 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

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

Elements Used:

C: 15-15 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

241.1334 241.1341 -0.7 -2.9 8.5 3.2 C15 H17 N2 O

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)

126.7335 1.013e0

126.7722 1.266e-2

126.8142 1.266e-2

126.8503 1.266e-2

126.8803 1.266e-2

127.0059 1.013e0

127.1932 1.025e0

127.2231 2.025e0

127.2738 2.025e0

127.3025 1.013e0

127.4436 1.013e0

127.4637 2.038e0

127.5514 2.025e0

127.6297 1.013e0

127.6538 1.013e0

127.6832 1.013e0

127.7073 1.013e0

127.7734 2.025e0

127.8695 1.013e0

128.0844 1.119e0

128.1763 2.532e-2

128.2199 1.025e0

128.2455 1.266e-2

128.2845 1.013e0

128.2999 1.266e-2

128.3116 1.266e-2

128.3808 1.013e0

128.4472 2.025e0

128.4803 1.013e0

128.5860 1.013e0

128.6055 2.532e-2

128.6430 1.013e0

128.7091 1.013e0

128.7276 1.266e-2

128.7758 1.266e-2

128.8962 1.013e0

128.9673 1.025e0

129.0157 1.051e0

129.1649 1.013e0

129.2101 1.013e0

129.2297 1.025e0

129.3491 1.013e0

129.3732 1.266e-2

129.3932 2.532e-2

129.4792 3.038e0

129.5580 1.013e0

129.6080 2.025e0

129.6274 1.013e0

129.6486 1.025e0

129.7306 1.013e0

129.7485 1.013e0

129.7696 1.013e0

129.8634 1.013e0

129.9696 1.266e-2

129.9907 1.266e-2

130.2233 2.051e0

130.2558 2.025e0

130.3575 3.038e0

130.3849 1.013e0

130.4045 2.532e-2

130.4334 2.532e-2

130.4639 2.532e-2

130.5859 5.063e-2

130.6199 1.025e0

130.6370 2.025e0

130.6762 1.013e0

130.7279 1.266e-2

130.7454 2.478e0

130.7642 3.038e0

130.8055 2.532e-2

130.8463 1.266e-2

130.8588 1.013e0

130.8980 1.013e0

130.9654 3.038e0

131.0226 2.025e0

131.0409 1.684e0

131.0856 4.104e1

131.1236 1.405e0

131.2100 1.038e0

131.2932 2.025e0

131.3451 1.013e0

131.4244 2.532e-2

131.4488 1.013e0

131.4747 2.532e-2

131.5453 3.798e-2

131.5674 1.013e0

131.6011 1.013e0

131.6302 2.025e0

131.6681 1.013e0

131.6805 1.266e-2

131.7386 1.013e0

131.8424 1.013e0

131.8628 3.038e0

131.9155 1.266e-2

131.9477 2.038e0

131.9886 1.013e0

132.1052 8.052e-1

132.1429 2.025e0

132.2025 1.013e0

132.2240 1.025e0

132.2696 1.025e0

132.2855 1.038e0

132.3583 2.025e0

132.3964 2.532e-2

132.4193 1.013e0

132.4547 2.025e0

132.4681 1.013e0

132.4925 1.266e-2

132.5349 2.038e0

132.5689 1.266e-2

132.6320 2.532e-2

132.6855 2.025e0

132.7084 1.025e0

132.7407 1.266e-2

132.8172 1.013e0

132.8385 1.013e0

132.8537 1.013e0

132.8784 1.013e0

132.9458 1.013e0

133.0373 1.252e0

133.0593 4.282e-2

133.0763 4.734e0

133.0929 5.792e0

133.1755 1.266e-2

