 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

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

Elements Used:

C: 11-11 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

192.1019 192.1025 -0.6 -3.1 5.5 10.9 C11 H14 N 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)

127.5243 1.266e-2

127.6070 1.025e0

127.6833 1.266e-2

127.7492 1.266e-2

127.8128 1.266e-2

127.9565 1.266e-2

127.9777 1.013e0

128.0727 4.402e0

128.0955 1.314e0

128.1432 6.076e0

128.1810 1.025e0

128.2307 1.266e-2

128.2424 1.013e0

128.2574 1.266e-2

128.3552 2.025e0

128.4703 1.038e0

128.4921 1.266e-2

128.5768 3.038e0

128.6070 1.266e-2

128.6523 1.013e0

128.6733 1.013e0

128.6928 2.532e-2

128.9386 1.266e-2

129.0066 1.025e0

129.0628 8.823e-1

129.1021 1.663e1

129.1452 3.063e0

129.1890 1.266e-2

129.2436 1.266e-2

129.2735 2.025e0

129.3387 2.025e0

129.5358 3.038e0

129.5790 1.013e0

129.6423 2.532e-2

129.7033 1.266e-2

129.7302 1.266e-2

129.8001 1.266e-2

129.8571 1.013e0

129.8696 1.013e0

129.9055 2.025e0

129.9482 2.025e0

129.9876 1.127e-1

130.0668 4.999e0

130.0971 1.461e2

130.1326 7.928e-1

130.1607 6.642e1

130.1919 8.101e0

130.2363 2.532e-2

130.2512 1.013e0

130.2723 1.013e0

130.2934 2.532e-2

130.3208 1.013e0

130.3332 1.013e0

130.3840 3.038e0

130.4757 4.051e0

130.5333 3.241e1

130.5580 2.532e-2

130.6183 1.025e0

130.6426 4.051e0

130.6932 2.051e0

130.7310 1.013e0

130.7553 1.013e0

130.8250 1.266e-2

131.0076 1.013e0

131.0335 2.889e-2

131.0884 3.107e1

131.1473 1.266e-2

131.1634 1.318e1

131.2265 2.038e0

131.2843 2.025e0

131.3513 1.013e0

131.4149 1.013e0

131.4582 1.013e0

131.4853 3.038e0

131.5036 2.532e-2

131.5320 4.063e0

131.6434 2.532e-2

131.7167 1.013e0

131.7385 1.266e-2

131.8510 2.532e-2

131.9808 2.025e0

132.0099 2.025e0

132.0611 3.226e0

132.0821 3.391e1

132.1563 1.013e0

132.2266 1.013e0

132.4098 2.025e0

132.4499 1.013e0

132.5019 1.266e-2

132.5476 1.266e-2

132.5689 1.013e0

132.6467 2.025e0

132.6697 1.266e-2

132.8534 1.013e0

132.8905 1.266e-2

132.9245 1.266e-2

133.0069 1.266e-2

133.0663 4.453e0

133.0843 2.736e0

133.1541 1.013e0

133.1881 1.013e0

133.2338 1.013e0

133.3626 1.013e0

133.3974 2.038e0

133.4548 1.025e0

133.5238 1.025e0

133.5517 2.038e0

133.5925 1.013e0

133.6145 2.025e0

133.7096 1.266e-2

133.7743 1.013e0

133.8353 2.025e0

133.8907 1.013e0

134.0300 3.024e0

134.0474 1.984e0

134.1298 3.114e0

134.2556 2.025e0

134.3504 3.038e0

134.5065 1.266e-2

134.5806 1.266e-2

134.6084 1.013e0

134.6512 1.013e0

134.7932 1.013e0

134.8363 1.013e0

134.8980 1.266e-2

