

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

458 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 69Ga: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

327.1695 327.1709 -1.4 -4.3 9.5 8.5 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)

153.4307 2.025e0

153.4713 3.038e0

153.5262 3.038e0

153.5605 7.203e0

153.6646 1.266e-2

153.6921 2.025e0

153.7994 1.266e-2

153.8813 1.038e0

153.9086 3.038e0

153.9972 1.266e-2

154.0107 1.266e-2

154.0470 7.751e0

154.1563 2.051e0

154.2244 1.266e-2

154.3009 1.013e0

154.3831 1.013e0

154.5553 1.013e0

154.7166 1.013e0

154.7399 1.025e0

154.7631 1.013e0

154.8324 1.013e0

154.8624 1.266e-2

154.9056 2.532e-2

155.1997 2.532e-2

155.3024 1.013e0

155.3486 1.013e0

155.4811 1.266e-2

155.5372 1.013e0

155.6138 1.266e-2

155.7180 4.063e0

155.7764 1.025e0

155.8092 1.266e-2

155.8521 1.013e0

155.8757 1.013e0

155.8894 1.266e-2

155.9651 1.025e0

155.9987 1.013e0

156.0515 3.955e0

156.1158 1.435e0

156.1809 1.013e0

156.2112 1.266e-2

156.2872 2.532e-2

156.4036 1.013e0

156.4363 2.025e0

156.4771 1.013e0

156.4981 1.025e0

156.6095 1.266e-2

156.8271 2.038e0

156.8548 2.025e0

156.8721 1.266e-2

156.9115 2.025e0

156.9333 4.051e0

156.9536 2.051e0

156.9888 4.051e0

157.0354 3.520e2

157.1313 4.120e0

157.2110 4.051e0

157.2669 1.025e0

157.2873 2.025e0

157.4235 5.063e-2

157.4752 1.013e0

157.5101 1.038e0

157.5853 1.025e0

157.6001 3.798e-2

157.6398 3.038e0

157.6746 5.063e0

157.7494 1.025e0

157.7678 2.038e0

157.8293 4.051e0

157.8627 1.266e-2

157.8839 1.025e0

157.9560 3.038e0

158.0388 4.721e1

158.0960 2.737e0

158.1639 3.051e0

158.2501 1.266e-2

158.2934 1.013e0

158.3399 2.532e-2

158.4274 1.013e0

158.4842 3.798e-2

158.5481 2.051e0

158.5911 1.266e-2

158.6487 3.038e0

158.6784 3.038e0

158.6981 1.266e-2

158.7286 1.266e-2

158.8152 1.038e0

158.8521 1.051e0

158.8848 3.798e-2

159.0322 3.543e1

159.1700 5.692e-1

159.2090 2.051e0

159.3012 1.013e0

159.3411 1.013e0

159.4521 1.266e-2

159.4790 1.266e-2

159.5030 2.532e-2

159.5353 8.861e-2

159.5793 1.266e-2

159.5930 1.013e0

159.6238 1.025e0

159.7258 1.025e0

159.7433 2.038e0

159.7742 2.025e0

159.8016 1.013e0

159.9487 1.013e0

159.9863 1.266e-2

160.0368 7.319e0

160.1596 1.211e0

160.1895 1.025e0

160.3927 1.013e0

160.4635 2.025e0

160.5932 3.038e0

160.6267 3.798e-2

160.7400 1.013e0

160.7568 1.266e-2

160.8953 3.038e0

160.9279 3.798e-2

160.9773 2.025e0

161.0258 1.013e0

161.0447 3.945e-1

161.0822 2.230e0

161.2592 2.532e-2

161.2856 1.266e-2

161.3434 2.025e0

161.3608 3.038e0

161.3958 3.038e0

161.4292 2.025e0

161.5020 1.013e0

