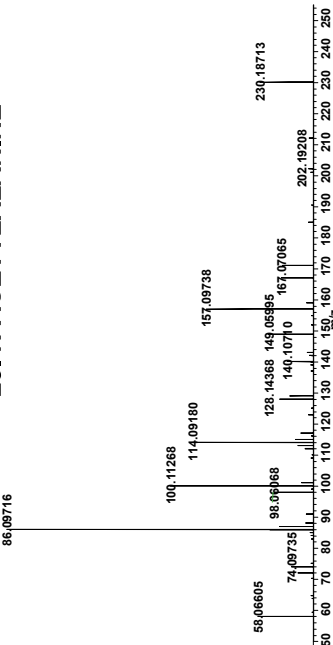
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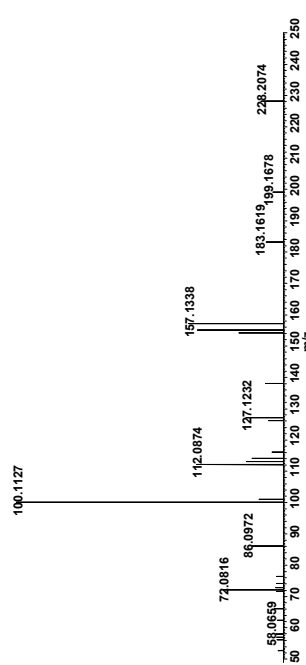
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23. N-ACETYLALANINE

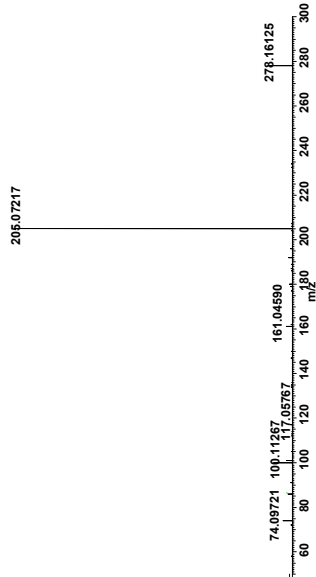


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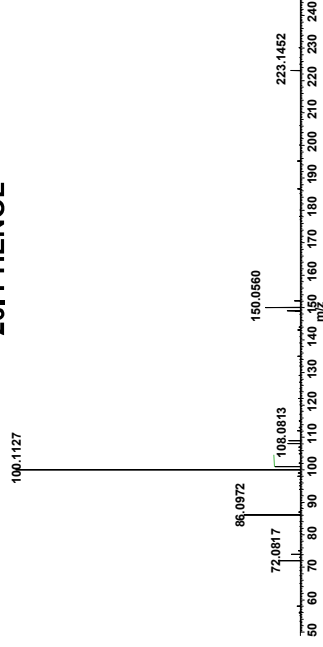


Supplementary Figure 7. MS/MS spectra for 250 derivatized metabolite standards

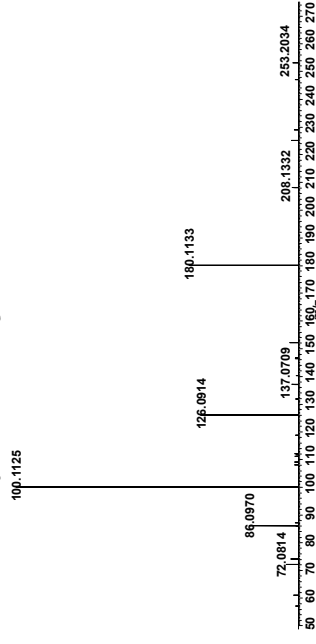
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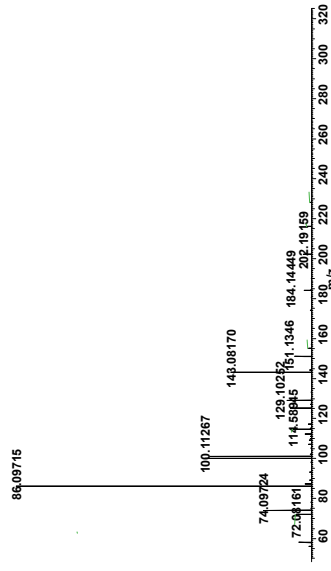
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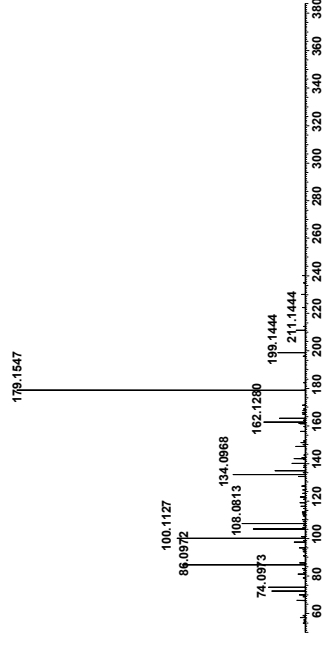
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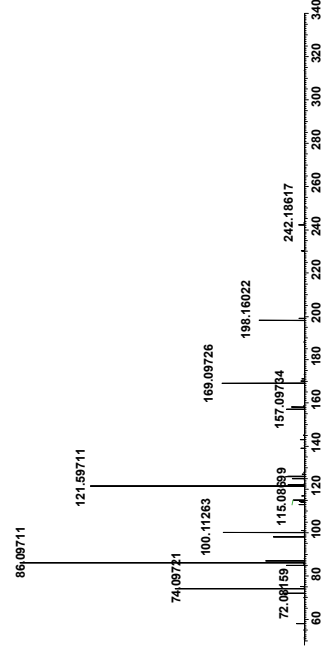
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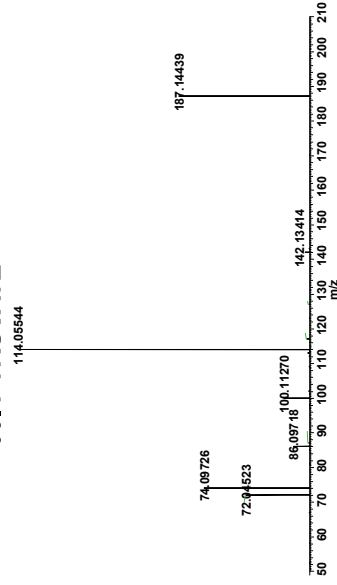
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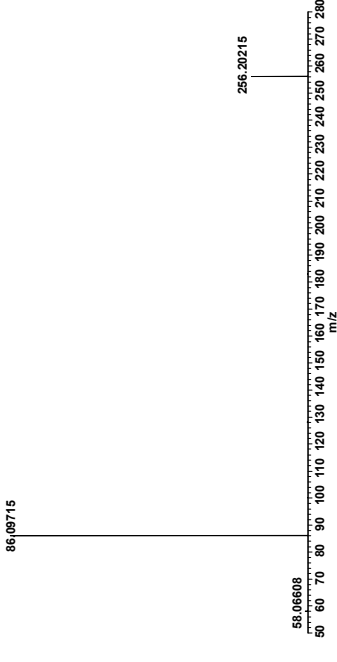
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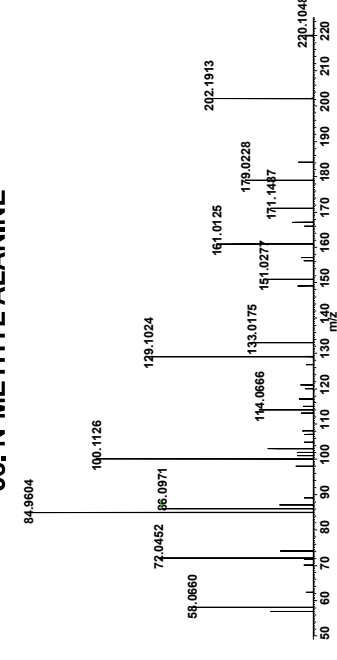
33. PYRUVATE



34. N-ACETYLPROLINE

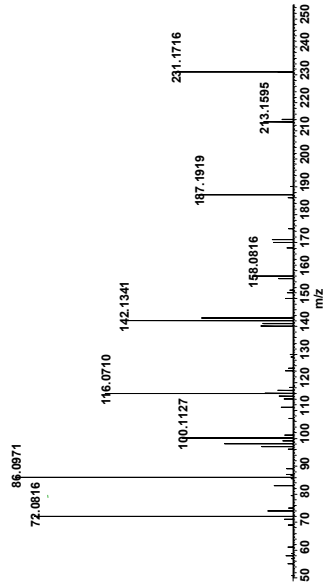


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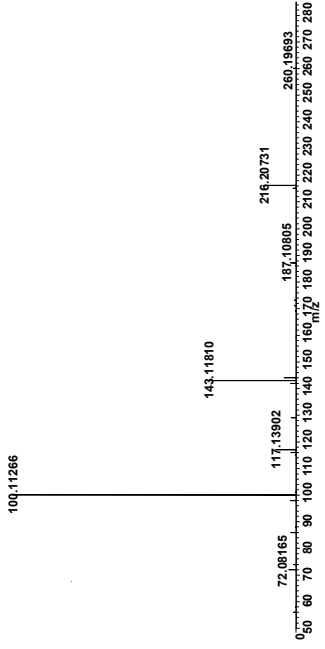


Supplementary Figure 8. MS/MS spectra for 250 derivatized metabolite standards

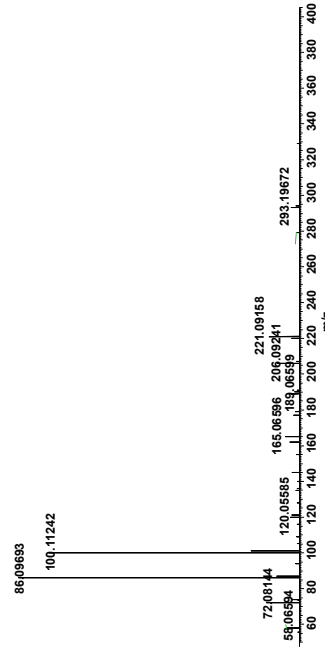
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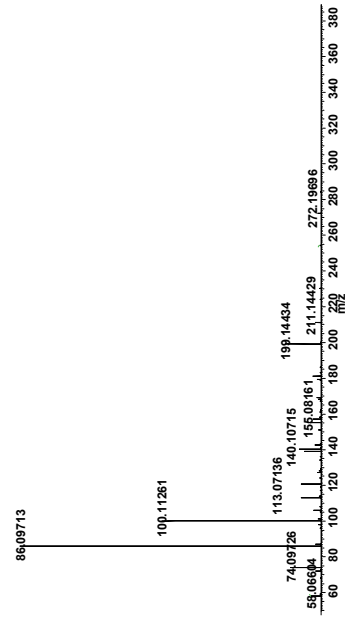
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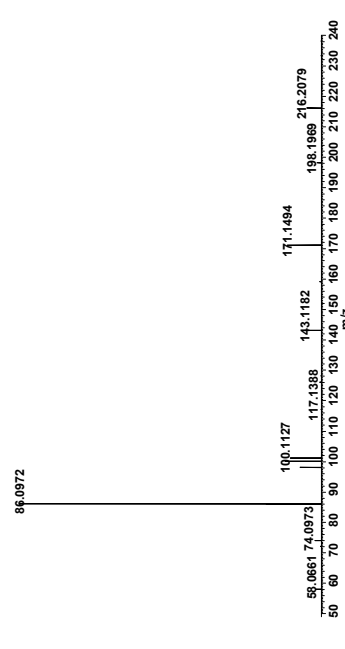
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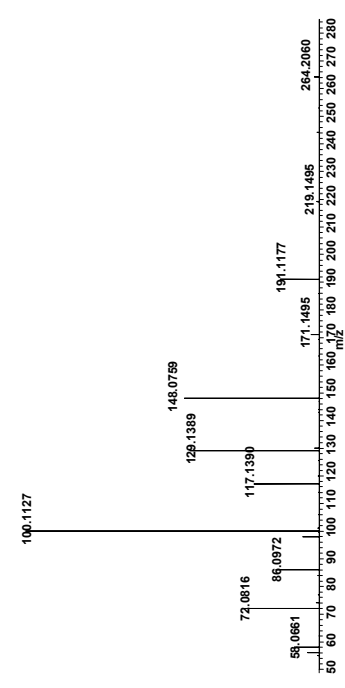
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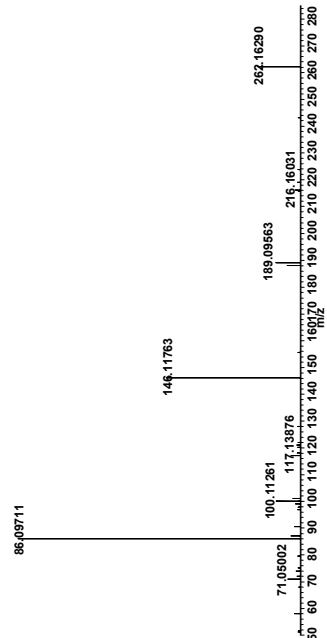
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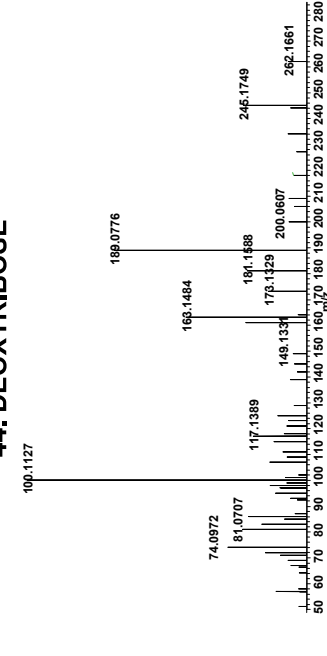
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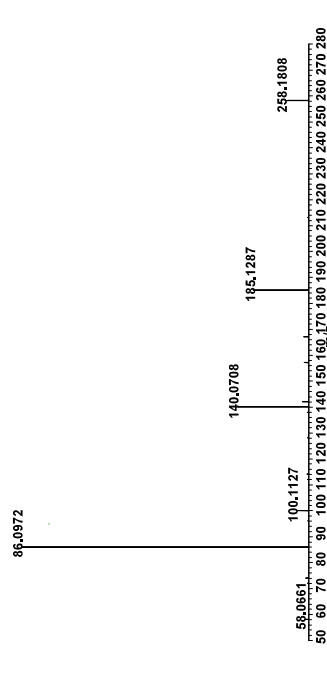
43. HISTIDINOL



44. DEOXYRIBOSE

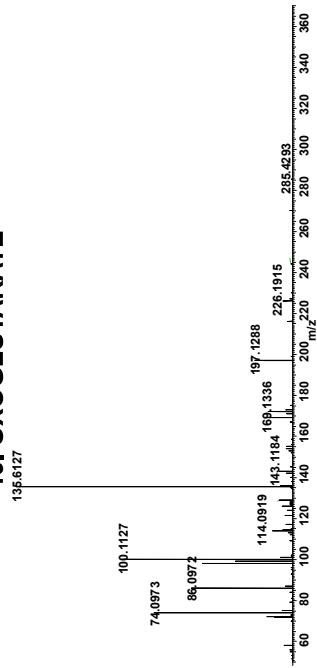


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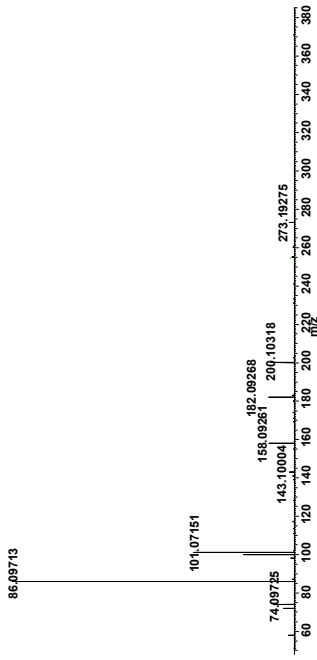


Supplementary Figure 9. MS/MS spectra for 250 derivatized metabolite standards

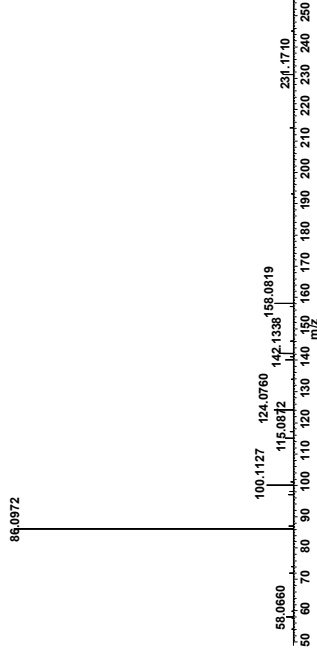
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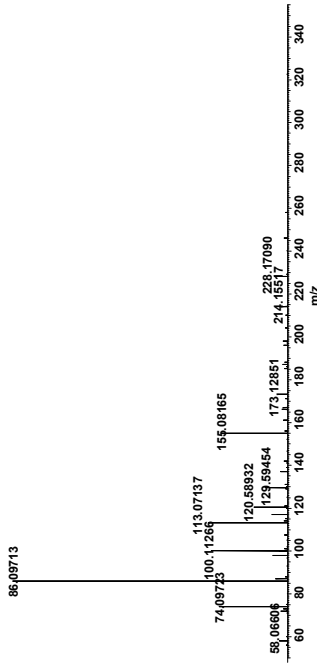
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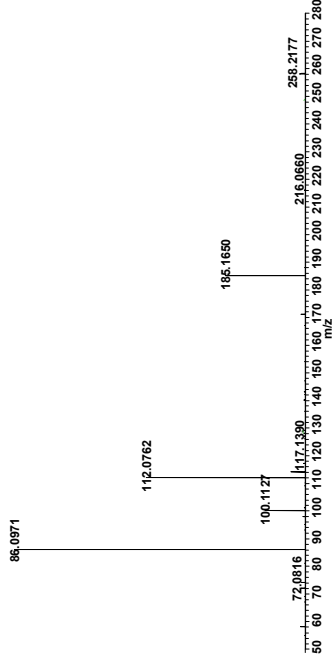
49. MONOETHYLMALONATE



