

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

717 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 56Fe: 0-1

Minimum: -15.0

Maximum: 5.0 15.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

260.0838 260.0842 -0.4 -1.5 8.5 0.4 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)

134.4968 2.025e0

134.5182 1.025e0

134.5368 1.266e-2

134.5523 1.013e0

134.6110 1.266e-2

134.6387 1.013e0

134.8006 2.025e0

134.8361 1.266e-2

134.9069 1.013e0

134.9689 1.025e0

135.0054 1.025e0

135.0244 1.266e-2

135.1753 1.266e-2

135.2053 3.038e0

135.2792 1.025e0

135.4448 1.266e-2

135.5203 2.025e0

135.7277 1.025e0

135.7542 1.013e0

135.7677 2.025e0

135.8407 1.013e0

135.9428 1.013e0

135.9922 1.013e0

136.1611 2.025e0

136.2559 1.013e0

136.2682 1.266e-2

136.4201 1.266e-2

136.5907 2.025e0

136.6172 2.532e-2

136.6416 3.798e-2

136.7184 1.266e-2

136.9204 1.013e0

136.9420 1.013e0

136.9700 1.013e0

136.9979 1.025e0

137.1166 1.882e0

137.2473 1.266e-2

137.2887 2.025e0

137.4775 1.266e-2

137.5317 3.798e-2

137.5679 1.013e0

137.5944 2.532e-2

137.6160 2.025e0

137.6646 1.266e-2

137.7096 2.532e-2

137.7456 1.013e0

137.7801 1.013e0

137.8451 2.532e-2

137.8858 1.266e-2

137.9170 3.038e0

138.0319 2.316e-1

138.1510 1.013e0

138.2014 1.013e0

138.2326 1.013e0

138.2696 1.013e0

138.3731 1.266e-2

138.4275 3.038e0

138.5015 1.266e-2

138.5576 1.013e0

138.6009 1.013e0

138.6202 1.266e-2

138.6860 1.013e0

138.7173 1.013e0

138.8734 1.013e0

138.9044 1.051e0

138.9455 1.013e0

138.9720 1.025e0

139.0268 1.025e0

139.0582 3.151e-1

139.1681 1.013e0

139.2432 1.013e0

139.2920 2.532e-2

139.3596 2.025e0

139.3764 1.025e0

139.4078 2.025e0

139.4657 1.266e-2

139.6227 1.025e0

139.7467 1.025e0

139.8208 2.025e0

139.8869 2.532e-2

139.9400 2.532e-2

139.9622 3.038e0

140.1196 3.394e0

140.2139 1.013e0

140.2425 1.266e-2

140.2826 1.266e-2

140.3399 1.266e-2

140.3997 1.013e0

140.4402 1.266e-2

140.5377 1.266e-2

140.5603 1.266e-2

140.6072 1.266e-2

140.6266 1.266e-2

140.6963 4.051e0

140.7300 1.013e0

140.7509 2.025e0

140.8042 1.025e0

140.8248 5.063e0

140.8909 1.013e0

141.1639 2.025e0

141.2525 3.038e0

141.3233 2.025e0

141.5100 1.266e-2

141.6082 1.025e0

141.7515 1.025e0

141.8326 1.013e0

141.8766 1.025e0

141.8982 3.038e0

141.9372 1.266e-2

141.9542 1.025e0

141.9721 1.013e0

142.2348 2.532e-2

142.2883 1.266e-2

142.3167 2.532e-2

142.4093 1.266e-2

142.4702 2.038e0

142.4880 1.025e0

142.5294 1.013e0

142.6523 3.038e0

142.7138 1.013e0

142.7820 2.025e0

142.7991 1.013e0

142.8503 2.532e-2

142.9007 1.266e-2

142.9771 1.266e-2

143.0359 2.713e0