134.9168 1.013e0

134.9321 1.266e-2

134.9957 1.025e0

135.0374 4.051e0

135.0737 1.039e1

135.0952 3.530e1

135.1417 2.025e0

135.2196 1.266e-2

135.2459 1.025e0

135.2752 1.013e0

135.3801 1.013e0

135.4422 1.013e0

135.4819 1.013e0

135.5065 1.266e-2

135.6648 1.013e0

135.6799 1.266e-2

135.7635 1.266e-2

135.7881 1.013e0

135.8939 1.025e0

135.9060 2.025e0

135.9274 1.013e0

135.9712 1.266e-2

135.9895 1.025e0

136.0117 2.461e0

136.0508 3.138e0

136.0725 4.051e0

136.0884 9.011e-1

136.1129 3.219e1

136.1847 1.013e0

136.2994 1.013e0

136.4924 1.266e-2

136.5076 1.266e-2

136.5323 1.266e-2

136.6240 1.025e0

136.7293 2.025e0

136.8866 1.266e-2

136.9146 1.013e0

137.0296 1.013e0

137.0467 2.532e-2

137.0786 4.705e0

137.1790 1.266e-2

137.2941 1.266e-2

137.3469 1.013e0

137.5181 1.266e-2

137.5525 1.013e0

137.5685 1.013e0

137.6309 1.266e-2

137.6429 1.013e0

137.6805 2.025e0

137.7070 2.025e0

137.8054 1.266e-2

137.8551 1.266e-2

137.9272 1.266e-2

137.9768 2.025e0

138.0049 1.013e0

138.0206 1.013e0

138.0385 2.038e0

138.0620 3.101e0

138.2076 1.013e0

138.2610 1.013e0

138.3327 1.013e0

138.4347 2.532e-2

138.4514 2.025e0

138.4956 1.013e0

138.5614 1.266e-2

138.6803 1.025e0

138.7396 1.013e0

138.7613 1.013e0

138.9396 1.013e0

139.0151 1.013e0

139.0465 1.013e0

139.0986 1.443e1

139.1904 1.013e0

139.2893 2.025e0

139.4301 1.025e0

139.4759 1.013e0

139.4928 2.532e-2

139.5168 1.266e-2

139.5470 3.038e0

139.5701 1.266e-2

139.5824 1.013e0

139.7207 1.013e0

139.7366 1.013e0

139.7803 1.013e0

139.7994 2.532e-2

139.8308 1.266e-2

139.8729 2.532e-2

139.9027 1.013e0

139.9849 1.266e-2

140.0821 1.208e1

140.1826 1.013e0

140.2083 1.013e0

140.2418 3.038e0

140.4599 1.266e-2

140.5511 1.025e0

140.5842 2.025e0

140.6000 3.038e0

140.6268 1.266e-2

140.6488 1.266e-2

140.7560 1.025e0

140.7966 1.013e0

140.8537 1.013e0

140.8726 1.013e0

140.9227 1.266e-2

140.9388 1.013e0

141.0019 1.266e-2

141.0694 1.535e0

141.1460 2.757e0

141.1944 1.013e0

141.2766 1.013e0

141.3003 2.025e0

141.3746 1.013e0

141.4107 5.063e-2

141.4438 1.266e-2

141.4695 1.013e0

141.5042 3.038e0

141.5390 1.266e-2

141.5512 1.266e-2

141.6273 1.013e0

141.7373 3.798e-2

141.8931 1.013e0

141.9198 2.025e0

141.9722 1.013e0

141.9847 1.013e0

142.0147 1.025e0

142.0311 3.031e0

142.0668 5.956e0

142.0994 3.996e1

142.1428 1.741e0

142.1906 1.013e0

142.2066 1.013e0

142.2414 1.013e0

142.2588 2.025e0

142.4186 1.018e0

142.5517 1.266e-2

142.6095 1.266e-2

142.6282 1.013e0

142.6566 1.013e0

142.7711 1.025e0

142.8410 1.266e-2

142.9962 1.266e-2

143.0125 1.013e0

