 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

684 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 Cl: 0-1 69Ga: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

260.0839 260.0842 -0.3 -1.2 8.5 169.2 C15 H15 N O Cl

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)

100.0878 2.949e0

100.0984 1.951e0

100.3525 1.266e-2

100.7011 3.798e-2

101.0063 6.184e0

102.1384 3.038e0

102.5430 2.532e-2

102.7489 1.108e0

103.6262 1.266e-2

103.7574 2.532e-2

103.8305 2.532e-2

104.3496 2.025e0

104.3859 2.051e0

104.5288 1.266e-2

104.5587 2.532e-2

104.5764 2.532e-2

104.5938 1.266e-2

104.6476 2.038e0

104.6838 3.089e0

104.7014 2.532e-2

104.7509 3.798e-2

104.9151 1.063e0

104.9576 6.734e-1

104.9702 3.089e0

105.0696 9.185e1

105.2092 6.127e0

105.4238 1.089e0

105.5438 3.798e-2

105.5730 2.343e0

105.6539 5.063e-2

105.7711 6.020e-1

105.7962 2.051e0

105.9579 3.798e-2

106.0771 7.618e1

106.1122 2.947e0

106.3458 1.038e0

106.5926 1.025e0

106.6432 3.798e-2

106.6611 1.266e-2

106.8655 3.798e-2

106.9001 2.532e-2

107.0186 1.418e0

107.2988 2.532e-2

107.3757 5.063e-2

107.4971 1.025e0

107.5650 3.798e-2

107.6010 1.038e0

107.8018 3.798e-2

107.8637 2.025e0

107.9658 1.025e0

108.2784 1.063e0

108.3168 3.798e-2

108.3422 2.051e0

108.3830 1.266e-2

108.5345 1.195e0

108.6952 2.038e0

108.8844 2.038e0

109.0684 4.256e0

109.2739 2.038e0

109.3286 5.063e-2

109.5494 2.532e-2

109.6372 1.266e-2

110.3839 2.532e-2

110.4635 2.532e-2

110.6270 1.038e0

110.7360 1.266e-2

110.9766 1.266e-2

111.0495 8.261e0

111.0853 5.855e0

111.2706 2.025e0

111.3333 1.355e0

111.4670 1.266e-2

111.6044 1.266e-2

111.7168 3.798e-2

112.6962 2.532e-2

112.7440 1.266e-2

113.2212 1.266e-2

113.4365 2.025e0

113.4789 1.025e0

113.7224 2.025e0

113.9094 2.532e-2

114.2078 1.266e-2

114.4976 1.013e0

114.5821 1.038e0

114.6111 1.025e0

114.6735 1.266e-2

114.9229 2.532e-2

114.9727 2.025e0

115.4701 1.038e0

115.7253 1.070e0

115.7889 1.266e-2

116.0441 1.381e0

116.6668 1.025e0

116.7027 1.266e-2

116.8033 2.532e-2

116.9375 2.038e0

116.9848 1.051e0

117.1610 2.532e-2

117.2329 2.025e0

117.2951 1.266e-2

117.4014 1.266e-2

117.8147 1.025e0

117.9159 1.025e0

117.9721 3.798e-2

118.0680 2.894e1

118.3995 1.266e-2

118.4921 1.266e-2

118.9005 2.532e-2

118.9503 1.038e0

119.1160 1.518e0

119.2521 2.063e0

119.2774 2.532e-2

119.3557 1.025e0

119.3806 3.565e-1

119.7725 1.424e-1

121.0947 2.216e0

121.1136 7.863e0

121.1315 7.726e-1

121.2883 8.532e-2

121.3814 1.051e0

121.4864 1.089e0

121.5423 2.063e0

122.4232 1.025e0

123.0439 3.406e0

123.1686 3.798e-2

