 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

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

Elements Used:

C: 12-12 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

206.1186 206.1181 0.5 2.4 5.5 1.5 C12 H16 N O2

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)

149.6805 1.266e-2

149.7807 2.025e0

149.8721 1.025e0

149.9536 1.266e-2

150.0738 1.013e0

150.1322 1.266e-2

150.1874 1.266e-2

150.2105 1.266e-2

150.2984 1.013e0

150.4124 1.013e0

150.4610 1.266e-2

150.4808 1.266e-2

150.5194 2.532e-2

150.5361 1.013e0

150.6127 2.025e0

150.6696 2.532e-2

150.7186 1.013e0

150.8099 2.532e-2

150.8314 2.025e0

150.8526 1.266e-2

150.8817 1.013e0

150.9337 1.013e0

150.9667 1.013e0

150.9930 1.013e0

151.0617 1.266e-2

151.1789 1.013e0

151.1939 2.025e0

151.2210 1.013e0

151.2741 1.013e0

151.3427 1.088e0

151.3633 2.532e-2

151.4112 1.266e-2

151.4273 1.013e0

151.4784 2.038e0

151.5384 1.013e0

151.5681 1.013e0

151.6320 1.025e0

151.6989 1.013e0

151.7153 1.266e-2

151.7576 1.013e0

151.8395 1.013e0

151.8983 1.013e0

151.9569 1.013e0

152.0622 1.266e-2

152.2196 1.266e-2

152.2519 1.266e-2

152.2850 1.013e0

152.4508 2.532e-2

152.5750 2.025e0

152.5950 1.025e0

152.6167 1.266e-2

152.6294 1.013e0

152.6688 1.266e-2

152.7081 1.266e-2

152.7710 1.013e0

152.8657 1.013e0

152.8986 2.532e-2

152.9219 1.013e0

152.9924 1.025e0

153.0596 1.266e-2

153.0830 1.013e0

153.1208 4.051e0

153.1718 1.013e0

153.2980 2.532e-2

153.3362 2.025e0

153.4151 1.013e0

153.4353 1.038e0

153.4642 2.532e-2

153.5005 1.013e0

153.5598 1.266e-2

153.6255 1.013e0

153.6978 2.025e0

153.7618 1.025e0

153.7801 2.025e0

153.8085 2.025e0

153.8692 1.266e-2

153.9114 4.051e0

153.9365 2.532e-2

154.1921 1.013e0

154.3013 1.013e0

154.3570 1.013e0

154.4202 1.266e-2

154.5012 2.532e-2

154.5755 1.266e-2

154.7997 1.266e-2

154.8399 1.013e0

154.9107 2.025e0

154.9933 2.025e0

155.1603 1.013e0

155.2263 1.013e0

155.2462 1.266e-2

155.3158 1.013e0

155.3956 1.266e-2

155.4669 2.025e0

155.4853 2.025e0

155.5479 1.266e-2

155.6474 2.025e0

155.6771 1.266e-2

155.6932 1.013e0

155.7839 1.038e0

155.8130 1.266e-2

155.8415 2.532e-2

155.8596 1.025e0

155.9874 3.038e0

156.0489 2.025e0

156.1108 4.063e0

156.1437 2.532e-2

156.1777 1.266e-2

156.2573 2.025e0

156.3211 2.532e-2

156.3592 2.038e0

156.3972 1.266e-2

156.4468 1.013e0

156.6930 1.025e0

156.7444 2.025e0

156.7883 1.051e0

156.8859 1.266e-2

156.9061 2.532e-2

156.9621 1.266e-2

157.0194 2.532e-2

157.1488 1.013e0

157.2423 1.013e0

157.2593 3.038e0

157.4038 2.025e0

157.6574 1.025e0

157.7256 1.013e0

157.7425 1.266e-2

