 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

904 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

327.1700 327.1709 -0.9 -2.8 9.5 29.7 C19 H23 N2 O3

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)

132.3374 2.063e0

132.3755 2.025e0

132.4196 2.038e0

132.4503 2.532e-2

132.4900 5.063e-2

132.5575 2.025e0

132.5907 2.532e-2

132.6505 1.025e0

132.6891 1.013e0

132.7088 2.532e-2

132.7837 1.266e-2

132.8235 1.013e0

132.8436 1.025e0

132.8814 2.532e-2

132.9003 1.266e-2

133.0846 7.881e0

133.1135 1.231e0

133.2682 1.266e-2

133.3290 1.266e-2

133.4491 1.013e0

133.5165 2.051e0

133.5534 1.266e-2

133.6937 1.038e0

133.7685 1.013e0

133.7914 1.155e-1

133.8176 1.025e0

133.8484 2.025e0

133.9251 1.266e-2

133.9742 2.532e-2

134.0130 2.025e0

134.0961 7.226e0

134.1896 1.266e-2

134.2123 2.038e0

134.2855 1.266e-2

134.3528 1.266e-2

134.6921 1.266e-2

134.8062 1.266e-2

134.9682 1.025e0

135.2692 2.532e-2

135.4468 1.025e0

135.5212 3.051e0

135.6898 1.266e-2

135.7145 1.025e0

135.7392 1.266e-2

135.8196 1.013e0

135.8489 3.038e0

135.8753 2.532e-2

136.0353 1.025e0

136.1047 1.096e0

136.3868 1.266e-2

136.4060 1.266e-2

136.4458 3.038e0

136.4848 1.025e0

136.5423 1.025e0

136.5797 1.266e-2

136.6029 2.532e-2

136.6357 1.266e-2

136.8773 2.038e0

136.9166 2.532e-2

137.0485 2.025e0

137.2354 1.013e0

137.5345 2.025e0

137.6341 1.266e-2

137.6874 1.266e-2

137.7216 1.266e-2

137.8193 1.025e0

137.8458 1.266e-2

137.9228 2.532e-2

138.0085 1.266e-2

138.0429 1.013e0

138.1990 3.038e0

138.2241 2.532e-2

138.3316 2.532e-2

138.3708 1.013e0

138.4832 1.013e0

138.6300 1.013e0

138.6678 1.013e0

138.6909 1.025e0

138.7304 1.013e0

138.7930 1.266e-2

138.8789 1.025e0

138.9024 1.013e0

138.9308 1.266e-2

138.9595 2.051e0

139.2222 1.266e-2

139.3098 1.266e-2

139.3292 1.266e-2

139.4337 2.025e0

139.5045 1.025e0

139.7399 1.013e0

139.7903 2.532e-2

139.8435 1.266e-2

139.9313 1.266e-2

139.9442 1.266e-2

140.0288 1.266e-2

140.3098 1.038e0

140.3692 1.013e0

140.4224 1.266e-2

140.6081 2.025e0

140.6873 1.266e-2

140.7553 1.038e0

140.8068 2.025e0

140.9062 2.025e0

141.1757 1.051e0

141.2328 2.532e-2

141.2547 1.013e0

141.2895 1.013e0

141.4505 1.266e-2

141.5330 1.266e-2

141.5929 1.025e0

141.7252 3.798e-2

141.8789 2.532e-2

141.9535 1.025e0

141.9728 1.025e0

142.3339 1.013e0

142.3461 1.013e0

142.4158 1.266e-2

142.4418 1.013e0

142.7553 1.266e-2

142.7916 1.025e0

143.0256 2.532e-2

143.1781 1.266e-2

143.4132 1.266e-2

143.6523 1.266e-2

143.9069 1.266e-2

144.0578 3.112e0

144.1312 2.672e0

144.2959 1.266e-2

