 Elemental Composition Report

Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 12-12 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 S: 0-1 56Fe: 0-1

Minimum: -15.0

Maximum: 5.0 15.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

218.0634 218.0640 -0.6 -2.8 7.5 2.3 C12 H12 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)

127.9021 1.013e0

127.9293 1.266e-2

128.2238 1.266e-2

128.6033 1.266e-2

128.7247 2.051e0

128.8081 1.013e0

128.8232 1.266e-2

129.1545 2.051e0

129.9322 1.025e0

130.3660 3.798e-2

130.5589 2.532e-2

130.7060 1.266e-2

131.0760 3.506e0

131.2776 1.013e0

132.1335 1.994e0

132.4081 1.038e0

132.7735 1.013e0

133.7658 2.532e-2

133.8841 1.038e0

133.9155 1.038e0

134.0561 1.152e0

134.1900 1.025e0

134.7893 1.013e0

134.9528 1.266e-2

135.3515 1.266e-2

135.5973 3.051e0

135.6252 5.063e-2

136.0958 1.703e1

136.3801 2.532e-2

136.4167 1.266e-2

137.1999 1.266e-2

137.4710 1.025e0

137.6129 1.038e0

137.9253 1.038e0

138.0905 2.475e0

138.1382 3.274e0

138.1604 2.532e-2

138.6040 1.266e-2

138.6450 1.013e0

138.8015 1.266e-2

138.9421 1.013e0

139.0841 1.391e0

139.3215 1.013e0

140.0749 3.465e0

140.1316 1.485e0

140.2705 1.266e-2

140.4311 2.532e-2

140.4875 2.025e0

141.3345 1.025e0

142.3644 1.013e0

142.4248 6.329e-2

142.8972 1.266e-2

143.1966 1.266e-2

143.2885 2.532e-2

143.5479 2.025e0

144.8762 3.063e0

145.1221 2.810e0

145.4033 2.532e-2

145.4336 1.025e0

145.9695 1.266e-2

146.1430 1.965e0

146.2345 2.532e-2

146.5769 2.532e-2

146.6410 1.266e-2

146.9288 3.798e-2

147.0503 1.537e0

147.1120 2.806e0

147.1425 1.964e0

147.2371 1.013e0

147.6518 3.051e0

147.7724 2.532e-2

148.0725 2.170e0

148.1377 1.071e0

148.2673 2.532e-2

148.4779 1.266e-2

148.5067 1.266e-2

149.1249 4.825e0

149.1873 1.013e0

149.2975 2.051e0

149.8176 1.266e-2

149.9127 2.063e0

150.0963 3.640e0

150.1605 1.025e0

150.4684 1.025e0

150.5077 2.532e-2

150.6480 1.266e-2

150.9543 1.038e0

151.9139 1.038e0

152.4010 1.266e-2

153.7491 1.013e0

153.9830 1.038e0

154.1178 2.010e0

154.6459 3.798e-2

155.4707 1.266e-2

155.5069 1.266e-2

155.9348 2.532e-2

155.9609 1.051e0

156.2921 3.798e-2

156.7974 2.532e-2

156.8646 2.038e0

157.6714 1.038e0

157.8080 1.013e0

158.2624 1.266e-2

158.6301 1.013e0

158.8109 1.266e-2

159.0323 3.045e0

159.5487 1.186e0

159.8440 1.266e-2

160.2069 1.266e-2

160.3416 1.266e-2

160.4422 1.266e-2

160.4729 1.266e-2

160.7013 2.532e-2

160.7791 1.266e-2

160.8523 1.038e0

160.9277 1.266e-2

161.0021 1.013e0

161.1401 2.025e0

161.3422 1.266e-2

161.8423 1.266e-2

162.1480 1.051e0

162.2430 1.025e0

162.4444 1.266e-2

162.5867 2.532e-2

162.8853 1.025e0

162.9735 1.025e0

163.3531 1.013e0

163.9642 1.038e0

164.2137 1.266e-2

164.2602 1.063e0

164.2984 1.266e-2

164.5725 1.038e0

164.5919 1.266e-2

164.6223 3.038e0

165.4282 2.532e-2

