 Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 19-19 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 56Fe: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

334.0886 334.0894 -0.8 -2.4 10.5 57.6 C19 H20 N O 56Fe

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)

148.0253 6.089e0

148.1586 1.013e0

148.1744 1.013e0

148.2652 2.025e0

148.2808 2.811e0

148.3234 1.013e0

148.3624 1.013e0

148.3882 1.013e0

148.4121 2.025e0

148.4303 1.013e0

148.4509 1.025e0

148.4724 1.013e0

148.4980 1.266e-2

148.5319 2.532e-2

148.5500 1.266e-2

148.6091 2.038e0

148.6368 3.038e0

148.6764 1.013e0

148.7087 1.013e0

148.7284 1.013e0

148.7541 3.038e0

148.7864 1.013e0

148.8518 2.025e0

149.1181 6.784e0

149.1914 2.532e-2

149.2246 1.266e-2

149.2622 2.025e0

149.3248 2.532e-2

149.3952 3.837e0

149.4325 1.013e0

149.4581 2.025e0

149.4819 2.025e0

149.5037 1.266e-2

149.5300 7.089e0

149.5652 1.266e-2

149.5998 3.038e0

149.6304 1.013e0

149.7406 1.266e-2

149.7663 3.038e0

149.8201 2.038e0

149.8366 1.038e0

149.8840 2.025e0

149.9246 2.532e-2

149.9518 2.025e0

150.1661 4.051e0

150.2210 4.063e0

150.2431 3.038e0

150.2714 2.532e-2

150.3121 2.532e-2

150.3755 1.013e0

150.4027 5.462e0

150.4210 1.013e0

150.4715 1.025e0

150.4897 1.013e0

150.5187 3.798e-2

150.5778 1.013e0

150.5908 1.266e-2

150.6235 2.025e0

150.6415 2.038e0

150.6625 1.266e-2

150.7168 2.025e0

150.7389 1.025e0

150.7830 1.013e0

150.8059 2.980e0

150.8404 2.532e-2

150.8631 5.031e0

150.8931 2.038e0

150.9085 2.532e-2

151.1255 3.400e0

151.1991 4.051e0

151.2271 2.532e-2

151.2828 1.013e0

151.3155 6.428e0

151.3940 2.749e0

151.4130 4.051e0

151.4469 6.101e0

151.4901 2.532e-2

151.5668 8.747e0

151.6557 1.266e-2

151.6855 4.202e0

151.7190 2.076e0

151.7792 2.038e0

151.8526 3.038e0

151.8941 1.266e-2

151.9501 2.025e0

152.1053 3.638e0

152.1553 5.838e0

152.1913 3.038e0

152.2353 3.038e0

152.2570 9.460e-1

152.3564 4.051e0

152.3934 2.038e0

152.4384 1.025e0

152.4906 1.266e-2

152.5736 2.025e0

152.6144 1.025e0

152.6469 1.025e0

152.7237 1.266e-2

152.8557 1.013e0

152.8784 2.025e0

152.9110 1.013e0

152.9511 2.025e0

152.9770 1.038e0

153.0914 2.475e0

153.1761 2.025e0

153.1967 2.002e0

153.2811 4.063e0

153.3450 2.025e0

153.3719 1.266e-2

153.4865 1.303e-2

153.5711 7.595e-2

153.6393 5.063e0

153.7538 2.025e0

153.7787 2.038e0

153.8032 2.025e0

153.8371 4.051e0

153.9314 1.013e0

153.9806 3.668e0

154.0337 3.038e0

154.0578 3.644e0

154.1646 2.038e0

154.2181 1.013e0

154.2316 1.013e0

154.2552 1.013e0

154.2749 3.038e0

154.3306 2.532e-2

154.3970 1.103e0