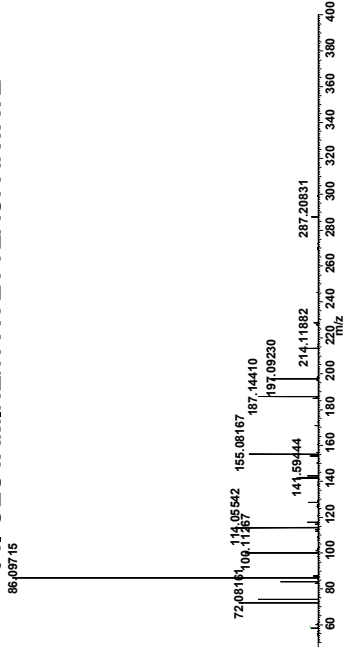
50. SERINE/MALATE



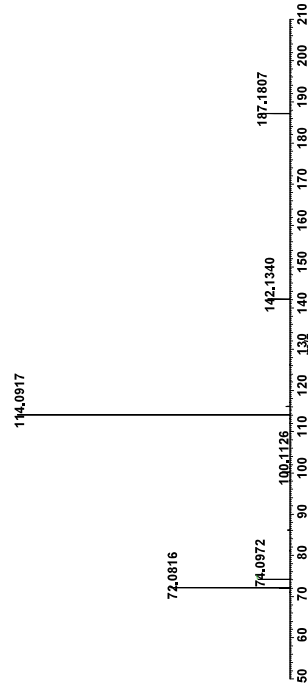
52. N-ACETYLPUTRESCINE/ 5-HYDROXYLYSINE



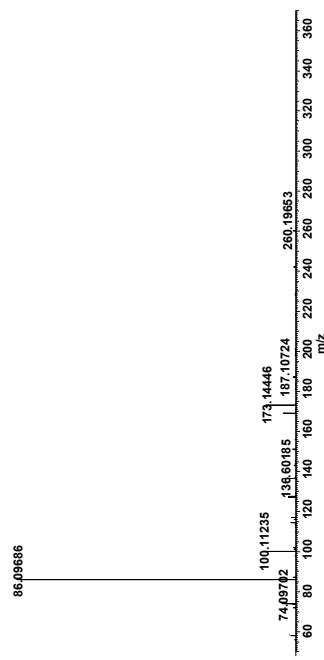
54. GLUTAMINE/N-ACETYLASPARTATE



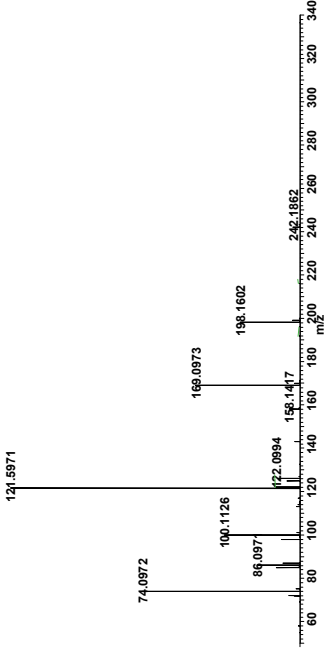
56. ISOBUTYRATE/BUTANOATE



58. THREONINE/ALLOTHREONINE/HOMOSERINE

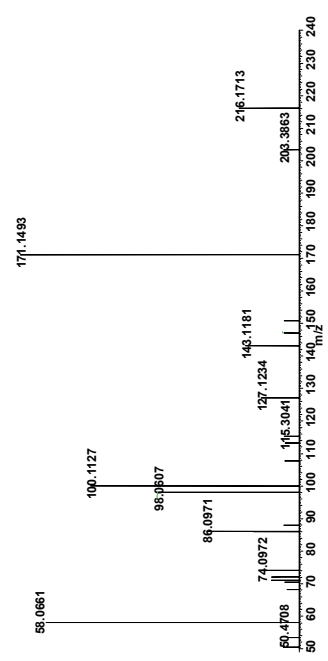


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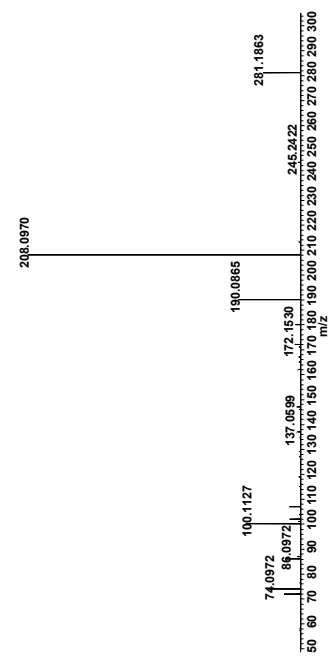


Supplementary Figure 10. MS/MS spectra for 250 derivatized metabolite standards

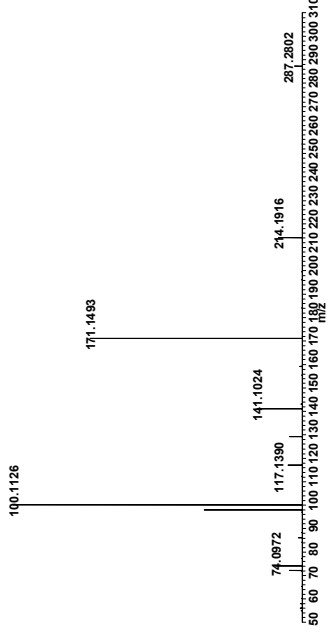
62. N-ACETYLGLYCINE



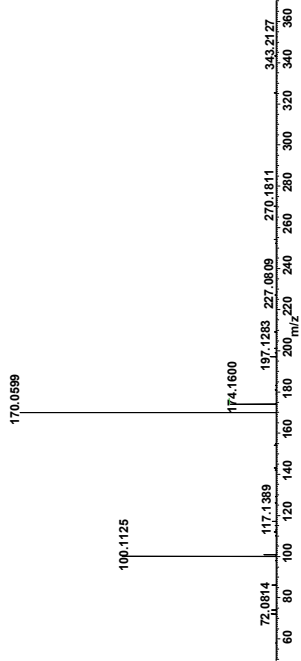
63. HOMOVANILLATE/ HYDROXYPHENYLLACTATE



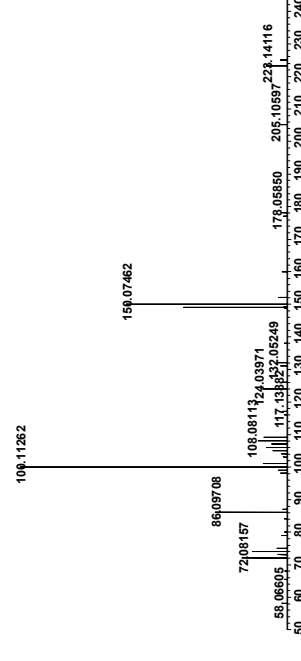
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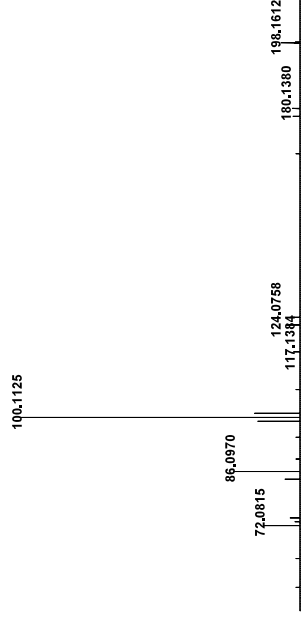
66. BIOTIN



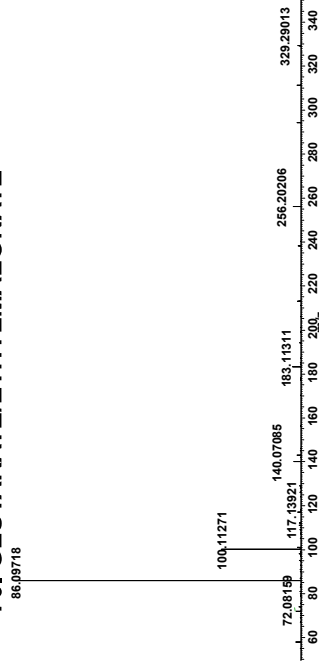
67. 2-HYDROXYPYRIDINE



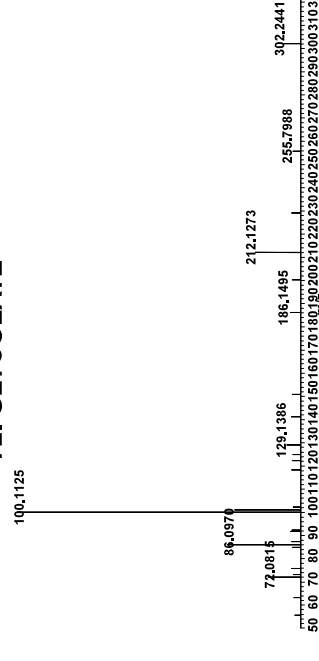
68. 1/3-METHYL-L-HISTIDINE



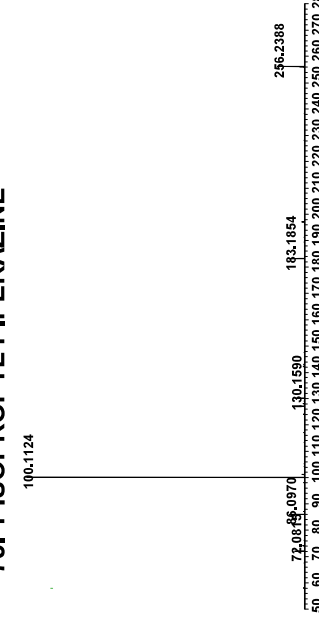
70. GLUTARATE/ETHYLMALONATE



72. GLYCOLATE

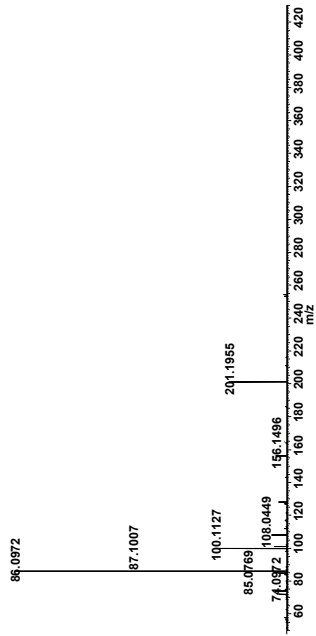


73. 1-ISOPROPYL PIPERAZINE

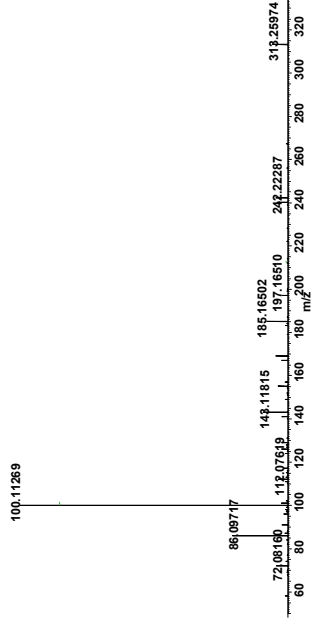


Supplementary Figure 11. MS/MS spectra for 250 derivatized metabolite standards

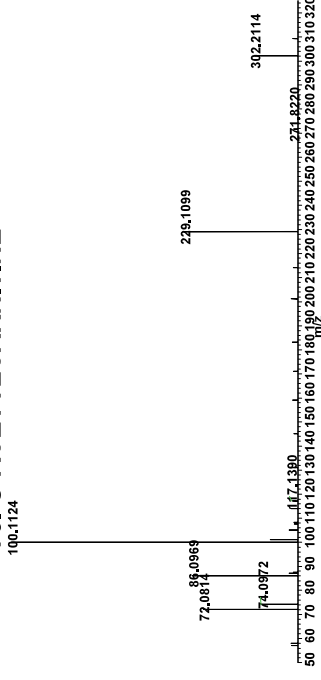
74. BUTYLAMINE/ PENTANOATE



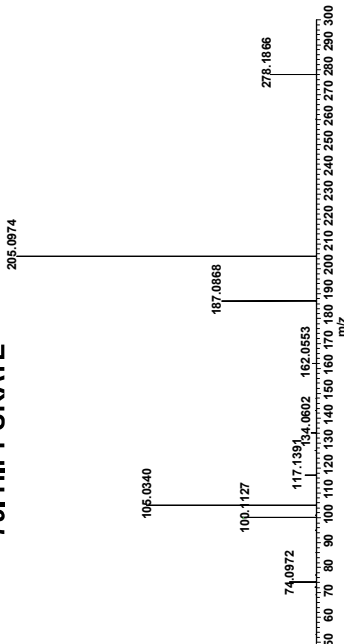
76. DETHIOBIOTIN/MALEATE



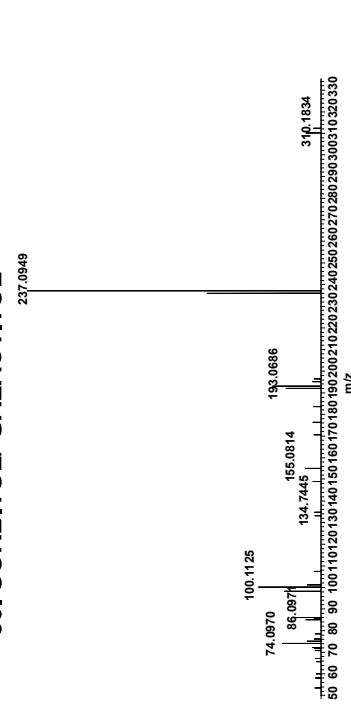
78. O-ACETYL CARNITINE



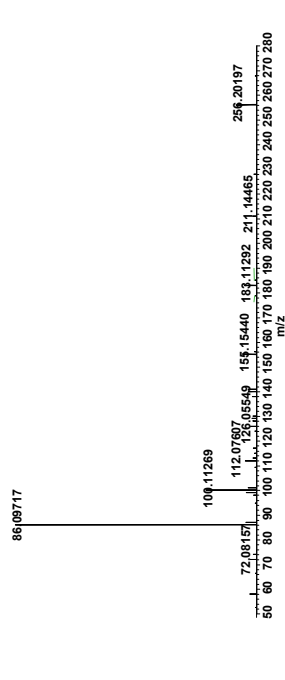
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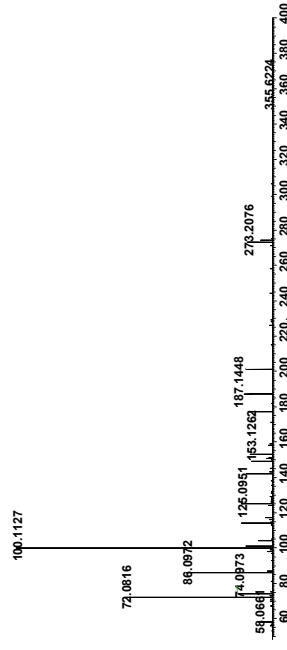
80. SORBITOL/ GALACTITOL



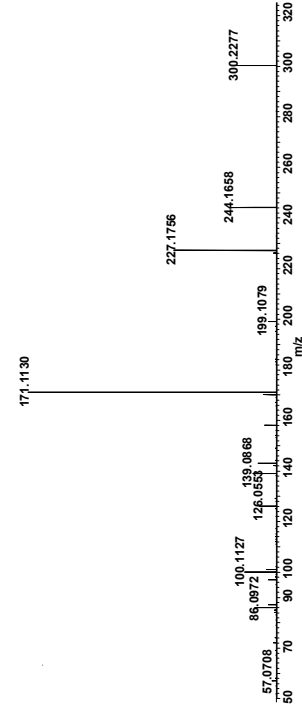
82. 1,3-DIAMINOPROPANE/AMINOISOBUTANOATE



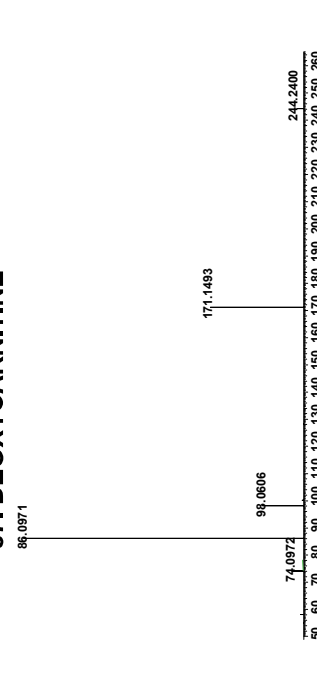
84. N-ACETYL SERINE/ O-ACETYL SERINE



86. GLYOXYLATE

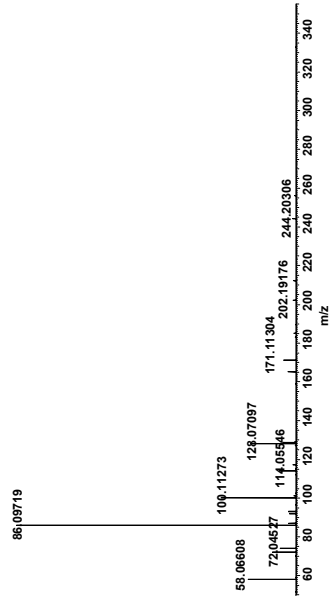


87. DEOXYCARNITINE

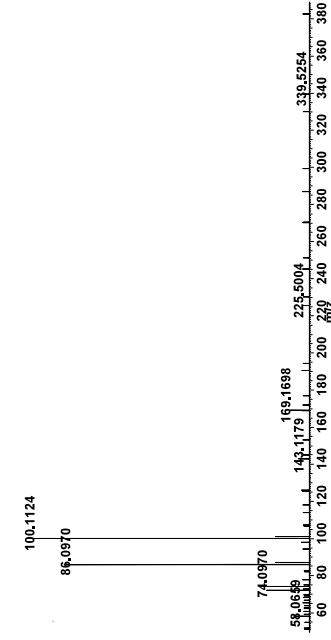


Supplementary Figure 12. MS/MS spectra for 250 derivatized metabolite standards

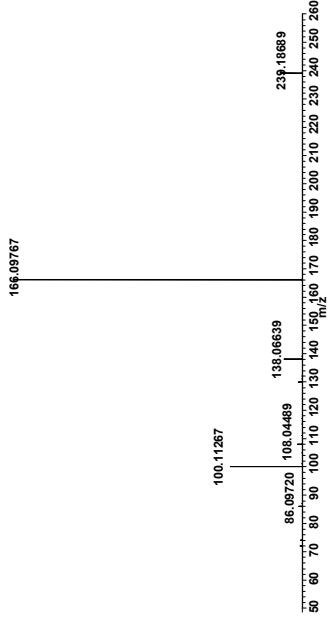
88. GAMMA-AMINO BUTYRATE/2-AMINOISOBUTYRATE



