 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

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

Elements Used:

C: 16-16 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 69Ga: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

293.1859 293.1865 -0.6 -2.0 5.5 3.8 C16 H25 N2 O3

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)

134.9115 1.013e0

134.9485 1.266e-2

135.1474 2.532e-2

135.1909 5.063e-2

135.3656 1.025e0

135.4239 2.025e0

135.7584 1.266e-2

135.8392 1.266e-2

135.8700 1.013e0

135.9068 1.013e0

135.9474 2.025e0

135.9673 2.532e-2

136.0722 1.086e0

136.1578 1.266e-2

136.1736 1.013e0

136.2933 2.025e0

136.3441 1.013e0

136.5889 2.532e-2

136.6201 1.013e0

136.6480 1.013e0

136.7292 1.266e-2

136.7462 1.025e0

136.8499 1.266e-2

136.8844 1.266e-2

136.9370 1.266e-2

137.0089 1.013e0

137.0370 2.947e0

137.1735 2.532e-2

137.2919 1.013e0

137.3447 1.013e0

137.3670 1.013e0

137.4501 1.038e0

137.5504 1.013e0

137.6660 1.013e0

137.6783 1.013e0

137.7111 1.025e0

137.7622 2.532e-2

137.8248 1.266e-2

137.9185 1.013e0

137.9465 1.013e0

137.9841 2.532e-2

138.0122 1.013e0

138.0307 4.610e-1

138.1026 6.135e0

138.1805 1.013e0

138.2169 1.396e0

138.2368 1.038e0

138.4090 1.266e-2

138.4444 5.063e0

138.5214 1.025e0

138.5462 1.013e0

138.5591 1.266e-2

138.6418 2.025e0

138.6619 2.025e0

138.6931 1.266e-2

138.7707 3.051e0

138.9346 1.013e0

138.9767 2.532e-2

139.0957 1.106e1

139.1297 3.015e-1

139.1791 1.266e-2

139.1945 1.266e-2

139.3642 1.266e-2

139.4173 1.025e0

139.5082 1.266e-2

139.5373 6.076e0

139.5866 1.266e-2

139.5992 1.266e-2

139.6998 1.025e0

139.7530 1.266e-2

139.8440 1.266e-2

139.9697 1.266e-2

140.1088 2.909e0

140.1979 2.025e0

140.2212 1.013e0

140.2971 1.013e0

140.4891 1.266e-2

140.5304 2.025e0

140.5521 1.266e-2

140.6281 2.025e0

140.6466 1.266e-2

140.7726 1.013e0

140.8671 1.013e0

140.9463 1.266e-2

141.0045 2.532e-2

141.0662 1.125e0

141.1065 7.482e0

141.1439 1.565e0

141.1824 4.051e0

141.2058 4.697e-1

141.2463 1.013e0

141.4243 1.025e0

141.5287 2.532e-2

141.5475 1.025e0

141.5651 1.013e0

141.6124 1.266e-2

141.6471 3.038e0

141.8276 1.013e0

142.1568 2.025e0

142.1850 1.025e0

142.2646 1.266e-2

142.3961 2.532e-2

142.5406 1.013e0

142.5569 3.798e-2

142.5925 1.025e0

142.6421 1.013e0

142.6958 1.013e0

142.7521 4.051e0

142.7819 2.025e0

142.7940 1.266e-2

142.8550 1.013e0

142.9626 3.798e-2

142.9986 3.798e-2

143.1254 1.292e1

143.2094 3.038e0

143.2836 1.038e0

143.3061 1.266e-2

143.3283 1.266e-2

143.4333 1.013e0

143.4758 3.798e-2

143.5286 2.025e0

143.5629 1.334e1