144.3574 2.532e-2

144.7067 2.025e0

144.7946 1.013e0

144.8358 1.266e-2

144.9609 1.266e-2

145.0849 7.466e0

145.1357 1.760e0

145.1801 1.025e0

145.2373 1.025e0

145.2955 2.025e0

145.3694 3.038e0

145.4924 1.013e0

145.5527 2.436e0

145.6075 1.013e0

145.7042 1.266e-2

145.8066 1.266e-2

145.8690 2.532e-2

145.9624 2.532e-2

146.1920 1.266e-2

146.3156 2.038e0

146.3511 4.051e0

146.4300 1.266e-2

146.5393 1.038e0

146.6166 2.532e-2

146.7832 1.266e-2

146.8584 2.038e0

146.8962 1.013e0

147.1656 3.798e-2

147.1896 2.038e0

147.2367 1.025e0

147.3654 1.038e0

147.5346 2.532e-2

147.6087 1.013e0

147.6573 1.013e0

147.6828 1.013e0

147.7560 2.025e0

147.8005 2.532e-2

147.8757 2.532e-2

147.9062 1.025e0

148.0805 1.105e-1

148.2296 2.532e-2

148.3072 1.025e0

148.3259 2.025e0

148.4557 1.266e-2

148.4790 2.532e-2

148.6763 1.013e0

148.7762 1.013e0

148.8090 1.013e0

148.8234 2.025e0

148.9260 1.266e-2

149.0478 1.242e0

149.2602 1.013e0

149.3247 1.266e-2

149.4969 1.013e0

149.5714 1.266e-2

149.6103 1.266e-2

149.6302 1.013e0

149.7048 1.266e-2

149.7247 1.025e0

150.1476 3.038e0

150.2646 2.038e0

150.3932 1.025e0

150.4439 1.266e-2

150.6644 3.798e-2

150.7288 2.532e-2

150.8609 1.013e0

151.1815 5.063e-2

151.3284 1.013e0

151.4000 2.532e-2

151.4576 1.038e0

151.6424 1.013e0

151.8582 5.063e-2

151.8842 2.038e0

151.9204 2.038e0

152.2233 3.038e0

152.2910 1.266e-2

152.3102 1.266e-2

152.4113 1.051e0

152.4480 2.025e0

152.7998 2.532e-2

152.8715 1.013e0

152.9242 1.013e0

153.3415 1.266e-2

153.4110 1.025e0

153.6053 1.266e-2

153.7680 2.025e0

153.8323 1.013e0

153.9379 1.266e-2

154.0538 2.010e0

154.2145 1.266e-2

154.2809 1.266e-2

154.3799 1.013e0

154.6328 3.798e-2

154.8922 1.013e0

155.0942 3.265e0

155.3189 1.013e0

155.4312 1.266e-2

155.4616 1.013e0

155.5231 2.532e-2

155.5609 1.013e0

155.7529 1.266e-2

155.7905 1.025e0

155.8421 1.038e0

155.8891 1.266e-2

156.1593 1.025e0

156.3043 1.266e-2

156.3885 2.025e0

156.5565 1.266e-2

156.7995 1.013e0

156.9711 3.051e0

157.1887 3.038e0

157.5191 1.025e0

157.6089 2.025e0

157.7520 1.013e0

157.8710 2.051e0

158.1663 2.025e0

158.2190 1.051e0

158.2616 1.025e0

158.2823 2.471e-1

158.3761 3.798e-2

158.5895 2.532e-2

158.6208 1.266e-2

158.6532 2.025e0

158.7282 1.013e0

158.7907 4.051e0

158.8486 1.013e0

158.8756 2.025e0

158.8993 1.266e-2

158.9427 1.266e-2

159.0013 2.051e0

159.1372 1.756e0

159.1636 2.532e-2

159.2048 2.038e0

159.2894 2.025e0

159.3931 2.532e-2

159.4994 1.013e0

159.5463 2.532e-2

159.7002 1.013e0

159.7540 1.013e0

159.7845 2.025e0

159.8750 1.266e-2

