 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

113 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 15-15 H: 0-200 N: 0-10 O: 0-15

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

226.1240 226.1232 0.8 3.5 8.5 8.4 C15 H16 N O

REPORT MASSES AS +/-5mDa, referenced against

Leucine Enkephalin @ 557.2802 (M+H, C13 isotope) and 556.2771 (M+H, C12 isotope) positive mode, 555.2645 (M-H, C13) and 554.2615 (M-H, C12) negative mode.

or Sulfadimethoxine @312.0840 (M+H, C13) and 311.0814 (M+H, C12) positive mode, 310.0684 (M-H, C13) and 309.0658 (M-H, C12) negative mode.

This software version MassLynx 4.1 is calibrated ignoring the electron in all cases.

ANALYSIS RUN USING: WATERS LCT PREMIER (ESI POSITIVE/ESI NEGATIVE)

148.3469 1.013e0

148.3600 1.266e-2

148.4346 1.266e-2

148.4895 1.266e-2

148.5839 1.266e-2

148.6092 1.013e0

148.6322 1.266e-2

148.6872 1.266e-2

148.8366 1.013e0

148.8561 3.038e0

148.9598 1.013e0

149.0372 1.013e0

149.0812 2.025e0

149.1763 1.013e0

149.2225 1.013e0

149.2512 1.266e-2

149.3909 1.266e-2

149.5373 1.266e-2

149.5535 1.013e0

149.6290 2.025e0

149.6867 1.013e0

149.7642 1.013e0

149.8138 1.266e-2

149.8788 2.025e0

150.0248 2.025e0

150.0931 1.266e-2

150.1157 2.025e0

150.1422 1.013e0

150.1973 1.013e0

150.2409 1.025e0

150.4008 2.025e0

150.4381 1.266e-2

150.5459 1.266e-2

150.5798 2.025e0

150.6045 1.013e0

150.6363 2.025e0

150.7281 1.266e-2

150.7513 1.025e0

150.9767 1.013e0

151.1557 1.266e-2

151.1723 1.266e-2

151.2145 1.013e0

151.2353 3.038e0

151.2802 1.266e-2

151.3128 1.266e-2

151.4798 1.013e0

151.5711 1.013e0

151.6270 1.266e-2

151.7056 1.013e0

151.7245 1.013e0

151.7443 1.266e-2

151.7872 1.013e0

151.8849 2.025e0

151.9736 1.013e0

152.0755 1.266e-2

152.0990 2.532e-2

152.1342 2.025e0

152.3114 1.266e-2

152.3371 1.013e0

152.4457 1.013e0

152.4912 1.013e0

152.5179 1.025e0

152.6292 2.025e0

152.7309 1.266e-2

152.7626 2.025e0

152.8819 1.025e0

152.9708 1.013e0

153.0729 1.266e-2

153.1318 1.266e-2

153.2007 1.266e-2

153.2930 1.266e-2

153.3129 1.266e-2

153.4244 1.266e-2

153.5197 1.013e0

153.5381 2.025e0

153.5699 1.013e0

153.5878 2.038e0

153.6585 1.013e0

153.6712 1.266e-2

153.7409 1.266e-2

153.8296 1.013e0

153.8791 1.266e-2

153.9281 1.013e0

153.9515 1.013e0

154.0122 2.532e-2

154.1230 1.025e0

154.1595 1.266e-2

154.2356 1.013e0

154.3079 1.013e0

154.5319 1.025e0

154.5587 1.266e-2

154.6178 1.266e-2

154.6830 3.063e0

154.8416 2.532e-2

154.8889 1.025e0

154.9389 1.013e0

155.0314 1.013e0

155.0507 1.013e0

155.1937 1.266e-2

155.2207 3.038e0

155.2763 1.013e0

155.3060 1.013e0

155.4002 1.025e0

155.4417 1.013e0

155.5841 1.013e0

155.6897 1.013e0

155.8195 1.266e-2

156.0453 1.266e-2

156.1743 1.013e0