157.8020 1.013e0

157.8510 2.025e0

157.9958 1.266e-2

158.0190 1.013e0

158.0898 1.013e0

158.2429 1.013e0

158.3735 1.266e-2

158.4107 2.532e-2

158.4905 2.025e0

158.5226 4.051e0

158.6742 1.013e0

158.7045 1.013e0

158.8301 2.025e0

159.0029 3.038e0

159.0764 1.013e0

159.1104 2.025e0

159.1412 2.532e-2

159.1734 1.013e0

159.2157 1.038e0

159.2376 1.013e0

159.3042 1.013e0

159.3398 2.532e-2

159.3910 1.266e-2

159.4892 1.038e0

159.5899 3.038e0

159.6196 1.025e0

159.7373 1.013e0

159.8648 1.013e0

159.8859 2.025e0

159.9252 1.013e0

160.0056 2.532e-2

160.0409 2.025e0

160.1366 1.013e0

160.2710 1.013e0

160.3016 1.013e0

160.3456 1.266e-2

160.3792 1.013e0

160.4582 2.025e0

160.5640 1.266e-2

160.6816 1.266e-2

160.7496 1.013e0

160.8104 1.038e0

160.9987 1.266e-2

161.0430 1.013e0

161.0678 2.532e-2

161.1165 1.013e0

161.1710 2.025e0

161.2078 1.013e0

161.2307 1.025e0

161.3330 1.266e-2

161.4339 2.532e-2

161.5012 1.266e-2

161.5961 1.266e-2

161.6132 1.266e-2

161.6731 1.266e-2

161.7039 1.266e-2

161.8423 1.013e0

161.9208 1.013e0

161.9536 3.038e0

161.9739 1.266e-2

162.0729 2.025e0

162.1094 1.266e-2

162.1500 1.013e0

162.1671 2.532e-2

162.2045 2.532e-2

162.2749 1.266e-2

162.3125 1.013e0

162.3295 1.266e-2

162.3602 1.013e0

162.3773 1.266e-2

162.4374 1.013e0

162.4716 1.013e0

162.5057 1.013e0

162.5313 2.025e0

162.5501 2.532e-2

162.5668 1.025e0

162.5999 1.013e0

162.7093 1.013e0

162.7393 2.025e0

162.7559 1.013e0

162.7865 1.013e0

162.8514 1.013e0

162.8685 1.013e0

162.9168 4.051e0

162.9834 1.025e0

163.0073 3.038e0

163.0603 2.025e0

163.0783 2.025e0

163.1120 1.013e0

163.1889 2.025e0

163.2215 1.013e0

163.3363 1.013e0

163.4247 1.013e0

163.4513 1.013e0

163.4890 1.013e0

163.5471 1.266e-2

163.5881 2.025e0

163.7169 2.025e0

163.8217 1.013e0

163.9245 1.013e0

163.9435 2.025e0

164.0088 1.013e0

164.1492 1.013e0

164.2577 1.013e0

164.3194 1.013e0

164.3399 1.013e0

164.4037 1.266e-2

164.4261 1.025e0

164.5694 1.025e0

164.7232 1.025e0

164.7522 1.013e0

164.7757 1.038e0

164.8299 1.013e0

165.0115 5.076e0

165.0552 1.013e0

165.0831 4.051e0

165.1152 1.025e0

165.1479 2.025e0

165.1652 1.025e0

165.2292 1.013e0

165.2513 2.025e0

165.3012 2.025e0

165.4267 2.038e0

165.4565 2.025e0

165.5146 2.025e0

165.6703 1.013e0

165.8555 1.013e0

165.8760 1.266e-2

165.8963 1.013e0

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166.1656 1.038e0

166.2124 1.025e0

166.2589 2.025e0

166.3002 1.266e-2

166.3174 1.025e0

166.3640 1.025e0

166.3829 2.025e0

166.5055 1.013e0

166.5228 1.013e0

166.6400 1.013e0

166.6705 1.266e-2

166.6875 1.266e-2