159.9191 1.013e0

159.9557 1.013e0

159.9771 3.798e-2

160.0092 2.025e0

160.0332 1.013e0

160.1219 1.656e0

160.1811 1.013e0

160.2079 1.013e0

160.2318 1.013e0

160.2466 2.025e0

160.2940 2.532e-2

160.3425 1.013e0

160.3953 1.038e0

160.4445 2.025e0

160.4876 1.266e-2

160.5344 1.013e0

160.6035 2.532e-2

160.6418 1.013e0

160.6868 5.063e0

160.7229 1.025e0

160.8424 1.025e0

160.9253 1.025e0

160.9695 2.568e-1

161.0259 1.013e0

161.0448 2.532e-2

161.1139 4.658e0

161.2593 2.532e-2

161.2891 1.013e0

161.4000 2.038e0

161.4207 1.013e0

161.4447 1.266e-2

161.4986 1.013e0

161.5921 1.025e0

161.6216 2.532e-2

161.6440 2.532e-2

161.6771 1.266e-2

161.7654 1.013e0

161.7926 4.051e0

161.8364 2.025e0

161.9196 2.025e0

162.1626 2.532e-2

162.2928 1.266e-2

162.3470 1.025e0

162.5980 1.013e0

162.6248 1.013e0

162.6927 1.266e-2

162.7232 2.025e0

162.8414 1.013e0

162.9061 1.013e0

162.9299 1.025e0

162.9649 2.051e0

163.1783 1.025e0

163.2162 2.333e0

163.2592 1.266e-2

163.2845 2.025e0

163.3370 1.266e-2

163.4392 1.266e-2

163.5278 1.025e0

163.5878 2.038e0

163.6635 1.013e0

163.6908 1.013e0

163.7142 1.025e0

163.8914 1.025e0

163.9199 1.038e0

164.0018 3.798e-2

164.2371 2.038e0

164.2743 2.038e0

164.3478 3.798e-2

164.4751 1.025e0

164.5573 1.428e0

164.7836 2.025e0

164.8115 1.025e0

164.9492 2.025e0

165.0157 1.013e0

165.1675 1.025e0

165.3115 2.038e0

165.3263 1.025e0

165.3676 1.013e0

165.3910 1.025e0

165.4677 1.025e0

165.4921 2.025e0

165.5483 3.038e0

165.7792 1.025e0

165.8015 1.266e-2

165.9385 2.532e-2

166.1033 2.324e0

166.1666 2.532e-2

166.1900 2.025e0

166.2945 1.266e-2

166.3413 2.025e0

166.3732 1.266e-2

166.4319 1.266e-2

166.5771 3.038e0

166.6099 2.051e0

166.6738 1.025e0

166.6968 2.532e-2

166.7599 2.038e0

166.7846 1.266e-2

166.8402 1.025e0

166.8638 1.266e-2

166.9647 2.532e-2

167.0048 1.013e0

167.0339 2.038e0

167.4787 1.013e0

167.5027 1.025e0

167.5515 1.013e0

167.6575 1.266e-2

167.6920 1.013e0

167.7413 1.038e0

167.8094 1.025e0

167.9180 3.051e0

168.1054 3.415e-2

168.1529 5.617e-1

168.2220 1.013e0

168.2947 2.025e0

168.3888 1.962e0

168.4368 3.038e0

168.4843 1.266e-2

168.5293 2.025e0

168.6740 1.025e0

168.7330 1.025e0

168.7705 2.025e0

168.8664 3.798e-2

168.8843 1.025e0

168.9228 1.013e0

168.9707 1.013e0

169.2220 3.798e-2

169.2577 1.266e-2

169.3502 3.038e0

169.5069 1.025e0

169.5862 1.013e0

169.6318 1.013e0

169.6673 2.532e-2

169.7593 3.038e0

169.9535 1.013e0

169.9860 2.532e-2

170.0053 1.013e0

170.2079 1.025e0

170.2520 1.025e0

170.3172 1.013e0

170.4554 3.063e0

170.4938 1.266e-2

