 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

104 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 S: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

246.0956 246.0953 0.3 1.2 7.5 1.3 C14 H16 N O S

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)

148.1892 1.013e0

148.3154 1.266e-2

148.3414 1.013e0

148.4102 2.025e0

148.4416 2.532e-2

148.5419 2.038e0

148.5999 1.266e-2

148.7201 1.025e0

148.7786 1.013e0

148.7959 2.532e-2

149.1800 1.013e0

149.1966 1.266e-2

149.2354 2.532e-2

149.3004 1.266e-2

149.4579 2.025e0

149.5070 3.038e0

149.5711 1.025e0

149.7260 1.266e-2

149.8269 1.266e-2

149.9475 1.013e0

149.9993 1.266e-2

150.0254 1.266e-2

150.0462 1.025e0

150.3750 2.532e-2

150.4846 2.532e-2

150.6567 1.266e-2

150.7369 2.532e-2

150.8302 1.266e-2

150.9186 1.013e0

151.1628 2.025e0

151.2824 2.532e-2

151.2966 1.013e0

151.3398 1.013e0

151.4215 1.013e0

151.6390 2.532e-2

151.7010 2.025e0

151.8036 1.266e-2

152.0040 1.013e0

152.2167 1.013e0

152.2334 1.266e-2

152.2672 1.025e0

152.3723 3.798e-2

152.4263 1.266e-2

152.4756 1.025e0

152.6172 1.013e0

152.6493 1.013e0

152.7314 1.025e0

152.8269 1.266e-2

152.8661 1.266e-2

152.9057 1.025e0

152.9645 2.025e0

153.1912 1.013e0

153.2545 1.025e0

153.5269 1.013e0

153.5896 1.013e0

154.0110 1.013e0

154.0808 1.266e-2

154.1760 1.013e0

154.4111 1.266e-2

154.4868 1.266e-2

154.5659 1.266e-2

154.5827 1.266e-2

154.6618 1.025e0

154.9229 1.266e-2

154.9821 1.266e-2

155.0055 1.013e0

155.2366 1.266e-2

155.3225 1.025e0

155.3428 1.013e0

155.5283 2.025e0

155.5517 1.013e0

155.6412 1.266e-2

155.8134 1.013e0

155.8402 1.013e0

155.9466 1.013e0

156.0159 1.266e-2

156.0377 5.063e-2

156.1591 3.798e-2

156.3843 1.013e0

156.4356 1.038e0

156.4806 1.013e0

156.6435 1.013e0

156.7562 1.266e-2

156.8301 1.266e-2

157.0396 2.051e0

157.1960 1.013e0

157.2230 1.266e-2

157.2493 1.266e-2

157.2723 1.266e-2

157.3296 1.266e-2

157.4753 1.025e0

157.7696 1.013e0

157.8430 1.266e-2

157.8633 1.013e0

157.9296 1.013e0

158.2535 1.266e-2

158.3238 1.266e-2

158.3468 1.266e-2

158.3739 2.532e-2

158.4440 1.266e-2

158.4876 1.266e-2

158.5348 2.038e0

158.6216 2.532e-2

158.7068 1.038e0

158.8509 2.532e-2

158.8913 2.532e-2

158.9935 1.266e-2

159.0343 1.038e0

159.1874 1.266e-2

159.3131 1.025e0

159.4763 1.266e-2

159.5008 1.025e0

159.5224 1.013e0

159.8353 1.013e0

159.9391 1.266e-2

159.9698 2.532e-2

160.0059 2.532e-2

160.2486 2.532e-2

160.3666 1.266e-2

160.3830 1.266e-2

160.4536 1.013e0

160.5110 1.266e-2

160.5831 2.532e-2

160.6588 1.013e0

160.8968 2.532e-2