143.0945 2.061e-1

143.1429 4.586e0

143.1935 1.025e0

143.2170 2.532e-2

143.3618 1.266e-2

143.4095 1.013e0

143.6204 1.038e0

143.6754 2.532e-2

143.6911 2.532e-2

143.7187 2.532e-2

143.7422 1.025e0

143.7691 1.013e0

144.1174 1.252e0

144.2300 1.038e0

144.2571 1.013e0

144.2812 1.025e0

144.3096 1.038e0

144.3433 1.266e-2

144.4551 1.266e-2

144.4696 2.025e0

144.4870 1.025e0

144.5555 2.532e-2

144.6191 2.532e-2

144.6723 1.013e0

144.7970 1.266e-2

144.8537 2.038e0

145.1776 1.266e-2

145.2235 1.038e0

145.2545 1.266e-2

145.3120 1.013e0

145.3347 1.266e-2

145.3517 2.025e0

145.3887 1.013e0

145.4338 1.013e0

145.4963 2.532e-2

145.5739 3.063e0

145.6040 1.266e-2

145.6394 1.013e0

145.6762 2.025e0

145.7191 1.013e0

145.7868 3.038e0

145.8508 1.013e0

145.8926 1.013e0

145.9053 1.266e-2

145.9395 1.025e0

146.0000 1.025e0

146.0207 1.266e-2

146.1011 1.433e0

146.1601 3.038e0

146.1911 1.266e-2

146.3069 2.025e0

146.3583 1.025e0

146.4053 3.798e-2

146.4949 1.025e0

146.6345 1.266e-2

146.6698 1.013e0

146.6962 1.025e0

146.7249 1.013e0

146.7906 1.025e0

146.8213 1.013e0

146.8408 1.266e-2

146.8844 2.532e-2

146.9402 1.266e-2

147.0827 1.499e0

147.1524 2.038e0

147.2406 1.013e0

147.2915 1.013e0

147.3435 1.013e0

147.3672 2.532e-2

147.3920 2.025e0

147.4108 2.532e-2

147.4307 1.013e0

147.4853 1.266e-2

147.5888 1.013e0

147.6046 1.266e-2

147.6434 1.266e-2

147.6680 2.532e-2

147.7484 3.038e0

147.7858 1.013e0

147.8217 4.051e0

147.8699 1.013e0

147.9342 1.013e0

148.0018 2.025e0

148.0938 1.030e1

148.1667 1.266e-2

148.2493 2.025e0

148.3972 1.266e-2

148.4259 1.013e0

148.4872 1.013e0

148.5640 2.025e0

148.6523 1.013e0

148.7349 2.025e0

148.7724 2.532e-2

148.8242 1.266e-2

148.8631 1.038e0

148.8779 2.025e0

148.9656 2.532e-2

148.9895 1.013e0

149.1616 1.266e-2

149.2038 1.266e-2

149.3438 1.025e0

149.4471 1.266e-2

149.5109 2.025e0

149.6426 1.266e-2

149.7156 3.051e0

149.7595 1.013e0

149.8374 1.013e0

149.8993 2.532e-2

149.9417 1.266e-2

149.9576 2.532e-2

150.0165 1.013e0

150.0788 6.704e0

150.2166 2.038e0

150.2470 1.025e0

150.2670 2.025e0

150.3260 2.532e-2

150.4463 2.532e-2

150.4720 2.532e-2

150.4988 1.013e0

150.5211 1.266e-2

150.6778 1.013e0

150.7005 1.038e0

150.7596 1.013e0

150.7919 2.532e-2

150.8144 1.266e-2

150.8511 2.025e0

150.9057 1.266e-2

150.9377 2.532e-2

150.9988 4.051e0

151.2456 3.959e0

151.4499 2.532e-2

151.4790 3.798e-2

151.7540 4.051e0

151.8506 2.532e-2

151.8721 3.798e-2

151.9023 3.798e-2

152.0181 1.013e0

152.1068 1.834e0

152.1738 2.038e0

152.2062 3.798e-2

152.2819 1.025e0

152.2966 2.532e-2

152.3161 3.038e0

