 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

876 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 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

311.1747 311.1760 -1.3 -4.2 9.5 5.9 C19 H23 N2 O2

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)

147.7692 5.063e-2

147.8169 2.532e-2

147.8622 1.266e-2

147.8835 2.038e0

147.9544 2.051e0

148.0288 2.532e-2

148.0789 2.843e-1

148.1149 6.100e1

148.2227 2.025e0

148.2404 1.013e0

148.2794 1.013e0

148.3052 1.013e0

148.3407 1.013e0

148.4002 3.038e0

148.4363 1.988e0

148.4604 1.266e-2

148.5009 1.025e0

148.5579 1.013e0

148.6516 2.691e0

148.6815 2.051e0

148.7066 1.266e-2

148.7388 1.266e-2

148.7570 2.025e0

148.7843 2.532e-2

148.8619 3.585e0

148.8852 1.266e-2

148.9496 2.025e0

148.9674 4.063e0

149.0280 8.849e0

149.0501 2.383e0

149.1063 2.470e0

149.1223 7.624e0

149.1638 1.013e0

149.2027 2.025e0

149.2738 1.025e0

149.3004 1.013e0

149.3815 1.013e0

149.4006 3.038e0

149.4204 1.266e-2

149.4443 2.532e-2

149.4983 1.266e-2

149.5324 5.063e0

149.5694 1.013e0

149.5993 2.038e0

149.6250 1.013e0

149.7095 1.013e0

149.7351 1.013e0

149.7807 2.031e0

149.8106 1.038e0

149.8330 3.798e-2

149.8736 2.025e0

149.9376 1.013e0

149.9715 4.051e0

150.0370 2.060e0

150.0971 2.984e0

150.1432 1.084e0

150.2576 4.051e0

150.3083 2.025e0

150.3295 2.025e0

150.3539 1.013e0

150.4158 1.013e0

150.4353 2.532e-2

150.4520 1.266e-2

150.4910 1.266e-2

150.5183 2.025e0

150.5824 1.013e0

150.6047 1.013e0

150.6961 3.038e0

150.7418 2.025e0

150.7894 3.038e0

150.8366 1.013e0

150.9097 1.025e0

150.9470 1.013e0

150.9966 2.107e0

151.0461 1.228e1

151.1092 5.889e-1

151.1496 2.794e0

151.1925 2.532e-2

151.2438 3.063e0

151.2672 4.051e0

151.2961 3.038e0

151.3396 1.013e0

151.4421 6.329e-2

151.4996 1.013e0

151.5479 8.152e0

151.5880 1.013e0

151.6221 4.051e0

151.6887 3.038e0

151.7646 1.025e0

151.8088 4.051e0

151.8337 1.013e0

151.8512 2.532e-2

151.8910 3.038e0

151.9480 1.266e-2

151.9714 2.532e-2

152.0140 1.025e0

152.0295 2.025e0

152.0498 2.674e0

152.0678 5.415e-1

152.1065 8.433e-1

152.1215 7.436e0

152.1885 2.051e0

152.2924 1.013e0

152.4001 1.013e0

152.4392 2.025e0

152.5020 3.038e0

152.5470 3.038e0

152.5939 1.013e0

152.6336 1.051e0

152.6582 4.569e-2

152.6824 1.013e0

152.7484 2.025e0

152.7708 1.266e-2

152.8075 1.013e0

152.8403 2.532e-2

152.8729 1.013e0

152.8964 2.025e0

152.9353 4.051e0

152.9639 3.038e0

153.0074 1.266e-2

153.0569 2.440e0

153.1385 1.845e0

153.1740 2.532e-2

153.2015 1.013e0

153.2200 1.025e0

153.3664 1.013e0

153.3856 1.013e0