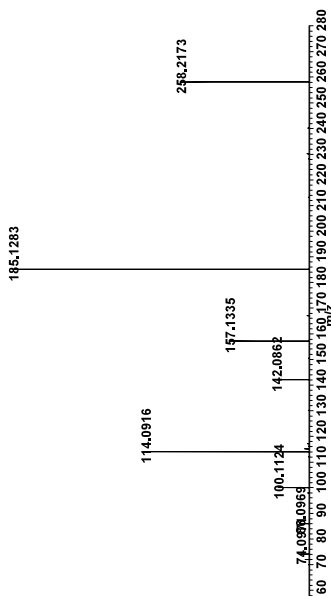
90. CADAVERINE



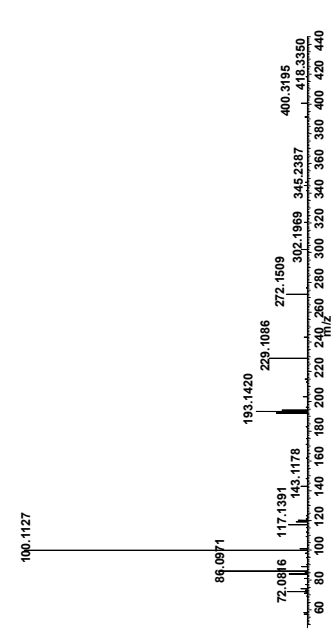
91. HISTAMINE



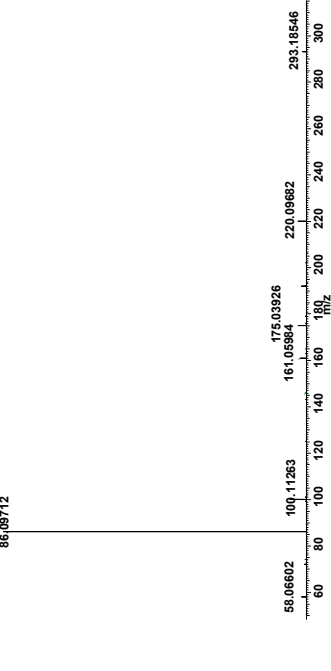
N-ACETYLPUTRESCINE



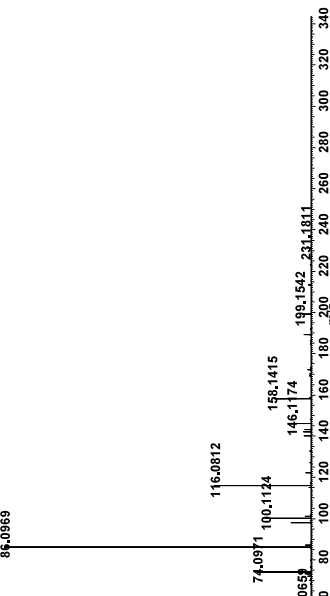
93. QUINATE



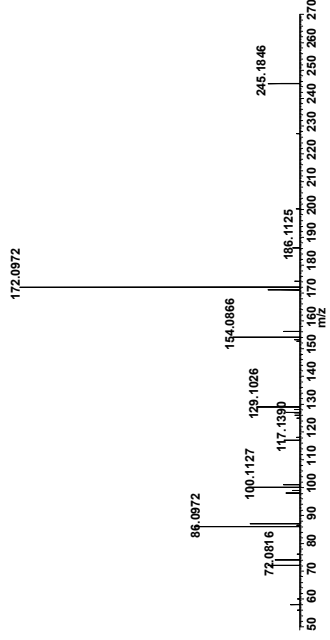
94. FERULATE



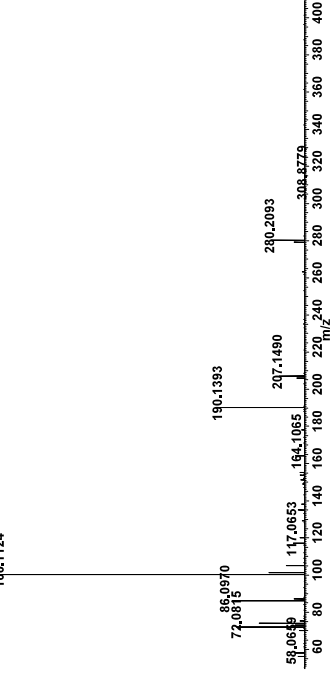
95. METHYLMALONATE



96. METHYL 4-AMINO BUTYRATE/ MONOMETHYLGLUTARATE

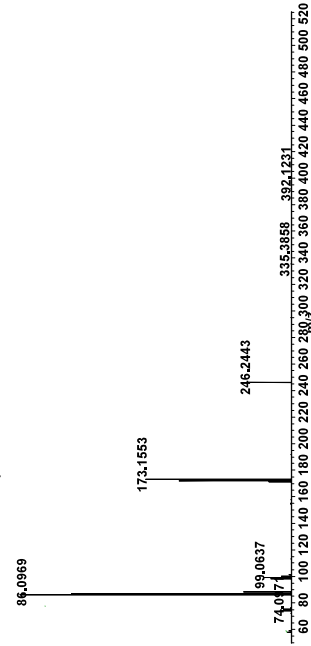


98. 3-AMINO-4-HYDROXYBENZOATE

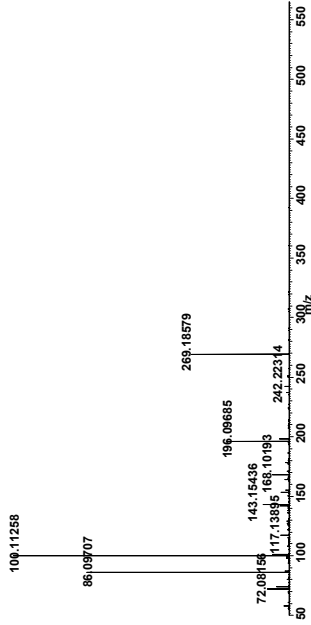


Supplementary Figure 13. MS/MS spectra for 250 derivatized metabolite standards

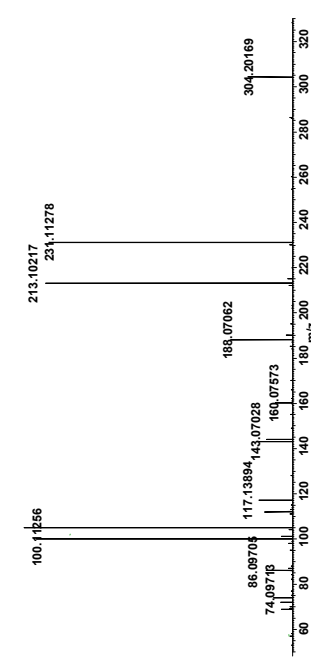
99. QUINOLINATE



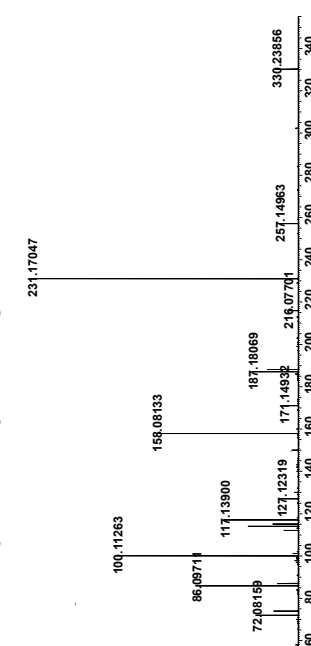
100. 3,4 DIHYDROXYMANDELATE



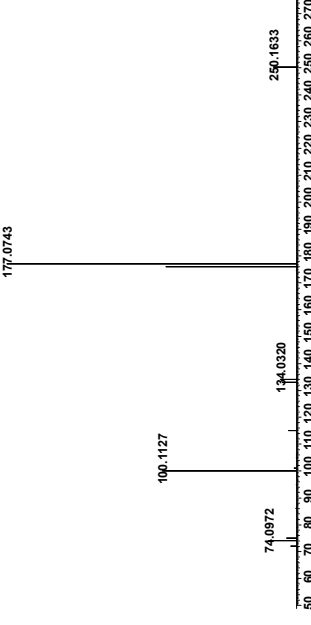
101. SEROTONIN



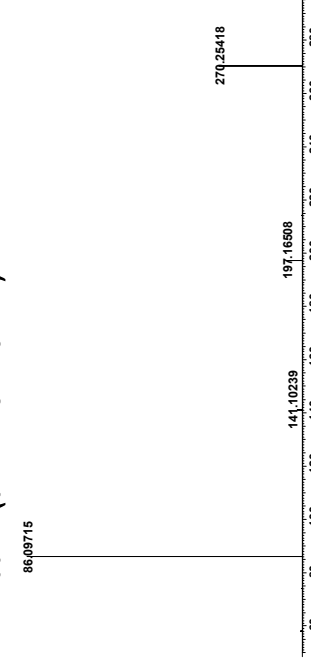
101. HYDROXYPYRUVATE



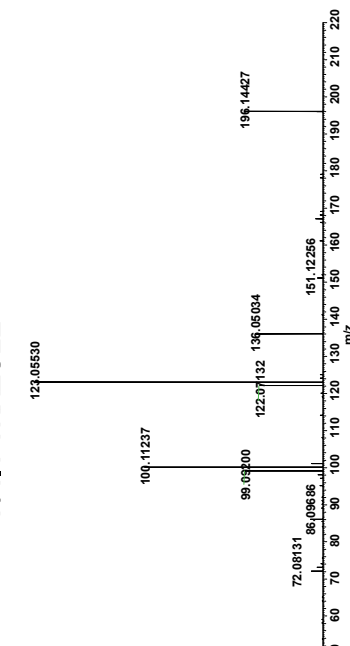
102. ERYTHRITOL



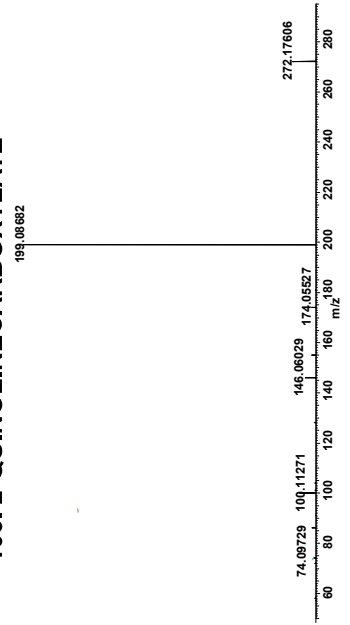
103. N-(3-AMINOPROPYL)PIPERIDNE



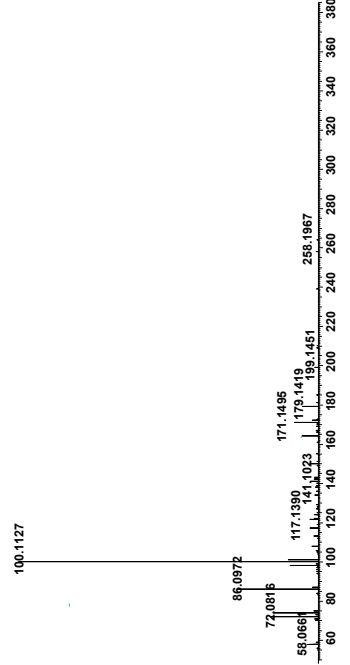
104. PYRAZOLE



105. 2-QUINOLINECARBOXYLATE

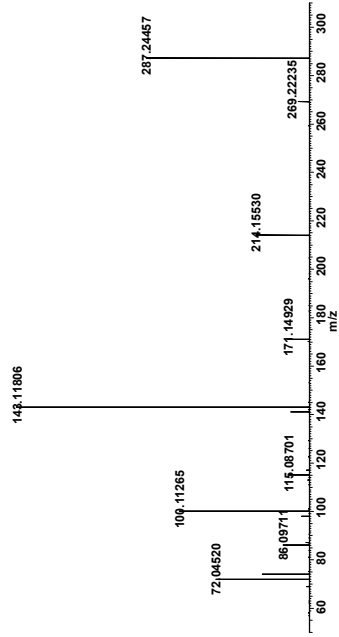


106. 5-AMINOLEVULINATE

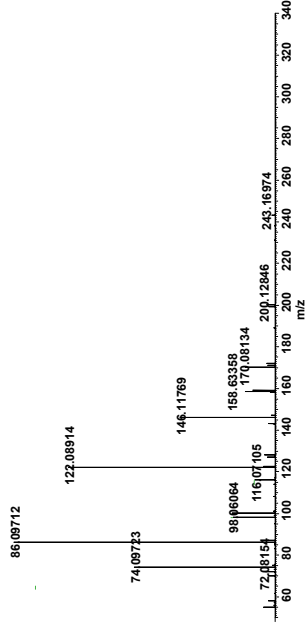


Supplementary Figure 14. MS/MS spectra for 250 derivatized metabolite standards

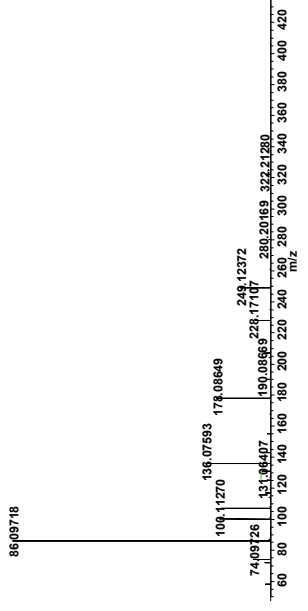
107. OXALATE/N-ALPHA-ACETYLLYSINE



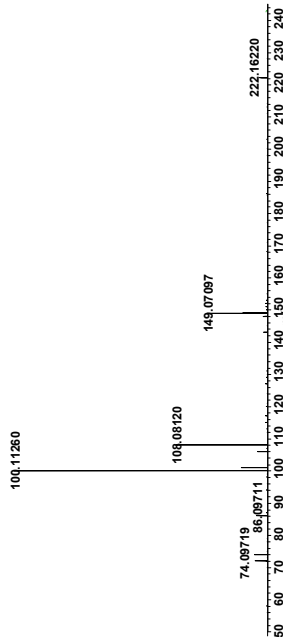
109. LACTATE



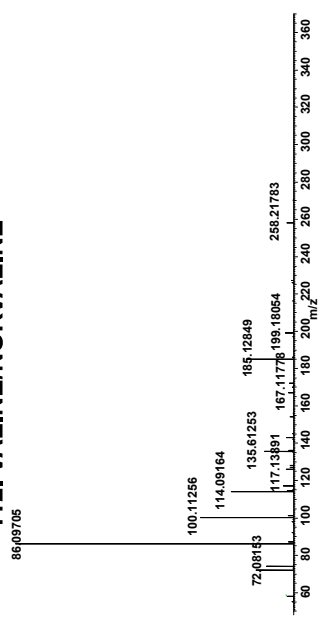
110. TYROSINE



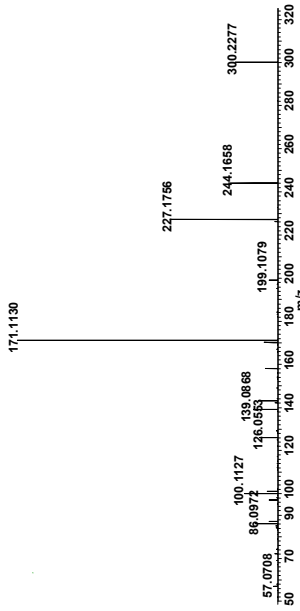
111. NICOTINATE



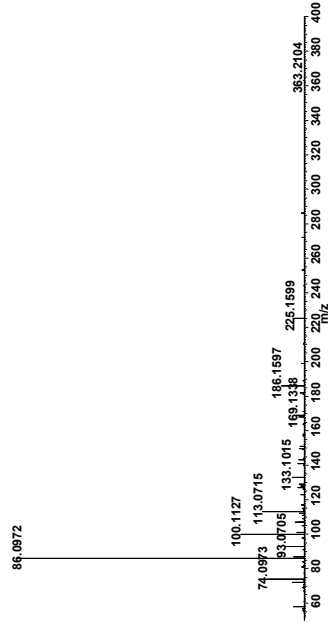
112. VALINE/NORVALINE



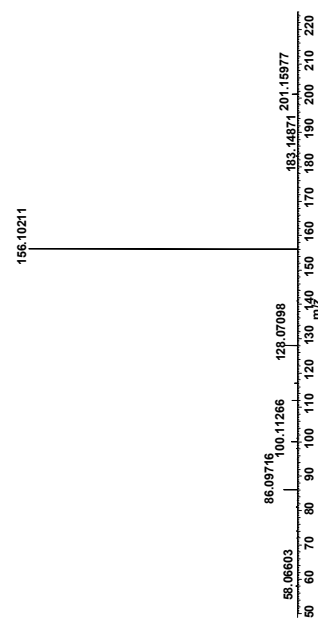
114. DIHYDROXYFUMARATE



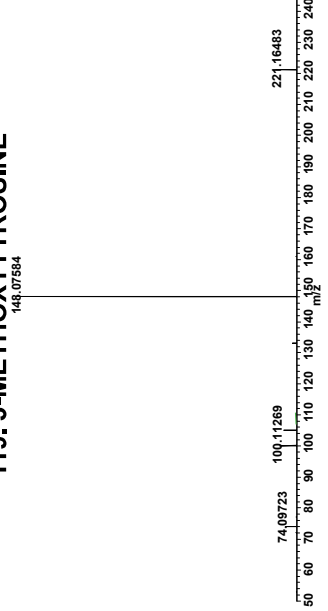
116. SUBERATE



117. ACETOACETATE/SUCCINATE SEMIALDEHYDE

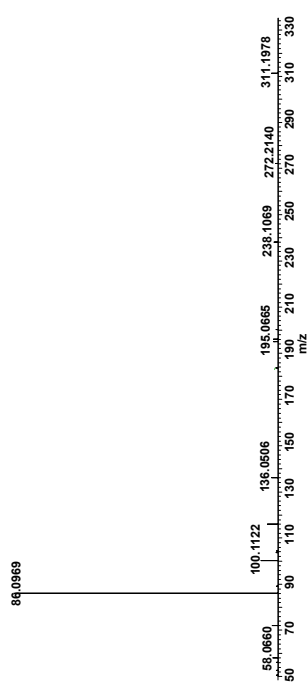


119. 3-METHOXYTYROSINE

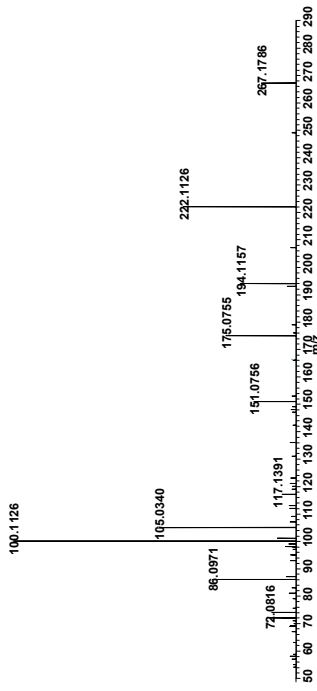


Supplementary Figure 15. MS/MS spectra for 250 derivatized metabolite standards

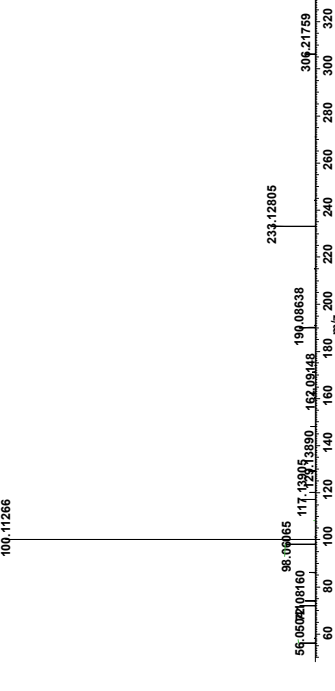
120. HOMOCYSTINE



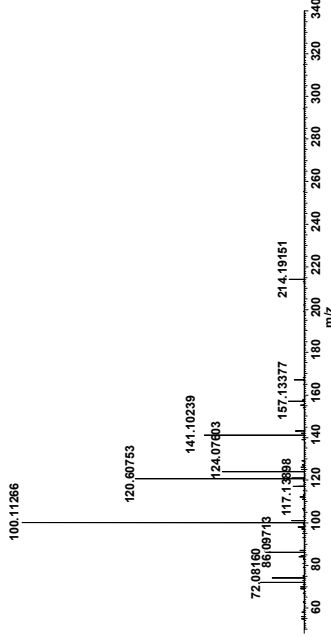
123. HOMOGENITISATE



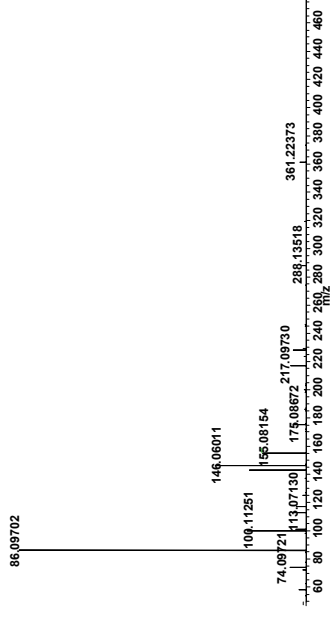
126. N-ACETYLPHENYLALANINE