133.2000 1.266e-2

133.2923 1.013e0

133.3413 1.266e-2

133.4393 1.013e0

133.4580 1.013e0

133.4855 1.266e-2

133.6084 1.266e-2

133.6685 2.532e-2

133.7342 1.266e-2

133.8806 2.025e0

133.8971 1.013e0

134.1433 2.025e0

134.2109 1.266e-2

134.2541 1.013e0

134.2911 1.266e-2

134.3279 1.013e0

134.3619 1.013e0

134.4585 2.025e0

134.4834 2.025e0

134.5006 1.013e0

134.6454 1.013e0

134.7068 1.013e0

134.7272 2.025e0

134.7652 3.038e0

134.7933 1.266e-2

134.8937 1.025e0

134.9449 1.013e0

134.9712 2.025e0

135.0283 1.013e0

135.0465 1.366e0

135.1481 2.025e0

135.1918 1.266e-2

135.2037 1.266e-2

135.2594 1.266e-2

135.2785 1.013e0

135.3214 1.266e-2

135.3397 1.266e-2

135.4523 3.038e0

135.6060 2.025e0

135.7206 2.025e0

135.8162 1.013e0

135.8288 1.013e0

135.8999 1.013e0

135.9155 1.025e0

136.0805 1.951e1

136.1502 3.038e0

136.2071 1.266e-2

136.2286 1.025e0

136.2955 2.025e0

136.3091 2.038e0

136.3808 1.013e0

136.3960 1.266e-2

136.4410 2.025e0

136.5294 3.038e0

136.5699 1.266e-2

136.5882 1.013e0

136.6848 2.025e0

136.6975 1.266e-2

136.7502 1.013e0

136.7934 4.051e0

136.8524 1.013e0

136.8652 1.013e0

136.9024 1.266e-2

136.9801 1.013e0

137.0369 3.148e0

137.1480 1.013e0

137.2286 1.013e0

137.3129 1.266e-2

137.3286 1.013e0

137.3411 1.266e-2

137.3773 3.038e0

137.4299 3.038e0

137.4534 1.013e0

137.4933 2.532e-2

137.6342 1.013e0

137.6526 1.013e0

137.7367 1.013e0

137.7791 2.025e0

137.7959 1.013e0

137.8176 1.013e0

137.8741 1.013e0

137.9521 1.266e-2

137.9942 1.025e0

138.0566 3.771e1

138.1024 2.468e0

138.1824 5.254e-1

138.2021 2.025e0

138.2455 1.013e0

138.2672 1.013e0

138.2896 1.266e-2

138.3015 1.013e0

138.3674 1.266e-2

138.3847 2.025e0

138.4144 1.266e-2

138.4644 1.025e0

138.5051 1.266e-2

138.5349 3.038e0

138.5896 1.266e-2

138.6299 1.266e-2

138.6675 1.013e0

138.7301 1.013e0

138.7462 1.266e-2

138.7790 2.025e0

138.8345 2.038e0

138.8546 5.063e0

138.9180 1.266e-2

138.9445 1.025e0

138.9839 1.013e0

138.9963 1.266e-2

139.0235 3.038e0

139.1672 1.025e0

139.2186 1.013e0

139.2315 1.266e-2

139.2780 2.025e0

139.3473 1.013e0

139.4101 1.013e0

139.4318 1.266e-2

139.4632 1.013e0

139.4978 1.266e-2

139.6064 2.025e0

139.6471 2.532e-2

139.6771 1.266e-2

139.7664 3.038e0

139.8626 1.266e-2

139.8999 1.266e-2

139.9189 1.013e0

139.9656 1.266e-2

139.9818 1.013e0

140.0003 1.013e0

140.0577 4.640e0

140.0824 8.739e0

140.1575 1.013e0

140.1831 1.266e-2

140.3060 1.266e-2

140.3455 4.051e0

140.5198 1.013e0

140.5577 2.025e0

140.5812 2.025e0

140.6111 1.013e0