160.9293 3.038e0

160.9627 3.063e0

161.2115 1.013e0

161.2714 3.038e0

161.2926 1.013e0

161.4617 1.025e0

161.6034 1.013e0

161.7691 1.013e0

161.7824 1.013e0

161.8836 1.013e0

161.9331 1.025e0

162.0017 1.266e-2

162.0222 1.013e0

162.1437 1.013e0

162.1641 1.013e0

162.1905 3.038e0

162.3130 1.013e0

162.4618 1.013e0

162.6585 1.266e-2

162.9159 1.013e0

162.9566 1.013e0

163.1227 1.266e-2

163.1398 1.013e0

163.1825 1.025e0

163.2220 1.266e-2

163.3095 1.013e0

163.4351 1.013e0

163.4680 3.038e0

163.6252 1.013e0

163.6627 2.025e0

163.6901 1.013e0

163.7226 1.025e0

163.7500 2.025e0

163.8021 1.013e0

163.8394 1.013e0

163.8873 1.013e0

163.9250 1.038e0

164.0676 2.025e0

164.1563 1.266e-2

164.5850 1.266e-2

164.7929 1.013e0

165.0316 2.532e-2

165.1175 1.038e0

165.2297 1.266e-2

165.3240 1.025e0

165.4997 3.038e0

165.5409 1.013e0

165.7011 1.013e0

166.0679 2.025e0

166.3368 2.025e0

166.3662 1.266e-2

166.5921 1.013e0

166.6812 1.013e0

166.7631 1.013e0

166.9321 1.266e-2

167.2358 2.532e-2

167.5333 2.532e-2

168.4399 2.532e-2

168.5039 1.025e0

168.5350 1.266e-2

169.3220 1.266e-2

169.3410 2.025e0

169.5335 1.025e0

169.6663 3.798e-2

169.7731 2.025e0

170.2395 1.266e-2

170.2843 1.266e-2

170.3257 1.013e0

170.4228 1.266e-2

170.5654 2.532e-2

170.6262 2.025e0

170.7913 2.025e0

170.8540 1.013e0

171.2491 1.266e-2

171.3153 1.013e0

171.5434 2.025e0

171.5695 1.013e0

171.6078 1.013e0

171.7611 2.532e-2

171.8029 1.266e-2

171.9458 1.013e0

172.0888 1.266e-2

172.1795 1.013e0

172.3784 2.532e-2

172.4237 1.266e-2

172.5178 1.266e-2

172.5667 2.532e-2

172.5876 1.013e0

172.7202 1.013e0

172.7481 1.266e-2

172.8773 1.266e-2

173.0101 2.532e-2

173.1744 1.013e0

173.2199 1.013e0

173.3319 2.025e0

173.3755 2.025e0

173.3983 1.266e-2

173.4752 1.013e0

173.6221 1.266e-2

173.6501 1.266e-2

173.6746 1.013e0

173.7375 1.013e0

173.8110 1.266e-2

173.9860 1.266e-2

174.0281 1.013e0

174.0631 1.013e0

174.1559 2.532e-2

174.2032 1.025e0

174.2242 1.013e0

174.2557 1.013e0

174.2977 1.266e-2

174.6243 1.266e-2

174.6525 1.025e0

174.6913 2.532e-2

174.8705 1.013e0

174.9161 1.266e-2

175.0319 1.025e0

175.0986 2.038e0

175.2389 1.266e-2

175.3231 1.266e-2

175.5046 1.038e0

175.5475 1.025e0

175.5916 3.798e-2

175.8146 1.025e0

175.9533 1.266e-2

176.1003 2.532e-2

176.4191 1.266e-2

176.4507 1.013e0

176.5461 2.025e0

176.6740 1.013e0

176.9557 3.038e0

177.0053 1.266e-2

177.1357 9.408e0

177.1667 2.025e0

177.2160 1.025e0

177.3779 2.038e0

177.8050 1.266e-2

177.8443 1.013e0

177.9719 1.013e0

178.1343 1.013e0