156.1945 1.013e0

156.2281 1.013e0

156.3244 1.266e-2

156.3601 1.266e-2

156.4632 1.013e0

156.7793 1.013e0

156.8925 1.013e0

156.9422 1.013e0

156.9654 1.266e-2

157.0193 1.013e0

157.0357 1.013e0

157.0720 1.013e0

157.2157 1.013e0

157.2389 1.266e-2

157.2717 1.025e0

157.3021 1.013e0

157.3389 1.013e0

157.4087 3.038e0

157.4551 2.532e-2

157.5884 2.025e0

157.6407 1.025e0

157.6816 1.266e-2

157.7424 1.013e0

158.0526 1.013e0

158.1461 1.266e-2

158.2087 3.798e-2

158.2428 1.266e-2

158.2901 1.013e0

158.5375 1.266e-2

158.5601 2.025e0

158.6143 1.025e0

158.6942 1.013e0

158.8985 1.266e-2

158.9760 1.013e0

159.2439 1.013e0

159.3210 1.266e-2

159.3977 1.013e0

159.4214 1.266e-2

159.4655 2.025e0

159.5184 1.013e0

159.5608 2.025e0

159.5997 1.013e0

159.6291 1.266e-2

159.6833 1.013e0

159.7403 1.013e0

159.7634 1.013e0

159.7959 3.038e0

160.0255 1.013e0

160.0807 3.038e0

160.1298 1.266e-2

160.2280 1.013e0

160.3031 2.025e0

160.3558 1.013e0

160.4122 1.266e-2

160.4292 1.013e0

160.4597 2.025e0

160.5536 2.038e0

160.5774 1.013e0

160.5961 2.025e0

160.6300 1.025e0

160.6531 1.025e0

160.7358 1.266e-2

160.8114 1.038e0

160.8638 1.013e0

160.9276 1.266e-2

161.0725 1.266e-2

161.1538 1.013e0

161.1742 1.013e0

161.2733 1.025e0

161.3193 1.013e0

161.4679 1.013e0

161.5415 1.013e0

161.6918 2.025e0

161.7633 2.532e-2

161.8353 1.013e0

161.9470 1.013e0

161.9669 1.013e0

162.1225 2.532e-2

162.1396 1.013e0

162.1788 2.532e-2

162.2010 1.266e-2

162.2548 1.266e-2

162.3123 1.025e0

162.4237 2.025e0

162.4509 1.266e-2

162.5897 1.266e-2

162.7324 1.266e-2

162.7981 2.038e0

162.8239 1.266e-2

162.8736 2.532e-2

162.9218 1.013e0

163.1249 7.418e1

163.1801 1.266e-2

163.2577 2.025e0

163.3532 1.266e-2

163.3977 1.013e0

163.4261 2.025e0

163.5284 2.038e0

163.5590 2.025e0

163.6997 1.013e0

163.7236 1.013e0

163.8370 1.025e0

163.8593 1.266e-2

163.8867 1.013e0

163.9684 1.266e-2

164.0481 1.025e0

164.1275 3.273e1

164.2095 1.013e0

164.3742 2.038e0

164.4327 2.025e0

164.5708 1.013e0

164.6492 1.025e0

164.7653 1.013e0

164.7922 1.266e-2

164.8435 1.013e0

164.9083 3.643e0

164.9431 1.025e0

165.0893 1.025e0

165.1469 5.758e0

165.1818 1.266e-2

165.3010 2.532e-2

165.3766 1.025e0

165.6431 2.532e-2

165.6666 1.013e0

165.6835 1.266e-2

165.8518 1.013e0

165.8892 1.013e0

165.9146 2.025e0

165.9485 1.025e0

166.1052 2.025e0

166.2690 1.013e0

166.2931 1.013e0

166.3344 1.013e0

166.4299 1.013e0

166.4708 1.266e-2

166.4950 2.532e-2

166.5803 2.038e0

166.6635 1.013e0

166.7211 1.013e0

166.7520 2.025e0

166.8141 2.025e0

166.9072 1.025e0

166.9449 1.266e-2

166.9991 1.013e0

167.2266 1.013e0

167.3460 1.013e0

167.5905 2.025e0

167.6865 1.013e0

167.8558 1.013e0

167.9636 2.025e0

168.0791 1.013e0

