 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

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

Elements Used:

C: 14-14 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

212.1075 212.1075 0.0 0.0 8.5 2773017.5 C14 H14 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)

150.9035 1.266e-2

150.9621 1.013e0

150.9948 1.266e-2

151.2119 2.532e-2

151.2561 2.532e-2

151.4419 1.013e0

151.4685 1.266e-2

151.5205 1.266e-2

151.5437 1.266e-2

151.5891 1.266e-2

151.6810 1.013e0

151.7363 1.266e-2

151.8366 1.025e0

151.8549 1.266e-2

151.8936 1.025e0

151.9162 3.038e0

152.1462 1.266e-2

152.2475 1.013e0

152.5870 2.025e0

152.6708 1.266e-2

152.7363 1.266e-2

152.7629 1.266e-2

152.8396 1.038e0

152.9543 2.025e0

153.0533 2.532e-2

153.0849 3.798e-2

153.1346 1.051e0

153.2783 1.013e0

153.3639 1.266e-2

153.3839 1.013e0

153.4201 1.266e-2

153.4378 1.025e0

153.6308 1.266e-2

153.8253 1.013e0

153.9321 3.798e-2

153.9885 2.532e-2

154.1571 2.532e-2

154.3201 1.266e-2

154.3925 1.025e0

154.4549 1.013e0

154.4883 1.013e0

154.5875 1.013e0

154.6450 2.532e-2

154.8184 1.013e0

154.8469 2.532e-2

154.9505 2.532e-2

155.0730 1.013e0

155.1756 1.266e-2

155.2683 2.025e0

155.3112 1.266e-2

155.5566 1.013e0

155.6886 1.013e0

155.7121 1.013e0

155.7439 2.025e0

155.7717 1.025e0

155.8566 1.025e0

155.8842 1.266e-2

155.9448 1.013e0

156.1059 2.038e0

156.3197 2.532e-2

156.3362 1.013e0

156.3858 1.266e-2

156.6740 3.798e-2

156.9149 2.025e0

157.1044 1.266e-2

157.1296 2.532e-2

157.2195 2.532e-2

157.4075 1.025e0

157.4638 1.266e-2

157.5198 2.038e0

157.6611 1.025e0

157.7496 2.532e-2

157.8344 1.013e0

157.8904 3.798e-2

157.9463 2.532e-2

158.0176 1.266e-2

158.0413 1.025e0

158.1313 1.266e-2

158.2279 2.025e0

158.4259 1.266e-2

158.4925 1.013e0

158.6664 1.013e0

158.7200 1.013e0

158.9341 1.266e-2

158.9772 2.038e0

159.0400 1.038e0

159.1703 1.025e0

159.1923 1.013e0

159.2859 1.013e0

159.5006 1.013e0

159.5410 1.013e0

159.5816 1.266e-2

159.6651 1.013e0

159.6990 1.266e-2

159.9102 1.266e-2

160.4109 1.266e-2

160.4857 1.266e-2

160.5173 1.025e0

160.6536 1.013e0

160.6802 1.266e-2

160.7176 1.266e-2

160.9281 2.025e0

161.2195 1.266e-2

161.5064 1.266e-2

161.5334 1.266e-2

161.6152 1.266e-2

161.6418 1.025e0

161.8443 1.013e0

161.9293 1.013e0

162.0900 1.025e0

162.1997 1.266e-2

162.2837 1.266e-2

162.3828 1.266e-2

162.4906 2.532e-2

162.5985 2.025e0

162.6293 1.266e-2

162.6481 2.532e-2

162.7748 1.013e0

162.8091 2.532e-2

162.9564 1.025e0

163.0230 1.266e-2

163.0966 2.532e-2

163.1926 1.266e-2

163.4299 1.266e-2

163.6297 2.025e0

163.7567 1.266e-2