161.5208 2.025e0

161.6215 2.025e0

161.6944 1.013e0

161.9143 1.038e0

162.1187 6.403e-1

162.2371 2.025e0

162.2646 2.532e-2

162.4384 1.266e-2

162.4660 1.013e0

162.5590 2.076e0

162.5928 1.025e0

162.6197 2.038e0

162.6347 2.532e-2

162.6726 1.013e0

162.6931 2.038e0

162.7197 1.013e0

162.7751 2.532e-2

162.9130 1.266e-2

163.1264 4.947e0

163.1903 1.025e0

163.2425 2.025e0

163.3000 1.013e0

163.4025 2.532e-2

163.4409 2.025e0

163.5483 1.266e-2

163.5613 1.013e0

163.6704 1.266e-2

163.7009 1.025e0

163.7856 1.038e0

163.9252 1.266e-2

163.9767 1.266e-2

164.0431 1.416e0

164.1316 1.160e0

164.1909 1.266e-2

164.2149 1.013e0

164.2434 1.025e0

164.2590 1.266e-2

164.2931 1.266e-2

164.3235 1.266e-2

164.3811 1.013e0

164.4769 1.013e0

164.5169 1.025e0

164.5379 1.013e0

164.6224 3.798e-2

164.6704 1.051e0

164.7364 2.532e-2

164.7872 2.025e0

164.8587 1.013e0

164.9098 2.532e-2

164.9458 2.532e-2

165.0756 1.415e0

165.2222 1.025e0

165.2548 2.025e0

165.3137 3.038e0

165.4766 1.013e0

165.4940 1.266e-2

165.5551 1.266e-2

165.7879 2.025e0

165.9521 1.266e-2

165.9658 1.013e0

165.9970 1.013e0

166.0145 1.013e0

166.0735 2.378e0

166.4289 1.013e0

166.4694 1.025e0

166.4937 1.266e-2

166.5180 1.013e0

166.5412 1.013e0

166.6235 1.013e0

166.6479 1.013e0

166.7874 5.063e0

166.8229 1.266e-2

166.8502 3.798e-2

166.8896 2.532e-2

167.0295 2.063e0

167.1749 2.025e0

167.2399 2.025e0

167.3553 1.013e0

167.4134 1.013e0

167.5653 4.051e0

167.6166 2.038e0

167.6446 1.013e0

167.6787 3.038e0

167.7305 1.013e0

167.8468 2.532e-2

167.9234 2.532e-2

167.9676 1.266e-2

168.0210 7.595e-2

168.0518 6.111e-3

168.1218 1.198e1

168.1649 4.675e-1

168.2641 2.025e0

168.3571 2.532e-2

168.4914 1.025e0

168.5316 4.063e0

168.5946 1.266e-2

168.7017 1.266e-2

168.8054 1.013e0

168.8508 1.013e0

168.8791 2.025e0

168.9299 1.013e0

169.1424 7.824e-1

169.1957 1.013e0

169.2615 1.013e0

169.3517 1.013e0

169.3716 2.025e0

169.4895 1.013e0

169.5899 1.013e0

169.6475 1.051e0

169.6902 1.013e0

169.7358 2.025e0

169.9295 1.025e0

169.9706 2.025e0

169.9897 2.532e-2

170.0390 1.139e-1

170.1029 4.060e0

170.2176 3.051e0

170.2484 1.266e-2

170.3682 2.025e0

170.5325 3.038e0

170.5635 6.076e0

170.6052 1.013e0

170.6561 3.063e0

170.7371 2.025e0

170.9248 1.013e0

171.0157 1.013e0

171.0566 2.819e0

171.0791 9.841e-1

171.1088 6.729e0

171.1482 5.069e0

171.2502 1.025e0

171.2932 1.266e-2

171.4360 1.013e0

171.4980 1.025e0

171.5247 3.798e-2

171.5632 2.025e0

171.7313 1.025e0

171.8324 2.025e0

171.9475 1.266e-2

171.9771 1.025e0

172.0035 2.532e-2

172.0531 2.832e0

172.1350 3.028e0

172.1530 5.161e0