168.1724 1.266e-2

168.1966 1.266e-2

168.2757 2.025e0

168.4686 1.266e-2

168.6330 2.025e0

168.7578 1.266e-2

168.8479 1.266e-2

168.9137 1.025e0

168.9933 1.266e-2

169.1725 1.266e-2

169.1896 1.013e0

169.2553 1.013e0

169.2952 2.025e0

169.4356 2.038e0

169.5847 2.025e0

169.6120 1.266e-2

169.6430 1.266e-2

169.7255 1.025e0

169.7706 1.013e0

169.8297 1.266e-2

169.8922 1.013e0

169.9286 2.532e-2

170.1213 2.532e-2

170.2128 1.025e0

170.2559 1.013e0

170.3215 1.266e-2

170.3421 1.025e0

170.3907 1.266e-2

170.4568 1.013e0

170.5246 2.025e0

170.6155 3.038e0

170.7080 2.038e0

170.7314 1.266e-2

170.8810 1.266e-2

170.9103 1.025e0

170.9365 1.013e0

170.9850 2.025e0

171.0334 2.025e0

171.0991 1.025e0

171.1649 1.025e0

171.2535 1.025e0

171.2796 1.266e-2

171.3075 1.013e0

171.3911 1.013e0

171.4485 2.025e0

171.4852 1.013e0

171.5165 1.013e0

171.5583 2.025e0

171.7568 1.025e0

171.8613 2.025e0

171.8819 6.642e-1

171.9799 1.266e-2

172.0078 2.025e0

172.0915 1.013e0

172.1299 1.013e0

172.2031 1.266e-2

172.3566 1.266e-2

172.4054 1.013e0

172.4717 1.013e0

172.5449 1.266e-2

172.6024 1.025e0

172.7036 2.025e0

172.7717 1.013e0

173.0023 1.013e0

173.0442 1.013e0

173.1946 2.025e0

173.2803 2.025e0

173.3765 1.013e0

173.4045 2.025e0

173.4866 1.025e0

173.5128 1.013e0

173.5915 2.025e0

173.7944 1.025e0

174.0062 1.266e-2

174.1813 2.025e0

174.2058 2.532e-2

174.4105 2.038e0

174.4756 1.013e0

174.5161 2.025e0

174.5718 3.038e0

174.6587 1.013e0

174.6799 1.013e0

174.7045 1.266e-2

174.7644 1.013e0

174.8206 1.013e0

174.9030 1.025e0

174.9994 1.266e-2

175.2240 1.013e0

175.2661 1.013e0

175.3382 2.532e-2

175.4636 1.013e0

175.4919 1.013e0

175.5520 2.532e-2

175.6152 2.025e0

175.7733 1.013e0

175.8822 1.013e0

175.9473 1.025e0

175.9843 1.025e0

176.0445 1.266e-2

176.1439 1.266e-2

176.4217 1.266e-2

176.4568 2.532e-2

176.6021 1.013e0

176.6199 1.266e-2

176.6801 1.266e-2

176.7469 1.013e0

176.7980 2.532e-2

176.8526 1.013e0

176.9652 1.013e0

177.1362 5.732e0

177.2451 1.266e-2

177.3103 2.532e-2

177.3649 1.266e-2

177.4824 1.013e0

177.7366 1.013e0

177.7970 1.013e0

177.8613 1.013e0

178.1104 2.025e0

178.1391 5.063e-2

178.3396 1.013e0

178.4704 1.013e0

178.5027 1.013e0

178.7051 1.013e0

178.7298 1.013e0

178.8475 1.266e-2

178.9328 1.013e0

178.9505 1.025e0

179.0036 1.013e0

179.0706 1.013e0

179.1037 3.038e0

179.3305 2.532e-2

179.4306 1.013e0

179.4630 1.266e-2

179.5443 1.013e0

179.5762 1.013e0

179.6151 1.025e0

179.7654 1.013e0

179.8362 1.013e0

179.8787 2.532e-2

179.9395 1.266e-2

179.9612 1.013e0

180.0538 1.266e-2

180.0822 1.013e0

180.1928 2.025e0

180.3141 2.025e0

180.4097 1.013e0

180.5072 1.013e0

180.7068 1.266e-2

180.8528 1.013e0

180.8955 1.266e-2