143.6192 5.063e-2

143.6809 8.419e-2

143.6926 2.532e-2

143.8315 2.025e0

143.8650 2.025e0

143.9056 4.051e0

144.0127 2.051e0

144.0691 3.179e0

144.1163 2.387e-1

144.1393 2.645e0

144.2586 2.532e-2

144.3015 1.025e0

144.3512 1.013e0

144.4787 2.038e0

144.5160 3.798e-2

144.7066 2.038e0

144.7924 1.266e-2

144.8912 1.266e-2

144.9102 1.266e-2

144.9296 1.266e-2

145.0621 4.361e0

145.3232 1.266e-2

145.3649 2.025e0

145.4066 1.013e0

145.4550 1.013e0

145.4836 1.025e0

145.5524 2.025e0

145.6084 1.266e-2

145.6672 1.038e0

145.8039 1.013e0

145.8507 2.532e-2

146.1640 2.532e-2

146.2074 1.051e0

146.2827 1.266e-2

146.6007 1.266e-2

146.7857 1.025e0

146.8325 1.013e0

146.8826 1.025e0

146.8973 2.532e-2

146.9295 1.013e0

146.9849 3.051e0

147.0726 2.768e0

147.0957 3.424e0

147.2083 2.025e0

147.3902 2.532e-2

147.5130 1.266e-2

147.7213 2.532e-2

147.8378 2.532e-2

147.8582 1.013e0

148.0359 2.051e0

148.0658 9.161e-1

148.2236 1.013e0

148.3300 1.266e-2

148.5051 1.013e0

148.5578 1.549e0

148.5713 2.025e0

148.6381 1.266e-2

148.6508 1.266e-2

148.7346 1.025e0

148.8984 2.025e0

148.9489 1.013e0

148.9798 1.025e0

149.0896 2.874e0

149.1024 1.239e0

149.2029 2.038e0

149.2426 1.025e0

149.2656 1.717e0

149.3709 1.013e0

149.3938 3.038e0

149.4855 2.038e0

149.6640 5.063e-2

149.7255 1.025e0

149.7494 3.038e0

149.8542 1.025e0

150.0130 1.293e0

150.0278 2.989e0

150.1580 2.038e0

150.1773 1.038e0

150.3414 1.025e0

150.4869 1.013e0

150.6921 1.266e-2

150.7087 1.266e-2

150.9323 2.532e-2

150.9814 2.532e-2

151.1484 2.130e0

151.1735 2.532e-2

151.2334 2.038e0

151.3024 2.025e0

151.3243 4.366e0

151.5026 3.006e-1

151.5806 1.013e0

151.6355 3.038e0

151.8231 2.025e0

151.9003 1.051e0

151.9673 1.013e0

152.3327 2.532e-2

152.3534 1.266e-2

152.3915 2.532e-2

152.4161 2.038e0

152.4912 1.063e0

152.5742 6.329e-2

152.6199 1.038e0

152.6975 3.038e0

152.7444 1.266e-2

152.8102 1.266e-2

152.8329 5.063e0

153.0441 8.797e0

153.1601 7.089e0

153.2017 3.038e0

153.2670 3.798e-2

153.3456 2.025e0

153.3961 3.051e0

153.4679 2.025e0

153.6286 1.013e0

153.6540 1.038e0

153.6780 1.013e0

153.7577 1.013e0

153.8037 1.266e-2

153.9420 1.013e0

154.0050 1.013e0

154.0440 3.167e0

154.1539 4.051e0

154.1716 3.038e0

154.2588 1.266e-2

154.5393 2.532e-2

154.6250 1.266e-2

154.7223 2.025e0

154.7904 1.013e0

154.8468 1.013e0

154.8963 1.025e0

154.9426 1.013e0

154.9754 2.038e0

155.0434 1.415e0

155.0812 5.981e-1

155.1165 5.390e0

155.2605 1.013e0

155.4834 3.051e0

155.5207 1.025e0

155.5911 1.013e0

155.6610 1.013e0

155.7243 1.013e0

155.8530 1.266e-2

155.9129 1.266e-2