140.6331 1.013e0

140.7847 1.013e0

140.8097 2.025e0

140.8663 1.013e0

140.9010 1.013e0

140.9140 1.013e0

140.9390 1.013e0

140.9519 1.266e-2

140.9866 2.532e-2

141.0271 1.013e0

141.0858 2.434e0

141.1012 2.853e0

141.1510 5.031e0

141.2090 2.532e-2

141.2390 1.013e0

141.2543 1.266e-2

141.2829 1.013e0

141.3069 2.025e0

141.3809 2.025e0

141.4501 1.013e0

141.4883 1.013e0

141.5135 1.266e-2

141.5611 1.013e0

141.5770 1.013e0

141.5927 1.266e-2

141.6688 1.266e-2

141.7004 1.266e-2

141.7320 1.266e-2

141.7506 1.266e-2

141.8835 1.266e-2

141.8965 2.025e0

141.9216 1.013e0

141.9881 1.013e0

142.0389 6.638e-1

142.0588 3.884e0

142.1624 2.532e-2

142.1941 1.013e0

142.2086 1.025e0

142.2477 1.013e0

142.2767 1.013e0

142.3840 3.038e0

142.4002 2.025e0

142.4334 2.025e0

142.4877 2.038e0

142.5333 1.013e0

142.6160 1.266e-2

142.6537 3.798e-2

142.7524 1.266e-2

142.8794 1.013e0

142.9046 1.266e-2

142.9210 2.532e-2

143.0029 1.013e0

143.1494 3.798e-2

143.1816 2.038e0

143.2077 2.025e0

143.2258 1.025e0

143.2543 1.013e0

143.3238 4.051e0

143.3495 1.266e-2

143.4008 1.013e0

143.4325 1.266e-2

143.4501 4.051e0

143.4708 1.266e-2

143.5181 3.038e0

143.5852 2.025e0

143.6512 4.063e0

143.6744 1.013e0

143.7193 1.266e-2

143.7604 1.013e0

143.7730 1.013e0

143.8064 2.025e0

143.8276 1.013e0

143.8594 1.266e-2

143.9295 1.266e-2

143.9417 1.266e-2

143.9709 1.013e0

144.0118 1.013e0

144.0791 1.562e0

144.1084 5.863e0

144.1473 3.038e0

144.2003 1.266e-2

144.3295 2.025e0

144.4075 1.013e0

144.4440 2.038e0

144.4623 1.013e0

144.4909 2.025e0

144.6314 1.266e-2

144.7271 1.266e-2

144.7686 1.013e0

144.8006 1.266e-2

144.8185 2.025e0

144.8785 3.038e0

144.9223 1.013e0

144.9607 1.013e0

145.0278 1.013e0

145.0811 2.537e0

145.2084 2.025e0

145.2346 1.025e0

145.2714 1.013e0

145.2838 1.013e0

145.3256 1.013e0

145.3739 1.266e-2

145.4200 3.038e0

145.4894 1.013e0

145.5337 2.532e-2

145.5532 1.266e-2

145.5752 1.266e-2

145.6016 1.013e0

145.6721 2.025e0

145.6941 1.013e0

145.7139 1.013e0

145.7679 1.013e0

145.7843 1.266e-2

145.8088 1.038e0

145.9506 2.025e0

145.9840 2.038e0

146.1235 4.707e-1

146.2493 1.266e-2

146.3075 1.013e0

146.3511 2.025e0

146.3947 1.025e0

146.4284 2.025e0

146.5132 1.013e0

146.5391 1.013e0

146.5933 1.013e0

146.6317 2.025e0

146.7289 1.013e0

146.7477 1.013e0

146.7642 1.013e0

146.9409 1.013e0

147.0249 1.013e0

147.0793 2.423e0

147.2684 2.025e0

147.3294 1.025e0

147.3441 1.025e0

147.5508 1.013e0

147.6349 1.013e0

147.6891 1.013e0

147.7312 1.013e0

147.7733 1.266e-2