165.4586 1.266e-2

165.7357 2.038e0

165.8721 2.532e-2

165.9312 1.013e0

166.2148 1.025e0

166.3155 2.038e0

166.8565 1.266e-2

167.1407 1.266e-2

167.1756 1.266e-2

167.3770 7.958e-1

167.4141 2.532e-2

167.5307 1.063e0

167.8770 2.532e-2

167.9085 1.051e0

167.9400 3.798e-2

168.2386 1.266e-2

168.4163 4.063e0

169.4367 3.798e-2

169.4920 1.013e0

169.7675 2.038e0

169.9024 3.798e-2

169.9373 1.025e0

169.9662 1.266e-2

170.0781 3.570e0

170.5254 3.051e0

171.3963 2.025e0

171.5980 1.013e0

171.8130 2.532e-2

171.9121 1.266e-2

172.2535 2.532e-2

172.4519 1.013e0

172.9512 1.051e0

172.9883 1.025e0

173.6054 1.013e0

174.7876 2.532e-2

174.8397 1.013e0

174.8574 1.266e-2

175.2360 2.025e0

175.4765 1.266e-2

175.6420 2.532e-2

175.8665 3.038e0

175.8881 2.532e-2

176.2905 1.266e-2

176.3438 1.266e-2

176.5288 2.025e0

176.8859 1.038e0

176.9329 2.532e-2

177.2739 2.025e0

177.3521 3.640e-1

177.3844 2.051e0

177.4386 1.266e-2

177.6527 1.025e0

177.6723 1.266e-2

177.8922 1.266e-2

178.3750 1.266e-2

178.4772 1.025e0

178.7814 2.532e-2

178.8747 1.013e0

179.0471 1.038e0

179.1953 1.013e0

179.3729 3.051e0

179.7891 1.266e-2

180.0476 1.025e0

180.4766 2.025e0

180.4997 1.266e-2

180.7534 1.013e0

180.8276 2.532e-2

181.3433 2.532e-2

181.4053 2.025e0

181.4640 1.013e0

181.5288 1.025e0

181.6078 2.025e0

181.7400 1.266e-2

182.9274 1.013e0

183.3172 2.532e-2

183.4166 1.266e-2

183.4545 2.532e-2

183.5465 1.266e-2

184.3746 1.266e-2

184.4652 1.266e-2

184.9330 2.532e-2

185.1125 2.226e0

185.2075 2.532e-2

185.2311 1.025e0

185.3606 1.038e0

185.7021 1.013e0

186.4011 1.025e0

186.5154 2.532e-2

186.6008 1.013e0

186.6371 1.266e-2

186.8587 1.266e-2

186.9932 1.266e-2

187.1906 2.038e0

187.2150 1.025e0

187.3153 1.038e0

187.3642 2.025e0

187.6334 2.532e-2

187.8164 3.038e0

187.8479 8.470e-1

187.9774 2.532e-2

188.4565 1.266e-2

188.9672 1.025e0

189.2838 5.063e-2

189.6113 1.266e-2

189.6879 1.013e0

189.7354 1.013e0

189.8195 3.038e0

190.0269 3.798e-2

190.0684 1.983e1

190.3617 2.532e-2

190.4683 1.266e-2

190.4958 2.025e0

190.6476 1.266e-2

190.7337 2.532e-2

190.8489 2.532e-2

190.8810 2.038e0

191.0783 7.886e0

191.1948 1.266e-2

191.7792 1.266e-2

191.8306 1.266e-2

192.3350 5.063e-2

192.4307 1.266e-2

192.5863 2.532e-2

192.9163 1.025e0

193.4828 2.025e0

193.6794 1.025e0

193.8119 1.025e0

193.8891 1.025e0

194.1920 6.329e-2

194.4708 1.025e0

194.6419 1.266e-2

194.9367 2.025e0

195.3497 1.013e0

195.6339 2.532e-2

195.7444 1.013e0

195.8755 2.532e-2

195.9801 1.907e0

196.0342 1.025e0

196.3796 3.798e-2

196.4211 2.025e0

196.4493 2.025e0

196.5441 1.025e0

196.5758 3.051e0

196.8306 1.266e-2

196.9038 2.532e-2

197.0223 3.038e0

197.1100 2.660e1

197.4261 2.025e0

197.6788 3.798e-2

197.8408 2.025e0

197.8742 2.532e-2

197.8927 2.532e-2

198.4696 3.038e0

198.5209 1.025e0