154.4792 1.013e0

154.5507 5.254e-2

154.6312 2.025e0

154.6710 1.038e0

154.6942 1.266e-2

154.7275 1.038e0

154.7570 1.266e-2

154.8398 5.063e0

154.8992 2.025e0

154.9252 1.013e0

154.9522 1.025e0

155.0951 1.003e0

155.2069 1.013e0

155.2295 1.013e0

155.2893 2.025e0

155.3645 1.025e0

155.3785 1.013e0

155.4021 1.013e0

155.4221 1.266e-2

155.4674 3.038e0

155.4878 2.025e0

155.5384 2.038e0

155.5578 1.013e0

155.5872 1.266e-2

155.6108 1.266e-2

155.6297 2.025e0

155.6673 2.025e0

155.7035 1.013e0

155.7203 1.013e0

155.7994 1.266e-2

155.8197 1.013e0

155.8333 1.013e0

155.8728 1.013e0

155.8864 1.013e0

155.9501 2.532e-2

155.9756 2.532e-2

156.0093 3.038e0

156.1315 1.139e0

156.2614 1.266e-2

156.3020 3.165e0

156.3645 3.038e0

156.4108 1.013e0

156.4368 1.013e0

156.4689 4.051e0

156.5553 2.038e0

156.5900 1.266e-2

156.6234 1.013e0

156.6622 3.038e0

156.7231 1.013e0

156.7529 1.013e0

156.7933 1.025e0

156.8159 1.013e0

156.8465 3.038e0

156.8596 1.025e0

156.8794 1.013e0

156.9031 1.013e0

156.9245 3.038e0

157.0760 3.097e0

157.1135 2.142e0

157.1401 1.591e-1

157.1676 5.063e-2

157.2073 2.532e-2

157.2337 2.038e0

157.2521 1.013e0

157.2860 1.013e0

157.3206 2.025e0

157.3427 1.266e-2

157.3841 2.025e0

157.4187 1.013e0

157.4722 1.013e0

157.5059 1.266e-2

157.5792 2.532e-2

157.6024 1.013e0

157.6296 1.025e0

157.6422 1.013e0

157.6978 2.038e0

157.7226 1.013e0

157.7540 4.063e0

157.8259 1.013e0

157.8599 1.025e0

157.8792 1.025e0

157.9291 1.013e0

157.9859 1.013e0

158.0030 1.013e0

158.0969 7.494e-1

158.1341 2.625e0

158.1767 1.038e0

158.2145 2.025e0

158.2471 1.025e0

158.2715 2.038e0

158.3005 2.532e-2

158.3285 2.532e-2

158.3573 4.051e0

158.4407 1.013e0

158.4796 2.025e0

158.5211 2.025e0

158.5530 2.532e-2

158.5676 1.013e0

158.5949 2.025e0

158.6794 1.025e0

158.6984 1.013e0

158.7502 2.025e0

158.8292 1.013e0

158.8776 2.025e0

158.8998 1.266e-2

158.9481 2.025e0

159.0285 1.063e0

159.2515 2.025e0

159.2812 1.013e0

159.3189 2.532e-2

159.3855 1.266e-2

159.4104 1.025e0

159.4790 2.051e0

159.5217 3.798e-2

159.5619 1.025e0

159.6208 1.025e0

159.6606 1.013e0

159.7261 2.025e0

159.7529 2.025e0

159.7746 1.013e0

159.8087 1.013e0

159.8267 3.038e0

159.9023 2.025e0

159.9249 4.076e0

159.9967 1.013e0

160.0452 4.151e-1

160.0722 5.846e-1

160.1613 1.013e0

160.1857 3.038e0

160.2099 2.532e-2

160.2742 5.063e0

160.3094 1.013e0

160.3360 1.266e-2

160.3966 1.013e0

160.4571 1.013e0

160.4978 1.013e0

160.5233 1.038e0

160.5636 1.025e0

160.7233 1.013e0

160.7521 1.025e0

160.7907 1.013e0

160.8898 2.532e-2