163.8489 3.798e-2

163.8889 1.266e-2

164.0879 1.025e0

164.1611 1.266e-2

164.1778 1.266e-2

164.2048 1.013e0

164.2905 1.013e0

164.4289 3.798e-2

164.6377 1.013e0

164.8457 1.266e-2

164.9281 2.532e-2

165.0160 1.013e0

165.1396 1.266e-2

165.1603 2.025e0

165.2143 1.266e-2

165.2929 1.266e-2

165.3994 1.266e-2

165.4163 2.532e-2

165.4465 1.013e0

165.5939 1.266e-2

165.6112 1.266e-2

165.7543 1.266e-2

165.7783 1.266e-2

165.8127 1.025e0

165.8948 1.266e-2

166.0419 1.013e0

166.3659 2.532e-2

166.6074 2.025e0

166.6928 1.266e-2

166.9268 1.025e0

167.0702 1.266e-2

167.1564 1.266e-2

167.1771 2.025e0

167.3672 1.025e0

167.4312 5.063e0

167.4898 1.266e-2

167.5689 1.266e-2

167.6957 2.025e0

167.7785 1.013e0

167.9113 1.025e0

167.9573 3.038e0

168.0779 2.532e-2

168.1263 2.025e0

168.3877 1.266e-2

168.4189 1.266e-2

168.5192 1.013e0

168.6677 1.013e0

168.7717 3.038e0

168.8433 1.013e0

168.8710 1.013e0

168.9748 1.266e-2

168.9921 1.013e0

169.0357 1.038e0

169.5454 1.266e-2

169.6384 1.013e0

169.6865 1.013e0

169.9291 1.013e0

170.2444 1.266e-2

170.2927 1.266e-2

170.4139 1.266e-2

170.4834 3.038e0

170.5251 1.013e0

170.5842 1.266e-2

170.6190 1.266e-2

170.6537 1.025e0

170.6780 1.013e0

170.7163 1.266e-2

170.7963 1.266e-2

171.0253 1.266e-2

171.0703 1.013e0

171.0980 1.013e0

171.1742 1.013e0

171.2054 1.266e-2

171.4213 1.266e-2

171.4839 1.013e0

171.6685 1.013e0

171.7417 1.266e-2

171.8253 1.013e0

172.0380 1.266e-2

172.2996 1.013e0

172.3675 2.025e0

172.4286 1.266e-2

172.4496 1.013e0

172.5472 1.025e0

172.7391 1.266e-2

172.9906 1.266e-2

173.0850 1.266e-2

173.1326 2.051e0

173.2083 1.038e0

173.4453 1.266e-2

173.5973 2.025e0

173.7740 1.013e0

173.8580 1.013e0

173.9035 1.013e0

173.9735 1.013e0

174.4603 1.013e0

174.5307 1.013e0

174.7209 1.266e-2

174.7597 1.013e0

174.7914 1.266e-2

174.8160 1.025e0

174.9561 2.532e-2

175.2404 1.266e-2

175.5790 1.025e0

175.6316 2.025e0

175.6597 1.025e0

175.8266 1.025e0

175.8951 2.532e-2

176.0008 1.013e0

176.1230 3.798e-2

176.1426 2.025e0

176.1990 1.266e-2

176.2288 2.025e0

176.3924 1.266e-2

176.4522 1.025e0

176.5121 1.013e0

176.6080 1.266e-2

176.8268 1.013e0

176.8550 1.013e0

176.9605 1.266e-2

177.1343 5.498e0

177.2016 1.266e-2

177.2422 3.051e0

177.2721 2.532e-2

177.3250 1.013e0

177.4848 1.266e-2

177.5169 1.266e-2

177.5380 1.266e-2

177.5779 3.038e0

177.6050 1.266e-2

177.6685 1.266e-2

177.7495 1.013e0

177.9346 1.266e-2

178.0934 1.266e-2

178.2520 1.025e0

178.3102 1.013e0

178.3562 1.013e0

178.4162 1.025e0

178.6208 2.025e0

178.9883 2.025e0

179.1521 1.266e-2

179.3329 1.266e-2

