

Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 16-16 H: 0-200 N: 0-10 O: 0-15 Na: 0-1 S: 0-1

Minimum: -1.5

Maximum: 5.0 7.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

290.1212 290.1215 -0.3 -1.0 7.5 101.1 C16 H20 N O2 S

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)

148.4097 4.051e0

148.4287 1.013e0

148.4613 2.025e0

148.4872 2.025e0

148.5228 1.013e0

148.5645 4.051e0

148.5975 1.013e0

148.6162 4.051e0

148.6657 1.013e0

148.7382 2.025e0

148.7523 2.025e0

148.7755 1.013e0

148.8014 1.013e0

148.8387 2.025e0

148.8569 1.013e0

148.8887 2.025e0

148.9167 2.025e0

148.9503 2.025e0

148.9643 3.038e0

149.0139 5.045e0

149.0966 4.091e0

149.1239 2.025e0

149.1482 1.013e0

149.1813 2.025e0

149.2142 3.038e0

149.2429 1.013e0

149.2552 1.013e0

149.2837 4.051e0

149.3396 2.025e0

149.3742 2.025e0

149.4145 2.025e0

149.4441 2.025e0

149.4893 1.013e0

149.5427 2.025e0

149.5691 2.025e0

149.6060 2.025e0

149.6420 1.013e0

149.6610 3.038e0

149.7157 4.961e0

149.7492 2.025e0

149.8109 1.013e0

149.8415 3.038e0

149.8743 3.038e0

149.9056 2.025e0

149.9227 2.025e0

149.9541 1.013e0

149.9769 2.025e0

150.0302 4.033e0

150.0922 3.970e0

150.1138 2.368e1

150.1526 2.025e0

150.1999 3.038e0

150.3108 2.025e0

150.3283 4.051e0

150.3902 2.025e0

150.4043 3.038e0

150.4261 1.013e0

150.4602 2.025e0

150.4814 1.013e0

150.5078 1.013e0

150.5290 5.063e0

150.5663 1.013e0

150.5882 2.025e0

150.6216 3.038e0

150.6414 1.013e0

150.6934 1.013e0

150.7132 1.013e0

150.7817 3.038e0

150.8170 1.013e0

150.8336 1.013e0

150.8637 3.038e0

150.9286 1.013e0

150.9541 1.013e0

150.9763 3.038e0

151.0318 8.611e1

151.0592 1.403e0

151.1109 2.663e0

151.1539 1.013e0

151.1919 3.038e0

151.2160 1.013e0

151.2480 1.013e0

151.2713 1.013e0

151.3266 1.013e0

151.3432 1.013e0

151.3707 3.984e0

151.4118 2.025e0

151.4571 1.013e0

151.4704 1.013e0

151.5312 2.114e1

151.5865 3.038e0

151.6213 4.051e0

151.6458 2.025e0

151.6628 3.038e0

151.6929 2.025e0

151.7244 2.025e0

151.7515 1.013e0

151.7715 1.013e0

151.8046 3.038e0

151.8549 3.359e0

151.8783 2.025e0

151.9287 2.025e0

151.9616 1.013e0

151.9994 5.058e0

152.0280 1.715e1

152.0497 1.295e1

152.1037 9.783e0

152.1382 2.025e0

152.1531 2.025e0

152.2026 3.075e0

152.2418 2.203e0

152.2630 1.013e0

152.3322 1.013e0

152.3627 2.025e0

152.3988 4.051e0

152.4539 4.051e0

152.4926 1.013e0

152.5308 5.063e0

152.5940 3.038e0

152.6100 2.406e0

152.6340 1.013e0

152.6638 3.038e0

152.7103 3.038e0

152.7902 3.038e0

152.8138 1.013e0

152.8487 2.025e0

152.8711 2.769e0

152.8941 3.038e0

152.9509 2.025e0

152.9652 1.013e0

152.9915 1.013e0

153.0290 5.073e0

153.0475 3.536e0

153.0872 1.026e0

153.1228 1.215e1

153.1725 1.013e0

153.2247 1.013e0

153.2673 3.038e0

153.3070 1.013e0

153.3336 1.013e0

153.3590 3.038e0

153.4315 3.038e0

153.4716 1.013e0

153.5117 1.013e0

153.5338 1.013e0

153.5505 1.013e0

153.5873 2.025e0

153.6035 2.025e0

153.6395 2.025e0

153.6682 4.666e0

153.7017 1.013e0

153.7618 1.013e0

153.8160 3.038e0

153.8933 1.013e0

153.9266 1.013e0

153.9601 5.063e0

154.0016 4.165e0

154.0234 2.013e0

154.1129 5.602e0

154.1572 1.013e0

154.1955 3.038e0

154.2329 1.013e0

154.2598 1.013e0

154.2953 2.025e0

154.3321 2.025e0

154.3584 1.013e0

154.4062 2.025e0

154.4263 2.025e0

154.4912 2.405e0

154.5172 4.051e0

154.5779 2.025e0

154.6096 1.013e0

154.6420 2.025e0

154.6721 1.013e0

154.7114 2.025e0

154.7328 3.038e0

154.7581 3.038e0

154.8071 1.013e0

154.8256 2.025e0

154.8887 4.008e0

154.9500 1.013e0

154.9727 2.025e0

154.9982 3.038e0

155.0259 1.013e0

155.0437 3.038e0

155.0949 3.234e0

155.1390 3.038e0

155.1996 2.025e0

155.2180 1.013e0

155.2468 4.051e0

155.2671 2.025e0

155.2906 2.025e0

155.3272 2.025e0

155.3931 4.051e0

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155.4727 1.013e0

155.5029 1.013e0

155.5189 1.013e0

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155.6382 3.038e0

155.6819 1.013e0

155.7360 2.025e0

155.7590 3.038e0

155.7845 1.013e0

155.8406 1.013e0

155.8693 2.025e0

155.8965 2.025e0

155.9351 2.025e0

155.9637 1.013e0

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156.0600 3.123e1

156.0908 1.682e0

156.1216 5.411e0

156.1363 3.589e0