160.9828 1.013e0

161.0132 3.038e0

161.1105 1.612e0

161.1658 1.051e0

161.1921 2.532e-2

161.2120 1.013e0

161.2849 4.051e0

161.3237 1.013e0

161.3403 1.266e-2

161.4484 1.013e0

161.4752 1.013e0

161.5109 2.532e-2

161.6005 1.013e0

161.6843 1.013e0

161.7084 1.013e0

161.7485 1.013e0

161.9112 2.025e0

161.9432 3.798e-2

162.0654 1.844e0

162.0961 2.362e0

162.2426 1.013e0

162.2895 2.532e-2

162.3240 1.025e0

162.3831 2.025e0

162.4201 2.025e0

162.4629 1.266e-2

162.4962 2.025e0

162.5117 1.025e0

162.5375 1.266e-2

162.5511 1.013e0

162.6871 2.038e0

162.7097 1.013e0

162.7407 1.013e0

162.8325 2.025e0

162.9082 2.025e0

162.9458 1.025e0

163.0377 2.025e0

163.0598 2.937e0

163.1237 4.316e1

163.2059 3.038e0

163.2394 2.025e0

163.2661 2.025e0

163.3460 3.038e0

163.3751 1.266e-2

163.4089 2.038e0

163.4449 3.798e-2

163.4868 1.013e0

163.5109 1.266e-2

163.5454 2.025e0

163.5822 3.038e0

163.6707 1.013e0

163.6881 1.266e-2

163.7076 1.013e0

163.7301 2.025e0

163.7770 2.025e0

163.8075 3.038e0

163.8547 3.038e0

163.8806 3.038e0

163.9321 1.013e0

163.9634 1.303e0

163.9874 2.025e0

164.0156 2.025e0

164.1089 4.416e1

164.1250 1.097e1

164.1706 1.013e0

164.2151 1.013e0

164.2524 1.025e0

164.2998 1.013e0

164.3273 1.025e0

164.3682 3.798e-2

164.3884 1.025e0

164.4230 1.013e0

164.4530 1.266e-2

164.4841 1.266e-2

164.5245 2.989e0

164.5721 3.198e0

164.6618 2.025e0

164.7298 3.798e-2

164.7582 2.025e0

164.8316 1.013e0

164.8556 1.013e0

164.8986 2.025e0

164.9318 4.051e0

164.9548 1.266e-2

164.9951 1.266e-2

165.1473 4.230e-2

165.1731 1.013e0

165.2176 1.013e0

165.2643 2.354e0

165.2805 4.051e0

165.3027 1.013e0

165.3509 1.266e-2

165.3794 2.051e0

165.4529 6.076e0

165.4734 1.266e-2

165.5166 2.038e0

165.5937 1.013e0

165.6688 1.266e-2

165.6994 1.013e0

165.7492 2.025e0

165.8088 1.266e-2

165.9082 2.025e0

165.9325 1.266e-2

165.9921 1.025e0

166.0113 1.013e0

166.0412 2.025e0

166.0642 2.110e0

166.0867 9.369e-1

166.2728 2.532e-2

166.3199 2.038e0

166.3502 1.266e-2

166.3875 2.025e0

166.4309 3.038e0

166.4612 3.123e0

166.4940 1.266e-2

166.6403 3.038e0

166.7400 2.038e0

166.7885 1.266e-2

166.8406 1.013e0

166.8898 2.025e0

166.9125 1.013e0

166.9569 1.266e-2

167.0069 3.051e0

167.0628 1.305e0

167.1979 1.013e0

167.2212 1.013e0

167.2350 1.266e-2

167.2973 2.025e0

167.3696 1.266e-2

167.4441 3.038e0

167.4893 3.038e0

167.5310 2.025e0

167.5598 3.038e0

167.6169 2.025e0

167.6655 4.051e0

167.7098 1.013e0

167.7509 2.025e0

167.7679 1.025e0

167.8063 1.266e-2

167.8471 1.266e-2

167.9072 1.038e0

167.9350 1.025e0