153.4978 2.025e0

153.5146 1.266e-2

153.5705 1.266e-2

153.6126 3.798e-2

153.6451 3.038e0

153.6896 2.038e0

153.7154 1.266e-2

153.7876 2.025e0

153.8898 1.266e-2

153.9130 1.266e-2

154.0118 1.051e0

154.0349 1.266e-2

154.1064 5.273e0

154.1375 1.087e1

154.2044 4.051e0

154.2194 4.051e0

154.2666 1.038e0

154.3582 3.038e0

154.3880 2.025e0

154.4639 3.038e0

154.4854 2.532e-2

154.5359 1.422e0

154.5595 1.013e0

154.5929 1.266e-2

154.6332 3.038e0

154.6572 1.025e0

154.6920 1.266e-2

154.7348 2.025e0

154.7757 3.038e0

154.8181 1.038e0

154.8603 1.025e0

154.8903 1.266e-2

154.9365 2.051e0

154.9691 2.025e0

155.0140 3.038e0

155.0323 1.013e0

155.1445 2.057e0

155.2115 1.266e-2

155.2442 3.038e0

155.3313 2.038e0

155.3605 2.025e0

155.4168 1.266e-2

155.4645 3.038e0

155.5108 3.038e0

155.5362 1.038e0

155.5692 1.013e0

155.6002 1.025e0

155.6286 1.266e-2

155.6482 1.013e0

155.6719 1.266e-2

155.6979 1.266e-2

155.7315 1.013e0

155.7441 1.013e0

155.8386 8.101e0

155.8672 2.025e0

155.8842 1.013e0

155.9102 2.532e-2

155.9393 1.025e0

155.9824 3.063e0

156.0821 1.001e1

156.1960 1.013e0

156.2272 2.025e0

156.2461 1.548e0

156.2854 1.013e0

156.3040 1.093e0

156.3778 3.038e0

156.4862 1.025e0

156.5048 2.025e0

156.5613 1.013e0

156.5832 1.799e0

156.6054 1.527e0

156.6281 2.025e0

156.6778 1.013e0

156.7361 1.025e0

156.7561 3.038e0

156.7894 1.025e0

156.8425 2.532e-2

156.8779 5.063e0

156.9473 2.025e0

156.9938 1.933e0

157.0389 1.080e2

157.1006 3.229e0

157.1704 1.266e-2

157.1967 3.038e0

157.2158 4.051e0

157.2804 2.025e0

157.3033 1.013e0

157.4005 3.038e0

157.4483 5.063e0

157.5158 3.038e0

157.5630 3.038e0

157.5865 1.013e0

157.6114 4.447e0

157.6413 1.748e0

157.6637 1.013e0

157.6873 1.013e0

157.7357 2.532e-2

157.7567 1.266e-2

157.7771 2.025e0

157.7986 2.038e0

157.8134 1.042e0

157.8339 1.266e-2

157.8839 1.013e0

157.9174 1.266e-2

157.9559 2.532e-2

158.0145 7.933e-1

158.0339 4.717e0

158.0971 6.798e-1

158.1171 1.732e0

158.1541 1.013e0

158.1977 1.745e0

158.2518 2.025e0

158.2694 2.025e0

158.3086 1.013e0

158.3632 3.038e0

158.4221 3.038e0

158.4526 2.038e0

158.5188 1.013e0

158.5540 2.025e0

158.5893 1.013e0

158.6274 2.025e0

158.6630 5.063e0

158.6928 1.266e-2

158.7211 3.038e0

158.7497 1.013e0

158.7819 2.025e0

158.8177 2.038e0

158.8658 2.038e0

158.9266 5.063e0

158.9642 1.266e-2

158.9841 1.266e-2

159.0336 1.144e1

159.0528 5.154e0

159.0921 5.913e0

159.1161 2.428e0

159.1499 1.698e0

159.1736 2.025e0

159.2322 1.025e0

159.2657 2.025e0

159.2824 1.013e0

159.3358 2.025e0

159.3560 2.051e0