123.2036 3.798e-2

123.2609 3.051e0

123.5547 1.266e-2

123.6964 2.532e-2

123.8251 2.025e0

123.9692 1.038e0

124.1023 3.216e0

124.2628 1.025e0

124.3966 3.798e-2

124.4796 3.798e-2

124.6312 3.798e-2

125.1312 1.469e0

125.1725 2.532e-2

125.4582 1.266e-2

125.5445 1.266e-2

125.6338 1.266e-2

125.7526 1.266e-2

126.1221 1.052e0

126.2328 1.266e-2

126.2511 1.266e-2

126.8339 1.038e0

126.9266 1.013e0

127.2528 1.025e0

127.3458 1.266e-2

127.5185 2.532e-2

127.6203 1.038e0

128.0058 3.051e0

128.0606 3.358e0

128.2582 3.038e0

128.2831 1.038e0

128.3219 5.063e-2

128.6171 1.266e-2

128.6382 1.266e-2

128.6988 1.266e-2

128.8039 1.266e-2

129.0008 5.063e-2

129.0357 2.376e0

129.2322 1.051e0

129.3008 3.798e-2

129.4111 2.051e0

129.4757 3.798e-2

129.4898 1.038e0

129.6242 2.532e-2

129.7530 1.025e0

129.8773 1.266e-2

130.0209 1.398e0

130.5963 3.798e-2

131.3136 5.063e-2

131.4192 2.063e0

131.8078 3.798e-2

132.0497 1.990e0

132.2222 1.013e0

132.2511 1.051e0

132.3412 1.013e0

132.4483 2.025e0

132.4924 2.025e0

132.5603 3.038e0

132.6310 2.038e0

132.7236 5.063e-2

132.9046 1.266e-2

132.9464 2.038e0

133.4779 1.266e-2

133.7215 2.051e0

133.8235 2.051e0

133.9142 1.025e0

134.0196 2.038e0

134.2802 2.025e0

134.3666 1.025e0

134.4062 1.266e-2

134.5677 2.038e0

134.6131 1.025e0

134.6686 1.266e-2

134.6805 1.266e-2

134.8039 1.038e0

134.8335 7.595e-2

135.1282 1.996e0

135.4391 3.038e0

135.6617 3.798e-2

135.7457 5.063e-2

135.8303 1.025e0

135.9427 2.130e-1

136.3265 2.532e-2

136.6240 2.532e-2

137.6174 1.038e0

137.8482 5.063e0

138.0788 4.561e0

138.1173 8.576e-1

138.2607 2.038e0

138.3818 2.532e-2

138.4394 2.532e-2

138.5893 2.038e0

138.6802 2.532e-2

138.8039 2.532e-2

139.0690 3.035e0

139.3239 1.266e-2

139.3447 2.038e0

139.6595 3.038e0

139.6877 1.013e0

140.1590 1.013e0

140.1938 1.266e-2

140.3212 2.532e-2

140.4035 2.532e-2

140.5448 1.025e0

140.6464 1.038e0

140.8428 1.266e-2

140.8711 1.266e-2

140.9155 3.038e0

141.1166 2.592e0

141.2153 1.266e-2

141.3069 1.013e0

141.3539 2.038e0

141.5919 2.038e0

141.6987 2.532e-2

141.7935 1.266e-2

141.9897 1.266e-2

142.0314 2.765e2

142.0885 2.401e0

142.1117 1.500e0

142.1396 1.726e0

142.2053 1.038e0

142.3766 1.266e-2

142.9981 1.719e0

143.0356 1.364e1

143.4132 2.532e-2

143.6218 1.013e0

143.7036 3.798e-2

144.0821 1.519e1

144.4321 1.266e-2

144.4966 1.038e0

144.5467 1.013e0

144.7547 2.532e-2

145.5674 9.285e-1

145.8047 2.532e-2

145.9431 1.266e-2

146.0465 6.058e0

146.0986 5.190e1

146.1570 6.329e-2

146.2865 1.266e-2

146.3092 1.266e-2

146.4151 2.038e0

146.5793 3.038e0