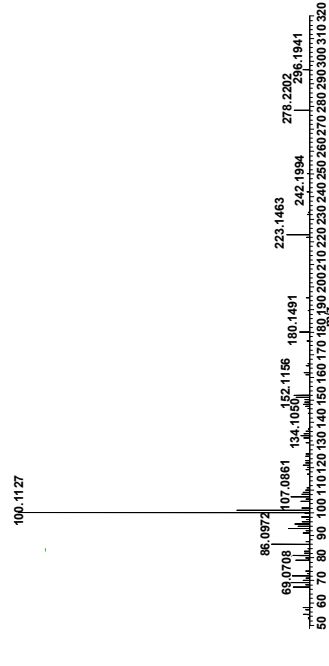
121. FUMARATE



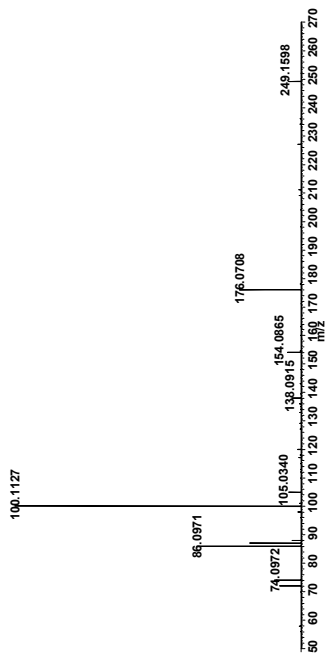
124. 5-HYDROXYTRYPTOPHAN



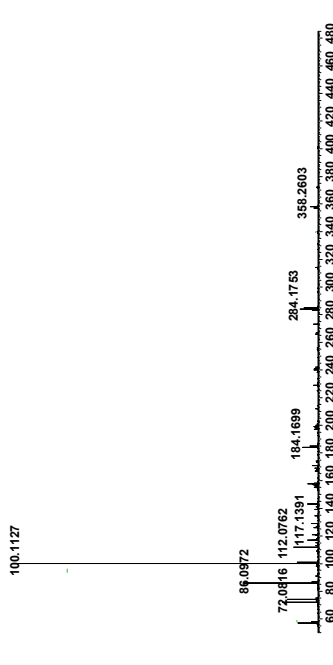
127. L-DOPA



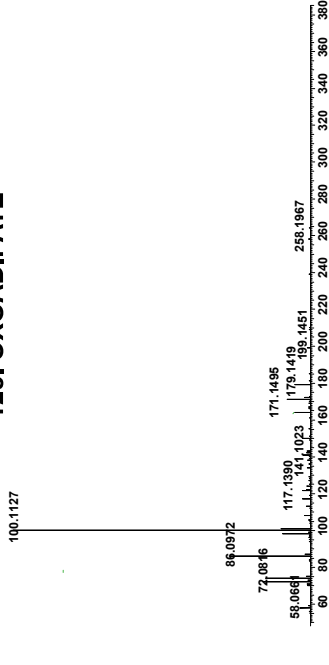
122. 4-FORMYL BENZOIC ACID



125. KETOLEUCINE

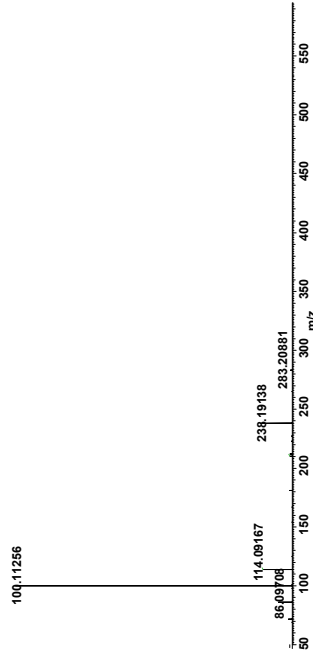


128. OXOADIPATE

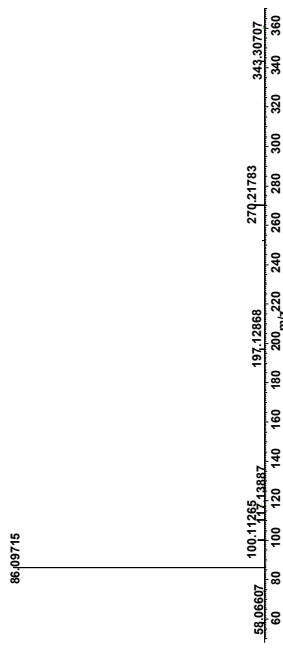


Supplementary Figure 16. MS/MS spectra for 250 derivatized metabolite standards

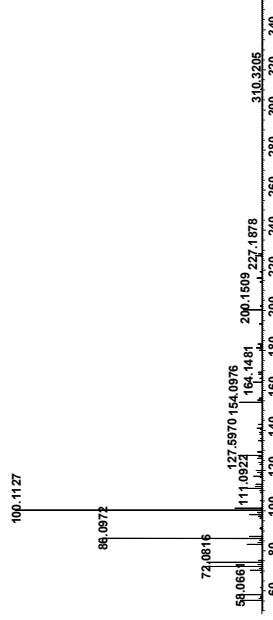
129. EPINEPHRINE/NORMETANEPHRINE



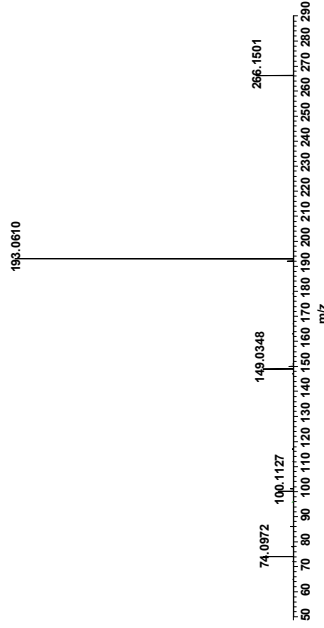
133. PUTRESCINE



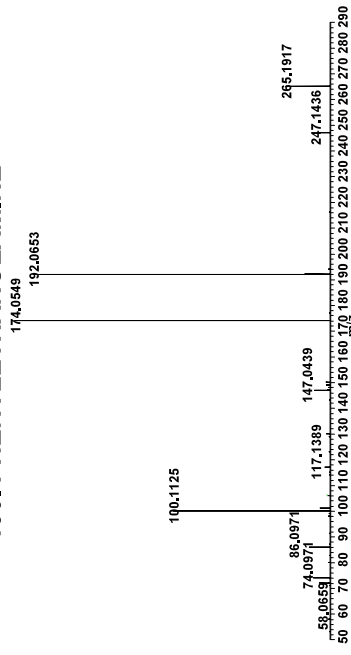
131. 2-METHYLMALEATE



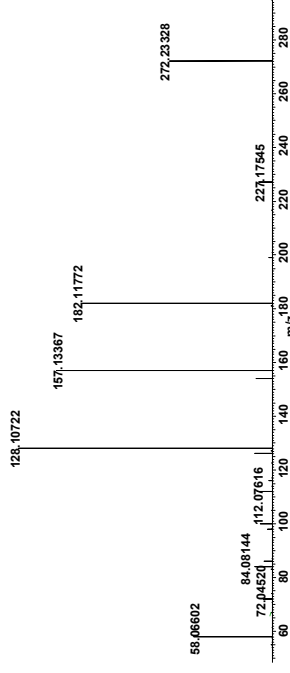
134. 2-NITROBENZOIC ACID



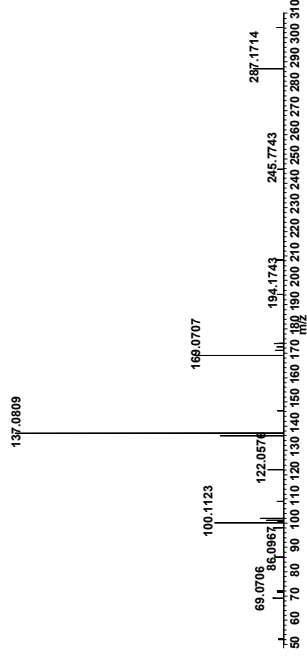
136. PHENYLETHANOLAMINE



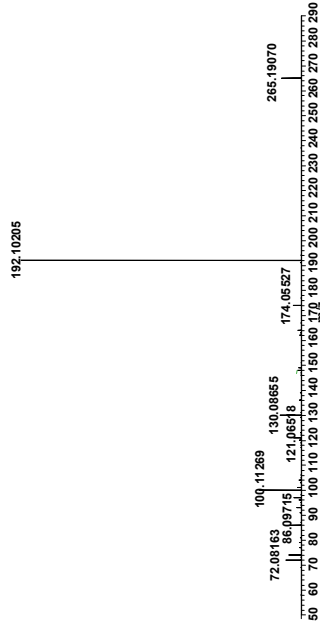
132. N-ACETYLLEUCINE



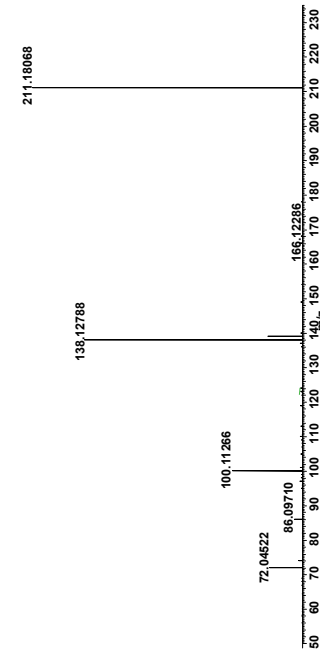
135. 1-HYDROXY-2-NAPHTHOATE



137. 3-(2-HYDROXYPHENYL)PROPANOATE

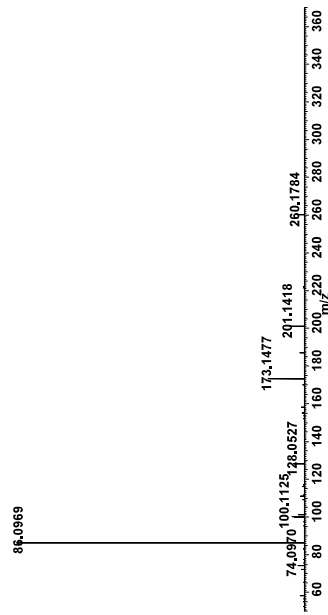


138. SORBATE

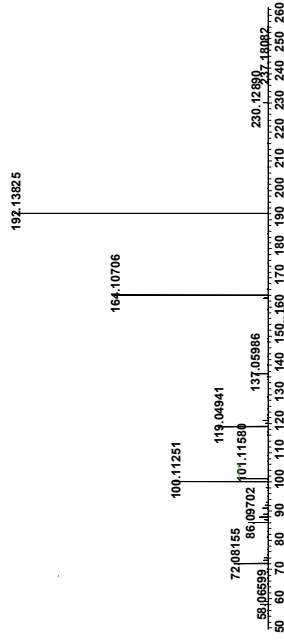


Supplementary Figure 17. MS/MS spectra for 250 derivatized metabolite standards

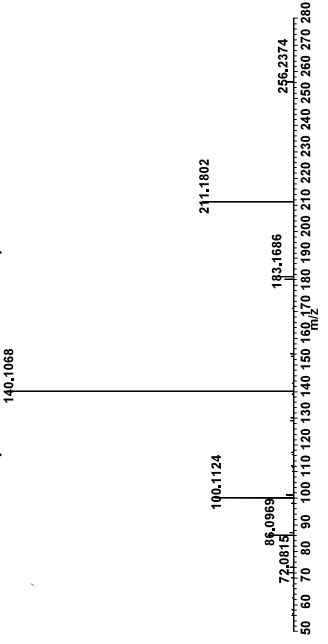
139. CITRAMALATE



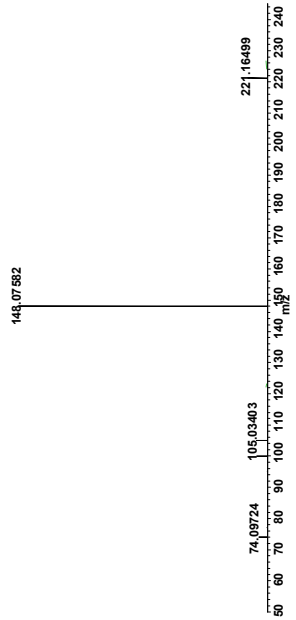
140. 2-AMINOPHENOL



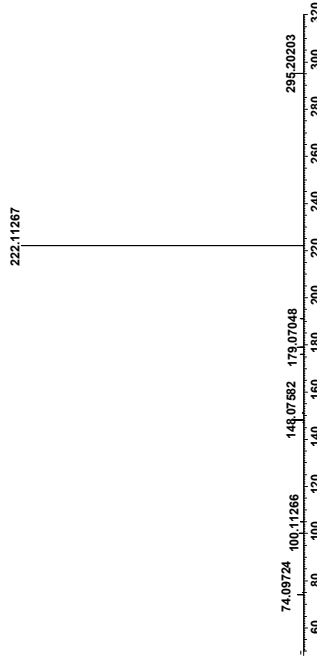
141. 1-(2-AMINOETHYL)PIPERIDINE



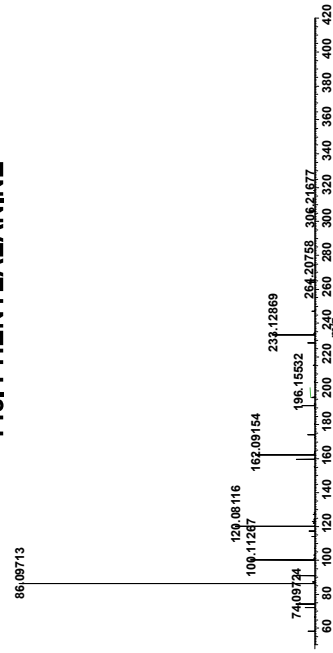
142. BENZOATE/ANILINE



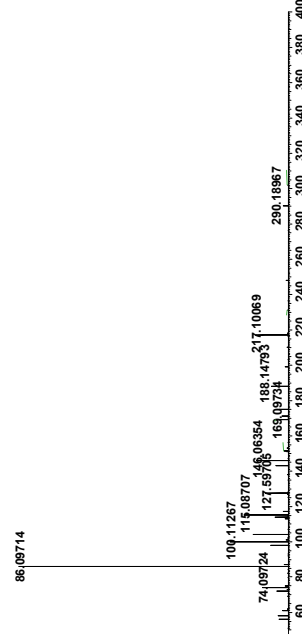
144. 3-METHOXYTYRAMINE



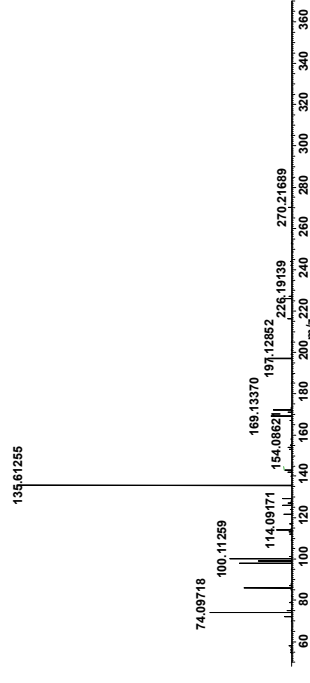
145. PHENYLALANINE



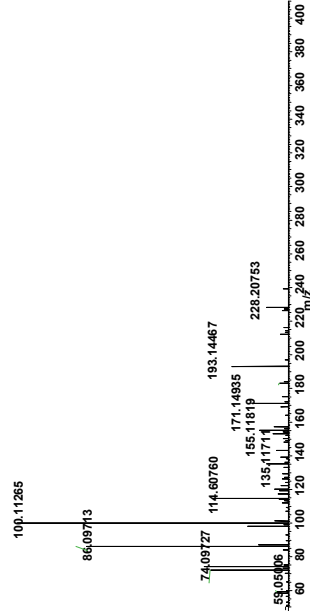
146. METHIONINE



147. 5-AMINOPENTANOATE/2-METHYLGUTARATE/ADIPATE

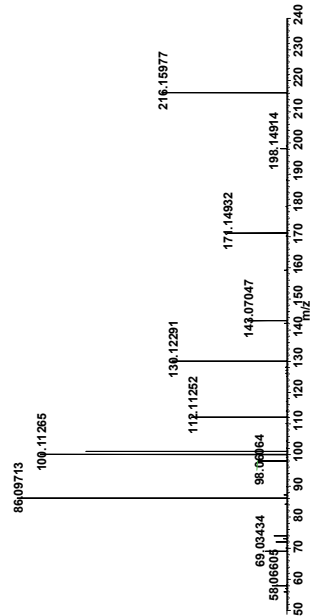


150. AZELATE

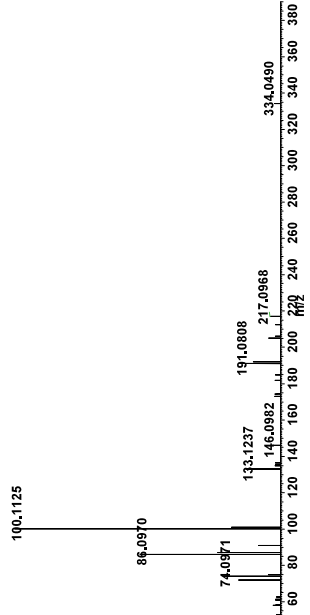


Supplementary Figure 18. MS/MS spectra for 250 derivatized metabolite standards

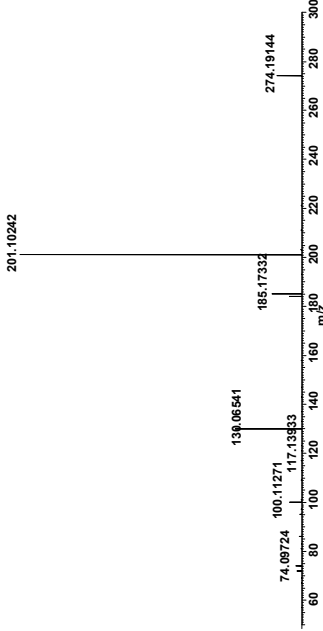
151. ACETOIN



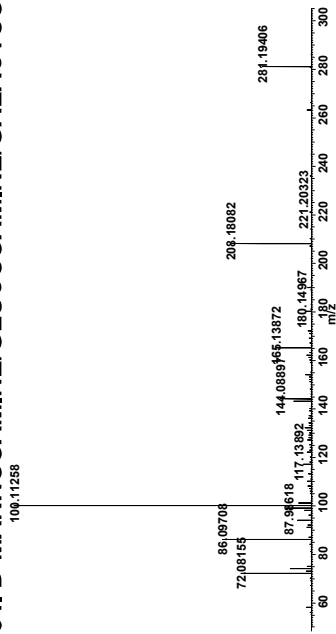
152. 2,4-PYRIDINEDIACARBOXYLIC ACID



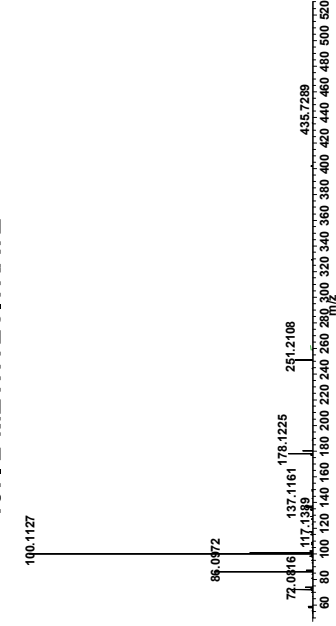
153. INDOLE-3-ACETATE



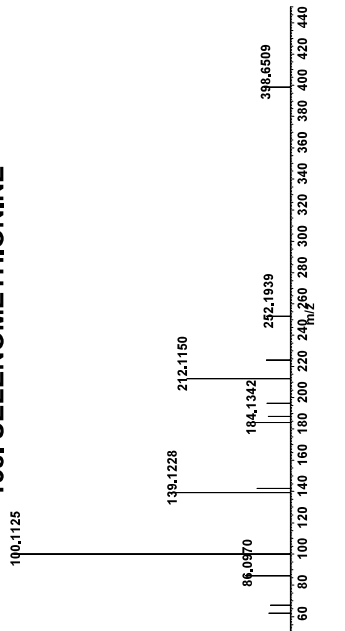
154. D-MANNOSAMINE/GLUCOSAMINE/GALACTOSAMINE



