

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 1000.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

232 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 56Fe: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 1000.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

320.2223 320.2226 -0.3 -0.9 5.5 2.3 C19 H30 N O3

REPORT MASSES AS +/-5mDa, referenced against

Leucine Enkelphalin @ 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.

49.7576 2.025e0

149.7874 1.013e0

149.8557 1.013e0

149.8714 1.013e0

149.8976 2.025e0

149.9381 2.025e0

150.0293 4.051e0

150.0762 1.013e0

150.0927 1.013e0

150.1321 1.013e0

150.1526 2.025e0

150.3993 1.013e0

150.4494 2.025e0

150.5162 2.025e0

150.5488 2.025e0

150.7767 1.013e0

150.7933 1.013e0

150.8199 1.013e0

150.8800 2.025e0

150.9203 4.051e0

150.9468 3.038e0

151.0434 1.070e1

151.0971 1.013e0

151.1258 1.013e0

151.1790 2.025e0

151.2475 1.013e0

151.2861 4.051e0

151.3044 2.025e0

151.3319 1.013e0

151.4023 2.025e0

151.4300 1.013e0

151.5571 1.013e0

151.5704 1.013e0

151.6070 1.013e0

151.6739 2.025e0

151.7143 1.013e0

151.8128 1.013e0

151.8516 1.013e0

151.8881 2.025e0

152.0238 2.025e0

152.0479 3.038e0

152.0665 2.942e0

152.0942 1.013e0

152.1452 3.038e0

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152.2126 1.013e0

152.2516 1.013e0

152.2782 1.013e0

152.3228 4.051e0

152.3823 1.013e0

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152.5175 1.013e0

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152.8833 2.025e0

152.9439 1.013e0

152.9996 1.013e0

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153.0754 2.025e0

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153.1316 1.013e0

153.1638 1.013e0

153.1929 3.038e0

153.2860 1.013e0

153.3217 1.013e0

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153.4797 2.025e0

153.5045 2.025e0

153.5395 1.013e0

153.5984 1.013e0

153.6317 1.013e0

153.7156 2.025e0

153.8253 2.025e0

153.8756 1.013e0

153.9771 1.013e0

154.0202 1.013e0

154.0403 1.013e0

154.0628 1.013e0

154.0759 1.013e0

154.1093 1.013e0

154.1359 2.025e0

154.1591 5.128e0

154.2641 1.013e0

154.3074 2.025e0

154.3433 1.013e0

154.3633 2.025e0

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154.4257 1.013e0

154.4948 1.013e0

154.5216 1.013e0

154.6208 1.013e0

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154.6765 2.025e0

154.7201 2.025e0

154.7462 1.013e0

154.7742 2.025e0

154.7959 1.013e0

154.8651 2.025e0

154.9119 1.013e0

155.0336 1.013e0

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155.9645 1.013e0

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156.1121 3.038e0

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184.8807 1.013e0

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185.9074 4.051e0

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186.6871 1.013e0

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186.8502 2.025e0

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186.9791 2.025e0

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187.1209 2.025e0

187.1636 1.013e0

187.2103 1.013e0

187.2533 1.013e0

187.4215 1.013e0

187.4757 1.013e0

187.5044 1.013e0

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