147.8285 1.013e0

147.8474 1.013e0

147.8771 1.266e-2

147.9102 2.038e0

147.9396 3.038e0

147.9608 1.013e0

148.0090 1.013e0

148.0343 9.824e-1

148.1643 1.266e-2

148.2327 1.013e0

148.2781 1.013e0

148.3102 1.266e-2

148.3291 1.266e-2

148.4399 1.266e-2

148.4849 1.013e0

148.4977 1.013e0

148.5331 1.266e-2

148.6034 2.025e0

148.6306 1.266e-2

148.7116 1.013e0

148.7521 2.532e-2

148.7992 1.013e0

148.8315 1.013e0

148.8703 3.038e0

149.2045 1.013e0

149.2384 1.025e0

149.2566 1.013e0

149.2789 1.013e0

149.3022 1.266e-2

149.3799 1.013e0

149.4089 1.266e-2

149.4412 1.013e0

149.5812 1.266e-2

149.6946 1.266e-2

149.7635 1.013e0

149.8247 1.013e0

149.8472 2.038e0

149.8804 1.025e0

149.9193 1.013e0

149.9424 1.266e-2

149.9583 1.013e0

149.9972 1.013e0

150.1781 2.025e0

150.2449 1.013e0

150.2845 2.025e0

150.3001 1.266e-2

150.3267 1.013e0

150.3624 1.013e0

150.3914 1.266e-2

150.5998 1.013e0

150.6131 1.013e0

150.6439 2.025e0

150.6946 1.013e0

150.7240 1.013e0

150.7502 2.025e0

150.8182 1.025e0

150.9228 4.051e0

150.9809 3.038e0

150.9945 1.025e0

151.0780 1.058e0

151.1078 3.946e0

151.2747 1.051e0

151.3216 1.013e0

151.3848 3.038e0

151.4078 7.089e0

151.4358 1.013e0

151.5830 5.063e-2

151.6446 3.798e-2

151.6948 2.025e0

151.7238 1.266e-2

151.8025 4.051e0

151.8289 1.013e0

151.8848 5.063e-2

151.9683 2.025e0

152.0791 4.174e0

152.1075 1.147e0

152.1610 2.025e0

152.1959 2.025e0

152.2725 2.025e0

152.2942 1.013e0

152.3210 2.898e-1

152.3478 2.532e-2

152.3761 1.025e0

152.4495 4.051e0

152.5537 1.316e1

152.5904 3.798e-2

152.6892 2.025e0

152.7760 1.013e0

152.7995 2.025e0

152.8421 1.013e0

152.8645 1.013e0

152.8914 2.025e0

152.9274 1.013e0

152.9733 1.266e-2

153.0461 5.626e0

153.1044 5.116e0

153.2218 1.025e0

153.2443 2.025e0

153.3054 2.532e-2

153.3874 1.013e0

153.4142 1.013e0

153.5630 1.051e0

153.6169 2.025e0

153.6344 1.013e0

153.6625 4.051e0

153.7172 2.025e0

153.7568 1.013e0

153.8096 1.013e0

153.8266 3.038e0

153.9178 1.266e-2

153.9310 1.013e0

153.9599 1.025e0

153.9805 1.025e0

154.0500 6.273e0

154.1498 2.624e0

154.1741 2.038e0

154.2245 1.013e0

154.2609 1.025e0

154.2875 1.266e-2

154.3010 1.013e0

154.4293 1.013e0

154.5199 2.025e0

154.5813 2.025e0

154.6015 1.266e-2

154.6605 2.025e0

154.8257 1.013e0

154.8476 1.025e0

154.8665 1.025e0

154.9501 1.025e0

155.0273 1.025e0

155.0910 7.773e0

155.1580 1.038e0

155.2032 2.025e0

155.2477 2.025e0

155.2724 1.013e0

155.2957 2.532e-2

155.3554 1.266e-2

155.4084 2.025e0

155.4649 1.266e-2

155.5490 2.025e0

155.5775 1.266e-2