180.9876 3.038e0

181.0567 1.013e0

181.0929 7.089e0

181.2304 2.025e0

181.2997 1.013e0

181.3569 1.013e0

181.4041 1.025e0

181.4584 1.038e0

181.5462 1.266e-2

181.6153 1.266e-2

181.7792 1.266e-2

181.8693 1.266e-2

181.8871 1.013e0

181.9298 2.025e0

181.9617 1.266e-2

181.9980 1.013e0

182.0199 1.266e-2

182.0985 1.013e0

182.2133 1.266e-2

182.3420 1.013e0

182.3999 1.025e0

182.4504 1.013e0

182.4824 1.013e0

182.5287 2.532e-2

182.7581 1.013e0

182.8020 1.013e0

182.8630 1.013e0

182.9200 1.266e-2

182.9705 1.266e-2

183.0498 1.013e0

183.1175 1.013e0

183.2154 1.013e0

183.3009 1.266e-2

183.4701 1.025e0

183.5099 1.266e-2

183.7444 1.013e0

183.7979 1.266e-2

183.8246 2.532e-2

183.8665 1.013e0

183.8958 2.025e0

183.9672 1.266e-2

184.0688 1.013e0

184.0956 1.025e0

184.2273 1.025e0

184.2631 1.013e0

184.3078 1.025e0

184.3675 1.266e-2

184.3896 1.013e0

184.4398 1.266e-2

184.6593 1.013e0

184.7071 1.013e0

184.8364 1.013e0

184.8623 1.013e0

184.9843 1.013e0

185.0397 1.013e0

185.0592 2.025e0

185.2915 1.013e0

185.4238 2.025e0

185.4657 1.013e0

185.9072 1.013e0

186.0264 1.013e0

186.1696 2.025e0

186.2304 2.532e-2

186.2842 1.013e0

186.3220 2.025e0

186.3677 1.025e0

186.4507 1.013e0

186.7482 1.013e0

186.7855 1.266e-2

186.8071 1.266e-2

186.8937 1.013e0

187.0060 1.266e-2

187.0355 1.266e-2

187.2785 1.013e0

187.3628 2.025e0

187.5663 1.013e0

187.6247 2.025e0

187.6770 2.532e-2

187.7271 1.013e0

187.7953 1.013e0

187.8134 1.266e-2

187.9783 1.266e-2

188.0106 1.013e0

188.0869 3.038e0

188.1741 1.013e0

188.2179 3.038e0

188.3160 1.266e-2

188.3385 1.013e0

188.4122 3.038e0

188.4663 1.266e-2

188.5461 1.013e0

188.7035 2.025e0

188.7366 1.266e-2

188.7581 1.013e0

188.9776 1.266e-2

189.1804 1.038e0

189.2186 1.266e-2

189.2510 1.013e0

189.2834 1.013e0

189.3209 1.013e0

189.3392 1.266e-2

189.3968 1.013e0

189.4634 1.013e0

189.5069 3.798e-2

189.6093 1.266e-2

189.7263 1.266e-2

189.7497 2.025e0

189.8217 1.013e0

189.9078 1.025e0

189.9352 1.013e0

190.0047 1.013e0

190.0777 1.013e0

190.0957 2.532e-2

190.1804 1.013e0

190.2651 1.025e0

190.3227 1.013e0

190.4366 2.025e0

190.5103 1.013e0

190.6868 1.266e-2

190.8956 1.266e-2

191.2664 1.266e-2

191.4128 1.266e-2

191.5789 1.013e0

191.6640 2.025e0

191.7109 1.013e0

191.9134 1.013e0

191.9419 1.038e0

192.2154 1.013e0

192.3076 2.532e-2

192.3782 1.266e-2

192.4226 1.038e0

192.5175 1.013e0

192.8643 1.266e-2

192.9049 1.013e0

192.9411 1.266e-2

193.0560 1.013e0

193.1287 6.329e-2

193.1634 1.013e0

193.2038 1.013e0

193.2379 2.038e0

193.2818 1.013e0

193.3144 1.266e-2

193.3477 1.013e0

193.4177 2.025e0

193.4591 1.013e0

193.5437 1.025e0

193.5845 1.025e0

193.7096 1.025e0

193.7913 1.013e0

193.8129 1.013e0

193.8593 3.038e0