152.3822 2.532e-2

152.4296 2.532e-2

152.4572 1.013e0

152.7647 1.038e0

152.8037 2.038e0

152.8516 1.266e-2

152.9122 2.038e0

152.9928 1.266e-2

153.0818 2.931e0

153.1574 3.243e0

153.1958 1.266e-2

153.2219 2.038e0

153.3410 3.051e0

153.4822 1.266e-2

153.5746 1.013e0

153.6471 2.025e0

153.6782 4.051e0

153.7162 3.038e0

153.7460 1.013e0

153.7802 2.025e0

153.9235 1.266e-2

154.0654 1.415e0

154.2272 1.013e0

154.2634 1.266e-2

154.3211 2.532e-2

154.4353 1.013e0

154.4505 2.532e-2

154.5259 3.038e0

154.5489 3.038e0

154.5738 1.013e0

154.6040 1.013e0

154.6536 2.025e0

154.7258 1.013e0

154.7560 1.013e0

154.7787 2.532e-2

154.8367 2.025e0

154.8553 1.266e-2

154.9143 1.013e0

154.9443 1.266e-2

154.9639 1.266e-2

154.9939 2.025e0

155.0351 2.025e0

155.1568 5.063e-2

155.1856 1.266e-2

155.2521 1.013e0

155.2883 1.266e-2

155.3943 1.013e0

155.4868 1.013e0

155.5300 1.266e-2

155.5861 1.266e-2

155.6493 1.013e0

155.6778 1.038e0

155.6956 1.266e-2

155.8417 2.051e0

155.9164 2.025e0

155.9350 1.013e0

155.9779 1.025e0

156.0112 3.051e0

156.1734 2.532e-2

156.2040 2.025e0

156.2666 1.266e-2

156.2797 1.013e0

156.3135 1.013e0

156.4063 2.532e-2

156.4392 1.266e-2

156.5312 2.038e0

156.5860 3.051e0

156.6739 1.025e0

156.7390 1.266e-2

156.8182 2.532e-2

156.9493 2.038e0

157.4244 1.266e-2

157.5048 1.013e0

157.6443 1.025e0

157.6614 1.013e0

157.6947 1.266e-2

157.7147 2.025e0

157.7531 2.038e0

157.8282 2.532e-2

157.9248 1.266e-2

157.9784 1.266e-2

157.9985 2.025e0

158.1156 1.460e-1

158.3132 1.013e0

158.3827 1.266e-2

158.4301 1.025e0

158.5267 1.013e0

158.5734 1.266e-2

158.7076 2.025e0

158.7781 1.266e-2

158.9052 2.532e-2

158.9453 1.013e0

159.1517 1.848e0

159.1764 1.013e0

159.2001 1.013e0

159.3005 1.013e0

159.3304 1.266e-2

159.4543 1.013e0

159.6093 1.013e0

159.6261 1.013e0

159.7301 3.038e0

159.7578 1.025e0

159.7906 2.532e-2

159.8681 1.013e0

159.9252 1.266e-2

160.0290 1.013e0

160.2361 2.025e0

160.3163 2.532e-2

160.3673 2.025e0

160.3954 1.013e0

160.4490 2.532e-2

160.4999 1.013e0

160.5805 1.266e-2

160.7947 2.025e0

160.8468 1.266e-2

160.9392 1.038e0

160.9627 1.025e0

161.0893 3.882e-1

161.1548 6.593e-1

161.2718 1.013e0

161.4002 1.013e0

161.4164 1.025e0

161.4577 2.532e-2

161.6058 1.266e-2

161.6569 1.013e0

161.7125 1.025e0

161.7454 1.025e0

161.8305 2.025e0

161.8920 3.038e0

161.9640 2.532e-2

162.0081 1.266e-2

162.1670 1.266e-2

162.1945 2.025e0

162.2143 1.013e0

162.2346 1.013e0

162.2587 1.013e0

162.2788 1.013e0

162.3038 2.038e0

162.4099 2.025e0

162.5903 1.013e0

162.6178 1.266e-2

162.8614 1.266e-2