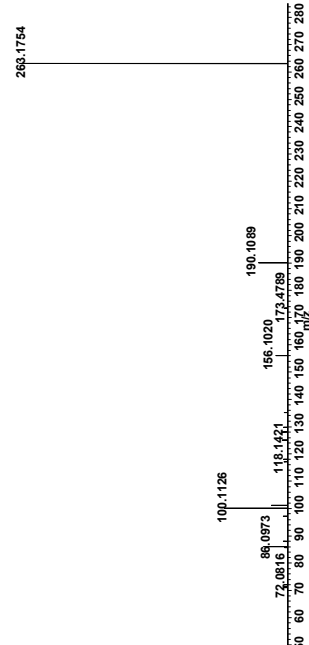
157. 2-METHYLCITRATE



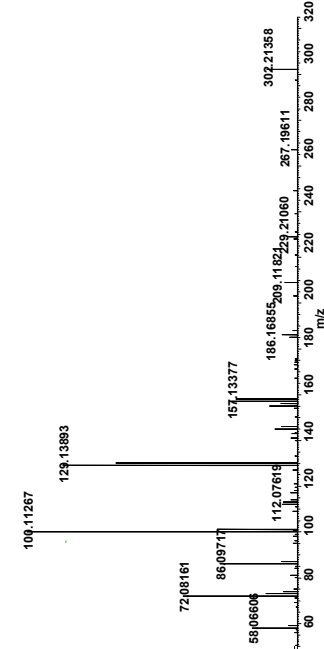
158. SELENOMETHIONINE



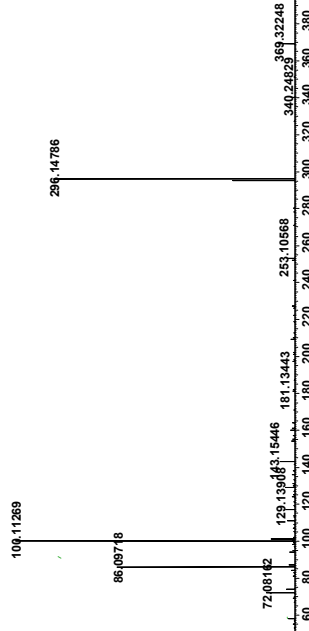
159. 4-AMINO ACETOPHENONE/ 4-COUMARATE



161. N-METHYLTRYPTAMINE

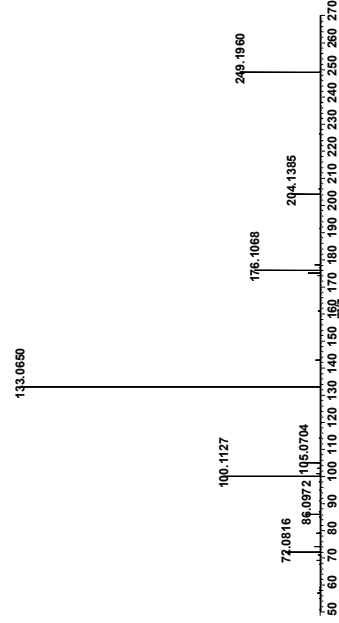


162. CYCLOHEXANE 1,2 DIAMINE

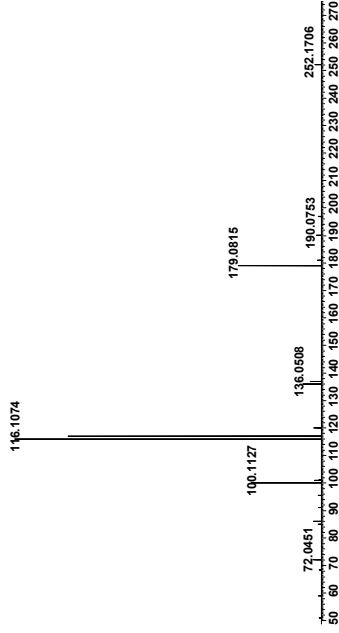


Supplementary Figure 19. MS/MS spectra for 250 derivatized metabolite standards

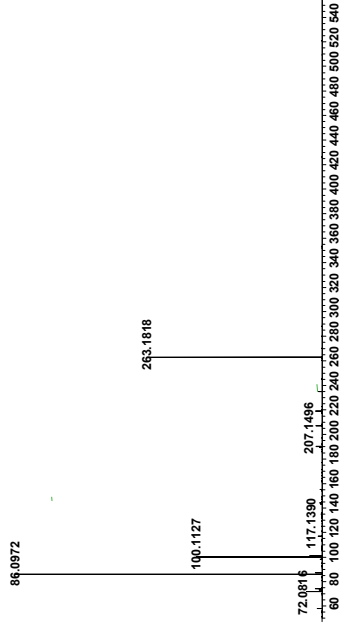
163. PHENETHYLAMINE



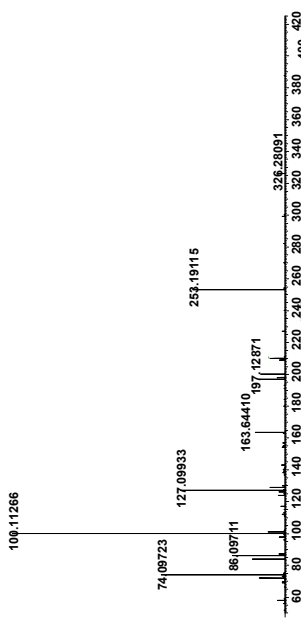
164. 3-HYDROXYANTHRANILATE



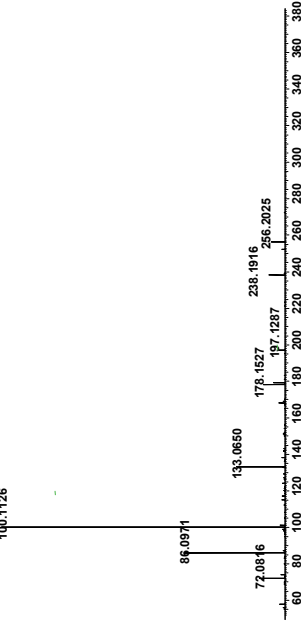
165. 3-DEHYDROSHIKIMATE



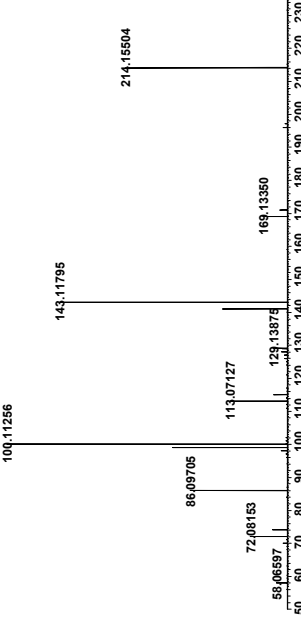
166. SEBACATE



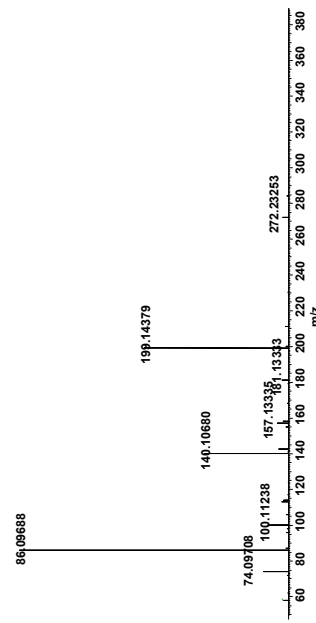
167. PIPECOLATE



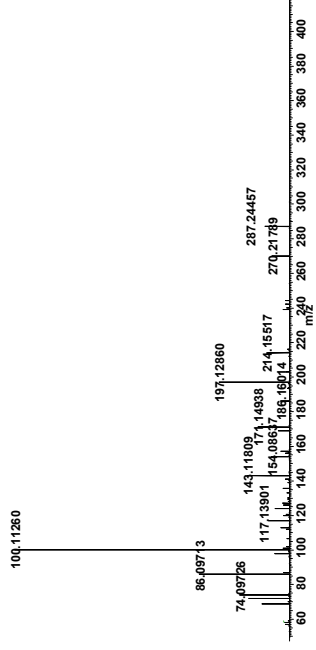
168. HEXANOATE



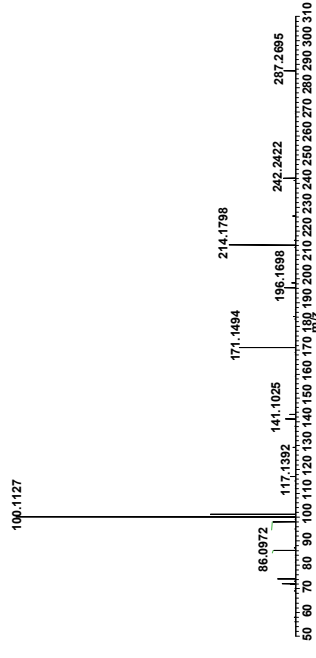
169. LEUCINE/ISOLEUCINE/NORLEUCINE



172. NORSPERMIDINE

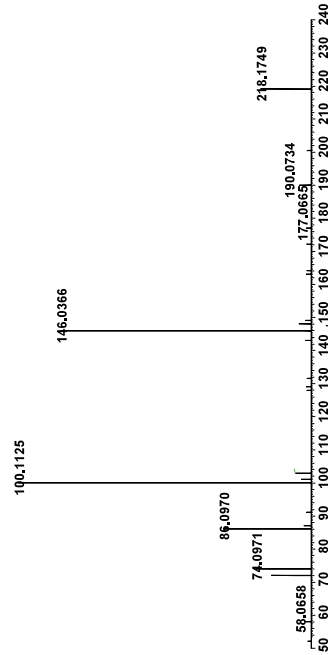


173. 10-HYDROXYDECANOATE

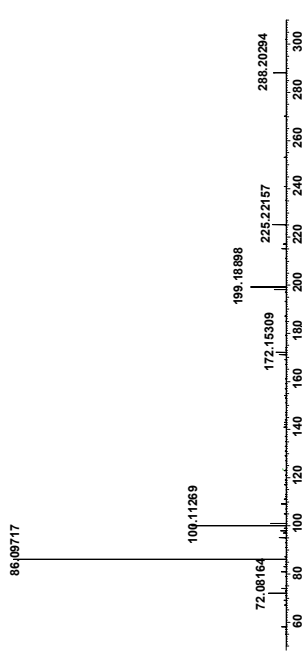


Supplementary Figure 20. MS/MS spectra for 250 derivatized metabolite standards

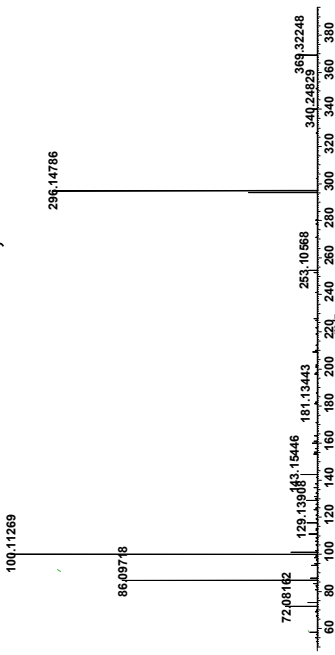
174. 2,3-BUTANEDIOL



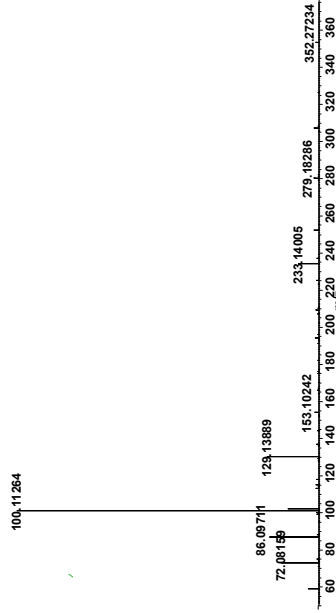
180. TRYPTAMINE



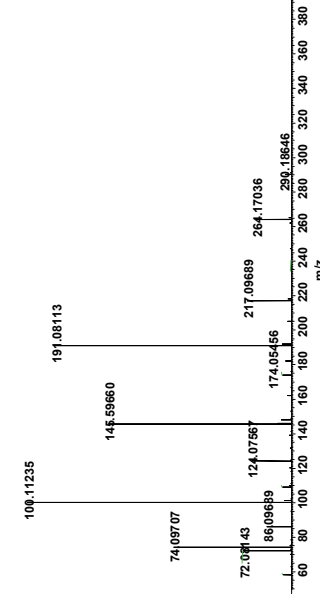
184. CYCLOHEXANE 1,4 DIAMINE



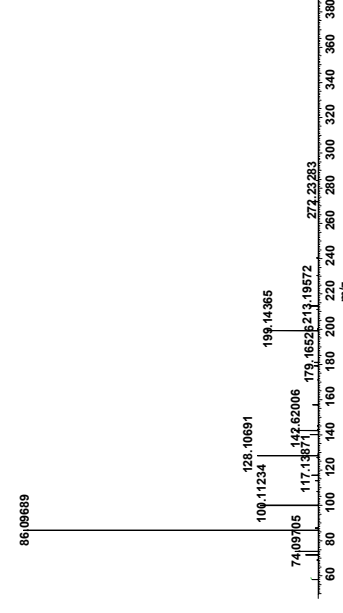
175. 4-IMIDAZOLEACETATE



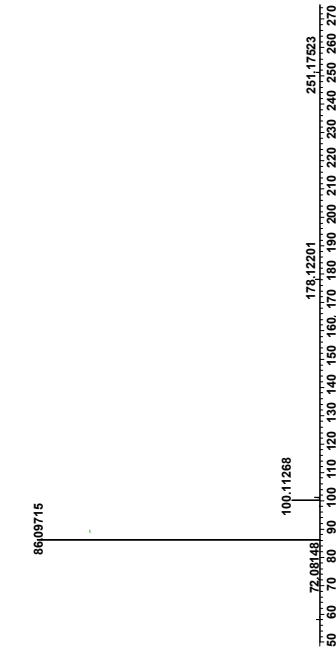
181. 4-AMINO BENZOATE/TRIGONELLINE



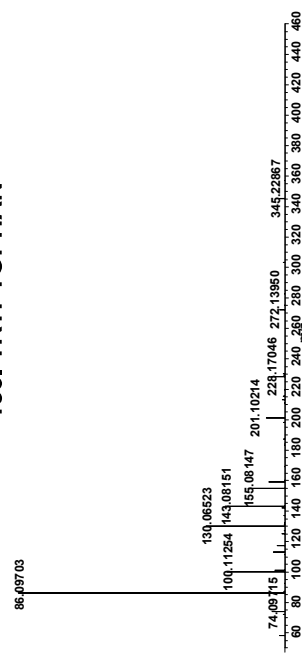
185. 6-AMINO CAPRIC ACID/6-CARBOXYHEXANOATE



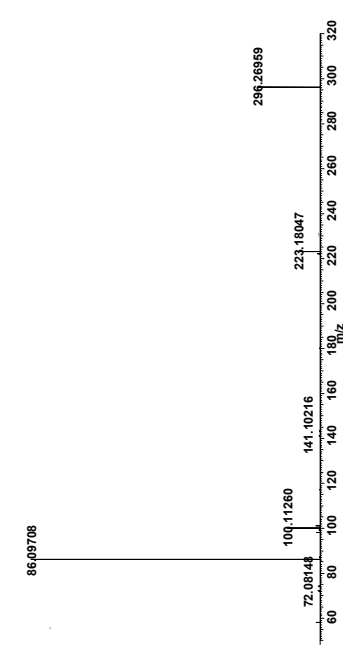
176. 2/3/P-HYDROXYPHENYLACETATE/MANDELATE



