

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

2183 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 26-26 H: 3-150 N: 0-20 O: 0-20 Na: 0-1 S: 0-2

Minimum: -1.5

Maximum: 5.0 10.0 1000.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

481.2267 481.2273 -0.6 -1.2 12.5 92.0 C26 H33 N4 O3 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.

PEAK LIST

147.2275 1.013e0

147.2496 1.013e0

147.2790 1.013e0

147.3272 1.013e0

147.3852 1.013e0

147.4211 3.038e0

147.4607 4.051e0

147.4979 1.013e0

147.5242 1.013e0

147.5372 1.013e0

147.5658 2.025e0

147.5855 1.013e0

147.6337 3.038e0

147.6628 1.013e0

147.6950 1.013e0

147.7210 1.013e0

147.7825 2.025e0

147.8358 2.025e0

147.8770 4.051e0

147.8989 1.013e0

147.9829 1.013e1

148.0636 3.522e0

148.1120 6.541e0

148.1714 2.025e0

148.1927 1.013e0

148.2109 2.025e0

148.2443 1.013e0

148.2774 3.038e0

148.3189 2.025e0

148.3639 1.013e0

148.3903 1.013e0

148.4352 1.013e0

148.4612 1.013e0

148.5016 2.025e0

148.5450 1.013e0

148.6032 1.013e0

148.6428 2.025e0

148.7075 1.013e0

148.7229 2.025e0

148.7674 2.025e0

148.8075 1.013e0

148.8370 1.013e0

148.9437 1.013e0

148.9668 2.025e0

148.9822 2.025e0

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149.0257 2.267e0

149.0955 3.869e0

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149.1768 1.013e0

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149.6173 2.025e0

149.6643 2.025e0

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149.7860 2.025e0

149.8295 2.025e0

149.8460 1.013e0

149.8886 1.013e0

149.9259 2.025e0

149.9539 2.025e0

149.9727 1.013e0

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150.0472 1.653e1

150.0872 2.343e0

150.1255 3.031e0

150.1700 3.038e0

150.2009 1.013e0

150.2175 1.013e0

150.2394 1.013e0

150.2560 2.025e0

150.3078 2.025e0

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150.3712 2.025e0

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150.4479 2.025e0

150.4661 2.025e0

150.4843 1.013e0

150.5178 2.025e0

150.5496 2.025e1

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150.6698 3.038e0

150.6880 2.025e0

150.7156 1.013e0

150.7349 2.025e0

150.7548 2.025e0

150.7948 2.025e0

150.8432 2.025e0

150.8701 2.025e0

150.9016 2.025e0

150.9206 3.038e0

150.9635 1.013e0

150.9899 3.038e0

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151.1249 2.597e0

151.1628 1.114e1

151.1996 7.089e0

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151.3327 1.013e0

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151.4211 2.025e0

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151.7327 2.025e0

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151.7979 5.063e0

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151.9214 2.025e0

151.9706 4.051e0

151.9950 2.025e0

152.0499 6.804e1

152.1341 1.051e0

152.1723 5.063e0

152.2028 5.063e0

152.2260 2.213e0

152.2458 2.025e0

152.2848 3.038e0

152.3167 2.025e0

152.3469 1.013e0

152.3635 1.013e0

152.3902 1.013e0

152.4290 1.013e0

152.4622 4.051e0

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152.5502 1.110e1

152.5684 9.189e0

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152.6388 1.013e0

152.6836 3.038e0

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174.9378 2.025e0

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177.1328 2.463e0

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