162.9395 1.013e0

162.9753 2.025e0

163.1350 3.916e0

163.1512 1.601e0

163.2107 1.266e-2

163.2348 1.025e0

163.2586 1.013e0

163.2785 1.013e0

163.3516 1.025e0

163.4036 3.038e0

163.5210 2.038e0

163.6017 1.013e0

163.6696 1.266e-2

163.7272 3.798e-2

163.7668 2.038e0

163.8439 3.038e0

163.9991 1.013e0

164.0197 1.025e0

164.1613 3.038e0

164.2720 1.266e-2

164.3605 1.266e-2

164.4795 1.266e-2

164.5038 1.013e0

164.6467 2.025e0

164.7252 2.025e0

164.7915 2.025e0

164.8338 1.266e-2

164.9025 2.025e0

164.9303 3.798e-2

165.0045 1.266e-2

165.0752 3.158e0

165.2164 1.266e-2

165.2852 1.013e0

165.4042 1.266e-2

165.4654 1.013e0

165.4966 1.013e0

165.5374 1.025e0

165.5752 1.266e-2

165.6086 2.038e0

165.6365 1.266e-2

165.6607 1.013e0

165.7637 1.266e-2

165.8449 3.051e0

165.8793 1.013e0

165.9684 1.025e0

166.0413 3.969e0

166.1036 1.213e0

166.2462 1.013e0

166.2885 2.532e-2

166.3214 1.013e0

166.3689 1.013e0

166.4651 2.532e-2

166.5891 1.013e0

166.6418 1.025e0

166.7641 1.013e0

166.8186 1.025e0

166.8799 1.013e0

166.9491 1.266e-2

166.9937 1.266e-2

167.0449 9.215e-1

167.1654 1.266e-2

167.2995 2.025e0

167.3406 2.025e0

167.4335 1.025e0

167.5754 2.532e-2

167.6537 1.013e0

167.6913 1.013e0

167.7755 2.025e0

167.8360 1.266e-2

167.9086 1.266e-2

167.9355 1.013e0

168.2493 1.013e0

168.3284 1.266e-2

168.4203 3.038e0

168.5215 3.038e0

168.6391 1.266e-2

168.6902 1.266e-2

168.7734 1.013e0

168.9012 1.266e-2

168.9186 1.013e0

168.9803 1.025e0

169.0535 7.862e-1

169.2053 1.013e0

169.2368 1.266e-2

169.2951 1.013e0

169.3300 1.025e0

169.3658 2.025e0

169.4409 1.013e0

169.5960 1.266e-2

169.6482 2.025e0

169.7033 1.013e0

169.7420 2.025e0

169.9339 2.025e0

169.9530 1.013e0

170.0247 2.038e0

170.0968 6.941e0

170.1392 1.359e0

170.1914 1.266e-2

170.2125 1.025e0

170.2883 1.266e-2

170.4798 1.013e0

170.5034 1.013e0

170.5738 2.025e0

170.6268 1.025e0

170.6742 1.630e-1

170.7184 2.025e0

170.7819 1.013e0

170.8297 1.013e0

170.8684 1.266e-2

170.9069 1.266e-2

170.9480 1.013e0

170.9761 1.025e0

171.0654 1.178e0

171.2143 2.532e-2

171.2513 3.038e0

171.2975 1.025e0

171.3228 5.063e0

171.3639 2.038e0

171.4246 1.266e-2

171.5042 2.025e0

171.5898 2.025e0

171.6155 1.266e-2

171.6719 1.266e-2

171.7214 2.025e0

171.9052 1.266e-2

171.9363 1.013e0

172.0060 1.025e0

172.0751 1.428e0

172.2431 1.266e-2

172.2784 1.013e0

172.3021 1.266e-2

172.3406 2.025e0

172.4115 1.038e0

172.4521 1.013e0

172.5038 3.798e-2

172.6271 1.266e-2

172.6616 2.532e-2

172.7187 2.038e0

172.7840 2.025e0

172.8186 1.013e0

172.8398 1.266e-2

172.9097 1.266e-2

172.9550 1.266e-2