183. TRYPTOPHAN

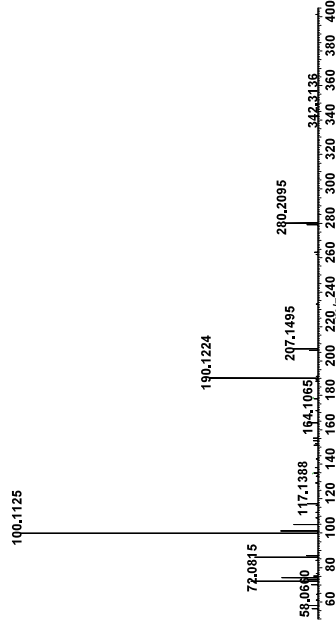


187. 1-CYCLOHEXYLPIPERAZINE

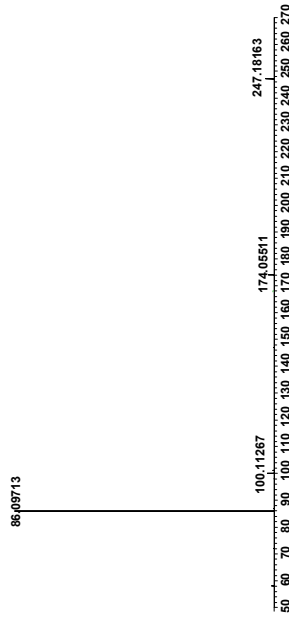


Supplementary Figure 21. MS/MS spectra for 250 derivatized metabolite standards

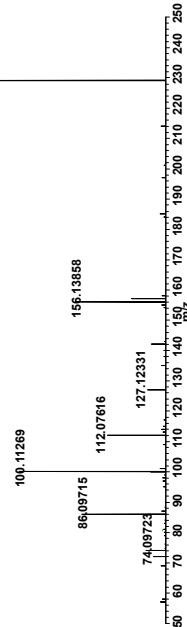
188. 3-SULFINOALANINE



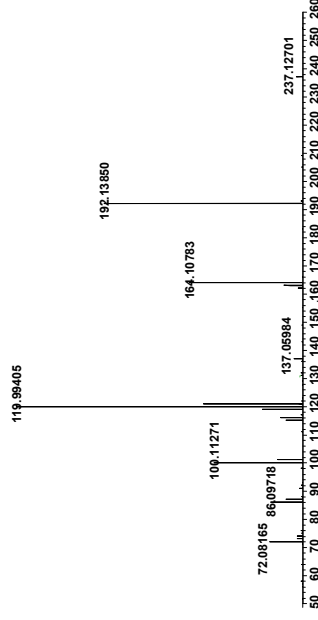
191. TRANS-CINNAMATE



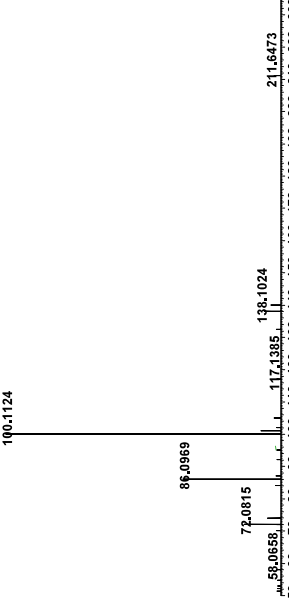
194. MONO METHYL FUMARATE



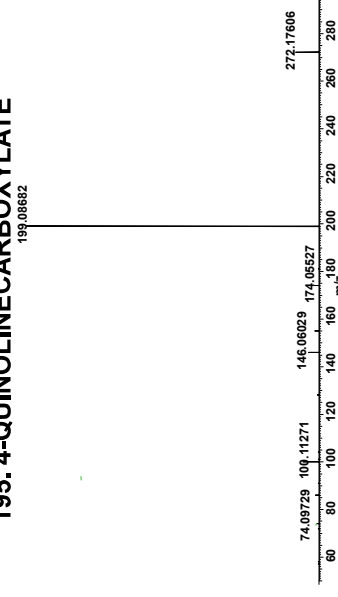
189. HYPOTAURINE



192. GLUCONATE



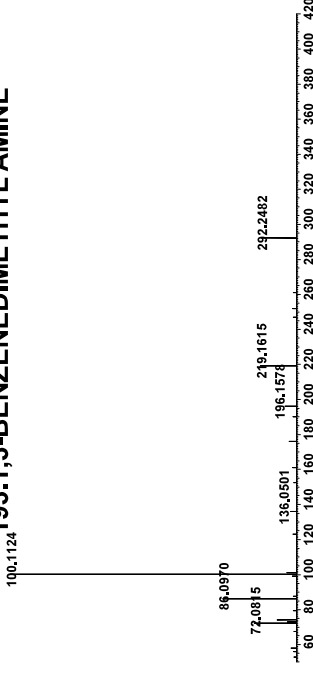
195. 4-QUINOLINECARBOXYLATE



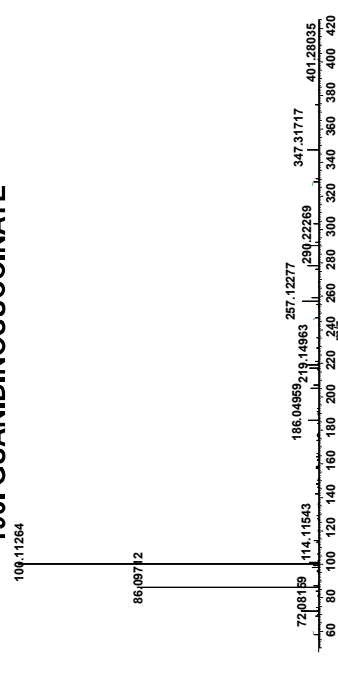
190. DOPAMINE



193. 1,3-BENZENEDIMETHYL AMINE

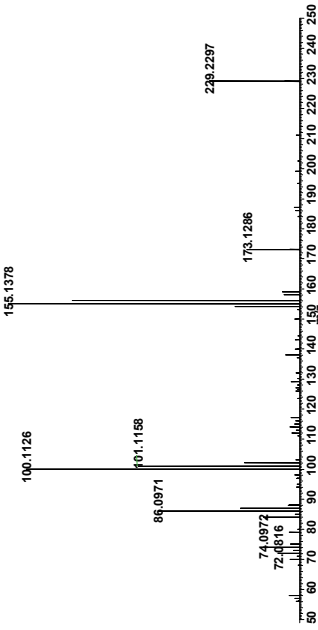


196. GUANIDINOSUCCINATE

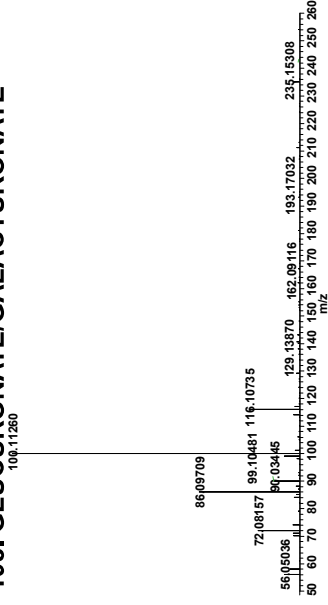


Supplementary Figure 22. MS/MS spectra for 250 derivatized metabolite standards

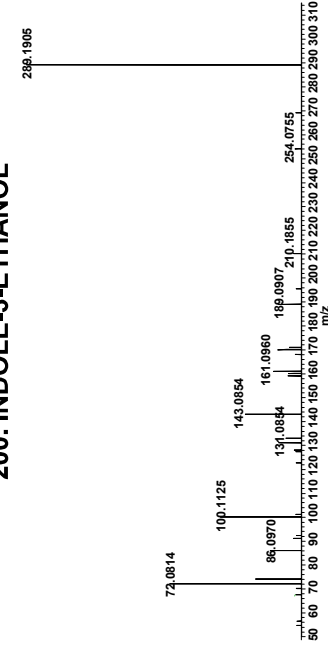
197. HEPTANOATE



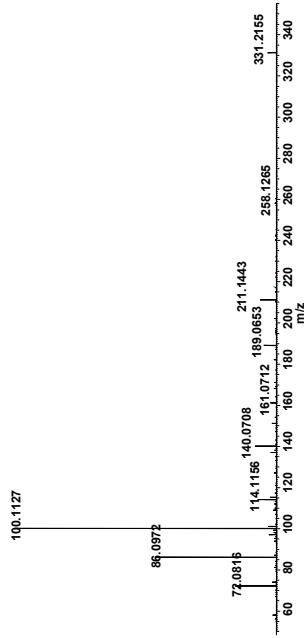
198. GLUCURONATE/GALACTURONATE



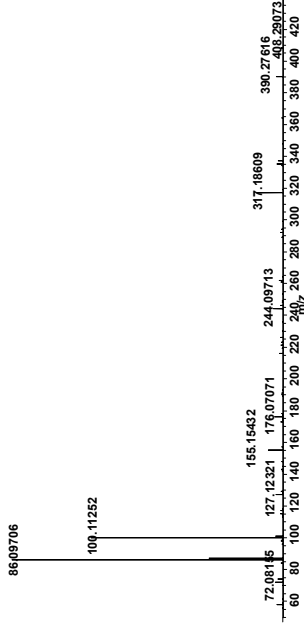
200. INDOLE-3-ETHANOL



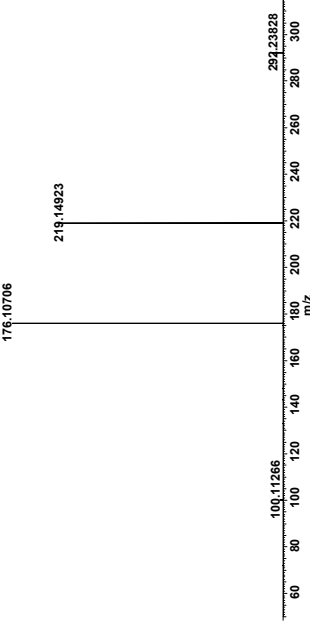
201. L-TRYPTOPHANAMIDE



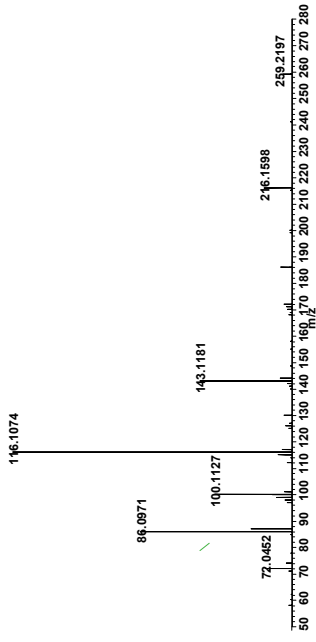
202. P-OCTOPAMINE



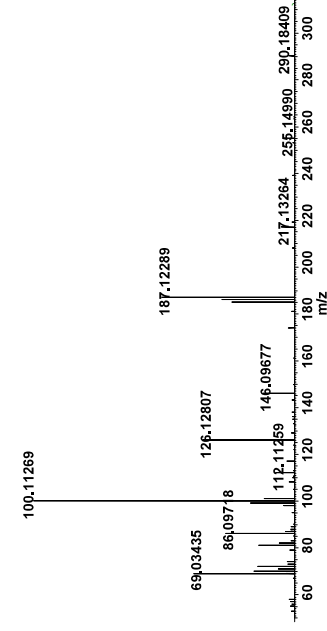
203. 4-(DIETHYLAMINO) BENZOIC ACID



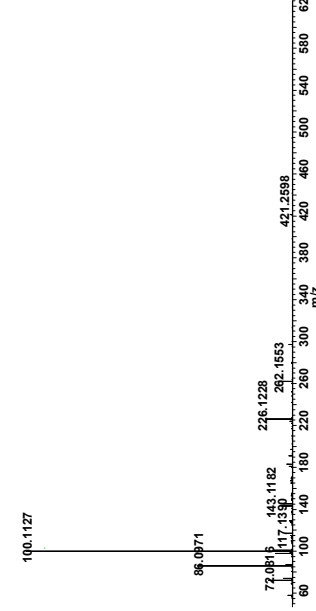
204. ETHYL 3-UREIDOPROPIONATE



205. 5-HYDROXYINDOLEACETATE

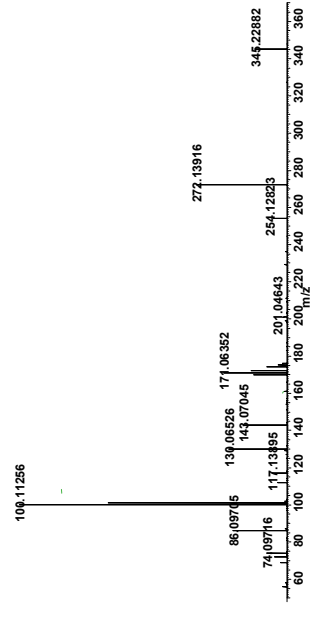


206. ANSERINE

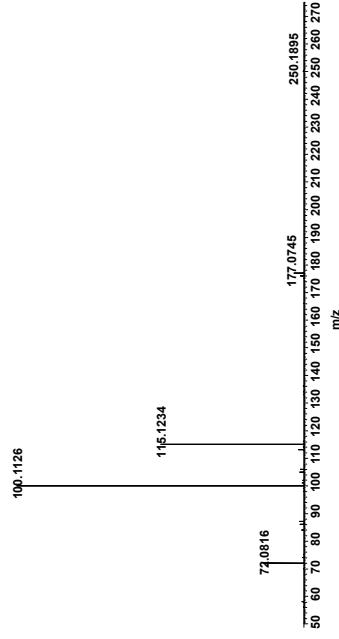


Supplementary Figure 23. MS/MS spectra for 250 derivatized metabolite standards

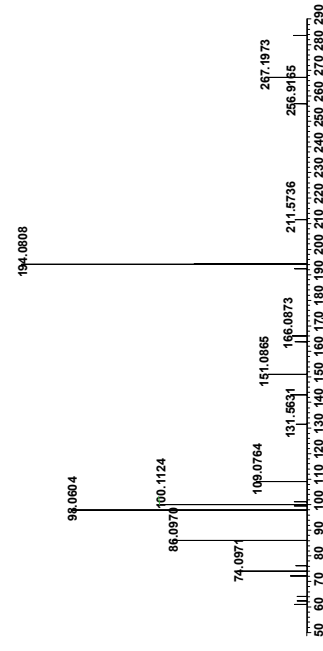
207. N-ACETYLTRYPTOPHAN



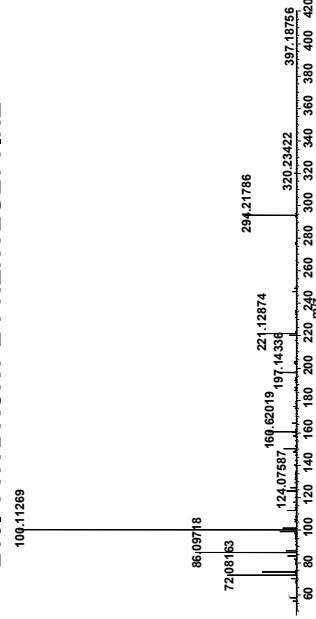
208. 1-PHENYLETHANOL



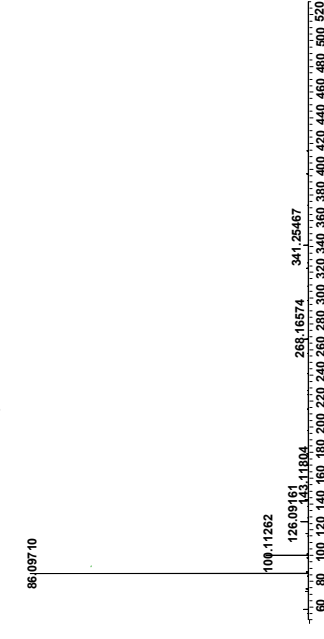
209. METHIONINE SULFOXIMINE



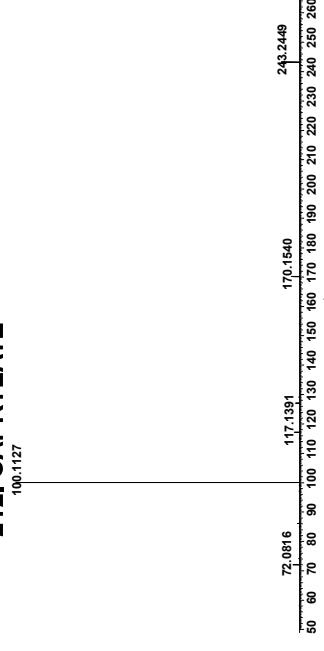
210. 4-HYDROXY-L-PHENYLGLYCINE



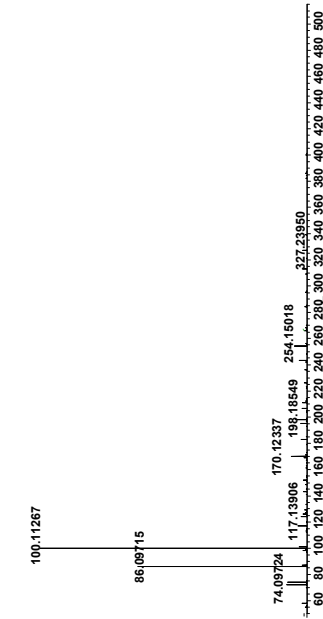
211. LYSINE



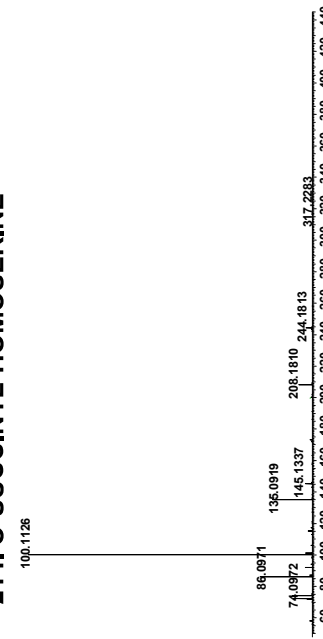
212. CAPRYLATE



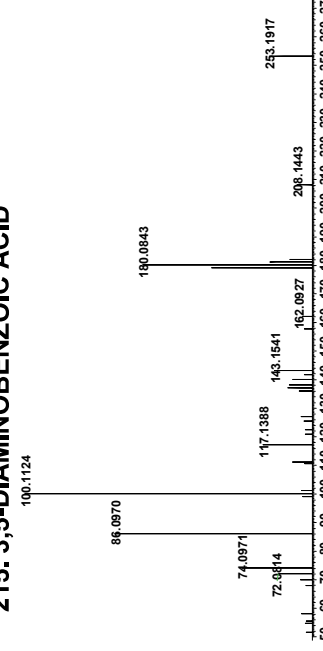
213. AMINOADIPATE



214. O-SUCCINYL-HOMOSERINE

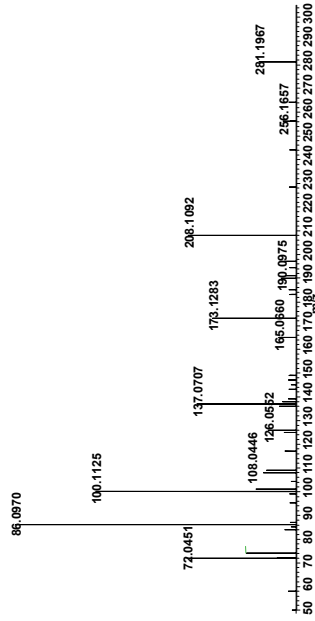


215. 3,5-DIAMINOBENZOIC ACID

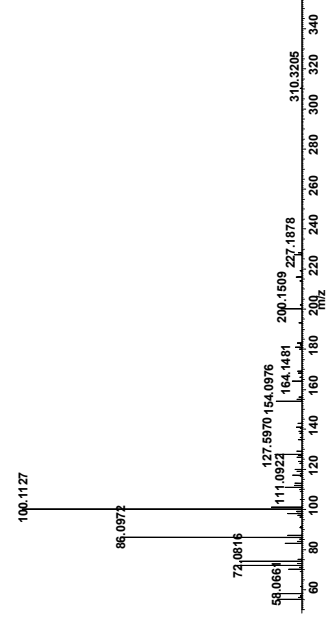


Supplementary Figure 24. MS/MS spectra for 250 derivatized metabolite standards

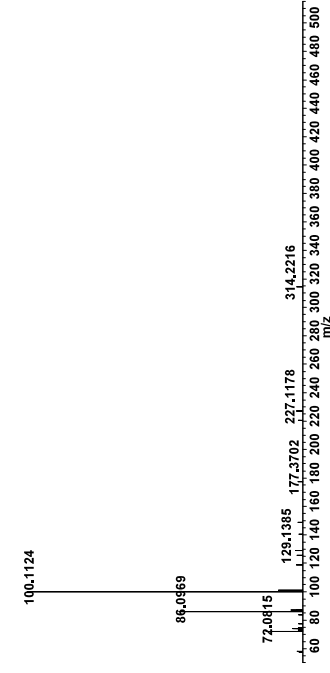
216. SALSOLINOL



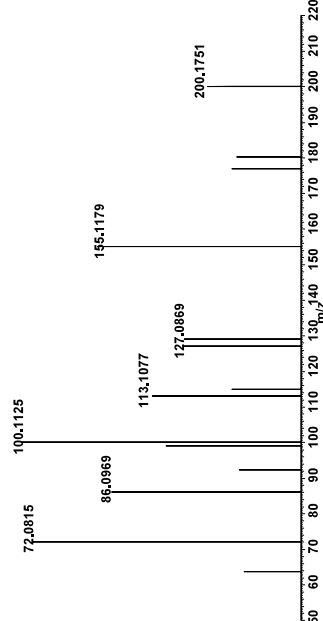
217. ITACONATE



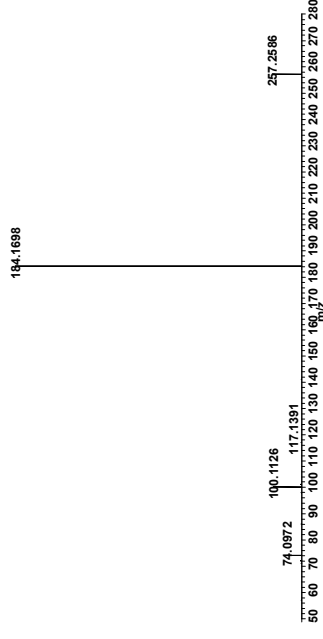
218. 3-HYDROXYMETHYLGLUTARATE



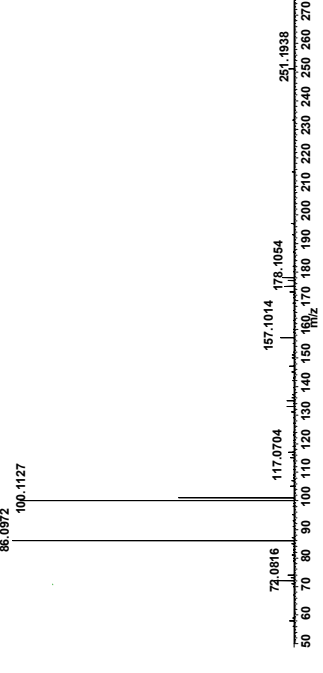
219. 1-AMINOCYCLOPROPANECARBOXYLATE



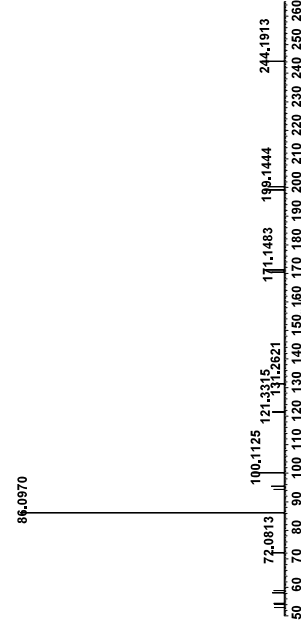
220. NONANOATE



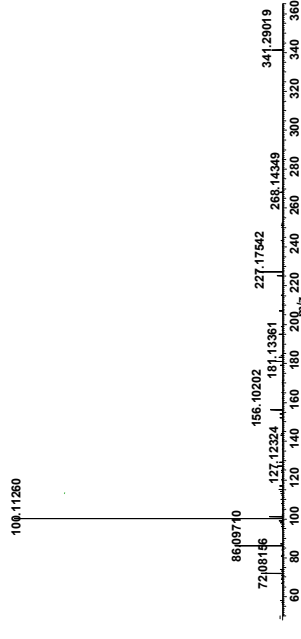
221. OXALOMALATE



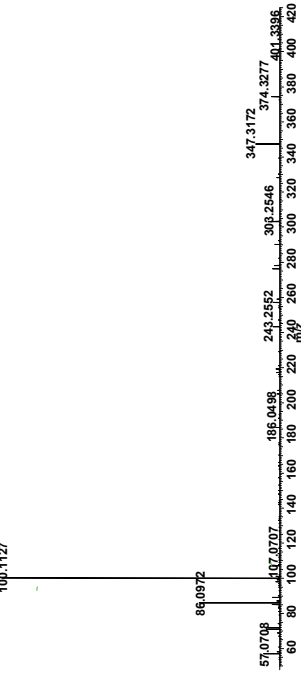
222. TRANS-4-CYCLOHEXANEDIOL



223. 3-METHYLGLUTACONATE

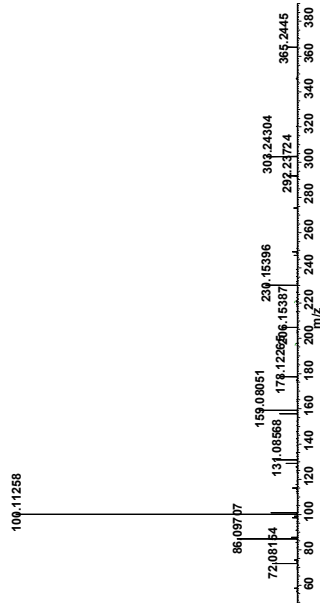


224. CITRULLINE

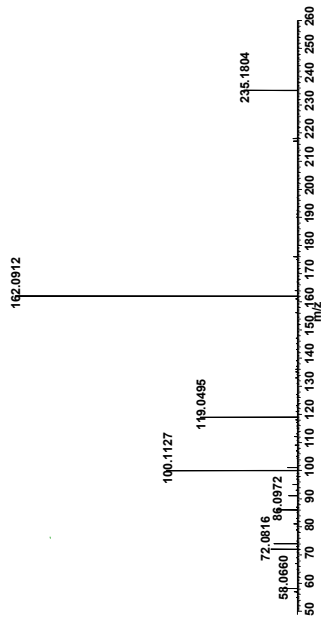


Supplementary Figure 25. MS/MS spectra for 250 derivatized metabolite standards

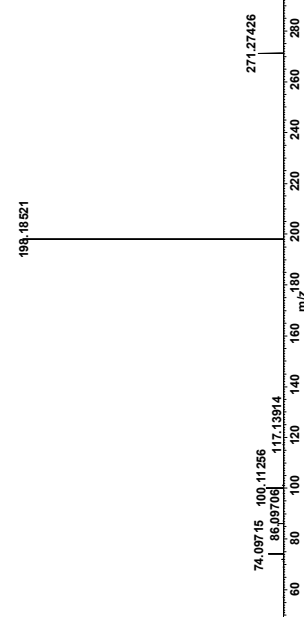
225. PYROCATECHOL/HYDROQUINONE



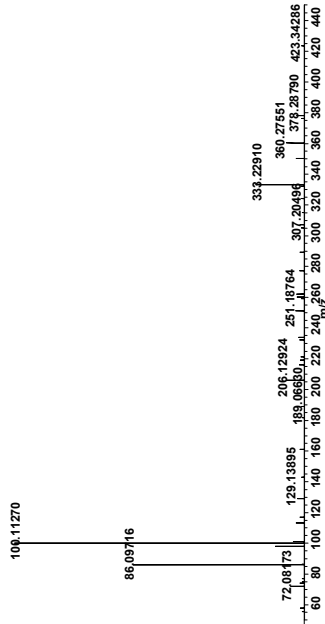
229. BENZYLAMINE



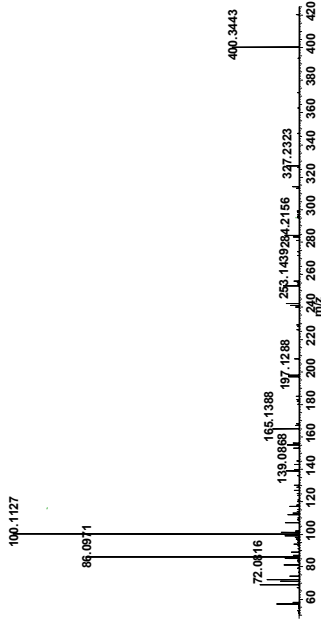
232. DECANOATE



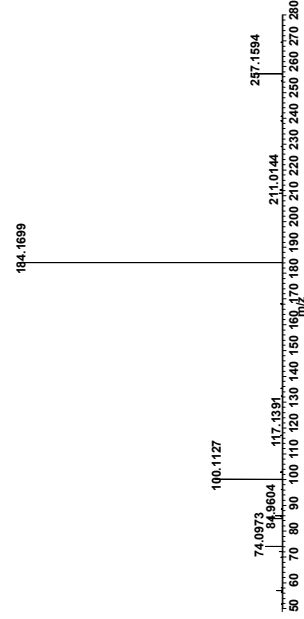
227. PORPHOBILINOGEN



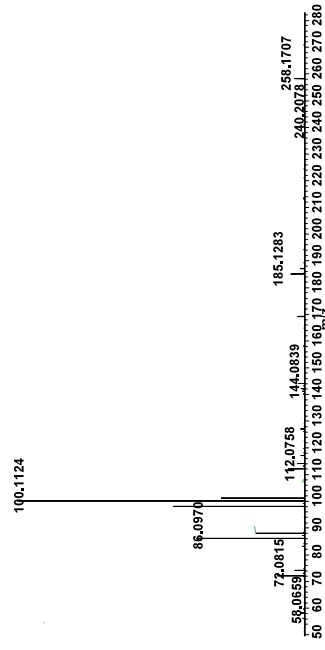
230. ARGININE



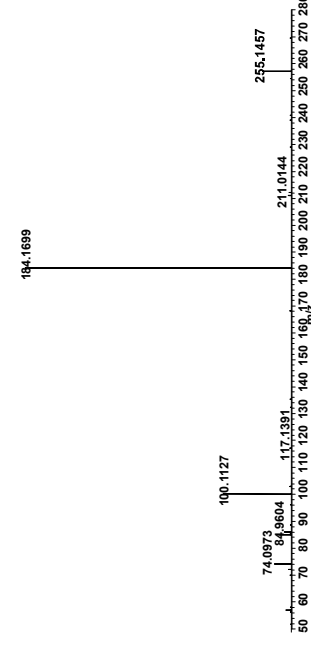
233. DIHYDROOROTATE



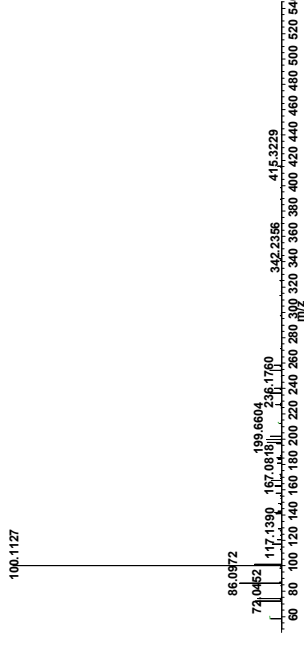
228. PANTOLACTONE



231. OROTATE

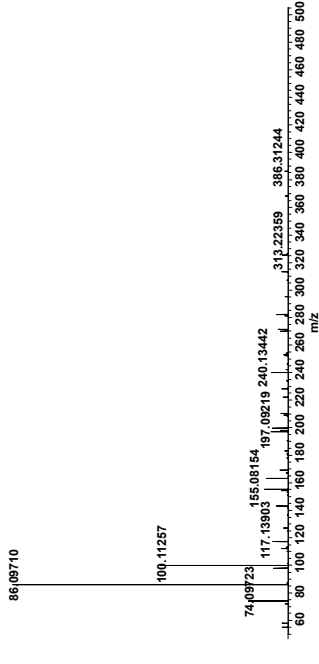


234. DIAMINOPIMELATE

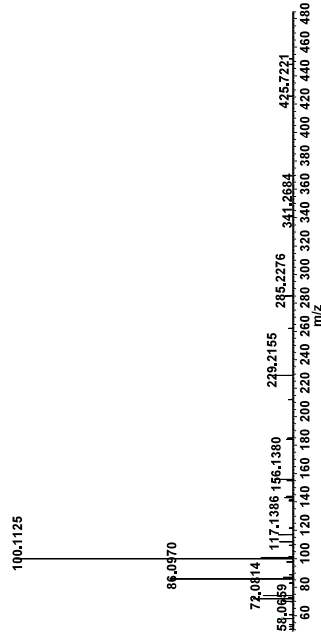


Supplementary Figure 26. MS/MS spectra for 250 derivatized metabolite standards

