 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

142 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: 0-15 I: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

226.1234 226.1232 0.2 0.9 8.5 0.8 C15 H16 N O

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)

149.0076 1.013e0

149.0305 1.013e0

149.0527 1.013e0

149.1109 2.430e1

149.1403 3.568e0

149.1924 1.013e0

149.2155 1.013e0

149.2932 2.025e0

149.3255 1.013e0

149.3856 4.051e0

149.4169 1.013e0

149.4421 1.013e0

149.5269 2.025e0

149.5561 1.013e0

149.6270 3.038e0

149.6568 1.013e0

149.7967 1.013e0

149.8368 2.025e0

149.8683 1.013e0

149.9013 3.038e0

149.9500 2.025e0

149.9858 3.038e0

150.0305 1.013e0

150.0436 1.013e0

150.0864 1.013e0

150.1139 8.574e0

150.1563 2.025e0

150.1770 1.013e0

150.2034 1.013e0

150.2619 1.013e0

150.3723 1.013e0

150.4119 1.013e0

150.4770 1.013e0

150.4956 3.038e0

150.5122 2.025e0

150.5621 1.013e0

150.5874 1.013e0

150.6073 1.013e0

150.6625 3.038e0

150.7574 1.013e0

150.8259 1.013e0

150.8488 1.013e0

150.8613 1.013e0

150.8944 1.013e0

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150.9464 1.013e0

150.9762 1.013e0

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151.7704 1.013e0

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151.8558 2.025e0

151.8878 1.013e0

152.0030 1.013e0

152.0750 1.013e0

152.1437 1.013e0

152.1695 1.013e0

152.1925 1.013e0

152.2473 4.051e0

152.3897 2.025e0

152.4386 1.013e0

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152.5695 1.013e0

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152.6450 1.013e0

152.6616 1.013e0

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152.8092 2.025e0

152.8359 1.013e0

152.8914 1.013e0

152.9936 2.025e0

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153.0424 2.025e0

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153.1774 1.013e0

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153.6499 2.025e0

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154.1701 2.025e0

154.2032 2.025e0

154.2266 2.025e0

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165.3657 2.025e0

165.4505 4.051e0

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171.1678 3.038e0

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171.2442 1.013e0

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173.1870 1.013e0

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174.3839 3.038e0

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174.8814 2.025e0

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175.4859 2.025e0

175.5177 2.025e0

175.5853 4.051e0

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175.6708 1.013e0

175.7956 2.025e0

175.8290 3.038e0

175.9413 1.013e0

175.9908 2.025e0

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176.0865 1.013e0

176.1326 1.013e0

176.1908 2.025e0

176.2312 1.013e0

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176.3191 1.013e0

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176.5034 4.051e0

176.5394 2.025e0

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176.7957 1.013e0

176.8608 2.025e0

176.9013 1.013e0

176.9347 2.025e0

176.9505 1.013e0

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177.1314 5.063e0

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177.2146 2.025e0

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179.1114 2.025e0

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179.2874 2.025e0

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