146.6383 1.063e0

146.6853 1.013e0

146.8497 1.038e0

146.9337 2.532e-2

147.0232 1.051e0

147.3574 1.025e0

147.4701 2.532e-2

147.5234 2.532e-2

147.5458 1.266e-2

147.6907 2.532e-2

148.3540 1.266e-2

148.5092 1.013e0

148.6711 1.266e-2

148.7233 1.025e0

148.7859 2.532e-2

148.8537 2.038e0

148.9463 2.025e0

149.0151 2.025e0

149.4494 2.532e-2

149.4805 2.532e-2

149.5819 1.038e0

149.6218 1.013e0

149.7719 3.038e0

149.8626 2.051e0

149.9566 2.532e-2

150.1408 1.325e0

150.3474 1.266e-2

150.4165 2.532e-2

150.6248 1.013e0

150.9962 1.013e0

151.0687 1.013e0

152.0282 3.342e1

152.5990 1.051e0

152.7335 2.532e-2

152.9425 1.013e0

153.0277 4.051e0

153.0871 2.532e-2

153.1674 1.025e0

153.4536 2.532e-2

153.7878 1.266e-2

153.8967 1.266e-2

154.0888 3.038e0

154.4176 3.798e-2

154.4670 1.266e-2

154.6573 3.798e-2

154.7214 2.025e0

154.7795 2.532e-2

154.9136 1.025e0

155.1724 3.798e-2

155.1998 1.025e0

155.2427 2.532e-2

155.3605 1.025e0

155.3855 2.038e0

155.4826 2.532e-2

155.5128 1.266e-2

155.7489 3.051e0

156.0273 1.220e1

156.2240 2.532e-2

156.4336 3.063e0

156.7270 1.051e0

156.7907 3.189e0

156.8241 1.025e0

156.8795 3.063e0

156.9211 4.114e0

157.0338 3.960e2

157.1115 2.817e0

157.1691 1.498e1

157.2194 4.540e0

157.3224 6.089e0

157.4799 3.089e0

157.5583 2.076e0

157.5896 1.051e0

157.6390 2.900e0

157.6700 1.244e1

157.7015 3.769e0

157.7523 1.013e-1

157.8043 2.038e0

157.8760 3.051e0

157.9147 4.101e0

157.9596 1.038e0

158.0401 6.435e1

158.3327 2.051e0

158.3573 1.268e0

158.3980 5.063e-2

158.4262 3.635e0

158.4699 1.038e0

158.5025 2.038e0

158.7175 4.076e0

158.7431 1.063e0

158.7686 2.532e-2

158.7943 1.654e0

158.8397 3.051e0

158.8858 1.025e0

158.9011 2.038e0

158.9615 1.266e-2

159.0013 5.063e-2

159.0338 9.913e1

159.1034 4.966e0

159.1640 2.063e0

159.2707 3.798e-2

159.3064 1.266e-2

159.4335 2.063e0

159.5141 1.266e-2

159.6830 5.063e-2

159.7670 1.038e0

159.9072 2.532e-2

159.9471 1.266e-2

160.0367 3.177e0

160.1024 2.063e0

160.2187 1.038e0

160.4485 3.038e0

160.6121 2.532e-2

160.6573 1.266e-2

160.7084 3.798e-2

160.7418 1.266e-2

160.9581 2.532e-2

161.0440 3.337e-1

161.1373 3.063e0

161.4396 1.013e0

161.5661 2.025e0

161.6024 1.051e0

161.6926 1.038e0

161.8279 2.532e-2

162.1488 1.830e0

162.2734 2.038e0

162.3117 2.532e-2

162.3966 2.532e-2

162.4608 1.266e-2

162.5251 2.051e0

162.6443 1.038e0

162.8466 1.013e0

162.8845 1.266e-2

162.9454 3.798e-2

163.0750 2.076e0

163.1250 3.130e1

163.3121 1.013e0

163.3404 5.063e-2

163.4882 1.038e0

163.5680 1.025e0

163.5871 1.266e-2

163.6756 1.013e0

163.7401 2.532e-2