168.0132 1.025e0

168.0504 1.904e0

168.0885 5.696e0

168.1663 6.203e-1

168.1991 2.025e0

168.2189 1.013e0

168.2723 3.038e0

168.3260 1.013e0

168.3522 2.025e0

168.3951 1.266e-2

168.4646 1.025e0

168.4982 2.025e0

168.5209 2.038e0

168.5947 2.025e0

168.6447 2.038e0

168.7020 1.013e0

168.7724 5.063e0

168.8056 1.013e0

168.8679 4.051e0

168.9040 2.025e0

168.9338 2.025e0

168.9885 2.532e-2

169.0130 1.025e0

169.0392 1.025e0

169.1784 2.025e0

169.2134 1.266e-2

169.2667 1.025e0

169.2942 2.038e0

169.3347 1.025e0

169.3485 2.025e0

169.3948 1.025e0

169.4336 2.038e0

169.4688 1.013e0

169.5003 2.025e0

169.5453 8.177e0

169.5937 1.013e0

169.6287 1.025e0

169.6544 1.025e0

169.6957 3.038e0

169.7645 1.025e0

169.7961 1.025e0

169.8179 1.038e0

169.8434 2.038e0

169.8704 1.266e-2

169.9351 2.025e0

170.0250 1.025e0

170.1289 2.028e0

170.1771 1.025e0

170.1996 1.266e-2

170.2452 1.013e0

170.2761 1.025e0

170.3422 3.798e-2

170.4217 1.013e0

170.4392 1.013e0

170.5116 2.025e0

170.5987 3.051e0

170.6227 1.025e0

170.6473 1.266e-2

170.6980 1.025e0

170.7479 1.013e0

170.7830 3.038e0

170.8105 1.013e0

170.8572 3.038e0

170.8841 2.626e0

170.9082 2.025e0

170.9439 1.025e0

170.9632 2.025e0

170.9966 1.025e0

171.0309 1.025e0

171.0920 1.296e0

171.1180 2.194e-1

171.1909 2.532e-2

171.2450 1.013e0

171.3224 3.798e-2

171.3689 3.038e0

171.4215 3.051e0

171.4668 3.038e0

171.5266 1.013e0

171.5689 2.532e-2

171.5951 3.038e0

171.6154 2.038e0

171.6433 2.038e0

171.6730 1.266e-2

171.7281 1.013e0

171.8181 3.038e0

171.8923 1.025e0

171.9163 4.051e0

172.0037 2.532e-2

172.0571 1.660e0

172.0887 3.321e0

172.1674 3.063e0

172.1967 1.025e0

172.2135 3.038e0

172.3133 3.038e0

172.4709 1.013e0

172.5151 2.025e0

172.5339 1.013e0

172.5612 1.266e-2

172.5825 2.025e0

172.6283 1.013e0

172.6561 1.266e-2

172.7540 2.025e0

172.7831 2.038e0

172.8005 2.067e0

172.8586 4.051e0

172.9060 2.025e0

172.9297 2.025e0

172.9579 2.532e-2

172.9870 2.038e0

173.0091 1.013e0

173.0683 4.445e0

173.1674 1.582e-1

173.2325 2.025e0

173.2582 2.038e0

173.2818 1.266e-2

173.3584 2.025e0

173.3902 2.025e0

173.4264 2.025e0

173.4489 2.025e0

173.4808 1.266e-2

173.5038 2.025e0

173.5733 3.038e0

173.6563 2.025e0

173.7148 3.038e0

173.7398 1.266e-2

173.7734 1.025e0

173.7964 1.266e-2

173.8410 1.013e0

173.8871 2.025e0

173.9469 1.266e-2

174.0237 1.266e-2

174.0856 3.255e0

174.2341 2.532e-2

174.2546 2.025e0

174.2795 1.013e0

174.3059 1.038e0

174.3468 1.266e-2

174.3641 1.013e0

174.3881 1.013e0

174.4199 1.266e-2

174.4552 1.025e0

174.5443 2.532e-2

174.5592 1.268e0