193.8801 2.532e-2

193.9799 1.266e-2

194.0435 1.013e0

194.0652 1.013e0

194.1469 2.038e0

194.2249 1.013e0

194.2503 1.266e-2

194.4138 1.266e-2

194.4872 1.013e0

194.5064 1.266e-2

194.7316 1.013e0

194.7769 1.013e0

194.8060 2.025e0

194.8242 1.013e0

194.9133 1.266e-2

194.9317 1.025e0

194.9859 2.025e0

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195.0951 1.013e0

195.1133 1.266e-2

195.2953 1.266e-2

195.3185 1.013e0

195.5970 1.013e0

195.6970 1.013e0

195.7452 3.076e0

195.8304 1.266e-2

196.0013 1.266e-2

196.0538 3.038e0

196.1745 2.025e0

196.3629 1.013e0

196.4446 1.266e-2

196.5420 1.013e0

196.5894 1.013e0

196.6285 1.038e0

196.7462 1.013e0

196.9512 1.013e0

197.0598 1.266e-2

197.2012 2.532e-2

197.2422 1.266e-2

197.3672 2.025e0

197.4777 1.013e0

197.5854 1.266e-2

197.7876 1.013e0

197.8209 1.266e-2

197.8392 1.013e0

197.9635 1.025e0

198.0421 1.266e-2

198.1315 1.013e0

198.5611 1.013e0

198.6755 2.025e0

198.7639 1.025e0

198.7970 1.013e0

198.9324 2.038e0

199.0074 1.025e0

199.2454 1.025e0

199.3497 1.025e0

199.3865 1.266e-2

199.4400 2.532e-2

199.5512 1.013e0

199.6299 1.013e0

199.7949 1.013e0

199.8246 1.013e0

199.9195 1.266e-2

200.0808 1.013e0

200.1780 1.013e0

200.3506 1.266e-2

200.4181 1.266e-2

200.5209 1.266e-2

200.5900 2.532e-2

200.7293 2.025e0

200.8549 1.013e0

201.1451 1.013e0

201.1719 2.532e-2

201.2509 1.013e0

201.4577 1.266e-2

201.5713 1.266e-2

201.5972 2.025e0

201.6320 1.013e0

201.7110 1.266e-2

201.7717 1.013e0

201.8562 2.025e0

201.9035 1.013e0

202.1163 2.532e-2

202.1946 1.013e0

202.3676 1.266e-2

202.6400 1.266e-2

202.6984 3.038e0

202.7874 1.013e0

202.8099 1.266e-2

202.8407 1.013e0

202.9053 1.013e0

202.9881 1.013e0

203.0220 1.013e0

203.0710 1.013e0

203.1208 1.025e0

203.1568 2.025e0

203.2664 1.025e0

203.3364 1.013e0

203.4642 2.038e0

203.4875 1.013e0

203.6554 1.013e0

203.7036 1.013e0

203.7719 1.266e-2

203.8603 1.013e0

203.9205 1.013e0

203.9476 3.038e0

204.0001 2.025e0

204.1113 4.051e0

204.2699 1.013e0

204.4028 1.013e0

204.4767 2.025e0

204.5806 1.013e0

204.6225 1.025e0

204.7943 1.013e0

205.0752 1.013e0

205.1662 3.038e0

205.2657 1.013e0

205.3879 1.013e0

205.4173 1.013e0

205.6726 2.025e0

205.7262 1.266e-2

205.7764 1.013e0

205.8852 3.038e0

205.9372 3.038e0

206.0062 2.532e-2

206.1039 1.013e0

206.1390 7.089e0

206.1718 2.606e0

206.1982 1.013e0

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206.3402 1.013e0

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276.8929 2.025e0

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278.3239 1.013e0

278.5723 1.266e-2

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278.8247 1.013e0

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