143.0618 7.329e1

143.1044 2.188e0

143.1195 4.873e0

143.1556 2.038e0

143.1907 1.266e-2

143.2142 2.025e0

143.2794 1.013e0

143.3559 2.249e0

143.3811 2.051e0

143.4193 1.013e0

143.4543 1.013e0

143.5407 1.013e0

143.5606 1.318e1

143.6261 2.532e-2

143.7826 1.013e0

143.8824 1.289e0

143.9219 4.063e0

144.0012 2.532e-2

144.0775 3.744e0

144.1093 6.380e0

144.1443 7.161e-1

144.1797 5.063e0

144.2604 1.013e0

144.3613 2.051e0

144.4621 1.013e0

144.4841 1.013e0

144.5707 1.266e-2

144.6949 1.013e0

144.7079 1.013e0

144.7266 1.266e-2

144.7447 1.025e0

144.7847 1.013e0

144.8371 2.025e0

144.8788 2.025e0

144.9384 1.025e0

144.9821 8.380e0

145.0045 3.587e0

145.0243 1.013e0

145.0992 5.804e-2

145.3016 2.025e0

145.3737 1.266e-2

145.3958 1.266e-2

145.4212 1.266e-2

145.4458 2.532e-2

145.4662 1.266e-2

145.5244 1.266e-2

145.6012 1.266e-2

145.6234 1.013e0

145.6425 1.266e-2

145.6719 1.013e0

145.7004 1.266e-2

145.8078 1.025e0

145.8545 1.013e0

145.9721 1.025e0

146.0209 1.266e-2

146.0744 3.460e1

146.1563 1.013e0

146.2860 2.532e-2

146.3073 1.013e0

146.4650 1.266e-2

146.4839 1.013e0

146.5274 2.025e0

146.5838 1.013e0

146.6581 1.266e-2

146.6760 3.798e-2

146.7607 1.013e0

146.8314 1.266e-2

146.8651 2.025e0

146.8987 1.013e0

146.9827 1.038e0

147.0565 1.506e0

147.1571 1.013e0

147.1793 1.025e0

147.2245 1.013e0

147.3472 2.025e0

147.3858 1.013e0

147.4794 1.013e0

147.5152 2.025e0

147.5341 1.013e0

147.5927 1.013e0

147.6535 1.013e0

147.8377 2.038e0

147.8859 1.013e0

147.9057 1.013e0

147.9545 1.025e0

148.0692 5.350e0

148.1133 2.740e1

148.1870 1.013e0

148.2745 1.266e-2

148.2959 1.038e0

148.4115 2.025e0

148.4752 2.532e-2

148.5204 1.013e0

148.5346 2.532e-2

148.5594 1.013e0

148.6238 1.013e0

148.7403 1.013e0

148.8867 1.266e-2

148.9360 2.025e0

149.0303 3.906e0

149.0580 1.403e0

149.1105 4.351e0

149.1521 1.266e-2

149.1815 1.013e0

149.2142 1.013e0

149.2282 2.025e0

149.2628 1.013e0

149.4053 1.013e0

149.4642 1.266e-2

149.4831 1.266e-2

149.5321 1.266e-2

149.5634 3.038e0

149.6604 2.025e0

149.7221 4.051e0

149.8994 1.025e0

149.9404 2.038e0

150.0036 1.266e-2

150.0480 1.537e1

150.0919 2.753e1

150.1283 1.738e1

150.2318 4.051e0

150.3685 1.013e0

150.4791 1.013e0

150.5484 1.051e0

150.5646 3.051e0

150.7113 2.051e0

150.8738 3.038e0

150.9993 2.025e0

151.0475 1.195e2

151.0935 3.468e0

151.1130 5.439e0

151.1472 3.117e0

151.1774 1.266e-2

151.2052 1.025e0

151.2298 1.025e0

151.2621 2.038e0

151.2920 3.038e0

151.3314 1.013e0

151.5510 3.443e1

151.5775 4.202e0

151.6252 1.266e-2

151.6744 2.532e-2