198.5413 5.063e-2

198.8752 1.013e0

199.0031 2.025e0

199.4495 1.038e0

199.6362 1.266e-2

199.6742 1.013e0

199.8145 2.532e-2

199.9614 2.025e0

200.0211 3.038e0

200.0625 6.893e0

200.4354 1.025e0

200.6475 1.266e-2

200.7036 5.063e-2

200.7535 1.266e-2

201.1079 1.854e0

201.4840 1.013e0

201.5107 1.038e0

201.6502 2.532e-2

201.9483 1.266e-2

202.0639 1.826e0

202.3187 1.013e0

202.4923 1.025e0

202.5399 2.532e-2

202.6425 3.038e0

202.7275 1.266e-2

202.8407 1.266e-2

202.8740 4.051e0

203.2281 2.051e0

203.2972 2.025e0

203.3626 1.013e0

203.4020 2.063e0

203.4299 2.025e0

203.5822 4.051e0

203.7365 1.025e0

203.8449 1.266e-2

203.9593 3.798e-2

204.2167 2.025e0

204.2509 1.266e-2

204.3553 1.025e0

204.3913 1.266e-2

204.4376 3.038e0

204.6236 1.266e-2

204.7405 5.063e-2

205.1595 1.258e-1

205.2395 1.013e0

205.5110 2.038e0

205.5663 1.013e0

205.6525 2.025e0

205.8082 1.025e0

206.0241 1.025e0

206.5227 1.834e0

206.5487 1.025e0

206.6081 2.025e0

206.7603 1.266e-2

206.8618 2.532e-2

206.8863 1.013e0

206.9708 2.025e0

207.1495 2.535e0

207.1965 1.266e-2

207.3150 1.013e0

207.4879 1.013e0

207.5520 2.532e-2

207.5831 1.266e-2

208.6658 2.532e-2

208.7506 1.038e0

209.1069 1.267e0

209.4252 2.532e-2

209.4629 1.013e0

209.5630 1.013e0

209.5945 5.063e-2

209.6876 1.025e0

209.8783 1.013e0

210.2713 1.013e0

210.3059 1.266e-2

210.5609 7.165e0

210.6728 2.038e0

210.7401 2.025e0

210.7874 1.013e0

210.9444 1.025e0

211.1416 2.737e0

211.2168 2.038e0

211.2452 1.038e0

211.3906 1.266e-2

211.5293 1.266e-2

211.7092 1.025e0

211.8153 1.266e-2

211.8778 1.025e0

212.2333 2.532e-2

212.6512 2.038e0

212.6990 3.798e-2

213.2604 1.013e0

213.3383 1.266e-2

213.4850 1.266e-2

213.5473 1.013e0

213.8151 2.532e-2

213.8836 2.532e-2

214.0358 3.943e0

214.3018 1.025e0

214.4235 2.025e0

214.4768 1.266e-2

214.7473 4.063e0

214.8080 1.013e0

214.9173 3.798e-2

215.0258 8.096e-1

215.0546 2.025e0

215.2725 1.038e0

215.3044 1.025e0

215.5792 3.798e-2

215.9033 1.025e0

216.2848 5.866e-1

216.3180 1.979e0

216.3479 4.114e0

216.3922 9.203e0

216.4350 1.014e1

216.4823 2.076e0

216.5305 1.185e1

216.5909 9.228e0

216.6253 7.029e0

216.6838 6.340e0

216.7108 1.656e0

216.7575 1.260e1

216.8357 5.513e0

216.8688 3.964e0

216.8970 2.063e0

216.9212 4.063e0

216.9676 1.442e1

217.0049 2.405e0

217.0846 1.760e1

217.1781 5.497e0

217.2237 3.419e0

217.2824 1.804e1

217.3197 1.141e1

217.3834 4.114e0

217.4762 1.624e1

217.5168 7.554e-1

217.5483 7.787e0

217.6002 3.541e0

217.6282 8.687e0

217.6730 1.855e1

217.6941 2.278e1

217.7406 1.482e1

217.7635 2.401e1

217.7914 2.035e1

217.8249 1.625e1

217.8603 3.845e1

217.9154 2.280e1

217.9477 3.949e1

218.0634 1.798e4

218.1576 1.420e0

218.1895 2.493e2

218.2306 2.348e2

218.2854 5.075e1

218.3214 7.219e1

218.3578 8.120e1

218.3900 1.795e2