174.5806 6.076e0

174.6636 3.038e0

174.7006 3.798e-2

174.7325 2.025e0

174.7715 2.025e0

174.8062 2.025e0

174.8517 3.038e0

174.8871 2.025e0

174.9753 2.038e0

175.0277 1.013e0

175.0454 1.266e-2

175.0823 1.284e-1

175.1913 2.025e0

175.2144 2.025e0

175.2355 2.025e0

175.3195 1.266e-2

175.4005 1.013e0

175.4211 1.266e-2

175.4388 1.013e0

175.4673 2.025e0

175.4894 2.038e0

175.5348 1.025e0

175.5760 1.013e0

175.6505 3.038e0

175.6897 2.025e0

175.7069 1.266e-2

175.7345 1.266e-2

175.7593 1.013e0

175.7859 1.051e0

175.8268 1.013e0

175.8551 1.013e0

175.8706 2.532e-2

175.9090 2.025e0

175.9498 1.013e0

175.9711 2.025e0

175.9980 3.798e-2

176.0414 2.038e0

176.1622 2.790e0

176.1967 1.266e-2

176.2209 1.266e-2

176.2778 1.266e-2

176.3275 1.266e-2

176.4684 3.038e0

176.5250 1.266e-2

176.5667 1.025e0

176.6272 1.025e0

176.6754 1.025e0

176.7719 1.013e0

176.7914 2.532e-2

176.8199 2.025e0

176.8691 3.038e0

176.9000 3.038e0

176.9343 1.013e0

176.9788 2.025e0

177.0618 1.956e0

177.1430 1.148e0

177.1847 6.076e0

177.2967 2.532e-2

177.3199 3.038e0

177.3626 2.025e0

177.4395 2.038e0

177.4986 1.025e0

177.5217 1.013e0

177.5467 1.013e0

177.5663 1.025e0

177.7165 1.025e0

177.7817 3.038e0

177.8155 1.013e0

177.8436 1.266e-2

177.8686 1.013e0

177.8998 3.038e0

178.0000 1.013e0

178.0288 4.140e0

178.2997 2.463e0

178.3442 1.013e0

178.3745 1.025e0

178.4572 1.013e0

178.4787 3.038e0

178.5162 1.025e0

178.5501 2.025e0

178.5788 1.266e-2

178.6033 1.013e0

178.6595 1.013e0

178.7007 2.025e0

178.7346 3.038e0

178.7596 1.013e0

178.7937 3.798e-2

178.8941 1.013e0

178.9335 2.038e0

179.0509 2.025e0

179.1152 1.579e1

179.2195 3.038e0

179.2504 1.266e-2

179.2906 1.025e0

179.3206 1.013e0

179.3571 3.051e0

179.3851 1.013e0

179.4424 1.013e0

179.4657 1.850e-1

179.4922 1.038e0

179.5807 2.025e0

179.6344 1.013e0

179.6702 2.025e0

179.7215 2.051e0

179.9136 3.038e0

179.9446 4.051e0

180.0236 1.038e0

180.0525 3.798e-2

180.0867 2.807e0

180.1997 1.025e0

180.2758 1.266e-2

180.3164 2.038e0

180.3650 1.013e0

180.3901 2.025e0

180.4127 4.051e0

180.4655 1.013e0

180.4927 3.038e0

180.5469 2.025e0

180.5857 4.051e0

180.6328 1.013e0

180.6722 1.266e-2

180.7154 2.051e0

180.7584 1.266e-2

180.8396 2.025e0

180.9150 1.266e-2

180.9473 2.025e0

181.0850 1.910e0

181.1274 2.359e0

181.2602 2.025e0

181.2799 1.266e-2

181.3339 3.038e0

181.4109 3.038e0

181.4618 3.798e-2

181.4906 1.013e0

181.5338 1.013e0

181.5976 3.038e0

181.6633 1.266e-2

181.8615 2.025e0

181.9352 2.532e-2

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