156.1612 2.814e0

156.1970 2.025e0

156.2323 1.013e0

156.2492 1.013e0

156.3141 3.503e0

156.3352 4.051e0

156.3636 4.051e0

156.3981 2.025e0

156.4317 2.025e0

156.4631 2.025e0

156.4843 2.025e0

156.5297 2.025e0

156.5549 2.025e0

156.5975 1.013e0

156.6177 2.025e0

156.6413 2.025e0

156.6695 4.051e0

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156.7309 1.013e0

156.7625 3.038e0

156.8020 4.531e0

156.8307 1.013e0

156.8669 1.013e0

156.9002 3.038e0

156.9305 1.013e0

156.9911 4.051e0

157.0812 3.134e1

157.1117 3.625e0

157.1570 1.013e0

157.1764 1.013e0

157.2436 2.025e0

157.2788 3.038e0

157.3046 3.038e0

157.3394 3.038e0

157.3672 3.038e0

157.3944 4.051e0

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157.5299 1.013e0

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157.9671 1.013e0

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158.0427 3.038e0

158.0683 3.946e0

158.0870 8.318e0

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158.1775 1.013e0

158.2112 3.150e0

158.2463 3.038e0

158.2855 3.038e0

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158.3862 2.025e0

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158.8095 1.013e0

158.8328 1.013e0

158.8565 1.013e0

158.8733 1.013e0

158.9201 1.013e0

158.9754 2.025e0

159.0243 2.025e0

159.0976 1.257e1

159.1517 3.038e0

159.1828 2.025e0

159.2116 1.013e0

159.2489 1.013e0

159.2721 1.013e0

159.2998 2.754e0

159.3238 2.025e0

159.3458 1.013e0

159.3730 2.025e0

159.4026 1.013e0

159.4361 1.013e0

159.4711 3.038e0

159.5136 1.013e0

159.5725 5.063e0

159.6210 4.051e0

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159.6924 3.038e0

159.7302 2.025e0

159.7669 4.051e0

159.7957 3.168e0

159.8290 2.025e0

159.8562 1.013e0

159.9193 3.038e0

159.9645 3.388e0

159.9926 3.038e0

160.0228 3.038e0

160.0402 1.013e0

160.0930 1.588e0

160.1083 2.629e0

160.1319 1.013e0

160.1614 1.013e0

160.2342 2.025e0

160.2495 2.025e0

160.3025 2.025e0

160.3405 2.419e0

160.3841 1.013e0

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160.4270 1.013e0

160.4983 1.013e0

160.5188 1.013e0

160.5387 1.013e0

160.5684 1.013e0

160.5854 1.013e0

160.6398 1.013e0

160.6602 1.013e0

160.6996 1.013e0

160.7167 1.013e0

160.7405 1.013e0

160.7745 1.013e0

160.7952 2.025e0

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160.8753 1.013e0

160.8990 1.013e0

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160.9741 2.025e0

161.0168 1.013e0

161.0873 1.376e0

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161.2062 2.025e0

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161.3342 1.013e0

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161.4964 1.013e0

161.5312 2.025e0

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161.5938 1.013e0

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161.7357 1.013e0

161.7971 1.013e0

161.8136 1.013e0

161.8980 1.013e0

161.9406 2.025e0

161.9657 1.013e0

161.9789 1.013e0

162.0496 6.506e0

162.0827 1.682e0

162.1251 1.103e1

162.1819 2.025e0

162.2125 1.013e0

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162.2713 3.038e0

162.3084 2.025e0

162.3529 2.025e0

162.3784 2.025e0

162.4196 3.038e0

162.4393 1.013e0

162.4945 2.298e0

162.5421 3.038e0

162.6422 1.013e0

162.6610 2.025e0

162.7479 1.013e0

162.7754 2.939e0

162.7929 2.025e0

162.8765 1.013e0

162.9056 2.025e0

162.9410 4.051e0

162.9619 3.038e0

162.9885 7.089e0

163.0661 8.920e0

163.1360 3.038e0

163.1850 1.013e0

163.2192 1.013e0

163.2466 2.025e0

163.2884 3.038e0

163.3205 1.013e0

163.3530 2.025e0

163.3735 2.025e0

163.4060 1.013e0

163.4354 4.051e0

163.4799 2.025e0

163.4971 2.025e0

163.5228 2.025e0

163.5655 2.025e0

163.5938 3.038e0

163.6367 1.013e0

163.6563 2.025e0

163.6840 1.013e0

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163.7542 4.051e0

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163.9361 1.013e0

163.9635 1.013e0

163.9874 5.063e0

164.0141 1.013e0

164.0655 9.632e0

164.1294 6.653e0

164.1814 2.025e0

164.2114 1.013e0

164.2541 5.063e0

164.2967 1.013e0

164.3619 2.025e0

164.3894 4.051e0

164.4222 2.025e0

164.4462 1.013e0

164.4891 2.025e0

164.5264 4.051e0

164.5560 1.013e0

164.6032 1.978e0

164.6200 2.025e0