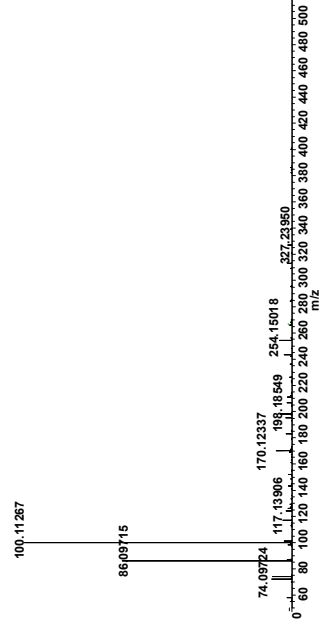
235. ASPARTATE



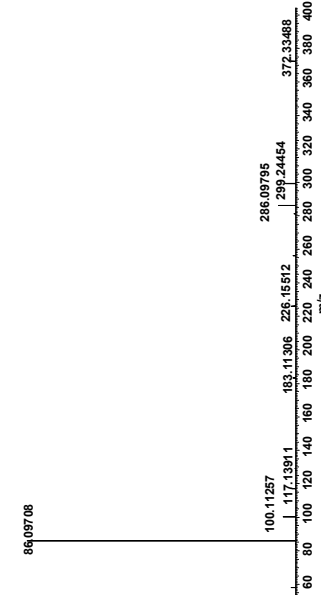
238. SPERMINE



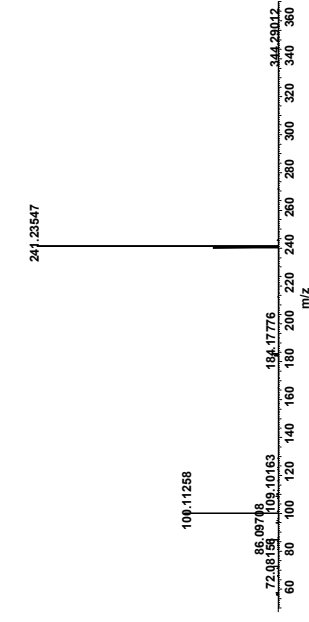
236. D-ORNITHINE



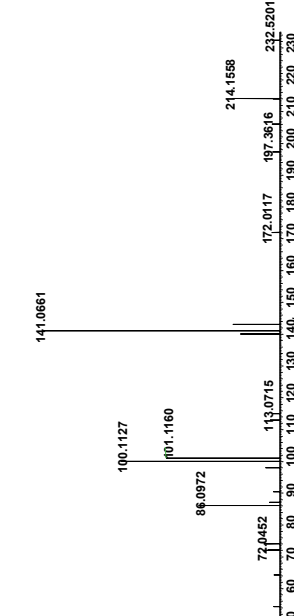
239. N1-ACETYLSPERMINE



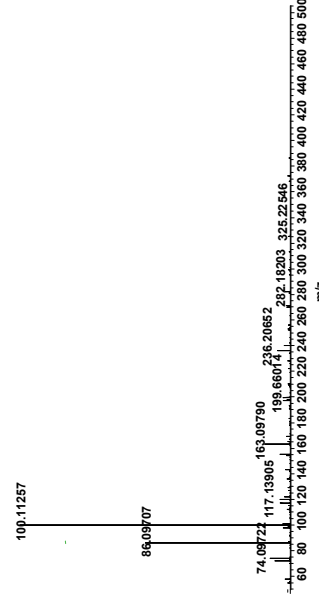
241. N-METHYLASPARTATE



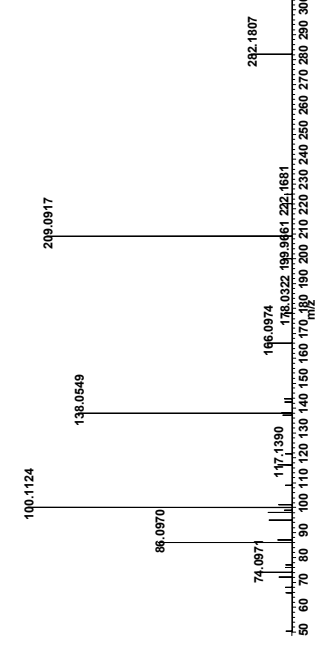
242. MALEAMATE



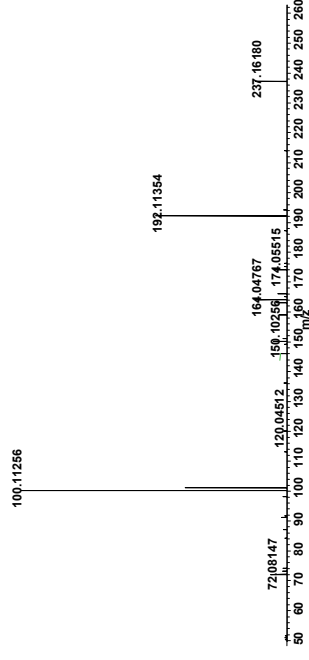
237. GLUTAMATE



240. 4-PYRIDOXATE

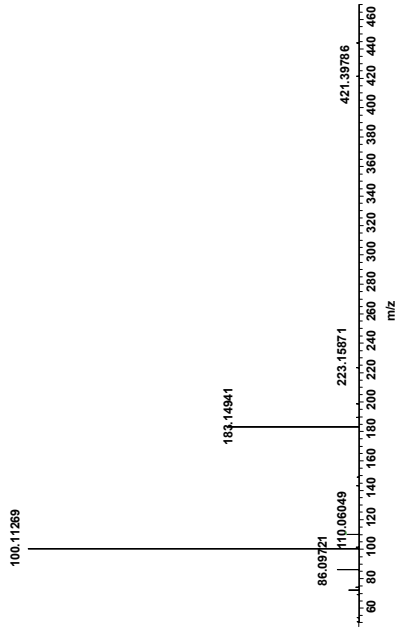


243. 4/3-HYDROXYBENZOATE/ SALICYLATE

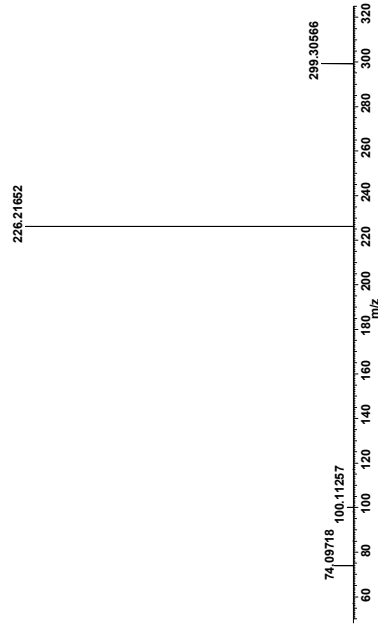


Supplementary Figure 27. MS/MS spectra for 250 derivatized metabolite standards

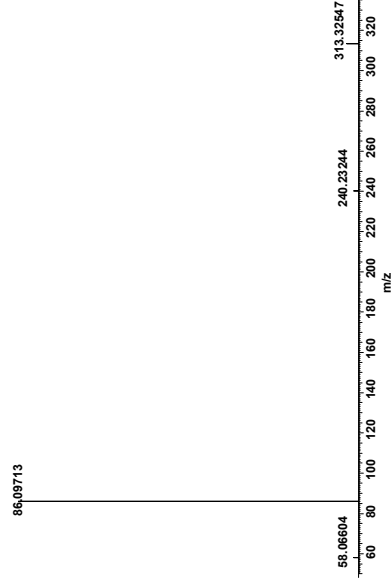
246. LAUROYL-CARNITINE



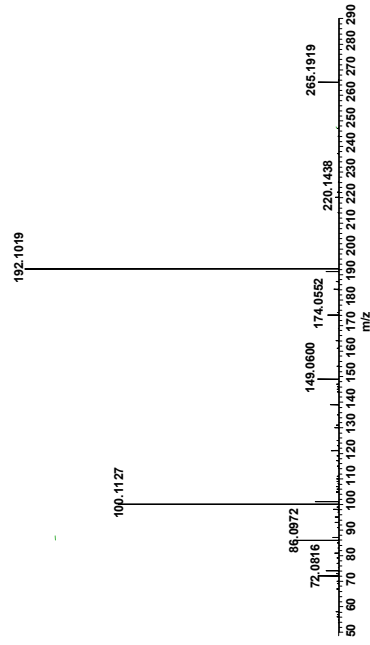
247. LAURATE



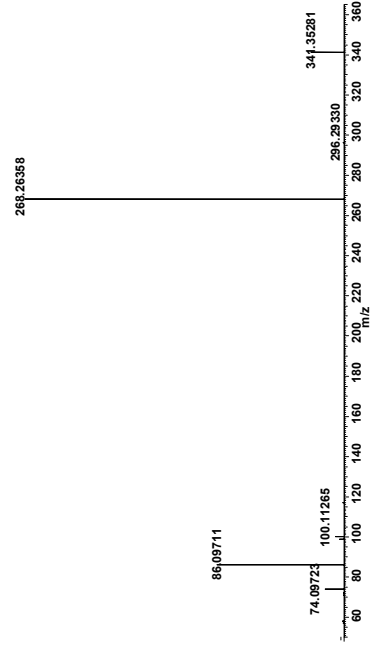
248. DODECYLAMINE



249. TYRAMINE



250. TETRADECYLAMINE



191	TRANS-CHINAMATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
192	GLUCONATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
193	1,3-BENZENE-DIMETHYLAMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	12.96	3.93	0.27	30000e390	
194	MONO-METHYL-FUMARATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	13	4.37	0.19	20000e390	
195	4-CYCLOHEXENECARBOXYLATE	12.84	0.18	0.18	2000e170	ND	ND	ND	ND	ND	12.28	2.83	0.27	40000e450	
196	GLUANIBENZOICACONATE	ND	ND	ND	ND	12.63	14.68	0.13	1000e110	ND	ND	ND	ND	ND	
197	HEPTANOATE	ND	ND	ND	ND	12.68	11.97	0.14	2000e220	13.24	7.26	0.19	14000e450	ND	
198	GALACTURONATE	12.58	0.21	0.21	8500e330	13.12	10.88	0.09	4000e370	13.45	2.77	0.19	8500e460	ND	
199	GLUCURONATE	12.56	0.21	0.21	8500e330	13.12	10.88	0.09	4000e370	13.45	2.77	0.19	8500e460	ND	
200	INDOLE-3-ETHANOL	ND	ND	ND	ND	ND	ND	ND	ND	ND	12.16	2.82	0.08	16000e1000	
201	1,3-BIS(3-TRIFLUOROMETHYLPHENYL)PROPANE	12.62	0.20	0.20	2300e170	13.04	8.95	0.19	1700e210	14.26	20.73	0.41	14500e270	ND	
202	PROPYLAMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
203	4-(BIS(3-TRIFLUOROMETHYLPHENYL)AMINO)BENZENOIC ACID	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
204	ETHYL 3-O-BETA-D-GALACTOPYRANOSYLATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
205	5-HYDROXYINDOLE-3-PYRUVATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	12.71	4.35	0.21	7200e450	
206	ASORBATE	ND	ND	ND	ND	11.34	22.25	0.10	9000e330	ND	ND	ND	ND	ND	
207	INACETYLTRYPTOPHAN	10.85	0.95	0.91	1700e24	12.41	11.91	0.11	1900e250	14.76	20.58	0.25	16000e470	ND	
208	1-PHENYLETHANOL	ND	ND	ND	ND	ND	ND	ND	ND	ND	13.77	7.43	0.31	8500e1400	
209	METHYLENE-BIS(SOXIMINE)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
210	4-HYDROXY-2-PHENYLGLYCINE	ND	ND	ND	ND	13.84	16.41	0.09	11000e110	14.49	32.31	0.31	12000e1100	ND	
211	LYSINE	12.73	0.41	0.10	1000e200	17.19	14.11	0.23	300e15	1.16	5.68	0.09	4400e270	ND	
212	CAPRYLATE	13.19	7.92	0.09	9000e120	13.62	18.32	0.20	3100e170	14.22	1.18	0.50	24000e360	ND	
213	AMINOACETATE	12.73	0.38	0.03	11000e400	ND	ND	ND	ND	ND	ND	ND	ND	ND	
214	OSHOIC(11)-HOMOSERINATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
215	3,5-DIAMINOBENZENOIC ACID	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
216	SALICINOL	ND	ND	ND	ND	15.58	7.64	0.08	5000e310	ND	ND	ND	ND	ND	
217	ITACONATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	13.05	7.14	0.27	8800e450	
218	4-HYDROXYMETHYLSULFARATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
219	1,4-BIS(3-CYCLOHEXYLANE)CARBOXYLATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