156.0784 5.692e0

156.2080 3.798e-2

156.3067 2.025e0

156.3683 2.025e0

156.4408 1.013e0

156.5310 1.266e-2

156.5573 1.013e0

156.7236 1.013e0

156.8867 1.013e0

157.0986 2.991e0

157.1835 1.266e-2

157.2610 1.025e0

157.7316 1.025e0

157.8129 1.013e0

157.8571 1.266e-2

157.9331 1.013e0

158.0943 1.910e0

158.1186 2.859e0

158.1926 1.025e0

158.4141 3.038e0

158.4648 1.013e0

158.5079 1.266e-2

158.6058 1.013e0

158.7831 1.013e0

158.8195 1.266e-2

158.8433 1.025e0

158.9971 1.013e0

159.1079 4.642e0

159.2248 1.013e0

159.4297 1.013e0

159.5352 2.438e0

159.5871 1.266e-2

159.6178 1.013e0

159.6594 1.025e0

159.6914 1.013e0

159.7335 2.025e0

159.7718 1.013e0

159.8630 1.013e0

159.8961 1.013e0

160.0490 3.060e0

160.0868 3.572e0

160.2000 2.025e0

160.2460 1.266e-2

160.3067 1.266e-2

160.3400 1.013e0

160.3902 1.266e-2

160.4073 1.013e0

160.5655 1.266e-2

160.6164 1.266e-2

160.7444 1.013e0

160.7575 1.266e-2

160.9090 1.266e-2

160.9765 1.013e0

161.0828 6.939e0

161.1185 3.634e0

161.1875 2.532e-2

161.2157 1.266e-2

161.2767 1.266e-2

161.3174 1.013e0

161.3441 1.013e0

161.4267 2.025e0

161.4747 2.038e0

161.5994 2.532e-2

161.7124 2.025e0

161.7731 1.013e0

161.7973 1.013e0

161.8758 1.025e0

161.9554 1.013e0

161.9828 2.025e0

162.0710 5.493e-1

162.1487 1.311e0

162.3923 1.266e-2

162.4209 1.025e0

162.6632 1.013e0

162.7035 1.013e0

162.9986 1.013e0

163.0210 3.038e0

163.1077 1.113e0

163.1618 1.025e0

163.1955 1.266e-2

163.2271 3.038e0

163.2620 2.532e-2

163.5793 1.013e0

163.6489 2.532e-2

163.7461 1.266e-2

163.8020 2.025e0

163.9028 1.266e-2

163.9431 1.266e-2

163.9776 1.266e-2

164.0801 1.969e0

164.1395 6.937e0

164.2305 2.532e-2

164.2550 2.409e0

164.3365 1.025e0

164.4340 1.013e0

164.5493 1.266e-2

164.6242 1.025e0

164.7234 1.013e0

164.8925 2.532e-2

165.0453 5.625e-1

165.1132 6.585e0

165.2084 2.025e0

165.2231 1.025e0

165.2660 2.025e0

165.3273 1.013e0

165.4241 3.798e-2

165.4671 1.266e-2

165.5596 1.013e0

165.6999 1.013e0

165.8033 1.051e0

165.8828 2.025e0

166.0880 5.395e0

166.4072 2.025e0

166.4495 1.266e-2

166.4877 1.266e-2

166.5561 1.013e0

166.5734 1.025e0

166.6868 1.013e0

166.8168 1.266e-2

166.9061 2.025e0

166.9442 1.013e0

167.0183 1.051e0

167.1056 1.879e0

167.1601 1.266e-2

167.2261 4.051e0

167.2495 2.025e0

167.3702 1.266e-2

167.3872 1.013e0

167.4387 2.532e-2

167.4732 1.266e-2

167.5072 2.025e0

167.5385 1.266e-2

167.5726 1.266e-2

167.6001 1.266e-2

167.6385 1.025e0

167.7139 1.266e-2

167.8859 1.013e0

167.9414 2.038e0

167.9780 3.038e0

168.0085 2.025e0

168.0302 1.025e0

168.0505 2.386e0

