 Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

387 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 17-17 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 I: 0-2

Minimum: -1.5

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

302.1387 302.1392 -0.5 -1.7 8.5 174.2 0.0 C17 H20 N O4

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.

144.8664 1.013e0

144.8947 1.013e0

144.9836 6.361e1

145.0232 6.076e0

145.0573 7.089e0

145.0973 7.947e0

145.1328 4.224e0

145.1542 1.013e0

145.1799 5.063e0

145.2110 4.051e0

145.2574 5.063e0

145.2869 3.038e0

145.3067 2.025e0

145.3421 4.051e0

145.3780 1.013e0

145.4074 3.038e0

145.4625 4.051e0

145.4916 3.038e0

145.5181 2.025e0

145.5416 3.038e0

145.5809 2.025e0

145.6058 1.013e0

145.7237 3.038e0

145.7938 2.025e0

145.8149 3.038e0

145.8560 3.735e0

145.8784 1.013e0

145.9203 1.013e0

145.9859 2.025e0

146.0185 2.025e0

146.0703 1.284e2

146.1318 3.873e0

146.1588 5.063e0

146.1794 3.384e0

146.1983 8.101e0

146.2319 3.038e0

146.2832 3.038e0

146.3346 1.013e0

146.3608 1.013e0

146.3928 5.063e0

146.4262 2.025e0

146.4487 2.025e0

146.4699 3.038e0

146.5007 3.038e0

146.5596 1.013e0

146.5859 2.025e0

146.6208 1.013e0

146.6422 4.051e0

146.6836 2.025e0

146.7651 3.038e0

146.7781 2.050e0

146.8076 1.013e0

146.8607 2.025e0

146.8828 4.051e0

146.9058 3.038e0

146.9525 2.750e0

146.9803 2.235e1

147.0264 1.013e0

147.0461 1.013e0

147.0720 4.583e0

147.0899 6.871e0

147.1539 2.025e0

147.1939 1.013e0

147.2218 2.025e0

147.2390 1.013e0

147.2661 3.038e0

147.3328 1.013e0

147.3661 2.025e0

147.3876 1.013e0

147.4134 1.013e0

147.4259 2.025e0

147.4456 2.025e0

147.5037 2.025e0

147.5341 2.025e0

147.5585 2.025e0

147.5867 2.025e0

147.6396 2.025e0

147.6747 1.013e0

147.6976 1.013e0

147.7475 2.025e0

147.8056 2.025e0

147.8238 2.025e0

147.8653 2.025e0

147.9152 2.025e0

147.9333 1.013e0

147.9839 4.051e0

148.0201 2.025e0

148.0714 4.689e0

148.1142 2.431e0

148.1272 1.924e0

148.1543 2.025e0

148.1889 1.013e0

148.2182 5.063e0

148.2404 1.013e0

148.2756 1.013e0

148.3003 2.025e0

148.3150 3.038e0

148.3775 3.038e0

148.4265 2.025e0

148.4880 2.025e0

148.5044 2.025e0

148.5769 1.013e0

148.6028 1.013e0

148.6209 2.025e0

148.6578 1.013e0

148.6959 2.025e0

148.7143 2.025e0

148.7389 1.470e0

148.7617 1.013e0

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148.8941 3.038e0

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148.9715 4.051e0

148.9919 2.025e0

149.0208 2.025e0

149.0350 3.038e0

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149.1167 1.741e0

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149.1799 1.013e0

149.2481 1.013e0

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149.3484 2.025e0

149.3780 1.013e0

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149.4429 3.038e0

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149.5762 1.013e0

149.6031 3.038e0

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149.6766 1.013e0

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149.7877 2.025e0

149.8263 1.013e0

149.8428 2.025e0

149.8813 1.013e0

149.9309 1.013e0

149.9520 3.038e0

150.0126 3.038e0

150.0478 1.013e0

150.0627 2.025e0

150.1256 4.055e1

150.1581 1.013e0

150.1954 3.038e0

150.2348 2.025e0

150.2849 2.025e0

150.3147 2.025e0

150.3456 3.038e0

150.3881 2.025e0

150.4515 1.013e0

150.4809 1.013e0

150.5051 2.025e0

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150.6536 4.051e0

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150.8789 1.013e0

150.9524 2.025e0

150.9702 1.013e0

150.9994 2.025e0

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151.0913 2.546e0

151.1088 2.965e0

151.1293 2.199e0

151.1663 1.013e0

151.1888 1.013e0

151.2194 3.038e0

151.2544 1.013e0

151.2702 2.025e0

151.2915 1.394e0

151.3186 3.038e0

151.3327 4.051e0

151.3826 6.184e0

151.3962 3.038e0

151.4473 2.025e0

151.5076 2.025e0

151.5492 2.835e1

151.5878 3.038e0

151.6142 3.038e0

151.6432 2.025e0

151.6747 6.076e0

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151.7517 1.013e0

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151.8350 4.814e0

151.9024 2.025e0

151.9492 5.458e0

151.9925 3.038e0

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152.1246 4.649e0

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152.2067 4.051e0

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152.2608 3.495e0

152.2918 2.025e0

152.3213 1.013e0

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152.4988 2.025e0

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155.7807 1.013e0