179.3505 1.266e-2

179.4760 2.038e0

179.5503 2.025e0

179.5963 1.013e0

179.6281 1.013e0

179.8174 1.025e0

179.9438 2.025e0

179.9922 1.025e0

180.0491 1.013e0

180.1395 1.025e0

180.3520 1.013e0

180.4051 1.025e0

180.5061 1.266e-2

180.5805 1.013e0

180.7129 1.013e0

181.0182 2.025e0

181.0978 1.933e1

181.1487 2.532e-2

181.1848 1.266e-2

181.2701 1.013e0

181.4625 1.038e0

181.5257 2.025e0

181.5558 1.266e-2

181.6177 1.266e-2

181.6552 2.025e0

181.6747 1.266e-2

181.7816 1.266e-2

181.8895 1.025e0

182.0077 1.013e0

182.0672 2.532e-2

182.0930 6.642e-1

182.1134 1.025e0

182.1792 1.266e-2

182.3035 2.025e0

182.3267 2.532e-2

182.4458 1.025e0

182.5471 2.532e-2

182.5959 1.025e0

182.7715 1.266e-2

183.1709 1.013e0

183.2142 1.266e-2

183.3691 1.013e0

183.4944 1.025e0

183.8324 1.013e0

183.8727 1.013e0

184.0855 1.013e0

184.1712 2.532e-2

184.9188 1.266e-2

184.9925 2.532e-2

185.0670 1.266e-2

185.1047 1.038e0

185.3347 1.013e0

185.3995 1.025e0

185.4423 1.013e0

185.4978 1.266e-2

185.7034 1.266e-2

185.8089 3.798e-2

185.8911 1.266e-2

186.0436 2.532e-2

186.1148 2.532e-2

186.1996 1.013e0

186.3224 1.013e0

186.3869 2.025e0

186.4317 1.266e-2

186.7218 2.025e0

186.8024 1.013e0

187.3107 1.013e0

187.3599 2.025e0

187.4603 1.266e-2

187.4855 1.013e0

187.5538 1.013e0

187.6923 1.266e-2

187.7798 1.013e0

188.0168 1.013e0

188.0955 2.051e0

188.2247 1.025e0

188.2862 2.532e-2

188.3814 1.013e0

188.5342 1.266e-2

188.6366 1.025e0

188.6582 1.266e-2

188.6833 1.266e-2

188.7245 1.266e-2

188.7859 1.025e0

188.8956 1.266e-2

188.9578 1.013e0

189.0323 2.532e-2

189.0558 1.266e-2

189.1492 1.025e0

189.2247 1.013e0

189.5423 1.013e0

189.5973 1.266e-2

189.6594 1.013e0

189.7433 1.013e0

189.8351 1.013e0

189.9162 1.266e-2

189.9540 2.532e-2

190.0034 1.013e0

190.0621 1.013e0

190.2000 2.038e0

190.2533 1.266e-2

190.2766 2.025e0

190.2965 1.025e0

190.4731 1.013e0

190.5110 2.532e-2

190.5489 1.013e0

190.6337 1.013e0

190.7041 1.013e0

190.9105 1.038e0

191.0307 1.266e-2

191.2726 1.013e0

191.3147 2.532e-2

191.4268 1.013e0

191.4749 2.025e0

191.5563 1.013e0

191.7767 1.266e-2

191.8445 2.025e0

191.8833 1.013e0

192.3731 1.013e0

192.4649 1.266e-2

192.5020 1.013e0

192.7971 1.025e0

192.8501 1.025e0

192.9148 1.013e0

193.2844 1.266e-2

193.3279 2.025e0

193.3876 1.266e-2

193.4616 2.532e-2

193.5575 2.025e0

193.6500 1.013e0

193.7086 1.013e0

193.7351 2.532e-2

193.8065 2.025e0

193.9157 2.025e0

193.9970 1.266e-2

194.0895 2.025e0

194.4344 1.266e-2

194.5979 1.266e-2

194.7015 1.266e-2

194.7640 1.266e-2

194.8722 1.266e-2

194.9086 1.266e-2