168.1129 7.975e0

168.1929 1.266e-2

168.2128 1.013e0

168.2475 1.266e-2

168.3059 1.013e0

168.3545 1.013e0

168.5720 1.266e-2

168.6234 1.266e-2

168.6769 1.025e0

168.7096 1.266e-2

168.8941 2.025e0

168.9718 1.266e-2

169.0066 1.013e0

169.0515 1.648e0

169.0898 2.248e0

169.1484 2.025e0

169.1671 2.532e-2

169.2070 1.266e-2

169.2589 1.266e-2

169.3353 1.266e-2

169.3524 1.266e-2

169.6012 3.798e-2

169.6424 1.038e0

169.6667 1.266e-2

169.7121 1.266e-2

169.7331 1.013e0

169.7774 1.013e0

169.8277 2.038e0

169.9339 1.013e0

169.9888 1.266e-2

170.0133 1.025e0

170.0379 4.051e0

170.1760 1.013e0

170.2317 1.013e0

170.2767 1.266e-2

170.5806 1.025e0

170.6541 3.798e-2

170.7538 1.025e0

170.8948 1.013e0

170.9788 3.038e0

171.1499 4.143e0

171.1883 5.089e0

171.2975 1.266e-2

171.4263 1.266e-2

171.4751 1.266e-2

171.5377 2.063e0

171.6138 1.266e-2

171.6385 1.266e-2

171.6772 1.013e0

171.8129 1.266e-2

171.8964 1.013e0

172.0770 1.579e0

172.1129 3.832e0

172.1448 1.815e0

172.1631 1.025e0

172.1933 2.038e0

172.2590 1.013e0

172.2835 2.532e-2

172.3282 2.025e0

172.5778 2.532e-2

172.7088 1.266e-2

172.7440 1.013e0

172.7823 1.266e-2

172.9497 1.013e0

173.1356 2.334e0

173.1616 1.453e0

173.2120 1.025e0

173.2331 1.013e0

173.5167 1.013e0

173.5563 1.038e0

173.6366 2.038e0

173.6568 1.266e-2

173.6846 1.266e-2

173.7085 1.266e-2

173.7864 1.266e-2

174.0305 2.038e0

174.2035 1.266e-2

174.2854 1.025e0

174.4169 1.025e0

174.4446 3.038e0

174.5105 1.025e0

174.5450 2.038e0

174.6033 1.266e-2

174.6423 1.025e0

174.7119 2.025e0

174.7896 1.266e-2

174.8523 1.013e0

175.0408 2.038e0

175.2704 1.266e-2

175.3644 2.025e0

175.4430 1.266e-2

175.5442 1.025e0

175.6249 5.063e0

175.6475 1.266e-2

175.6867 1.013e0

175.7247 1.013e0

175.7670 1.013e0

175.8238 2.038e0

175.8588 3.798e-2

175.9806 2.025e0

176.0194 3.038e0

176.0948 9.474e-1

176.1800 1.013e0

176.2677 1.266e-2

176.3888 1.025e0

176.4726 1.013e0

176.5343 2.025e0

176.5533 1.013e0

176.6065 3.051e0

176.6385 1.013e0

176.6882 1.013e0

176.7349 2.025e0

176.7974 3.038e0

176.8579 1.266e-2

176.9109 3.038e0

176.9500 3.038e0

177.0256 3.051e0

177.1067 5.221e0

177.1364 5.966e-1

177.1838 1.038e0

177.2219 1.013e0

177.2705 1.013e0

177.2991 1.266e-2

177.5188 1.013e0

177.5580 1.025e0

177.7029 1.013e0

177.7385 1.266e-2

177.7708 2.532e-2

177.8006 1.025e0

177.9531 1.025e0

178.0041 1.266e-2

178.0364 1.038e0

178.0619 1.650e0

178.0980 1.378e0

178.1307 5.932e0

178.1644 1.335e1

178.2627 1.266e-2

178.3556 1.013e0

178.3771 1.266e-2

178.4102 2.025e0

178.5293 1.266e-2

178.7138 1.266e-2