166.7470 1.025e0

166.8832 1.013e0

166.9757 1.013e0

167.0319 1.025e0

167.0509 1.013e0

167.1699 1.025e0

167.2523 2.025e0

167.3324 1.266e-2

167.4257 1.013e0

167.4464 1.266e-2

167.5224 2.025e0

167.5722 1.025e0

167.5942 2.025e0

167.6350 1.013e0

167.7420 1.013e0

167.7627 1.013e0

167.8076 3.038e0

167.8526 1.013e0

167.9167 2.038e0

167.9416 1.266e-2

167.9776 2.025e0

168.0171 1.266e-2

168.0621 1.013e0

168.1243 1.266e-2

168.1830 1.266e-2

168.2211 1.266e-2

168.2931 1.266e-2

168.3085 2.025e0

168.3822 1.013e0

168.4826 1.013e0

168.5563 2.038e0

168.6107 3.038e0

168.6452 1.266e-2

168.7684 1.013e0

168.9105 1.013e0

169.0630 2.532e-2

169.2124 1.025e0

169.3665 1.266e-2

169.3856 1.025e0

169.4913 2.025e0

169.5677 2.532e-2

169.6021 2.025e0

169.6227 1.266e-2

169.6707 2.025e0

169.7224 1.266e-2

169.7813 1.013e0

169.8473 2.025e0

169.9930 1.266e-2

170.0173 1.013e0

170.1528 1.013e0

170.2184 1.025e0

170.2666 1.013e0

170.3096 1.025e0

170.3563 1.013e0

170.3858 2.025e0

170.4606 1.013e0

170.7143 1.266e-2

170.8117 1.038e0

170.8587 2.025e0

170.9160 1.266e-2

170.9644 1.266e-2

171.0424 2.025e0

171.1410 1.266e-2

171.2609 3.038e0

171.2939 2.025e0

171.3322 1.013e0

171.3531 2.025e0

171.3810 1.013e0

171.4158 1.013e0

171.4628 2.025e0

171.4906 2.025e0

171.6317 1.013e0

171.6491 1.013e0

171.7362 1.266e-2

171.7606 1.013e0

171.7850 1.013e0

171.8059 1.266e-2

172.0116 1.013e0

172.0900 1.025e0

172.1162 1.013e0

172.1597 3.038e0

172.3674 1.266e-2

172.4476 1.025e0

172.4736 2.025e0

172.5452 1.025e0

172.6219 1.013e0

172.6585 2.025e0

172.7057 1.025e0

172.7895 2.025e0

172.8628 1.013e0

172.8943 1.266e-2

172.9138 3.038e0

172.9397 1.266e-2

172.9816 1.013e0

173.1248 3.038e0

173.1494 2.025e0

173.2762 3.038e0

173.2964 1.266e-2

173.4293 1.013e0

173.4974 2.025e0

173.5744 2.025e0

173.7230 1.013e0

173.7510 2.025e0

173.7685 1.013e0

173.8210 1.013e0

173.8875 1.025e0

173.9295 1.266e-2

173.9628 2.025e0

174.1641 1.013e0

174.2727 1.013e0

174.2972 1.266e-2

174.4163 1.266e-2

174.4425 2.532e-2

174.5217 1.266e-2

174.5534 1.013e0

174.5815 1.013e0

174.6168 1.013e0

174.7048 2.532e-2

174.8385 2.025e0

174.8981 1.013e0

175.0641 3.038e0

175.1945 2.025e0

175.2594 1.013e0

175.3508 1.013e0

175.4233 2.025e0

175.4816 1.266e-2

175.5099 1.025e0

175.5347 1.266e-2

175.5630 2.532e-2

175.6015 1.013e0

175.6331 2.038e0

175.6671 2.038e0

175.7209 1.266e-2

175.7631 2.025e0

175.8194 1.013e0

175.9691 3.038e0

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176.0378 2.532e-2

176.3623 1.013e0

176.3799 1.013e0

176.5315 1.170e0

176.5527 1.013e0