170.5305 2.025e0

170.7013 1.038e0

170.7580 1.013e0

170.9243 1.013e0

171.0388 5.063e-2

171.2432 5.063e0

171.3625 1.266e-2

171.3901 1.266e-2

171.4537 2.532e-2

171.5085 1.266e-2

171.5887 2.038e0

171.6331 4.554e0

171.7137 1.266e-2

171.8513 2.025e0

171.8777 1.266e-2

171.9403 1.266e-2

172.0554 6.076e0

172.1963 2.532e-2

172.2924 5.063e0

172.4599 1.025e0

172.5197 1.025e0

172.5518 2.532e-2

172.6936 1.038e0

172.7536 1.266e-2

172.7745 2.532e-2

172.9205 1.025e0

172.9751 2.051e0

173.0226 1.025e0

173.1555 2.310e0

173.2914 1.266e-2

173.3226 2.532e-2

173.4697 1.025e0

173.5435 1.266e-2

173.6834 1.266e-2

173.6970 1.013e0

173.7534 2.025e0

173.7817 1.013e0

173.9985 1.266e-2

174.0429 1.038e0

174.2504 2.025e0

174.2861 2.532e-2

174.6057 1.013e0

174.6235 1.013e0

174.6650 3.038e0

174.7884 1.266e-2

174.8429 3.798e-2

174.9497 1.013e0

174.9775 1.266e-2

175.0525 1.173e0

175.2417 1.013e0

175.3260 1.013e0

175.3651 1.266e-2

175.5182 2.025e0

175.5547 1.266e-2

175.7028 1.013e0

175.7428 2.025e0

175.9102 1.266e-2

175.9333 2.532e-2

176.0542 2.838e0

176.0741 2.532e-2

176.1145 1.161e0

176.1456 5.007e0

176.2047 3.798e-2

176.3480 1.013e0

176.5397 1.025e0

176.6118 2.038e0

176.6373 2.532e-2

176.7678 1.013e0

176.7891 1.013e0

176.8471 3.038e0

176.9409 2.038e0

176.9978 2.532e-2

177.1407 1.253e0

177.1817 1.013e0

177.2084 2.532e-2

177.3300 2.025e0

177.3769 2.051e0

177.4340 1.025e0

177.4784 1.266e-2

177.5176 1.038e0

177.5408 1.025e0

177.5818 1.013e0

177.7195 1.013e0

177.8358 1.266e-2

177.8609 2.532e-2

177.9215 3.038e0

177.9573 1.013e0

178.0148 2.025e0

178.0487 1.013e0

178.0905 4.514e-1

178.2188 2.532e-2

178.2580 2.025e0

178.2848 1.025e0

178.3668 1.051e0

178.4146 3.051e0

178.5281 1.013e0

178.5555 1.038e0

178.5887 1.266e-2

178.6132 1.266e-2

178.6366 1.098e0

178.6590 3.038e0

178.6832 1.317e0

178.7411 3.038e0

178.8684 1.266e-2

178.8971 2.532e-2

178.9132 2.532e-2

179.0433 2.025e0

179.1200 1.461e1

179.3631 2.532e-2

179.4131 2.025e0

179.5837 1.025e0

179.6409 1.038e0

179.6696 1.266e-2

179.7075 5.063e-2

179.7971 1.025e0

179.9046 1.266e-2

179.9749 1.038e0

180.1744 8.285e-1

180.6106 1.025e0

180.9392 5.089e0

181.1787 2.532e-2

181.2205 5.063e-2

181.2542 1.013e0

181.4044 1.013e0

181.4918 2.532e-2

181.5849 1.051e0

181.6249 2.532e-2

181.9157 3.798e-2

181.9742 1.013e0

182.0031 2.025e0

182.1899 3.466e-1

182.2860 1.025e0

182.3437 1.025e0

182.3636 1.025e0

182.4620 2.051e0

182.5448 3.038e0

182.7531 1.013e0

182.8349 1.013e0

182.9120 1.025e0

182.9499 2.532e-2

183.0616 1.013e0