195.0577 1.266e-2

195.1939 1.025e0

195.2258 2.025e0

195.4178 1.013e0

195.5027 1.038e0

195.7498 1.025e0

195.9745 1.266e-2

196.2095 1.266e-2

196.2377 3.038e0

196.3423 1.013e0

196.4171 1.013e0

196.5738 1.266e-2

196.6147 1.266e-2

196.6849 1.266e-2

196.7160 1.266e-2

196.9656 1.013e0

197.0378 2.025e0

197.1920 1.266e-2

197.2740 1.266e-2

197.3453 2.532e-2

197.5657 4.051e0

197.6720 2.532e-2

197.7377 2.532e-2

197.7653 2.025e0

197.8236 1.266e-2

197.8506 3.038e0

197.9843 2.532e-2

198.0400 2.532e-2

198.1851 3.798e-2

198.4362 2.532e-2

198.5116 1.025e0

198.5381 1.013e0

198.7476 1.266e-2

198.9314 2.025e0

198.9679 1.013e0

199.0738 2.532e-2

199.2238 1.013e0

199.2425 1.013e0

199.3884 1.025e0

199.4220 1.013e0

199.4406 1.013e0

199.4824 1.266e-2

199.5080 1.266e-2

199.6582 2.532e-2

199.7681 1.013e0

199.8653 1.013e0

200.0011 1.013e0

200.2704 1.013e0

200.3806 1.013e0

200.4364 1.266e-2

200.4668 2.038e0

200.5274 1.013e0

200.5988 1.266e-2

200.7071 2.025e0

200.8843 1.013e0

201.0331 1.025e0

201.1781 1.013e0

201.2230 2.532e-2

201.4269 1.266e-2

201.6604 1.013e0

201.7027 1.266e-2

202.0510 2.025e0

202.1255 1.013e0

202.1774 1.266e-2

202.3711 3.038e0

202.4421 3.038e0

202.4845 1.266e-2

202.5746 1.013e0

202.6575 1.266e-2

202.7406 1.266e-2

202.8010 1.013e0

203.0480 2.532e-2

203.1609 1.266e-2

203.2450 1.266e-2

203.3538 1.266e-2

203.4922 2.025e0

203.7144 1.266e-2

203.9514 1.025e0

204.2664 2.025e0

204.3819 1.266e-2

204.4092 1.266e-2

204.7362 1.013e0

205.2240 2.025e0

205.5495 1.266e-2

206.0382 1.266e-2

206.2049 1.266e-2

206.4160 1.013e0

206.5353 2.532e-2

206.6007 3.038e0

206.6578 1.025e0

206.8125 1.266e-2

206.8351 2.025e0

207.0382 1.266e-2

207.0993 1.013e0

207.1724 1.013e0

207.2056 1.013e0

207.2558 1.013e0

207.3133 1.013e0

207.4743 1.266e-2

207.5081 1.013e0

207.5767 1.013e0

207.7073 2.038e0

207.7457 1.025e0

207.8107 1.266e-2

207.8720 1.013e0

207.9498 4.051e0

208.4311 1.266e-2

208.6691 1.266e-2

208.7733 1.266e-2

208.8495 1.013e0

208.9173 2.025e0

209.0076 1.266e-2

209.2141 1.266e-2

209.2962 1.266e-2

209.6418 1.013e0

209.7150 1.013e0

210.1670 2.025e0

210.2964 2.025e0

210.5425 1.025e0

210.5636 2.532e-2

210.6396 1.266e-2

210.7122 1.025e0

210.7589 1.013e0

210.9665 1.013e0

210.9940 1.013e0

211.0369 3.038e0

211.0709 2.051e0

211.1398 4.051e0

211.1901 1.013e0

211.2329 2.025e0

211.3450 2.025e0

211.3843 1.266e-2

211.4802 1.013e0

211.5046 1.038e0

211.7724 2.025e0

211.9559 1.013e0

212.0448 1.266e-2

212.1075 1.723e2

212.1605 2.434e0

212.2856 1.038e0

212.3197 3.038e0

212.3638 2.025e0

