

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 15-15 H: 0-200 N: 0-10 O: 0-14 Na: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

258.1613 258.1606 0.7 2.7 7.5 2.2 C15 H20 N3 O

FOR BEST FIT M+CH3CN+H ADDUCT SELECTED

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.

149.8456 3.038e0

149.8947 2.025e0

149.9124 2.025e0

149.9355 3.038e0

149.9567 1.013e0

149.9824 1.013e0

150.0155 1.013e0

150.0557 2.025e0

150.0955 3.038e0

150.1339 2.025e0

150.1554 1.013e0

150.2072 1.013e0

150.2285 2.025e0

150.2707 2.025e0

150.3014 2.025e0

150.3275 1.013e0

150.3759 2.025e0

150.4321 1.013e0

150.4488 3.038e0

150.4792 2.025e0

150.5493 2.025e0

150.5784 1.013e0

150.6177 2.025e0

150.6469 1.013e0

150.6845 2.025e0

150.7415 1.013e0

150.7713 1.013e0

150.7934 1.013e0

150.8198 1.013e0

150.8464 1.013e0

150.9016 2.025e0

150.9402 1.013e0

150.9726 3.038e0

151.0098 3.038e0

151.0497 3.038e0

151.0805 1.013e0

151.1460 2.025e0

151.1664 3.274e0

151.2125 3.038e0

151.2310 1.013e0

151.2709 2.025e0

151.2949 2.775e0

151.3185 3.038e0

151.3680 1.013e0

151.4063 2.025e0

151.4533 2.025e0

151.4815 2.025e0

151.5087 1.013e0

151.5302 2.025e0

151.5622 4.051e0

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151.6228 3.038e0

151.6401 3.038e0

151.6655 3.038e0

151.7224 3.038e0

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151.9736 1.013e0

152.0002 1.013e0

152.0574 3.038e0

152.0795 6.076e0

152.1476 1.013e0

152.1640 1.013e0

152.2196 1.013e0

152.2394 1.013e0

152.2817 1.013e0

152.3567 4.051e0

152.3886 2.025e0

152.4159 1.013e0

152.4425 2.025e0

152.4592 1.013e0

152.5212 1.013e0

152.5446 2.025e0

152.5683 2.025e0

152.6326 1.013e0

152.6705 2.025e0

152.7310 1.013e0

152.7758 2.025e0

152.7917 2.025e0

152.8165 1.013e0

152.8331 1.013e0

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152.9741 2.025e0

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153.0194 3.038e0

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153.2091 2.025e0

153.2442 2.025e0

153.2818 4.051e0

153.3487 1.013e0

153.3953 1.013e0

153.4167 2.025e0

153.4509 1.013e0

153.4709 1.013e0

153.5022 2.025e0

153.5265 1.013e0

153.5837 3.038e0

153.6071 2.025e0

153.6372 2.025e0

153.6911 3.038e0

153.7346 2.025e0

153.7868 2.025e0

153.8085 2.025e0

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153.9583 2.025e0

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154.0708 3.038e0

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154.1398 1.013e0

154.1714 4.051e0

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154.2550 2.025e0

154.3013 2.025e0

154.3248 1.013e0

154.3687 4.051e0

154.4171 1.013e0

154.4613 2.025e0

154.5029 1.013e0

154.5253 3.038e0

154.5411 3.038e0

154.5655 1.013e0

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154.9108 2.025e0

154.9392 1.013e0

154.9612 3.038e0

154.9867 2.025e0

155.0428 4.051e0

155.0843 3.038e0

155.1456 3.038e0

155.2111 4.051e0

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155.2933 1.013e0

155.3094 1.013e0

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155.8012 2.025e0

155.8273 3.323e0

155.8629 2.025e0

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156.0456 1.013e0

156.0755 4.051e0

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156.1761 2.025e0

156.2113 2.025e0

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156.2883 3.038e0

156.3076 1.013e0

156.3412 4.051e0

156.3617 5.111e0

156.4023 2.025e0

156.4372 1.013e0

156.4734 2.025e0

156.5264 3.038e0

156.5842 4.051e0

156.6152 2.025e0

156.6547 4.778e0

156.6998 6.076e0

156.7470 3.038e0

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156.8130 1.013e0

156.8378 4.051e0

156.9045 4.051e0

156.9723 2.025e0

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157.1270 4.051e0

157.1428 4.051e0

157.1703 2.182e0

157.1973 9.114e0

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157.2939 3.038e0

157.3114 3.328e0

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157.4669 2.025e0

157.4986 7.089e0

157.5307 2.025e0

157.5496 2.843e0

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158.6774 2.025e0

158.7040 4.300e0

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158.8285 2.025e0

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158.8793 2.025e0

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158.9219 3.038e0

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160.6372 2.025e0

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161.3693 1.013e0

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161.8389 1.013e0

161.8611 2.025e0

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161.9174 1.013e0

161.9539 1.013e0

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163.1577 9.114e0

163.2833 2.025e0

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163.3432 1.013e0

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165.5885 2.025e0

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165.7729 3.038e0

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166.1462 2.025e0

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168.2245 3.038e0

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168.2931 1.013e0

168.3391 2.025e0

168.3979 2.025e0

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168.4602 2.025e0

168.5103 2.025e0

168.5605 2.025e0

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168.9728 1.013e0

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169.1967 2.025e0

169.2442 4.051e0

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169.3284 1.013e0

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173.0481 2.025e0

173.0787 4.051e0

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173.1775 2.025e0

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173.7943 4.051e0

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173.8779 3.038e0

173.9137 3.038e0

173.9383 2.025e0

173.9908 2.025e0

174.0530 5.063e0

174.0797 7.089e0

174.1256 2.025e0

174.1484 2.025e0

174.1677 1.013e0

174.1887 1.013e0

174.2210 3.038e0

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174.2973 1.013e0

174.3333 3.038e0

174.3762 4.051e0

174.4294 3.038e0

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174.7648 1.013e0

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175.9144 4.051e0

175.9335 3.038e0

175.9646 2.881e0

175.9947 3.038e0

176.0307 2.025e0

176.0485 2.025e0

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