183.2235 1.266e-2

183.3416 1.013e0

183.5197 3.051e0

183.6144 1.038e0

183.6682 1.025e0

183.7271 1.266e-2

183.9071 1.266e-2

183.9324 3.798e-2

184.0444 1.013e0

184.2392 1.025e0

184.3624 1.051e0

184.4986 1.266e-2

184.5528 1.266e-2

184.6703 2.532e-2

184.7385 3.038e0

184.7917 2.025e0

184.8386 2.025e0

184.9752 1.266e-2

184.9966 2.025e0

185.1646 1.218e0

185.2935 1.266e-2

185.4258 1.025e0

185.5000 1.025e0

185.7714 1.266e-2

185.8436 1.266e-2

185.9158 1.266e-2

186.3402 2.532e-2

186.3656 1.013e0

186.4091 1.266e-2

186.4345 1.013e0

186.4600 1.025e0

186.4817 1.266e-2

186.5870 1.013e0

186.7532 3.038e0

186.7796 1.013e0

186.9140 3.798e-2

186.9540 1.266e-2

187.1976 2.025e0

187.2813 2.025e0

187.3605 1.038e0

187.4668 2.532e-2

187.6015 1.266e-2

187.6451 1.266e-2

187.6997 1.266e-2

187.7325 1.266e-2

187.7689 1.266e-2

187.8154 1.038e0

187.8599 1.013e0

187.9473 2.025e0

188.1013 2.230e-1

188.1672 1.659e0

188.2897 2.532e-2

188.3170 2.532e-2

188.3662 1.013e0

188.4354 2.025e0

188.5794 2.038e0

188.6797 1.025e0

188.7016 1.013e0

188.7563 1.013e0

188.8366 2.532e-2

188.8767 1.266e-2

188.9122 1.038e0

189.1624 1.080e0

189.2014 1.013e0

189.2344 1.266e-2

189.5222 1.025e0

189.6376 1.013e0

189.6705 1.013e0

189.7508 1.025e0

189.9774 1.038e0

190.0506 1.266e-2

190.2300 1.938e0

190.2484 3.798e-2

190.3258 1.266e-2

190.3496 1.025e0

190.5368 2.025e0

190.5953 2.532e-2

190.6373 7.595e-2

190.6740 1.013e0

190.7839 3.798e-2

190.8299 2.051e0

190.9095 5.089e0

191.0847 9.257e-1

191.1538 2.960e0

191.2972 2.123e0

191.3652 3.038e0

191.5244 1.051e0

192.0299 1.677e-1

192.6705 1.272e0

192.7475 2.016e0

192.7938 3.950e0

192.8238 6.290e0

192.8755 1.524e1

192.9172 7.230e0

192.9898 4.388e0

193.3096 2.396e0

193.4246 6.329e-2

193.5402 1.392e-1

193.7241 1.085e1

193.8735 1.051e0

193.8969 2.689e-1

193.9396 1.038e0

194.0047 4.051e0

194.0239 2.134e0

194.1158 1.899e1

194.2619 2.187e0

194.2960 3.798e-2

194.8759 3.163e0

195.0112 2.025e0

195.0315 2.025e0

195.0784 2.826e0

195.1185 1.004e2

195.2262 4.872e0

195.3062 1.038e0

195.3915 2.532e-2

195.4776 1.038e0

195.5496 2.101e0

195.7022 2.532e-2

195.8042 3.798e-2

195.8393 2.038e0

195.9474 2.532e-2

196.1213 2.171e1

196.1572 7.819e-1

196.3766 1.266e-2

196.6076 1.013e0

196.6810 2.025e0

196.7129 1.266e-2

196.8239 1.038e0

197.0504 3.038e0

197.1338 1.599e0

197.2419 1.266e-2

197.2711 4.051e0

197.3373 2.038e0

197.4028 2.025e0

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198.3326 2.532e-2

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