212.4589 1.013e0

212.6254 1.266e-2

212.6662 1.051e0

212.6893 8.689e-1

212.7191 2.532e-2

212.7554 2.532e-2

212.8482 2.532e-2

212.8969 2.038e0

213.0421 2.025e0

213.1158 4.787e1

213.1988 1.266e-2

213.2656 1.266e-2

213.3819 1.013e0

213.4474 1.013e0

213.5413 1.266e-2

213.6180 1.266e-2

213.7969 2.025e0

213.8317 1.266e-2

213.8553 1.266e-2

213.8869 3.798e-2

213.9584 2.532e-2

214.2667 1.013e0

214.4018 2.025e0

214.5051 1.013e0

214.7848 2.532e-2

214.8806 2.025e0

215.0495 1.013e0

215.0809 1.013e0

215.1264 3.038e0

215.2525 1.266e-2

215.3415 2.025e0

215.3727 1.266e-2

215.4159 2.025e0

215.7850 3.038e0

215.8333 1.266e-2

215.8689 1.013e0

215.9462 1.013e0

216.0007 1.013e0

216.2153 1.266e-2

216.3130 2.532e-2

216.3377 1.266e-2

216.3898 2.025e0

216.4902 1.013e0

216.7518 1.013e0

216.7742 1.266e-2

216.9268 1.266e-2

217.0543 3.038e0

217.2793 1.013e0

217.3077 1.266e-2

217.3565 2.532e-2

217.5617 2.025e0

217.6790 1.025e0

217.7187 1.013e0

217.7514 2.532e-2

217.7883 1.266e-2

217.8094 1.266e-2

217.9032 1.013e0

218.2481 1.013e0

218.5463 2.025e0

218.6209 1.266e-2

218.6644 1.266e-2

218.7589 1.266e-2

218.9863 1.013e0

219.1660 1.038e0

219.1897 2.038e0

219.2343 1.013e0

219.3911 2.025e0

219.5350 1.025e0

219.5623 2.025e0

219.6153 1.266e-2

219.7309 1.013e0

219.9295 2.532e-2

219.9749 1.266e-2

220.0920 1.013e0

220.1699 2.532e-2

220.2664 1.266e-2

220.4746 1.013e0

220.5854 1.013e0

220.7295 2.532e-2

220.9296 1.266e-2

221.0632 1.013e0

221.1380 1.266e-2

221.3011 3.038e0

221.3520 1.266e-2

221.7687 2.532e-2

221.9480 1.013e0

222.0317 1.266e-2

222.0693 2.038e0

222.1778 1.013e0

222.2559 2.025e0

222.3927 1.266e-2

222.5940 1.266e-2

222.8695 2.025e0

223.3004 1.013e0

223.3830 1.013e0

223.4956 1.013e0

223.5181 1.266e-2

223.5788 1.266e-2

223.6840 2.025e0

223.7180 1.266e-2

223.7501 2.532e-2

223.8007 1.013e0

223.8399 1.266e-2

223.8799 1.013e0

224.0477 1.025e0

224.0952 1.266e-2

224.1325 1.051e0

224.1791 2.532e-2

224.4830 2.025e0

224.7699 1.025e0

224.8043 1.025e0

225.1303 1.025e0

225.2696 1.266e-2

225.2900 1.013e0

225.4852 1.013e0

225.6572 2.025e0

225.9603 3.038e0

226.0619 2.025e0

226.1367 1.013e0

226.1900 1.025e0

226.2339 2.025e0

226.3715 1.013e0

226.4268 1.013e0

226.4816 2.532e-2

226.7082 1.266e-2

226.8319 1.013e0

226.8878 1.266e-2

227.1518 1.266e-2

227.3776 1.025e0

227.4197 1.013e0

227.4485 1.266e-2

227.5077 1.266e-2

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227.8487 1.025e0

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228.5470 1.266e-2

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