163.7977 1.266e-2

163.8551 1.025e0

163.8829 1.025e0

164.1120 5.197e1

164.2365 1.266e-2

164.2881 1.038e0

164.3029 1.051e0

164.5912 1.038e0

164.7277 1.013e0

164.7785 2.025e0

164.9355 6.329e-2

164.9802 1.013e0

165.0347 1.266e-2

165.3186 2.038e0

165.3420 2.025e0

165.3809 2.025e0

165.4396 1.126e0

165.4853 2.532e-2

165.6105 2.038e0

165.7281 1.038e0

165.8993 1.013e0

165.9606 1.013e0

166.1319 1.013e0

166.1631 3.798e-2

166.2245 2.532e-2

166.3083 2.038e0

166.4789 3.463e0

166.5777 2.038e0

166.6600 1.025e0

166.6993 1.025e0

166.8660 1.051e0

166.9900 1.038e0

167.3258 1.025e0

167.3642 1.038e0

167.5533 3.798e-2

167.6695 1.266e-2

167.7676 2.532e-2

167.8798 2.025e0

168.0089 3.798e-2

168.0789 3.063e0

168.2171 1.266e-2

168.3467 1.025e0

168.4258 2.532e-2

168.4962 2.532e-2

168.5259 2.532e-2

168.6208 1.025e0

168.7744 1.025e0

168.8594 1.025e0

169.0354 4.063e0

169.1529 1.013e0

169.3918 1.038e0

169.5088 1.266e-2

169.5801 2.038e0

169.7340 2.532e-2

169.8788 2.038e0

170.0708 4.051e0

170.2501 2.038e0

170.3401 1.038e0

170.3882 2.532e-2

170.4267 2.532e-2

170.6268 3.051e0

170.9315 2.025e0

170.9910 2.025e0

171.0282 4.228e0

171.1272 2.532e-2

171.1821 1.038e0

171.2843 1.266e-2

171.4625 1.266e-2

171.5104 1.038e0

171.5585 1.038e0

171.8001 2.025e0

171.8288 2.532e-2

171.8480 1.266e-2

172.3785 1.025e0

172.4355 3.798e-2

172.7097 3.038e0

172.7833 2.025e0

172.8036 2.532e-2

173.3829 1.025e0

173.9249 2.038e0

174.2424 1.266e-2

174.4249 1.025e0

174.7340 2.038e0

174.7678 2.038e0

174.7974 1.266e-2

174.8810 2.038e0

174.9451 2.532e-2

175.0026 2.532e-2

175.0274 2.532e-2

175.3952 1.013e0

175.4723 1.013e0

175.6520 1.266e-2

175.6876 1.266e-2

175.7857 1.266e-2

175.8426 1.266e-2

175.8699 2.051e0

175.9585 1.013e0

176.0369 5.063e-2

176.1825 2.038e0

176.4664 1.266e-2

176.5387 2.532e-2

176.5542 1.025e0

176.8339 1.266e-2

176.8865 1.266e-2

177.3517 2.025e0

177.7399 2.322e0

177.9094 1.266e-2

178.3710 1.025e0

178.7719 1.266e-2

178.8706 1.013e0

179.1125 4.051e0

179.4404 2.532e-2

179.8996 1.266e-2

179.9749 1.013e0

180.1057 1.399e0

180.4240 2.532e-2

180.7240 1.013e0

180.8860 2.025e0

180.9596 1.266e-2

181.1344 2.532e-2

181.2420 1.025e0

181.2986 3.038e0

181.3247 1.025e0

181.5677 1.266e-2

181.6001 1.013e0

181.6638 8.238e-1

181.7111 1.266e-2

181.7929 1.266e-2

182.4327 2.038e0

182.7318 2.532e-2

182.9467 2.532e-2

183.0604 5.291e0

183.5893 1.266e-2

183.6074 1.266e-2

183.6830 1.266e-2

183.7509 1.013e0

183.8120 3.038e0

183.8588 2.025e0

184.0964 1.038e0

184.5153 2.038e0

184.6925 1.266e-2