178.7566 1.266e-2

178.8539 2.051e0

179.0807 2.241e0

179.1742 2.025e0

179.1902 1.025e0

179.2332 1.013e0

179.3822 1.266e-2

179.5122 2.532e-2

179.6171 1.013e0

179.7807 1.266e-2

179.8324 2.025e0

179.9256 2.025e0

179.9897 2.025e0

180.0998 2.740e0

180.1769 1.025e0

180.2057 1.025e0

180.2658 1.013e0

180.6549 2.025e0

180.6728 1.266e-2

180.7302 1.266e-2

180.7518 1.266e-2

180.7909 2.025e0

181.0976 3.103e0

181.1175 2.191e0

181.1815 2.266e0

181.4128 2.025e0

181.5273 1.013e0

181.5991 1.013e0

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181.7226 1.025e0

181.7527 1.013e0

181.7847 1.013e0

181.8027 1.025e0

181.9035 1.013e0

181.9737 1.025e0

181.9981 1.839e0

182.0336 3.051e0

182.1274 6.785e0

182.2261 1.013e0

182.2458 2.532e-2

182.4662 1.266e-2

182.5849 2.532e-2

182.6857 1.266e-2

182.8078 1.013e0

182.8256 1.025e0

182.9891 1.716e0

183.0217 1.499e0

183.0826 4.630e0

183.1171 5.259e-1

183.1914 4.051e0

183.2945 2.025e0

183.3501 1.013e0

183.4043 1.013e0

183.4277 2.532e-2

183.6173 1.013e0

183.7416 2.038e0

183.7714 1.266e-2

183.8831 1.266e-2

183.9048 1.266e-2

183.9450 1.596e0

183.9734 1.025e0

184.0457 1.266e-2

184.1269 6.540e0

184.1618 2.072e0

184.2656 2.025e0

184.4057 1.013e0

184.4890 1.013e0

184.5704 2.025e0

184.5903 1.013e0

184.6771 1.013e0

184.7146 4.341e0

184.7531 1.013e0

184.7857 1.025e0

184.8111 1.013e0

184.8687 2.025e0

184.9549 1.013e0

185.0065 3.038e0

185.0935 6.515e0

185.1150 2.900e0

185.2948 1.013e0

185.5703 2.025e0

185.6970 1.013e0

185.7926 2.025e0

186.0329 1.013e0

186.0949 2.987e0

186.1854 1.013e0

186.2634 2.025e0

186.3197 1.013e0

186.4794 1.266e-2

186.6029 1.013e0

186.6828 1.266e-2

186.8136 1.266e-2

186.8336 1.025e0

186.8609 1.025e0

187.0117 1.025e0

187.0481 2.025e0

187.1157 3.963e0

187.1428 1.378e0

187.3099 2.532e-2

187.4100 1.013e0

187.5919 1.013e0

187.6465 1.013e0

187.6975 1.266e-2

187.8795 1.266e-2

187.9414 1.266e-2

187.9728 1.051e0

188.0236 2.038e0

188.0843 6.500e-1

188.1243 1.375e0

188.2145 2.025e0

188.3202 1.013e0

188.3457 1.025e0

188.3967 1.013e0

188.5863 1.013e0

188.6547 4.051e0

188.7322 1.266e-2

188.8465 3.038e0

188.9110 1.025e0

188.9620 3.798e-2

189.0037 3.038e0

189.1039 6.627e-1

189.2138 2.025e0

189.2614 1.013e0

189.2981 1.266e-2

189.4411 2.025e0

189.4742 1.266e-2

189.5256 1.013e0

189.6300 4.051e0

189.6719 1.013e0

189.7449 1.013e0

189.7741 1.266e-2

189.8637 2.025e0

189.9350 1.013e0

189.9807 5.063e-2

190.0319 2.051e0

190.1021 1.832e0

190.1396 4.157e0

190.2498 2.025e0

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