218.4235 5.292e1

218.4522 1.202e2

218.4890 1.769e2

218.5450 6.584e1

218.5818 7.527e1

218.6154 1.189e2

218.6691 1.330e2

218.6927 7.331e1

218.7601 1.660e2

218.8055 9.068e1

218.8388 1.751e2

218.8918 7.638e1

218.9262 7.739e1

218.9904 8.946e1

219.0691 2.665e3

219.1309 3.573e1

219.1682 1.231e2

219.2487 7.449e1

219.3168 4.258e1

219.3523 5.514e1

219.3810 3.877e1

219.4127 1.339e1

219.4626 5.517e1

219.4913 1.339e1

219.5346 5.719e1

219.6097 1.040e1

219.6360 5.421e1

219.6661 3.681e1

219.7302 1.316e2

219.7905 3.783e1

219.8499 1.342e1

219.9052 1.943e1

219.9537 3.886e1

220.0169 5.931e1

220.0629 1.064e3

220.1992 5.635e1

220.2655 3.791e1

220.3028 1.546e1

220.3546 1.746e1

220.3777 1.146e1

220.4219 1.747e1

220.4625 7.789e1

220.4864 4.942e1

220.5375 7.391e1

220.5821 5.944e1

220.6388 3.397e1

220.6755 5.747e1

220.7424 3.899e1

220.8097 7.400e1

220.9398 5.853e1

221.0057 2.052e1

221.0658 2.348e2

221.1200 7.510e1

221.1595 1.553e1

221.2497 1.854e1

221.4795 4.760e0

221.5991 1.088e0

221.6276 3.051e0

221.7273 1.266e-2

221.7615 1.038e0

221.8091 1.376e0

221.8787 3.190e0

221.9274 1.051e0

222.0672 1.122e1

222.2780 1.038e0

222.3720 3.038e0

222.4576 3.798e-2

222.4996 5.063e0

222.7236 1.004e0

222.8539 1.038e0

222.9245 2.532e-2

222.9500 1.742e0

223.3730 1.038e0

223.4109 2.532e-2

223.4418 1.051e0

223.5435 2.089e0

223.6074 3.798e-2

223.7541 9.581e-1

223.8532 2.038e0

224.3865 2.532e-2

224.4586 7.449e-2

224.7703 1.051e0

224.8839 2.532e-2

224.9275 3.798e-2

225.2179 3.038e0

225.5502 2.532e-2

225.8159 2.532e-2

225.8544 1.038e0

225.9644 3.038e0

226.3003 2.025e0

226.3410 1.266e-2

226.4409 1.025e0

226.6859 1.038e0

227.9788 1.013e0

228.0149 7.661e0

228.4626 1.025e0

229.0046 1.016e0

229.1546 3.593e0

230.4603 1.266e-2

230.6629 1.266e-2

230.7071 2.532e-2

231.0878 2.756e1

231.2167 3.798e-2

231.3767 1.266e-2

231.6030 1.025e0

231.8513 1.266e-2

232.3727 1.025e0

232.4067 2.025e0

232.5233 1.013e0

232.5511 4.076e0

232.9280 1.266e-2

233.0226 2.081e0

233.5971 1.025e0

233.9213 3.798e-2

234.0184 8.647e-1

234.0593 2.933e1

234.5334 1.025e0

234.6297 1.266e-2

234.7689 1.038e0

234.9396 1.266e-2

235.0928 1.996e2

235.2711 2.025e0

235.5872 2.532e-2

235.6620 3.369e0

236.0959 3.458e1

236.2650 2.025e0

236.4530 3.038e0

236.5364 1.025e0

237.0411 7.072e0

237.3448 3.798e-2

237.5652 2.025e0

237.8114 1.266e-2

238.1298 5.182e0

238.1811 2.344e0

238.4263 1.025e0

238.5358 1.038e0

238.6968 1.266e-2

238.9311 1.266e-2

238.9606 2.532e-2

239.1700 1.254e0

239.3951 4.051e0

239.4661 1.013e0

239.9037 3.063e0

239.9780 5.063e-2

240.0504 1.932e1

240.2879 2.532e-2

240.5049 3.798e-2

240.6388 1.013e0

240.6654 2.532e-2

240.8369 1.266e-2

241.2867 1.038e0

241.4175 5.063e-2

241.7302 3.798e-2

241.8955 1.038e0

241.9977 2.955e0

242.4167 1.025e0