176.5882 1.013e0

176.6130 1.025e0

176.6558 1.013e0

176.6735 1.013e0

176.7403 1.013e0

176.8847 1.266e-2

177.1222 1.013e0

177.1472 3.324e0

177.2490 1.013e0

177.2710 1.038e0

177.3019 1.013e0

177.3652 1.266e-2

177.4006 1.013e0

177.4399 1.025e0

177.5431 1.266e-2

177.6100 2.038e0

177.6348 3.038e0

177.7370 1.266e-2

177.7581 1.013e0

177.7794 1.013e0

177.8617 1.013e0

177.8796 1.266e-2

177.9220 1.266e-2

177.9741 2.038e0

178.0296 2.025e0

178.0526 1.266e-2

178.1248 7.967e0

178.3294 1.266e-2

178.3630 2.025e0

178.4513 2.025e0

178.6206 1.266e-2

178.6630 1.013e0

178.7196 1.013e0

178.7507 4.051e0

178.7868 1.266e-2

178.8499 2.051e0

178.9465 1.038e0

178.9951 1.025e0

179.0261 3.038e0

179.0710 1.266e-2

179.1166 1.038e0

179.2071 1.013e0

179.2778 1.038e0

179.3697 1.266e-2

179.3950 1.013e0

179.4418 1.013e0

179.4686 2.025e0

179.6546 1.013e0

179.7411 1.013e0

179.7870 2.025e0

179.8792 1.013e0

179.9362 1.013e0

179.9688 1.013e0

180.0189 1.266e-2

180.1095 8.139e0

180.1696 2.532e-2

180.2070 5.063e0

180.3571 1.013e0

180.4897 1.266e-2

180.5688 4.051e0

180.6494 1.266e-2

180.6917 3.038e0

180.7681 1.013e0

180.8035 1.013e0

180.8284 1.013e0

180.8479 2.025e0

180.8922 1.266e-2

180.9285 1.013e0

181.0314 2.038e0

181.0536 1.266e-2

181.0969 4.662e1

181.1467 2.025e0

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181.2361 1.013e0

181.3367 2.038e0

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181.6408 2.532e-2

181.7779 2.025e0

181.8662 1.266e-2

181.9321 2.532e-2

182.0020 1.266e-2

182.2319 1.013e0

182.2501 1.013e0

182.3854 1.013e0

182.4273 2.025e0

182.4580 1.266e-2

182.6174 1.025e0

182.6518 1.266e-2

182.8244 1.013e0

182.8421 1.025e0

182.8599 2.025e0

182.8920 2.532e-2

182.9222 2.025e0

182.9929 1.013e0

183.1162 2.025e0

183.1469 1.176e0

183.1689 1.266e-2

183.2212 1.025e0

183.2461 2.025e0

183.3120 1.013e0

183.4242 1.013e0

183.4670 1.013e0

183.5029 1.013e0

183.5486 1.025e0

183.6291 1.013e0

183.6505 1.013e0

183.6830 1.266e-2

183.7161 1.266e-2

183.7466 3.798e-2

183.8091 1.025e0

183.8269 1.013e0

183.8633 1.025e0

183.9213 1.266e-2

183.9713 2.025e0

184.0694 1.013e0

184.0978 1.013e0

184.2204 1.013e0

184.2815 1.013e0

184.3315 1.013e0

184.3533 2.025e0

184.3863 1.013e0

184.4456 2.532e-2

184.4725 1.025e0

184.5045 1.266e-2

184.5524 1.266e-2

184.5812 2.025e0

184.6313 1.013e0

184.6598 1.013e0

184.7001 1.013e0

184.8517 2.025e0

184.9097 1.266e-2

185.1898 2.532e-2

185.2384 1.266e-2

185.4911 2.038e0

185.5387 1.025e0

185.5583 2.025e0

185.9732 1.266e-2

186.0525 1.013e0

186.0748 1.013e0

186.1189 6.076e0