151.7463 1.266e-2

151.7952 1.013e0

151.8318 1.013e0

151.9296 1.025e0

151.9594 1.013e0

152.0515 3.636e1

152.1988 2.063e0

152.2824 2.038e0

152.3395 1.013e0

152.3557 1.013e0

152.4141 1.038e0

152.4900 1.266e-2

152.5447 3.063e0

152.7757 1.266e-2

152.9797 1.013e0

153.0461 1.242e1

153.0683 4.012e-1

153.1418 1.966e1

153.1872 3.826e0

153.2118 2.291e0

153.2380 1.038e0

153.2965 3.038e0

153.3889 3.038e0

153.4792 1.013e0

153.5110 2.025e0

153.5478 3.038e0

153.6508 1.013e0

153.6764 1.038e0

153.7054 2.025e0

153.7629 1.266e-2

153.8633 3.038e0

153.9500 3.038e0

153.9970 1.013e0

154.0263 1.013e0

154.0622 2.764e-1

154.0959 4.483e0

154.1432 9.611e0

154.1630 4.051e0

154.1915 1.266e-2

154.2343 1.013e0

154.2939 1.013e0

154.3266 2.025e0

154.3828 1.013e0

154.4818 1.266e-2

154.5415 1.025e0

154.5708 1.038e0

154.6169 1.013e0

154.6506 1.266e-2

154.7065 1.013e0

154.9019 1.013e0

154.9262 2.025e0

154.9875 1.266e-2

155.0420 1.818e0

155.0619 1.506e0

155.0860 1.357e0

155.1128 2.447e0

155.1352 3.444e0

155.1660 1.266e-2

155.1961 1.013e0

155.2220 1.013e0

155.2685 1.025e0

155.4510 1.013e0

155.4922 2.532e-2

155.5334 1.013e0

155.5706 1.266e-2

155.6310 3.038e0

155.6735 2.025e0

155.7465 2.038e0

155.8569 2.532e-2

155.9319 1.266e-2

155.9681 1.013e0

155.9957 3.038e0

156.0179 1.266e-2

156.0510 4.258e0

156.0768 1.698e1

156.1182 2.893e0

156.1457 3.929e0

156.1772 1.266e-2

156.2286 1.025e0

156.4633 1.025e0

156.5990 1.266e-2

156.7481 1.875e0

156.7823 1.266e-2

156.8423 3.038e0

156.9487 1.013e0

156.9851 1.013e0

157.0418 1.223e1

157.0638 7.132e0

157.1020 5.426e0

157.1634 2.025e0

157.1803 2.025e0

157.2014 1.013e0

157.2218 1.266e-2

157.2448 1.266e-2

157.2750 1.013e0

157.3329 3.038e0

157.4003 2.025e0

157.5018 1.013e0

157.5568 1.025e0

157.5914 1.013e0

157.6084 1.013e0

157.6980 1.013e0

157.7269 2.025e0

157.7957 2.532e-2

157.8853 1.013e0

157.9421 1.266e-2

158.0022 2.025e0

158.0939 2.592e0

158.1212 1.704e0

158.1556 4.672e0

158.1963 1.025e0

158.2200 6.076e0

158.2845 2.038e0

158.5203 1.266e-2

158.5737 1.013e0

158.5941 1.013e0

158.6588 3.038e0

158.7341 1.266e-2

158.8615 1.122e0

158.9165 2.025e0

158.9525 1.266e-2

159.0470 1.519e0

159.0780 3.428e0

159.1029 1.398e-1

159.1225 3.401e0

159.1563 1.013e0

159.1969 3.051e0

159.2131 1.025e0

159.2542 1.266e-2

159.4250 1.025e0

159.5458 1.013e0

159.5721 1.266e-2

159.6496 2.025e0

159.7168 1.266e-2

159.7874 1.013e0

159.8777 1.266e-2

159.9335 2.025e0

160.0514 2.216e0

160.2489 2.025e0

160.3051 1.013e0

160.5237 1.013e0

160.5704 1.266e-2

160.5842 1.013e0