220	INDANONATE	14.14	5.57	0.12	1100e170	14.71	7.98	0.08	1500e270	16.23	5.80	0.24	1200e350	ND	
221	ORACONATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
222	TRANS-3-CYCLOHEXANEDIOL	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
223	3-METHYLGLUTAMONATE	14.13	19.58	0.08	2100e170	ND	ND	ND	ND	ND	13.38	5.81	0.35	36000e460	
224	GIBBERULINE	14.52	7.50	0.41	8500e300	ND	ND	ND	ND	ND	ND	ND	ND	ND	
225	HYDROXYMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
226	PROCATENOL	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
227	PORPHORBILINOGEN	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
228	PROTOLACTONE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
229	BENZYLAMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	13.4	17.84	0.18	71000e340	
230	ACRIBINE	12.74	7.40	0.07	3800e190	ND	ND	ND	ND	ND	14.1	18.76	0.28	10000e270	
231	GRODATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
232	DECANOATE	15.08	24.34	0.08	1000e48	15.56	22.24	0.03	2800e190	16.24	0.85	0.26	13000e1100	ND	
233	DIHYDROPROTATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
234	DIBENZOPIRONE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
235	ASPARTATE	12.74	13.49	0.15	8700e110	17.16	17.35	0.08	3500e490	14.27	5.49	0.21	34000e460	ND	
236	D-CYTHINE	12.73	5.24	0.20	1100e490	17.16	12.80	0.18	3000e110	ND	ND	ND	ND	ND	
237	GLUTAMATE	12.73	8.21	0.10	1100e140	17.13	4.09	0.07	2000e160	13.89	11.49	0.29	11000e1100	ND	
238	PROBIDE	12.73	7.66	0.10	1000e250	17.15	12.83	0.08	1500e110	ND	ND	ND	ND	ND	
239	N-ACETYLSPERMINE	12.74	9.07	0.03	8500e300	12.61	8.93	0.08	1600e200	ND	ND	ND	ND	ND	
240	4-PROPYLATE	9.52	21.40	0.27	9000e200	13.29	3.84	0.09	8100e300	ND	ND	ND	ND	ND	
241	3-METHYLASPARTATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
242	MALEAMATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
243	4-HYDROXYBENZONATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
244	SALICYLATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
245	5-HYDROXYBENZONATE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
246	LAURYL-CARBITINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
247	LAURATE	ND	ND	ND	ND	24.36	17.81	0.05	2900e440	14.43	6.84	0.24	41000e500	ND	
248	DOCECYLAMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	20	4.42	0.65	17000e260	ND
249	TRIAMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
250	TETRADECYLAMINE	ND	ND	ND	ND	ND	ND	ND	ND	ND	26.05	14.16	0.33	30000e160	ND
Average			11.27	0.79	2300e420		13.82	0.35	9300e530		7.76	0.30	24000e1100		

Supplementary Table 4. Comparison of Peak width at half height (second) for capLC-ESI-MS and CE-ESI-MS

#	Analyte	capLC-ESI-MS	CE-ESI-MS TM	Fold change
1	GLYCINE	4.2	6.4	1.53
2	ALANINE	4.2	6	2.14
3	PYRUVATE	5.6	7.8	1.38
4	OXOSULFURATE	5.4	6.4	1.56
5	MALATE	10.4	12	1.15
6	SERINE	10.4	12	1.15
7	GLUTAMINE	4.6	6.4	1.83
8	THREONINE	4.2	6	2.14
9	SUCONATE	3.8	7.8	2.17
10	LACTATE	9	6.4	0.83
11	TYROSINE	5.4	6	1.67
12	VALINE	6	7.8	1.30
13	FUMARATE	4.8	6.4	1.75
14	LEUCINE	6	6	1.00
15	ISOLEUCINE	6	6	1.00
16	TRYPTOPHAN	5.4	6.4	1.56
17	LYSINE	5.4	11.4	2.11
18	ASPARTATE	5.4	11.4	2.11
19	GLUTAMATE	5.4	11.4	2.11
20	ASORINE	10.8	6	0.83
21	ASPARAGINE	7.8	6.4	1.08
22	GLUTAMINE	4.8	6	1.88
23	PHENYLALANINE	5.4	6	1.67
24	METHIONINE	5.4	7.8	1.44
25	PROLINE	9.37	18	1.96

133 Huang, T.; Ambruster, M.; Lee, R.; Wu, D. S.; Edwards, J. L. Metabolic analysis of mammalian cells and human tissue through one-pot two-stage derivatizations using a heartless capillary electrophoresis-electrospray ionization-mass spectrometry. *J. Chromatogr. A* 2018, 1587, 219-225.