159.3801 1.013e0

159.5219 5.609e0

159.5468 1.038e0

159.5843 2.025e0

159.6134 5.076e0

159.6524 3.051e0

159.7222 1.013e0

159.7715 3.038e0

159.8020 3.798e-2

159.8344 2.038e0

159.9095 3.038e0

159.9402 1.266e-2

159.9693 3.798e-2

160.0279 1.266e-2

160.0567 1.037e0

160.1186 3.396e0

160.1539 1.782e0

160.1827 2.025e0

160.2076 2.532e-2

160.2406 3.051e0

160.2595 1.013e0

160.2955 2.025e0

160.3133 2.025e0

160.3578 2.532e-2

160.3977 2.025e0

160.4250 3.038e0

160.4420 1.786e0

160.4651 1.266e-2

160.4856 1.013e0

160.5427 2.025e0

160.5667 3.038e0

160.5964 1.266e-2

160.6267 1.266e-2

160.6553 2.025e0

160.7210 1.013e0

160.7382 2.025e0

160.7643 1.025e0

160.8125 2.025e0

160.8610 2.025e0

160.8802 4.051e0

160.9302 1.013e0

160.9656 3.038e0

161.0077 1.013e0

161.0355 4.051e0

161.1295 3.144e0

161.1675 2.038e0

161.1929 6.076e0

161.2160 2.025e0

161.2522 2.532e-2

161.2708 1.025e0

161.3009 1.013e0

161.3332 2.025e0

161.4153 1.013e0

161.4291 1.013e0

161.4601 2.025e0

161.5018 2.532e-2

161.5275 1.266e-2

161.5494 4.063e0

161.6015 1.013e0

161.6690 1.266e-2

161.7061 2.025e0

161.7581 3.038e0

161.7824 2.025e0

161.8147 3.038e0

161.8717 1.013e0

161.9021 1.013e0

161.9292 2.707e0

161.9835 3.076e0

162.0374 1.025e0

162.0590 9.179e-1

162.0819 3.898e0

162.1063 1.938e0

162.1505 5.526e0

162.1864 1.013e0

162.2099 2.025e0

162.2646 2.038e0

162.3303 4.051e0

162.3915 6.282e0

162.4187 5.856e0

162.4556 3.038e0

162.4755 2.038e0

162.5008 1.025e0

162.5232 2.025e0

162.5520 1.013e0

162.5666 2.025e0

162.6047 2.532e-2

162.6231 1.013e0

162.6552 2.025e0

162.6856 4.051e0

162.7144 1.013e0

162.7315 1.013e0

162.7653 1.013e0

162.8012 6.076e0

162.8951 9.114e0

162.9241 7.594e0

162.9492 2.806e0

162.9941 6.076e0

163.0260 5.076e0

163.0549 6.969e0

163.1196 1.825e3

163.2198 1.359e1

163.2736 1.861e2

163.3357 7.101e0

163.3619 4.790e0

163.3914 2.063e0

163.4237 2.624e0

163.4689 8.029e0

163.5038 5.804e0

163.5317 1.073e1

163.5755 3.038e0

163.5926 4.793e0

163.6098 6.775e0

163.6565 8.101e0

163.6787 5.851e0

163.6953 2.952e0

163.7399 3.051e0

163.7642 6.076e0

163.7894 3.063e0

163.8096 3.038e0

163.8463 2.853e0

163.8805 6.376e0

163.9155 4.063e0

163.9437 3.038e0

163.9595 3.316e0

163.9841 3.038e0

164.0212 3.559e0

164.0721 2.710e0

164.1115 2.759e2

164.1275 3.905e2

164.1929 5.644e0

164.2160 3.038e0

164.2397 2.051e0

164.2587 2.025e0

164.2844 1.266e-2

164.3181 1.266e-2

164.3353 1.013e0

164.4409 2.532e-2

164.4829 4.456e0

164.5066 3.051e0

164.5292 7.601e-1

164.5567 1.266e-2

164.5901 3.038e0

164.6273 5.076e0