242.6437 5.063e-2

242.6914 2.532e-2

242.8550 2.532e-2

242.9028 1.013e0

243.7255 1.025e0

243.7653 1.266e-2

243.8499 2.038e0

243.9658 2.532e-2

244.3028 2.532e-2

244.4289 1.266e-2

244.4954 1.266e-2

244.7570 1.038e0

244.8893 3.798e-2

245.3102 1.266e-2

245.3775 1.266e-2

245.5011 1.266e-2

245.8553 8.016e-1

245.8851 5.063e-2

245.9365 2.051e0

246.0111 2.453e0

246.0389 1.353e0

246.3062 2.025e0

246.6503 2.025e0

247.0854 2.124e0

247.4215 1.266e-2

247.5509 1.013e0

247.6293 1.266e-2

247.6841 2.532e-2

247.8647 1.266e-2

247.9186 1.266e-2

248.1609 9.166e-1

248.2283 2.532e-2

248.3131 2.038e0

248.5687 2.025e0

248.7898 1.013e0

248.9401 1.266e-2

249.0316 1.336e0

249.1110 9.212e1

249.5264 3.798e-2

249.5791 1.063e0

249.6980 2.025e0

249.8737 1.038e0

249.9010 1.266e-2

250.0916 2.751e1

250.1568 2.569e0

250.1988 3.158e0

250.3134 1.266e-2

250.5364 1.266e-2

250.6746 1.266e-2

250.7862 2.025e0

250.9122 2.025e0

250.9806 6.807e0

251.0350 3.004e0

251.1061 5.155e0

251.1984 3.149e0

251.3352 1.038e0

251.6148 1.051e0

251.9459 5.063e-2

252.3617 2.532e-2

252.7360 1.266e-2

252.8628 1.266e-2

252.9596 8.861e-2

253.1991 1.612e0

253.5296 3.038e0

253.7168 1.025e0

253.9914 2.539e0

254.1768 1.911e0

254.2758 1.266e-2

254.4139 1.025e0

254.5006 2.532e-2

254.8438 2.297e-1

255.2844 2.063e0

255.4808 1.013e0

255.5252 2.532e-2

255.8162 1.025e0

256.0218 3.719e1

256.1562 2.578e0

256.2033 3.375e0

256.3854 1.266e-2

257.0238 1.014e0

257.6322 1.025e0

257.7562 2.025e0

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374.3570 8.035e-1

374.4511 3.063e0

374.5695 1.322e2

374.6798 1.051e0

374.7375 1.038e0

374.7894 3.203e0

375.0652 9.698e1

375.2297 2.283e0

375.2852 5.639e-1

375.3192 5.188e-1

375.4210 4.885e0

375.5052 3.586e0

375.5688 4.418e1

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375.8632 2.038e0

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376.4651 5.076e0

376.5758 1.170e1

376.7865 2.025e0

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377.2187 2.631e0

377.3268 1.717e0

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377.4756 1.051e0

377.7014 2.532e-2

377.8484 1.013e0

378.1944 1.116e0

378.2751 5.019e0

378.4081 1.025e0

378.4824 1.266e-2

378.8770 1.266e-2

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381.1223 8.143e0

381.2921 1.114e0

381.5843 3.103e0

381.7028 2.532e-2

382.1124 9.111e0

382.3643 9.406e-1

382.5534 1.523e-1

382.7074 1.013e0

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383.6000 8.994e-1

383.6678 1.025e0

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383.8285 3.051e0

383.8944 1.013e0

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385.9554 2.558e0

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397.8561 1.266e-2

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