186.2524 1.013e0

186.3903 1.013e0

186.5175 1.266e-2

186.5640 1.013e0

186.5873 1.025e0

186.6368 1.013e0

186.6625 1.266e-2

186.7582 3.066e0

186.8471 1.013e0

186.8757 2.025e0

186.9868 2.025e0

187.1107 1.038e0

187.1927 1.013e0

187.2252 1.013e0

187.3198 1.013e0

187.3921 1.266e-2

187.4507 1.013e0

187.4835 1.013e0

187.5105 2.532e-2

187.5379 2.051e0

187.5668 2.025e0

187.6288 2.532e-2

187.6541 1.013e0

187.7384 1.025e0

187.7743 1.013e0

187.8400 1.013e0

187.8797 1.051e0

187.9450 1.013e0

188.0292 2.025e0

188.0489 2.025e0

188.2225 1.013e0

188.2915 1.266e-2

188.3938 1.013e0

188.4100 2.025e0

188.4810 2.025e0

188.5178 1.266e-2

188.5358 1.013e0

188.5794 1.266e-2

188.6081 2.038e0

188.6442 4.051e0

188.6885 1.013e0

188.7110 1.013e0

188.7408 1.266e-2

188.8864 2.025e0

189.0559 2.025e0

189.2480 2.025e0

189.2986 1.266e-2

189.3175 1.013e0

189.3758 1.013e0

189.4242 1.038e0

189.7143 2.532e-2

189.7577 2.532e-2

189.8952 3.798e-2

189.9583 2.038e0

190.0202 1.013e0

190.0706 2.575e0

190.1809 1.266e-2

190.2585 2.025e0

190.2981 1.013e0

190.3560 3.051e0

190.4117 2.025e0

190.5109 3.038e0

190.6245 1.013e0

190.6569 1.013e0

190.7382 1.013e0

190.8212 2.532e-2

191.0176 1.266e-2

191.0882 1.025e0

191.1316 1.013e0

191.1605 1.013e0

191.1858 1.025e0

191.2554 1.038e0

191.3219 1.266e-2

191.4323 1.013e0

191.4621 1.013e0

191.4838 2.025e0

191.5183 2.025e0

191.6085 1.013e0

191.6455 2.025e0

191.6971 2.025e0

191.7259 1.266e-2

191.8146 1.013e0

191.8628 1.025e0

191.8922 1.013e0

191.9498 3.038e0

192.0243 1.266e-2

192.0729 1.013e0

192.1092 1.013e0

192.1646 1.266e-2

192.2602 1.025e0

192.3933 1.013e0

192.4222 3.038e0

192.5145 1.013e0

192.6104 1.013e0

192.6658 2.025e0

192.7245 1.266e-2

192.7766 1.013e0

192.7987 1.013e0

192.8848 3.038e0

193.0306 1.013e0

193.0564 1.266e-2

193.0886 1.025e0

193.1230 1.266e-2

193.2045 1.025e0

193.3331 1.013e0

193.3711 1.266e-2

193.4256 1.025e0

193.4556 1.266e-2

193.5325 2.025e0

193.6286 1.013e0

193.7067 1.266e-2

193.7629 1.013e0

193.8064 1.013e0

193.8363 2.025e0

193.9496 2.532e-2

194.1158 2.025e0

194.1729 2.025e0

194.2254 1.013e0

194.2655 2.532e-2

194.3007 2.025e0

194.3255 1.013e0

194.3545 1.013e0

194.3873 1.266e-2

194.5919 2.532e-2

194.6177 1.013e0

194.6638 2.025e0

194.6921 1.025e0

194.7449 1.025e0

194.7696 1.266e-2

194.8095 2.038e0

194.8662 1.013e0

194.8994 1.266e-2

194.9176 2.025e0

194.9418 2.532e-2

195.2167 2.025e0

195.2621 3.038e0

195.3219 2.025e0

195.4212 2.025e0

195.4857 1.038e0

195.6905 1.266e-2

195.7532 1.013e0

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