164.6683 6.329e-2

164.7184 5.497e0

164.7679 2.038e0

164.8059 2.038e0

164.8625 2.404e0

164.9012 4.051e0

164.9213 1.013e0

164.9642 4.706e0

164.9844 6.724e0

165.0090 4.063e0

165.0805 7.089e0

165.1137 2.678e1

165.1303 4.159e1

165.1777 2.025e0

165.1992 3.051e0

165.2379 3.038e0

165.2641 3.038e0

165.2894 4.844e0

165.3279 1.013e0

165.3721 3.880e0

165.4486 3.866e0

165.5127 1.013e0

165.5363 1.013e0

165.5636 3.038e0

165.5931 1.025e0

165.6249 2.025e0

165.6457 1.266e-2

165.6770 2.025e0

165.7172 1.063e0

165.7382 3.038e0

165.7725 1.013e0

165.7943 2.025e0

165.8147 1.393e0

165.8440 3.765e0

165.8886 1.013e0

165.9160 2.051e0

165.9611 2.649e0

166.0083 7.089e0

166.0354 9.009e-2

166.0633 1.013e0

166.0951 4.809e0

166.1201 1.001e1

166.1447 6.441e0

166.1783 3.051e0

166.2207 1.013e0

166.2450 1.013e0

166.2721 1.013e0

166.3059 3.051e0

166.3356 2.038e0

166.3973 2.025e0

166.4270 2.025e0

166.4674 1.013e0

166.4917 1.013e0

166.5239 3.871e0

166.5514 2.025e0

166.5809 2.025e0

166.7072 1.013e0

166.7316 1.013e0

166.7615 7.089e0

166.8040 6.041e-1

166.9032 1.013e0

166.9275 1.266e-2

166.9446 1.266e-2

166.9838 1.025e0

167.0468 1.025e0

167.0634 3.220e0

167.0853 2.025e0

167.1006 1.475e0

167.1798 1.025e0

167.1972 1.025e0

167.2189 1.266e-2

167.2383 6.223e-1

167.2587 2.532e-2

167.3541 2.267e0

167.4427 2.025e0

167.4769 2.025e0

167.5017 2.038e0

167.5531 1.013e0

167.5797 1.013e0

167.6088 3.038e0

167.6426 2.025e0

167.6787 3.798e-2

167.7092 2.025e0

167.7285 1.013e0

167.7566 2.025e0

167.8899 1.266e-2

167.9244 1.013e0

167.9611 1.038e0

168.0004 1.266e-2

168.0250 3.860e0

168.0481 1.266e-2

168.0823 4.051e0

168.1130 6.535e0

168.1473 3.945e0

168.1983 3.038e0

168.2411 1.013e0

168.2655 1.013e0

168.3024 1.051e0

168.3481 1.013e0

168.3691 2.025e0

168.4012 2.025e0

168.4395 4.051e0

168.4779 1.025e0

168.5273 2.025e0

168.5482 1.013e0

168.5791 3.038e0

168.6493 3.038e0

168.7206 1.013e0

168.7486 2.025e0

168.7655 2.025e0

168.8103 2.532e-2

168.8903 3.038e0

168.9104 1.013e0

168.9639 2.038e0

169.0281 1.266e-2

169.0481 2.038e0

169.0937 2.566e0

169.1130 1.379e0

169.1413 2.514e0

169.2180 2.025e0

169.2459 1.013e0

169.2659 1.266e-2

169.2921 1.051e0

169.3461 2.025e0

169.4446 2.025e0

169.4839 5.063e-2

169.5330 2.025e0

169.5567 1.038e0

169.6846 1.025e0

169.7231 1.013e0

169.7608 1.266e-2

169.8009 3.038e0

169.8871 2.025e0

169.9274 1.266e-2

169.9568 2.025e0

169.9981 2.025e0

170.0329 3.038e0

170.0682 4.051e0

170.0933 2.025e0

170.2305 2.025e0

170.2768 3.038e0

170.3339 3.038e0

170.3879 1.013e0