178.1880 1.013e0

178.2418 1.013e0

178.5251 2.532e-2

178.5894 1.266e-2

178.7642 2.025e0

178.9620 1.266e-2

179.2147 1.266e-2

179.2996 1.025e0

179.4887 1.013e0

179.6373 1.013e0

179.8230 1.266e-2

179.9171 2.025e0

180.0406 1.013e0

180.3435 1.013e0

180.3630 2.532e-2

180.4036 1.025e0

180.7113 1.266e-2

180.7438 1.013e0

180.9020 2.532e-2

181.0612 1.266e-2

181.0984 2.948e1

181.5154 1.013e0

181.6161 2.038e0

181.7909 4.051e0

181.9149 2.038e0

182.0711 1.013e0

182.1671 1.266e-2

182.2398 1.013e0

182.2612 2.532e-2

182.2967 1.013e0

182.4692 1.025e0

182.6162 2.025e0

182.6843 2.025e0

182.7307 1.266e-2

182.7555 1.013e0

182.8320 1.266e-2

182.9032 1.266e-2

182.9494 1.266e-2

183.0189 2.025e0

183.0615 1.266e-2

183.1621 1.266e-2

183.3198 1.266e-2

183.4033 1.013e0

183.5512 1.013e0

183.6145 1.038e0

183.6616 2.025e0

183.7330 2.025e0

183.9540 1.013e0

184.1878 1.013e0

184.2660 2.532e-2

184.3721 1.013e0

184.4230 1.013e0

184.5345 1.013e0

184.6631 1.038e0

184.7460 2.025e0

184.7764 1.013e0

184.8410 1.266e-2

185.0611 3.798e-2

185.1888 1.013e0

185.2068 1.266e-2

185.2425 1.013e0

185.3406 1.013e0

185.4160 1.266e-2

185.6733 1.266e-2

185.7448 1.013e0

185.8253 2.532e-2

185.8504 1.266e-2

185.9156 1.013e0

186.3032 1.013e0

186.3761 4.051e0

186.4660 1.013e0

186.5843 1.025e0

186.6039 1.266e-2

186.6299 1.013e0

186.6631 2.025e0

186.8584 1.266e-2

186.9641 1.013e0

187.0717 2.025e0

187.1039 1.025e0

187.1307 3.038e0

187.2342 3.798e-2

187.3279 1.013e0

187.4106 1.266e-2

187.5128 1.013e0

187.7712 1.025e0

187.7964 1.013e0

187.9274 1.266e-2

188.0513 1.266e-2

188.2848 1.266e-2

188.5256 1.013e0

188.7628 1.025e0

188.8170 1.013e0

188.8905 1.266e-2

189.0363 1.266e-2

189.1196 1.038e0

189.2049 1.266e-2

189.2702 1.266e-2

189.4015 1.266e-2

189.4201 2.025e0

189.4897 1.013e0

189.5334 2.025e0

189.7238 1.013e0

190.0815 3.051e0

190.1491 1.266e-2

190.2590 1.013e0

190.3059 2.532e-2

190.3578 1.266e-2

190.3942 1.013e0

190.8947 2.532e-2

190.9372 1.266e-2

191.0691 1.013e0

191.2121 1.013e0

191.3453 1.266e-2

191.3652 2.025e0

191.4442 1.013e0

191.5242 1.266e-2

191.6295 2.532e-2

191.7121 1.266e-2

192.1589 3.038e0

192.2454 1.013e0

192.5078 1.266e-2

192.5440 2.532e-2

192.6400 1.266e-2

192.6875 1.038e0

192.7695 1.266e-2

192.8538 1.013e0

192.8730 1.266e-2

192.9388 1.266e-2

192.9841 1.013e0

193.0401 1.025e0

193.1529 1.013e0

193.4099 2.532e-2

193.4601 1.013e0

193.5258 2.025e0

193.6258 1.038e0

193.8106 1.013e0

193.8518 4.051e0

193.8886 1.013e0

194.0483 2.532e-2

194.2625 1.013e0

194.3477 2.532e-2