160.6448 1.013e0

160.6887 1.266e-2

160.8402 1.013e0

160.8746 2.025e0

160.8939 1.266e-2

160.9544 1.013e0

160.9992 1.013e0

161.0797 7.483e0

161.3297 1.013e0

161.3492 1.013e0

161.4825 2.025e0

161.5152 1.025e0

161.5529 8.601e0

161.6160 1.013e0

161.6469 1.013e0

161.7128 2.025e0

161.7329 2.025e0

161.7477 1.013e0

161.7752 1.013e0

161.8239 2.025e0

161.8497 1.013e0

161.8829 1.025e0

162.0758 2.036e0

162.0965 3.894e-1

162.1193 7.045e-1

162.2112 1.266e-2

162.2878 1.038e0

162.3531 1.013e0

162.3840 1.013e0

162.4276 1.013e0

162.6308 1.013e0

162.6756 1.266e-2

162.6922 1.013e0

162.7158 1.013e0

162.7458 3.038e0

162.8145 1.013e0

162.8616 2.025e0

162.9056 1.266e-2

162.9329 1.266e-2

163.0964 7.002e0

163.1214 3.121e0

163.2196 2.532e-2

163.2603 1.025e0

163.3064 3.038e0

163.3432 1.013e0

163.4829 4.051e0

163.5307 1.013e0

163.5506 1.013e0

163.6853 1.025e0

163.7048 1.025e0

163.8057 1.013e0

163.8542 3.038e0

163.9277 1.013e0

164.0372 1.013e0

164.0738 3.533e1

164.1115 2.622e1

164.1493 6.850e-1

164.1770 1.405e0

164.2140 1.266e-2

164.2619 1.013e0

164.3217 5.063e0

164.4711 2.025e0

164.4953 1.025e0

164.5873 2.532e-2

164.7047 1.013e0

164.7254 1.266e-2

164.8754 1.013e0

164.9332 1.266e-2

164.9760 1.025e0

165.0099 1.025e0

165.0741 9.646e0

165.1175 1.121e0

165.2750 1.266e-2

165.3241 2.025e0

165.4234 2.025e0

165.5685 1.013e0

165.6332 2.025e0

165.6644 1.266e-2

165.6959 2.038e0

165.7327 1.013e0

165.7535 1.013e0

165.7836 2.025e0

165.8009 1.025e0

165.9445 1.266e-2

165.9808 2.025e0

166.0251 2.532e-2

166.0523 4.261e0

166.0885 1.702e1

166.3392 1.013e0

166.3656 2.025e0

166.4005 2.532e-2

166.4347 1.013e0

166.4816 3.038e0

166.5269 1.266e-2

166.5994 1.266e-2

166.7504 1.266e-2

166.8732 1.013e0

167.0884 3.697e0

167.1552 1.013e0

167.1935 1.013e0

167.2515 1.013e0

167.3061 1.013e0

167.4023 1.013e0

167.4233 2.025e0

167.4782 2.025e0

167.5231 1.013e0

167.5405 1.013e0

167.6212 2.025e0

167.6537 1.013e0

167.7705 2.025e0

167.9289 1.013e0

167.9600 1.013e0

167.9984 1.013e0

168.0582 1.773e0

168.0739 2.735e0

168.1151 6.721e0

168.1351 5.090e-1

168.1810 1.025e0

168.2181 1.038e0

168.4006 1.013e0

168.5940 3.038e0

168.6184 1.013e0

168.6498 1.266e-2

168.7377 2.025e0

168.7718 2.025e0

168.8489 3.038e0

168.8823 2.038e0

168.9998 2.025e0

169.0743 1.397e0

169.0895 1.735e0

169.1603 1.266e-2

169.1775 1.266e-2

169.2352 2.025e0

169.3162 1.266e-2

169.3780 2.025e0

169.5451 2.533e-2

169.5768 2.038e0

169.6416 1.266e-2

169.6720 1.013e0

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