172.2707 2.038e0

172.4618 2.532e-2

172.4953 2.025e0

172.5372 2.532e-2

172.5858 1.266e-2

172.6351 1.266e-2

172.6938 1.013e0

172.7467 1.013e0

172.7680 1.266e-2

172.8372 1.266e-2

172.8614 1.051e0

172.9057 2.051e0

172.9717 5.063e0

173.0124 1.266e-2

173.0434 1.025e0

173.2499 1.266e-2

173.2936 2.532e-2

173.3405 1.013e0

173.5372 1.025e0

173.5577 1.013e0

173.5833 2.038e0

173.6595 1.013e0

173.7696 2.025e0

173.8478 1.013e0

173.9845 1.266e-2

174.1633 2.044e0

174.2374 1.266e-2

174.3005 2.532e-2

174.3810 2.532e-2

174.4550 1.025e0

174.5113 1.266e-2

174.5422 1.013e0

174.7958 1.013e0

174.8480 1.013e0

174.9433 1.013e0

174.9813 1.013e0

175.0374 3.798e-2

175.0858 4.924e0

175.1195 1.148e0

175.1671 9.039e-1

175.3228 1.013e0

175.6006 2.025e0

175.6897 3.038e0

175.7171 1.013e0

175.7393 1.025e0

175.7911 2.532e-2

175.8740 2.532e-2

175.9176 1.266e-2

175.9780 1.266e-2

176.0101 2.532e-2

176.0415 1.051e0

176.1844 1.025e0

176.2104 1.266e-2

176.2606 2.038e0

176.3866 1.013e0

176.4682 2.532e-2

176.4967 1.013e0

176.5480 2.038e0

176.6841 1.266e-2

176.7221 1.266e-2

176.9198 1.266e-2

177.0196 2.025e0

177.0408 2.025e0

177.1116 5.003e-1

177.1738 1.269e0

177.2212 1.025e0

177.2559 1.013e0

177.3073 1.025e0

177.4609 1.013e0

177.5429 1.266e-2

177.5963 1.013e0

177.8649 1.013e0

177.8827 1.013e0

177.9130 2.025e0

177.9684 3.038e0

178.0643 3.764e0

178.1377 3.808e0

178.1636 1.891e0

178.3155 1.266e-2

178.4112 1.013e0

178.5290 5.063e-2

178.5963 1.013e0

178.6417 1.266e-2

178.7094 2.532e-2

178.7523 1.025e0

178.9190 1.266e-2

178.9860 1.326e0

179.0171 2.240e1

179.1433 4.090e0

179.1635 1.482e0

179.2377 4.051e0

179.2924 2.025e0

179.5202 1.266e-2

179.5378 1.013e0

179.5697 1.013e0

179.6271 1.266e-2

179.6495 1.038e0

179.6700 1.013e0

179.7167 1.013e0

179.7905 1.013e0

179.8979 1.266e-2

180.1301 4.073e-1

180.1654 1.964e0

180.2405 1.013e0

180.4545 1.013e0

180.7466 2.233e0

180.7877 2.038e0

180.9058 2.532e-2

181.0476 6.329e-2

181.0894 5.683e0

181.1104 5.173e0

181.2317 1.051e0

181.2547 1.013e0

181.3193 1.013e0

181.4349 2.025e0

181.4941 1.025e0

181.6163 1.266e-2

181.7591 2.025e0

181.8020 1.266e-2

181.8704 1.025e0

181.9063 1.013e0

181.9351 1.013e0

182.0248 6.076e0

182.0588 1.638e0

182.1239 3.149e0

182.1955 3.038e0

182.2721 2.025e0

182.4761 1.013e0

182.4993 2.025e0

182.5445 1.266e-2

182.5697 1.266e-2

182.6994 1.013e0

182.7427 1.013e0

182.7608 1.013e0

182.7821 1.266e-2

182.9287 1.013e0

182.9870 2.228e0

183.0261 1.013e0

183.0557 2.471e0

183.0773 1.837e0

183.1216 1.986e0

183.1523 2.773e0

183.1920 1.266e-2

183.4649 1.013e0