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155.8919 3.038e0

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155.9514 2.025e0

155.9765 2.025e0

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158.8478 2.025e0

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159.1653 1.013e0

159.1949 3.038e0

159.2520 2.025e0

159.2893 2.025e0

159.3218 2.025e0

159.3829 2.025e0

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160.3476 3.038e0

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160.4377 2.025e0

160.4540 2.025e0

160.4881 1.013e0

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160.7914 3.038e0

160.8169 2.025e0

160.8683 2.025e0

160.8998 3.038e0

160.9569 1.013e0

160.9735 2.025e0

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161.0406 2.025e0

161.0780 2.263e0

161.1018 1.054e0

161.1668 8.101e0

161.2299 1.013e0

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161.3240 1.013e0

161.3894 3.038e0

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161.4997 1.013e0

161.5168 1.013e0

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161.8912 2.025e0

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162.7820 1.013e0

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163.1215 7.107e0

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163.2707 1.013e0

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163.3242 2.025e0

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163.6643 1.013e0

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163.7219 1.013e0

163.7698 1.013e0

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163.8179 1.013e0

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163.8780 1.013e0

163.9535 2.025e0

163.9866 3.038e0

164.0384 1.013e0

164.0994 5.923e0

164.1456 9.254e0

164.1720 4.276e0

164.1887 2.025e0

164.2344 3.038e0

164.2936 2.025e0

164.3427 3.038e0

164.3783 4.051e0

164.4182 2.025e0

164.4467 1.013e0

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165.1084 2.302e1

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165.3321 2.025e0

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165.5955 2.025e0

165.6436 2.025e0

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166.2201 1.013e0

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166.2745 1.013e0

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166.3236 3.038e0

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166.3916 2.025e0

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166.6901 2.025e0

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166.8215 2.025e0

166.8836 2.025e0

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167.3728 1.013e0

167.3931 2.025e0

167.4209 2.025e0

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167.5694 1.013e0

167.5953 2.025e0

167.7096 1.013e0

167.7355 2.025e0

167.8012 2.025e0

167.8323 2.025e0

167.8789 1.013e0

167.9291 2.025e0

167.9959 1.013e0

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168.0728 3.038e0

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168.3748 1.013e0

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168.5057 2.025e0

168.5299 1.013e0

168.5714 1.013e0

168.5922 3.038e0

168.6476 2.025e0

168.6649 1.013e0

168.7408 2.025e0

168.7784 1.013e0

168.8230 2.025e0

168.8609 1.013e0

168.8817 1.013e0

168.8990 1.013e0

168.9457 4.051e0

169.0466 5.063e0

169.0885 2.199e0

169.1041 1.258e0

169.1456 6.003e0

169.1726 1.013e0

169.2531 2.025e0

169.2995 1.013e0

169.3412 1.013e0

169.3967 1.013e0

169.4366 2.025e0

169.4730 1.013e0

169.4921 2.025e0

169.5163 2.025e0

169.5485 6.391e0

169.6083 1.013e0

169.6292 1.013e0

169.6568 1.013e0

169.7256 1.013e0

169.7463 1.013e0

169.7875 1.013e0

169.8220 1.013e0

169.8428 2.025e0

169.9401 2.025e0

169.9713 1.013e0

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170.0347 3.038e0

170.0937 5.874e0

170.1348 1.054e0

170.1796 3.038e0

170.2388 1.013e0

170.3043 2.025e0

170.3388 1.013e0

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170.4286 1.013e0

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170.4944 1.013e0

170.5370 3.038e0

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170.6075 2.025e0

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170.9222 1.013e0

170.9570 1.013e0

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171.0410 7.946e0

171.0810 7.990e0

171.1130 5.324e0

171.1514 2.109e1

171.1877 7.089e0

171.2143 4.051e0

171.2656 1.013e0

171.3228 2.025e0

171.3419 1.013e0

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171.6607 2.025e0

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