170.4193 1.013e0

170.4819 1.266e-2

170.4987 1.013e0

170.5760 1.266e-2

170.6029 1.013e0

170.6203 2.532e-2

170.6625 1.013e0

170.6903 1.266e-2

170.7630 1.013e0

170.8081 1.266e-2

170.8812 1.013e0

170.9243 2.025e0

171.0303 1.013e0

171.0438 1.266e-2

171.0861 2.025e0

171.1125 1.719e0

171.1538 2.922e0

171.1771 3.798e-2

171.2078 1.013e0

171.2910 1.013e0

171.3165 3.038e0

171.4156 1.427e0

171.4696 3.038e0

171.5801 1.013e0

171.5954 2.025e0

171.7153 1.013e0

171.7689 4.051e0

171.7996 3.051e0

171.8302 1.013e0

171.8600 2.025e0

171.8846 1.051e0

171.9250 1.013e0

171.9802 1.266e-2

172.0083 1.266e-2

172.0671 1.266e-2

172.0895 4.648e0

172.1241 1.938e0

172.1557 4.513e0

172.1818 4.051e0

172.2155 1.025e0

172.2491 2.314e0

172.2774 3.051e0

172.3781 2.532e-2

172.5037 1.013e0

172.5871 1.025e0

172.6100 2.532e-2

172.6492 1.038e0

172.7339 1.025e0

172.7617 2.038e0

172.8245 2.038e0

172.8526 1.266e-2

172.8862 2.025e0

172.9100 2.532e-2

172.9537 3.038e0

173.0349 4.051e0

173.0740 3.659e0

173.1370 2.230e0

173.1738 1.013e0

173.1948 1.266e-2

173.2160 3.038e0

173.2531 2.025e0

173.2974 2.038e0

173.4191 3.038e0

173.4854 1.266e-2

173.5085 2.038e0

173.5468 2.532e-2

173.5707 1.063e0

173.6326 1.013e0

173.6628 2.025e0

173.7204 1.038e0

173.7374 2.025e0

173.7780 2.025e0

173.8352 1.013e0

173.8722 2.025e0

173.8972 3.038e0

173.9307 1.013e0

173.9894 1.266e-2

174.0328 3.038e0

174.0865 3.038e0

174.1305 2.389e0

174.1644 1.092e1

174.1898 2.025e0

174.2145 1.013e0

174.2487 1.266e-2

174.3018 1.266e-2

174.3284 2.025e0

174.3479 1.013e0

174.3996 2.025e0

174.5164 3.942e0

174.5560 1.025e0

174.5827 1.437e0

174.6161 3.038e0

174.6494 1.013e0

174.6893 1.025e0

174.7619 1.013e0

174.8072 2.025e0

174.8422 1.266e-2

174.8741 1.013e0

174.9203 1.025e0

174.9616 1.013e0

175.0040 1.013e0

175.0323 1.266e-2

175.1005 3.038e0

175.1200 2.402e0

175.1581 8.681e0

175.1906 2.025e0

175.2270 5.103e0

175.2450 1.025e0

175.2762 1.025e0

175.3206 2.025e0

175.3667 1.013e0

175.4473 1.063e0

175.5496 2.025e0

175.6090 1.013e0

175.6321 2.025e0

175.6640 2.025e0

175.7746 1.266e-2

175.8030 1.025e0

175.8906 1.013e0

175.9118 2.025e0

175.9669 2.025e0

175.9864 2.038e0

176.0102 3.051e0

176.0542 2.532e-2

176.1035 3.834e0

176.1202 1.497e0

176.1715 3.942e0

176.2064 2.025e0

176.2308 1.170e0

176.2527 4.051e0

176.2978 3.051e0

176.3144 1.025e0

176.3931 2.025e0

176.4909 1.013e0

176.5157 2.025e0

176.5538 3.798e-2

176.5785 1.013e0

176.6212 1.266e-2

176.6940 2.025e0

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