183.5226 1.266e-2

183.7707 1.013e0

184.0160 1.266e-2

184.1096 1.397e-1

184.1717 6.247e-1

184.2076 2.025e0

184.2917 2.025e0

184.4810 1.013e0

184.5931 1.013e0

184.7053 1.013e0

184.7705 2.025e0

185.0029 2.025e0

185.0476 2.532e-2

185.0879 2.524e0

185.1232 1.012e1

185.1503 3.314e0

185.2144 1.266e-2

185.2543 1.013e0

185.3394 2.532e-2

185.3937 1.025e0

185.5133 2.025e0

185.6022 1.013e0

185.6203 1.266e-2

185.6473 2.532e-2

185.6963 1.266e-2

185.8226 1.013e0

185.8569 2.532e-2

185.8840 1.013e0

185.9381 1.266e-2

186.0358 2.025e0

186.1336 1.760e0

186.3686 3.038e0

186.5005 1.266e-2

186.6385 2.532e-2

186.7002 1.013e0

186.9801 1.266e-2

187.0346 1.013e0

187.0538 2.038e0

187.1163 8.727e0

187.1437 2.175e0

187.1801 1.013e0

187.2310 2.532e-2

187.5330 1.038e0

187.7805 2.025e0

187.8597 2.038e0

187.8860 1.266e-2

187.9152 1.013e0

188.0465 2.038e0

188.1429 2.381e-1

188.1747 8.377e-1

188.2284 1.013e0

188.2502 1.013e0

188.3887 1.013e0

188.6889 3.038e0

188.9176 1.013e0

189.0480 3.076e0

189.0991 1.398e0

189.1181 3.213e-1

189.2167 1.013e0

189.5432 1.266e-2

189.6128 1.013e0

189.6638 2.038e0

189.7077 1.266e-2

189.8392 1.266e-2

189.8831 1.013e0

189.9178 2.532e-2

189.9526 2.532e-2

189.9818 2.051e0

190.0295 7.101e0

190.0558 3.569e0

190.0986 7.572e0

190.1571 3.015e0

190.2417 2.025e0

190.3437 1.051e0

190.4149 1.013e0

190.5283 1.013e0

190.6143 2.025e0

190.6564 1.013e0

190.7040 1.266e-2

190.7736 1.025e0

190.9732 5.100e0

191.0025 6.064e0

191.0939 1.121e0

191.1630 6.036e0

191.3439 3.038e0

191.3747 3.038e0

191.4079 3.038e0

191.4807 2.025e0

191.5194 1.266e-2

191.6231 1.013e0

191.6451 1.013e0

191.6778 3.051e0

191.7542 3.038e0

191.8138 1.013e0

191.8633 2.025e0

191.8798 1.013e0

191.9256 3.798e-2

191.9458 1.013e0

191.9818 2.063e0

192.0218 2.051e0

192.0773 1.157e1

192.1064 4.181e0

192.2098 2.532e-2

192.2612 1.025e0

192.3939 3.038e0

192.4991 1.013e0

192.5658 1.013e0

192.6061 1.266e-2

192.6833 1.266e-2

192.7348 1.266e-2

192.8118 1.013e0

192.9688 4.063e0

192.9918 1.025e0

193.0945 2.273e0

193.1411 1.409e1

193.1810 1.013e0

193.2312 1.025e0

193.2738 1.025e0

193.3702 1.266e-2

193.4383 2.025e0

193.4659 1.013e0

193.5946 3.798e-2

193.8006 1.025e0

193.8282 1.266e-2

193.9262 2.532e-2

193.9729 2.532e-2

193.9991 1.013e0

194.0488 2.025e0

194.2003 4.051e0

194.2501 1.013e0

194.4944 2.532e-2

194.5576 2.025e0

194.6288 1.266e-2

194.7670 2.025e0

194.9954 2.025e0

195.0619 1.013e0

195.1211 2.700e1

195.2259 1.266e-2

195.2480 2.025e0

195.4136 3.798e-2

195.4541 2.025e0

195.4933 1.013e0

195.5238 3.798e-2

195.6446 1.266e-2