194.3958 1.025e0

194.4203 2.532e-2

194.4595 1.038e0

194.5421 1.025e0

194.6329 2.532e-2

194.8513 2.025e0

194.8760 2.025e0

195.0522 2.532e-2

195.0708 1.013e0

195.1071 1.025e0

195.1412 2.025e0

195.2927 2.025e0

195.4236 1.025e0

195.5273 1.266e-2

195.6164 1.025e0

195.7538 1.013e0

195.7875 2.025e0

195.8601 2.532e-2

196.2044 1.013e0

196.3046 1.266e-2

196.3338 1.266e-2

196.4978 1.266e-2

196.5688 1.013e0

196.8040 1.013e0

196.8664 1.266e-2

196.9718 1.013e0

197.0793 1.266e-2

197.1578 1.013e0

197.1742 1.025e0

197.3293 1.013e0

197.6488 1.025e0

197.7755 2.025e0

197.8222 1.013e0

197.9007 1.266e-2

197.9720 1.013e0

198.0049 1.025e0

198.3397 2.025e0

198.3905 1.013e0

198.7614 1.025e0

198.9465 1.025e0

198.9666 1.266e-2

199.4681 2.025e0

199.4944 1.603e0

199.5373 1.025e0

199.6642 1.266e-2

199.7028 1.025e0

199.7925 1.013e0

199.8494 1.266e-2

199.8786 3.038e0

199.9538 1.266e-2

200.2289 1.266e-2

200.3619 2.532e-2

200.4159 1.013e0

200.5061 1.266e-2

200.7131 1.266e-2

200.7590 1.266e-2

200.7847 1.266e-2

200.9848 1.013e0

201.0032 1.266e-2

201.0335 1.266e-2

201.1960 2.025e0

201.2677 1.266e-2

201.3354 1.266e-2

201.3613 1.266e-2

201.6962 3.038e0

201.8079 1.025e0

201.8289 1.266e-2

201.8705 1.266e-2

201.8966 1.013e0

202.1877 1.013e0

202.2437 1.013e0

202.2675 1.266e-2

202.9287 1.025e0

202.9895 1.266e-2

203.0724 1.266e-2

203.2770 1.013e0

203.5694 2.025e0

203.6900 1.013e0

203.9409 1.013e0

204.0462 1.013e0

204.3432 1.013e0

204.3802 1.013e0

204.5970 2.038e0

204.6663 1.266e-2

204.7115 3.798e-2

204.9285 1.266e-2

205.1142 1.013e0

205.1789 1.266e-2

205.6056 1.266e-2

205.6359 1.013e0

205.6741 2.532e-2

205.7425 1.013e0

205.7830 2.025e0

205.9147 1.013e0

205.9313 2.025e0

206.1775 1.013e0

206.2962 1.013e0

206.3256 2.025e0

206.3535 2.532e-2

206.4794 1.013e0

206.5128 1.266e-2

206.6053 1.266e-2

206.9521 2.038e0

207.1210 1.038e0

207.2909 1.025e0

207.4685 1.013e0

207.4994 3.798e-2

207.5285 2.038e0

207.6562 1.013e0

208.1734 1.013e0

208.2273 1.266e-2

208.3145 1.266e-2

208.6028 1.013e0

208.6257 1.013e0

208.6990 2.532e-2

208.7942 1.266e-2

208.9133 1.266e-2

208.9487 2.025e0

209.1980 1.266e-2

209.2864 1.013e0

209.4829 2.532e-2

209.5249 1.013e0

209.6039 1.025e0

209.7194 1.025e0

209.7975 1.266e-2

209.8515 2.532e-2

209.9849 1.025e0

210.0373 3.038e0

210.2099 1.025e0

210.2411 1.266e-2

210.2953 1.013e0

210.3175 1.266e-2

210.4146 1.025e0

210.5529 2.038e0

210.7147 1.025e0

210.8807 1.266e-2

210.9093 2.025e0

210.9386 1.013e0

210.9773 1.266e-2

211.0077 1.266e-2