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164.6713 1.013e0

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164.8028 2.025e0

164.8449 1.013e0

164.8725 1.013e0

164.8931 2.025e0

164.9171 1.013e0

164.9910 2.025e0

165.0127 1.013e0

165.0557 8.615e0

165.0922 4.618e1

165.1332 5.967e0

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165.1974 1.013e0

165.2329 4.051e0

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165.3600 3.038e0

165.3867 2.025e0

165.4056 1.013e0

165.4332 2.025e0

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165.4967 4.051e0

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165.6775 2.025e0

165.7812 1.013e0

165.8293 1.013e0

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166.0877 6.624e0

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166.1932 3.038e0

166.2397 3.038e0

166.2775 2.025e0

166.2982 1.013e0

166.3464 3.038e0

166.3705 3.038e0

166.4481 3.038e0

166.5138 1.013e0

166.5345 2.025e0

166.5621 2.025e0

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166.6517 2.025e0

166.6793 2.025e0

166.7268 1.013e0

166.7641 3.038e0

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166.9433 1.013e0

166.9743 1.013e0

166.9922 3.038e0

167.0283 3.038e0

167.0574 1.506e0

167.1064 1.949e0

167.1455 1.013e0

167.1788 4.051e0

167.2007 1.013e0

167.2421 1.013e0

167.2629 1.013e0

167.2902 1.013e0

167.3105 1.013e0

167.3309 1.013e0

167.3525 3.038e0

167.3718 1.013e0

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167.4824 1.013e0

167.5204 1.013e0

167.5376 1.013e0

167.5662 3.038e0

167.5860 1.013e0

167.6187 4.051e0

167.6609 1.013e0

167.6881 2.025e0

167.7124 1.013e0

167.7660 2.025e0

167.7919 1.013e0

167.8385 2.025e0

167.8921 1.013e0

167.9369 1.013e0

168.0051 1.013e0

168.0256 2.025e0

168.0531 2.025e0

168.0824 4.065e0

168.1070 9.128e0

168.1288 4.051e0

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168.2659 2.025e0

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168.5141 4.051e0

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168.6624 2.025e0

168.6961 3.038e0

168.7278 2.025e0

168.7602 1.013e0

168.8062 5.063e0

168.8428 1.013e0

168.8775 1.013e0

168.8983 1.013e0

168.9297 4.051e0

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169.4461 2.025e0

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169.5745 2.025e0

169.6110 1.013e0

169.6832 1.013e0

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169.9918 4.051e0

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170.0520 4.024e0

170.0791 3.599e0

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170.7056 1.013e0

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170.8725 2.025e0

170.9177 1.013e0

170.9438 2.025e0

170.9734 2.025e0

171.0134 1.297e1

171.0549 3.356e0

171.0897 1.586e0

171.1393 1.516e1

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171.8773 2.025e0

171.9157 1.013e0

171.9436 2.025e0

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172.7532 1.013e0

172.7811 1.013e0

172.8056 1.013e0

172.8859 1.013e0

172.9208 1.013e0

172.9488 2.025e0

172.9916 4.051e0

173.0110 5.949e0

173.0582 5.660e1

173.1202 2.866e0

173.1454 3.038e0

173.1636 2.025e0

173.1934 2.025e0

173.2213 1.013e0

173.2514 4.051e0

173.2887 3.038e0

173.3104 2.025e0

173.3402 5.063e0

173.3681 2.025e0

173.4206 1.013e0

173.4660 2.025e0

173.4897 3.038e0

173.5427 5.063e0

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173.7153 3.038e0

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173.8194 2.025e0

173.8369 2.025e0

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173.9330 3.038e0

173.9804 4.051e0

174.0376 7.374e1

174.0800 2.881e0

174.1086 1.234e1

174.1415 2.025e0

174.1870 1.013e0

174.2098 2.025e0

174.2763 2.025e0

174.3026 2.025e0

174.3364 3.038e0

174.3814 2.025e0

174.4104 3.038e0

174.4342 2.025e0

174.4605 1.013e0

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174.5222 2.025e0

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174.6824 1.013e0

174.7263 3.038e0

174.7668 1.013e0

174.8088 1.013e0

174.8474 2.025e0

174.8930 1.013e0

174.9175 2.025e0

174.9561 1.013e0

175.0087 1.013e0

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