172.9761 1.266e-2

173.0771 3.806e0

173.1488 1.425e0

173.1784 1.013e0

173.2340 1.038e0

173.3024 2.025e0

173.3396 1.013e0

173.3819 1.013e0

173.4496 1.025e0

173.4761 1.038e0

173.6930 1.266e-2

173.7280 1.013e0

173.7795 2.253e0

173.8077 2.025e0

173.8262 1.013e0

173.8504 1.013e0

173.9628 1.025e0

173.9870 1.176e0

174.1014 2.926e0

174.1767 1.013e1

174.3629 2.025e0

174.4257 1.013e0

174.4434 1.025e0

174.4611 1.013e0

174.5767 1.266e-2

174.6121 1.025e0

174.6370 1.266e-2

174.6678 1.025e0

174.7030 1.013e0

174.7207 1.013e0

174.8327 1.266e-2

175.1039 6.295e0

175.2970 1.266e-2

175.3218 1.266e-2

175.4079 1.025e0

175.4269 1.013e0

175.4891 2.025e0

175.7989 2.025e0

175.8780 1.266e-2

176.1614 4.100e-1

176.2253 1.038e0

176.2801 1.266e-2

176.3014 1.013e0

176.3786 1.013e0

176.3996 1.013e0

176.4353 1.266e-2

176.4743 1.013e0

176.5549 2.532e-2

176.5833 1.266e-2

176.6012 1.266e-2

176.6509 1.266e-2

176.7072 1.013e0

176.7384 2.038e0

176.7635 1.266e-2

176.9259 1.013e0

176.9509 1.013e0

177.0260 2.051e0

177.1483 1.177e0

177.2025 2.532e-2

177.3436 1.013e0

177.4075 1.266e-2

177.4283 1.025e0

177.4492 2.025e0

177.4956 1.013e0

177.5134 1.025e0

177.6195 1.013e0

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177.7135 2.025e0

177.7653 1.013e0

177.8350 1.025e0

177.8620 2.025e0

177.9512 1.025e0

178.0127 1.013e0

178.0575 6.947e0

178.1181 3.203e0

178.2214 2.025e0

178.2823 1.013e0

178.3484 1.025e0

178.3996 1.266e-2

178.4416 1.013e0

178.6126 1.266e-2

178.6331 1.051e0

178.8152 2.038e0

178.9251 1.013e0

178.9644 1.013e0

179.0639 4.970e0

179.3821 2.025e0

179.4717 2.025e0

179.4945 1.266e-2

179.5366 2.025e0

179.5544 2.038e0

179.5991 2.038e0

179.6904 1.013e0

179.7367 1.013e0

179.8073 1.013e0

179.8288 1.013e0

179.9040 1.266e-2

179.9255 1.266e-2

179.9651 2.025e0

179.9878 1.025e0

180.0095 3.798e-2

180.0729 1.730e0

180.1054 1.347e0

180.1291 1.738e0

180.2110 1.266e-2

180.2640 1.266e-2

180.4731 2.038e0

180.5035 2.025e0

180.6064 1.266e-2

180.6566 1.266e-2

180.6978 2.025e0

180.7768 2.025e0

180.9604 2.025e0

180.9825 1.051e0

181.0961 4.063e0

181.1281 4.699e0

181.1951 3.326e0

181.2950 3.038e0

181.4285 2.532e-2

181.4894 2.025e0

181.5271 2.532e-2

181.5469 1.266e-2

181.6044 1.266e-2

181.8153 1.266e-2

181.8369 1.266e-2

181.9520 1.266e-2

182.0235 1.063e0

182.0542 3.038e0

182.1738 1.266e-2

182.2566 2.532e-2

182.3034 2.025e0

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182.3611 1.266e-2

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374.7803 1.266e-2

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