184.7505 2.532e-2

184.9092 3.798e-2

185.2143 2.532e-2

185.5096 2.025e0

185.5549 2.532e-2

185.6093 1.025e0

185.6415 3.051e0

185.9116 2.038e0

185.9326 1.013e0

186.0166 4.089e0

186.0662 4.051e0

186.3352 2.532e-2

186.4115 1.025e0

186.4877 2.025e0

186.6746 1.038e0

187.0919 3.038e0

187.3018 1.038e0

187.3473 2.532e-2

187.4583 1.025e0

187.6693 2.532e-2

187.6912 2.532e-2

187.7179 2.845e0

187.9197 2.038e0

188.2665 2.532e-2

188.3030 1.013e0

188.3640 3.798e-2

188.4178 1.025e0

188.4816 2.025e0

188.6858 2.532e-2

188.7952 1.266e-2

188.8887 4.063e0

188.9320 2.025e0

189.1782 1.266e-2

189.5119 2.532e-2

189.5743 1.013e0

189.6364 2.532e-2

189.8135 2.532e-2

189.9589 1.038e0

190.0164 2.038e0

190.2399 2.157e0

190.6032 1.025e0

190.6854 1.038e0

190.7649 3.051e0

190.8484 1.025e0

191.0144 2.025e0

191.1561 1.114e0

191.8989 1.051e0

192.1166 5.063e-2

192.1472 1.101e0

192.3098 1.038e0

192.4895 2.025e0

192.6097 2.532e-2

192.8210 1.013e0

192.9549 1.013e0

193.0229 1.025e0

193.0847 4.051e0

193.1357 8.152e0

193.2136 2.038e0

193.4124 2.532e-2

193.5328 1.051e0

193.8998 1.266e-2

194.1997 1.266e-2

194.2368 1.266e-2

194.4178 2.038e0

194.5108 1.025e0

194.6104 1.051e0

194.7963 1.266e-2

194.8335 2.532e-2

194.9566 3.798e-2

195.1474 1.833e0

195.1998 1.025e0

195.2386 2.532e-2

195.3106 2.025e0

195.4007 1.051e0

195.4353 1.266e-2

195.4596 2.025e0

195.5614 1.266e-2

195.6641 2.038e0

195.8826 2.905e-1

195.9142 1.266e-2

196.0819 1.013e0

196.2998 2.532e-2

196.4508 1.025e0

196.5196 2.025e0

196.5926 1.038e0

196.6477 1.013e0

196.6939 3.063e0

196.7562 1.025e0

196.7747 1.025e0

197.0576 2.532e-2

197.0894 2.532e-2

197.1650 2.846e0

197.2296 1.266e-2

197.5316 1.266e-2

197.5544 1.266e-2

197.6182 1.013e0

197.7353 2.532e-2

197.8738 2.532e-2

198.2092 1.266e-2

198.3340 3.798e-2

198.4649 2.532e-2

198.4816 1.013e0

198.6021 1.266e-2

198.7023 2.025e0

198.7358 1.266e-2

198.8450 1.013e0

198.9952 1.038e0

199.0638 3.038e0

199.1641 1.768e0

199.2199 1.266e-1

199.5448 2.532e-2

199.6321 1.266e-2

199.8120 2.051e0

200.1111 2.381e1

200.1961 1.063e0

200.3383 1.025e0

200.3854 3.798e-2

200.4962 2.063e0

200.6620 1.266e-2

200.6847 1.266e-2

200.7079 1.266e-2

200.7390 1.038e0

200.7653 3.798e-2

200.8506 1.025e0

200.9449 1.025e0

201.0146 2.532e-2

201.2568 3.798e-2

201.2876 2.532e-2

201.4245 1.038e0

201.5500 4.051e0

201.5949 3.051e0

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201.6808 1.051e0

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203.8746 1.025e0

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