211.1449 1.025e0

211.1926 1.266e-2

211.2451 1.025e0

211.9849 1.266e-2

212.4146 1.266e-2

212.4424 1.013e0

212.4787 1.025e0

212.5485 2.532e-2

212.6550 2.532e-2

212.6952 2.532e-2

212.8056 1.025e0

213.0683 3.051e0

213.1821 1.266e-2

213.4031 1.266e-2

213.4311 1.266e-2

213.7612 1.025e0

214.0442 2.532e-2

214.1148 2.532e-2

214.1846 1.266e-2

214.2975 2.025e0

214.3272 1.013e0

214.3762 2.532e-2

214.4137 1.266e-2

214.4937 2.532e-2

214.6277 1.013e0

214.8962 1.013e0

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215.1648 1.266e-2

215.2998 1.025e0

215.4413 1.013e0

215.5510 2.025e0

215.7108 2.025e0

216.1755 1.013e0

216.5350 1.013e0

217.0858 1.013e0

217.2385 1.013e0

217.4120 1.266e-2

217.4457 2.367e0

217.5910 1.266e-2

217.6194 1.266e-2

217.6885 3.798e-2

217.7288 1.013e0

217.8382 2.025e0

217.9524 2.038e0

218.0995 2.025e0

218.1722 2.025e0

218.2231 1.266e-2

218.2816 1.266e-2

218.4894 1.266e-2

218.6234 2.532e-2

218.6595 1.266e-2

218.8906 1.266e-2

218.9579 1.266e-2

218.9803 1.266e-2

219.0786 1.266e-2

219.1035 1.266e-2

219.1758 3.038e0

219.2326 1.013e0

219.3366 1.025e0

219.4180 2.532e-2

219.6102 1.266e-2

219.6650 1.013e0

219.6861 1.266e-2

219.9137 1.266e-2

220.0435 1.266e-2

220.2653 1.013e0

220.3276 1.013e0

220.4031 1.266e-2

220.4621 1.013e0

220.4963 2.038e0

220.5406 1.013e0

220.6099 2.532e-2

220.7299 1.013e0

220.7772 1.013e0

220.9016 5.063e0

220.9396 1.013e0

220.9667 1.013e0

220.9946 1.266e-2

221.2160 1.025e0

221.2828 1.013e0

221.3264 1.266e-2

221.3572 2.025e0

221.4213 1.013e0

221.8770 1.013e0

221.9716 3.038e0

222.1804 1.266e-2

222.4902 1.013e0

222.6365 1.266e-2

222.8246 1.025e0

222.8587 1.025e0

222.9199 3.051e0

222.9978 1.266e-2

223.1804 1.266e-2

223.2355 1.013e0

223.2868 1.266e-2

223.5571 1.013e0

223.6046 1.025e0

223.8161 1.013e0

224.1530 1.013e0

224.2330 1.266e-2

224.3612 3.051e0

224.5150 1.266e-2

224.6027 2.038e0

224.6466 1.266e-2

224.7857 1.266e-2

224.8220 1.266e-2

224.8561 2.532e-2

224.9173 1.266e-2

224.9381 1.266e-2

224.9731 1.013e0

225.0890 1.025e0

225.1247 2.532e-2

225.4478 1.013e0

225.5002 1.025e0

225.5243 6.649e-2

225.5907 1.013e0

225.6196 1.266e-2

225.6561 1.013e0

225.6827 1.266e-2

225.8982 1.013e0

226.1789 1.266e-2

226.2931 3.798e-2

226.4383 1.266e-2

226.6014 1.013e0

226.6380 1.013e0

226.7508 1.013e0

227.3745 1.266e-2

227.6864 1.266e-2

227.8523 4.051e0

227.9598 2.025e0

228.0516 2.025e0

228.0930 1.266e-2

228.1331 1.266e-2

228.2548 2.025e0

228.3686 1.013e0

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