195.6737 3.038e0

195.7608 1.266e-2

195.8606 1.013e0

195.8790 1.013e0

196.0016 9.441e0

196.0592 3.798e-2

196.1254 1.109e1

196.2962 1.013e0

196.3849 1.013e0

196.5660 2.025e0

196.6196 1.266e-2

196.7722 2.038e0

196.8640 2.025e0

196.9450 1.013e0

196.9671 1.266e-2

197.0670 2.025e0

197.0863 2.473e0

197.1281 3.935e0

197.1886 3.585e0

197.4982 2.025e0

197.5999 2.532e-2

197.6212 2.038e0

197.6536 1.266e-2

197.6962 2.038e0

197.7204 3.051e0

197.7507 1.038e0

197.8110 1.266e-2

197.9598 1.266e-2

198.0924 1.301e1

198.1301 2.861e0

198.1705 8.603e-2

198.2407 1.013e0

198.2723 2.025e0

198.4280 1.266e-2

198.5889 1.266e-2

198.6375 2.025e0

198.7209 2.025e0

198.7455 1.013e0

198.8229 2.532e-2

198.8582 2.025e0

198.8972 2.532e-2

198.9715 2.051e0

199.1318 3.641e0

199.2925 1.013e0

199.3555 2.025e0

199.4197 3.038e0

199.4503 1.013e0

199.6156 1.266e-2

199.6493 2.532e-2

199.9091 1.013e0

199.9407 2.532e-2

200.1195 1.131e1

200.1868 4.051e0

200.2921 1.013e0

200.3367 1.013e0

200.6146 6.076e0

200.6493 1.013e0

200.7060 1.025e0

200.7308 2.038e0

200.8149 1.266e-2

200.8722 4.051e0

200.9320 1.266e-2

200.9563 2.025e0

200.9857 3.063e0

201.1168 5.165e0

201.1675 1.077e0

201.2449 1.025e0

201.2859 1.013e0

201.3271 1.013e0

201.4106 1.013e0

201.5467 4.051e0

201.5933 2.532e-2

201.7013 1.013e0

201.7722 1.266e-2

201.7989 1.266e-2

201.8221 1.266e-2

201.9460 1.013e0

202.0351 1.025e0

202.0631 1.266e-2

202.1032 1.239e0

202.1565 2.384e0

202.1732 2.192e0

202.2793 1.266e-2

202.3578 1.266e-2

202.4791 1.013e0

202.5522 2.038e0

202.6228 1.013e0

202.7478 1.266e-2

202.8804 1.266e-2

202.9365 1.025e0

202.9957 2.025e0

203.1564 6.408e-1

203.2280 2.038e0

203.3008 1.013e0

203.3587 2.532e-2

203.4222 2.532e-2

203.4921 3.798e-2

203.7401 1.266e-2

203.8636 1.025e0

203.9367 3.038e0

203.9606 1.266e-2

203.9963 2.532e-2

204.0357 1.038e0

204.1743 3.205e0

204.3554 1.013e0

204.4689 1.013e0

204.6703 1.013e0

204.6965 1.266e-2

204.7920 1.013e0

204.8257 1.013e0

204.8839 1.013e0

204.9587 1.266e-2

205.0631 6.826e0

205.1300 2.398e0

205.1513 1.346e0

205.1845 2.474e0

205.2414 3.051e0

205.2905 1.266e-2

205.3513 2.025e0

205.5193 1.013e0

205.5793 1.266e-2

205.6618 2.025e0

205.7364 1.013e0

205.9039 1.266e-2

205.9628 2.532e-2

205.9842 1.954e0

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335.7464 2.025e0

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336.5542 1.013e0

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336.9420 2.177e0

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340.5660 2.025e0

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