155.6155 2.025e0

155.6568 3.038e0

155.6771 1.013e0

155.7234 1.013e0

155.7427 1.013e0

155.7894 1.013e0

155.8362 1.013e0

155.9289 1.013e0

155.9455 1.266e-2

155.9651 1.266e-2

156.0182 1.266e-2

156.1227 1.979e0

156.1432 1.946e0

156.1742 1.266e-2

156.2141 1.266e-2

156.2726 3.038e0

156.3075 1.013e0

156.3833 1.013e0

156.4003 1.013e0

156.4450 2.025e0

156.4800 1.025e0

156.5236 1.013e0

156.5518 4.051e0

156.5733 1.013e0

156.7009 1.025e0

156.7160 1.013e0

156.8925 1.013e0

156.9188 1.013e0

156.9390 1.013e0

156.9854 1.013e0

157.0722 8.983e-1

157.1672 2.532e-2

157.2468 2.025e0

157.3355 1.266e-2

157.3617 1.013e0

157.4121 1.025e0

157.4687 1.013e0

157.5521 1.013e0

157.6709 3.038e0

158.0009 2.025e0

158.0936 1.034e1

158.1213 2.415e0

158.1696 1.013e0

158.4070 4.051e0

158.4774 2.025e0

158.5105 1.013e0

158.5432 3.798e-2

158.5724 2.532e-2

158.6650 1.013e0

158.6809 1.013e0

158.7083 1.013e0

158.7516 1.266e-2

158.7886 1.266e-2

158.8220 1.013e0

158.8721 1.013e0

158.9290 1.013e0

158.9825 1.013e0

159.0631 4.532e0

159.1526 3.737e0

159.2136 1.013e0

159.3684 1.013e0

159.4152 1.013e0

159.4585 1.013e0

159.5027 1.266e-2

159.5241 4.051e0

159.5727 1.013e0

159.6236 1.013e0

159.6534 1.013e0

159.7206 1.013e0

159.7478 1.013e0

159.7674 1.013e0

159.7879 1.013e0

159.9054 1.013e0

159.9963 1.266e-2

160.0363 4.051e0

160.1140 8.489e-1

160.2026 1.025e0

160.2451 1.013e0

160.2682 2.025e0

160.3219 1.013e0

160.3858 1.013e0

160.3996 1.013e0

160.4738 1.013e0

160.5207 1.013e0

160.5777 1.266e-2

160.6155 2.025e0

160.6777 1.025e0

160.7732 1.013e0

160.7989 2.025e0

160.8372 1.266e-2

160.9653 3.038e0

161.0030 1.266e-2

161.0258 1.013e0

161.0819 6.742e0

161.1669 3.051e0

161.2387 1.013e0

161.2790 1.013e0

161.3027 1.013e0

161.3335 1.266e-2

161.4446 2.532e-2

161.4793 1.025e0

161.5122 1.013e0

161.6098 1.266e-2

161.6978 1.266e-2

161.7928 2.038e0

161.9177 1.013e0

161.9315 1.013e0

161.9889 2.025e0

162.0152 1.013e0

162.0359 1.013e0

162.1143 2.227e0

162.2388 1.266e-2

162.3202 1.013e0

162.3568 2.025e0

162.3879 1.013e0

162.4248 1.013e0

162.4590 1.013e0

162.4764 1.013e0

162.5199 1.013e0

162.5478 3.038e0

162.5739 1.013e0

162.6251 3.038e0

162.6760 1.013e0

162.7507 1.013e0

162.7978 1.025e0

162.8644 3.038e0

162.8975 1.038e0

163.0115 1.266e-2

163.0322 2.025e0

163.1308 3.896e0

163.2209 3.038e0

163.3000 1.266e-2

163.3172 1.013e0

163.3678 1.013e0

163.4184 1.013e0

163.4702 1.013e0

163.5036 1.013e0

163.5480 1.013e0

163.6375 1.025e0

163.6738 1.013e0

163.7624 1.013e0

163.7890 1.013e0

163.8097 1.013e0

163.8620 2.025e0

163.8983 1.266e-2

163.9387 2.025e0

163.9577 2.025e0

163.9933 1.013e0

164.1702 1.266e-2

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386.9433 3.038e0

387.0724 2.025e0

387.2514 1.470e0

387.3524 3.038e0

387.4247 3.038e0

387.6321 2.025e0

387.7214 1.013e0

387.9489 2.025e0

387.9934 1.013e0

388.0877 4.051e0

388.4024 1.013e0

388.4850 1.013e0

388.5508 2.025e0

388.6936 3.038e0

388.8087 1.013e0

388.8846 1.013e0

388.9656 2.025e0

389.0193 3.038e0

389.0599 4.051e0

389.1165 6.005e0

389.2655 2.238e1

389.3431 3.495e0

389.4227 2.025e0

389.4843 2.038e0

389.5462 3.038e0

389.6544 1.013e0

389.7008 1.013e0

389.7374 2.025e0

390.0885 3.035e0

390.1301 3.979e0

390.2310 4.289e0

390.2890 5.325e0

390.3670 2.025e0

390.4654 4.051e0

390.6487 3.038e0

390.8047 1.013e0

390.8831 2.532e-2

390.9318 2.025e0

390.9829 1.013e0

391.0333 1.013e0

391.1828 4.025e0

391.2892 6.143e1

391.4349 2.051e0

391.5751 1.013e0

391.6475 2.025e0

391.7334 2.025e0

391.7858 2.025e0

391.9168 2.619e0

391.9622 3.038e0

392.0804 1.266e-2

392.1408 9.950e-1

392.2936 2.096e1

392.3721 2.025e0

392.4694 1.013e0

392.5495 1.013e0

392.6015 1.013e0

392.6595 1.013e0

392.6919 1.013e0

392.8706 3.038e0

392.9857 2.025e0

393.0188 3.038e0

393.0991 4.051e0

393.3930 1.013e0

393.5282 3.038e0

393.5919 1.013e0

393.6804 1.013e0

393.7869 1.013e0

393.9322 4.051e0

394.0882 2.025e0

394.1837 2.940e0

394.4995 1.013e0

394.7987 2.025e0

394.9412 3.038e0

394.9778 3.051e0

395.0480 1.038e0

395.1233 1.025e0

395.3223 1.013e0

395.4169 3.038e0

395.4887 1.266e-2

395.5455 2.025e0

395.5799 4.051e0

395.6570 1.013e0

395.8575 1.013e0

396.0178 1.038e0

396.1096 2.025e0

396.1696 2.025e0

396.2191 1.230e-2

396.2828 2.992e0

396.3824 2.025e0

396.5070 1.013e0

396.6096 1.013e0

396.6944 1.266e-2

396.7553 2.025e0

396.7997 1.013e0

396.8558 1.013e0

396.9822 4.051e0

397.1092 9.114e0

397.2775 1.086e0

397.3380 2.025e0

397.3797 1.025e0

397.4178 1.013e0

397.5375 2.025e0

397.5976 3.038e0

397.6594 2.025e0

397.8575 2.532e-2

397.9064 3.038e0

397.9824 4.076e0

398.0367 1.013e0

398.1070 2.025e0

398.1411 2.025e0

398.1798 3.503e-1

398.2401 6.323e0

398.2800 8.558e0

398.3571 1.038e0

398.5133 2.025e0

398.6003 2.025e0

398.7599 1.013e0

398.8399 1.013e0

398.9128 1.013e0

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399.0912 5.063e0

399.2191 2.279e0

399.3158 7.137e0

399.3903 1.013e0

399.4713 2.025e0

399.5940 1.013e0

399.7432 1.013e0

399.7858 1.013e0