 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

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

Elements Used:

C: 13-13 H: 0-200 N: 0-10 O: 0-15

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

198.0923 198.0919 0.4 2.0 8.5 0.8 C13 H12 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)

145.9333 1.013e0

145.9624 3.038e0

145.9880 1.013e0

146.0169 3.038e0

146.0719 1.007e2

146.1081 2.025e0

146.1504 2.025e0

146.1936 1.013e0

146.2141 3.038e0

146.2675 1.013e0

146.2898 1.013e0

146.3252 1.013e0

146.3706 1.013e0

146.4797 1.013e0

146.5147 2.025e0

146.5775 2.025e0

146.6273 1.013e0

146.6534 1.013e0

146.6723 1.013e0

146.6950 1.013e0

146.7497 1.013e0

146.7778 2.025e0

146.8109 1.013e0

146.8272 2.025e0

146.8491 1.013e0

146.8852 1.013e0

146.9527 3.038e0

146.9814 2.025e0

147.0394 1.013e0

147.0719 7.089e0

147.1105 1.013e0

147.1376 2.025e0

147.1619 1.013e0

147.2134 1.013e0

147.2522 1.013e0

147.2648 1.013e0

147.3195 1.013e0

147.3392 1.013e0

147.3714 1.013e0

147.4071 1.013e0

147.5199 2.025e0

147.5551 1.013e0

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147.6228 1.013e0

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147.7881 2.025e0

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147.9766 2.025e0

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148.0334 1.013e0

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148.8428 1.013e0

148.8699 2.025e0

148.9153 2.025e0

148.9847 1.013e0

149.0211 2.025e0

149.0612 2.025e0

149.0989 1.013e0

149.1376 2.025e0

149.1700 2.025e0

149.1894 1.013e0

149.2224 1.013e0

149.2510 1.013e0

149.2873 1.013e0

149.3616 1.013e0

149.3890 2.025e0

149.4105 1.013e0

149.4328 1.013e0

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149.5370 1.013e0

149.6102 4.051e0

149.6887 2.025e0

149.7022 1.034e0

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149.8670 2.025e0

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149.9855 2.025e0

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150.0769 1.013e0

150.1971 2.025e0

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150.3957 1.013e0

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150.4957 2.025e0

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154.0789 2.025e0

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154.1362 2.025e0

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154.2516 3.038e0

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175.9245 2.025e0

175.9660 3.038e0

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176.9957 2.025e0

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177.1581 3.038e0

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177.9976 2.025e0

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179.2740 2.025e0

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179.6868 1.013e0

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180.1108 1.013e0

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180.4605 2.025e0

180.5463 1.013e0

180.5889 1.013e0

180.6816 1.013e0

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181.8731 1.013e0

181.9982 2.025e0

182.0273 1.013e0

182.1014 3.038e0

182.2640 1.013e0

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396.9256 3.038e0

396.9823 2.025e0

397.0149 2.025e0

397.0860 3.038e0

397.1718 7.968e0

397.2224 2.025e0

397.3098 2.025e0

397.4199 2.025e0

397.6159 2.025e0

397.6599 1.013e0

397.7563 2.025e0

397.9128 2.025e0

397.9604 1.115e0

398.0854 5.063e0

398.1987 3.038e0

398.2908 2.025e0

398.4772 1.013e0

398.6597 1.013e0

398.7705 3.038e0

398.8424 2.025e0

398.9059 3.896e0

399.0435 1.013e0

399.2162 4.051e0

399.2874 2.025e0

399.3301 3.038e0

399.5096 3.038e0

399.8130 1.013e0

399.8902 2.025e0

399.9446 1.013e0

400.0653 2.025e0

400.2109 8.101e0

400.3543 1.013e0

400.4348 2.025e0

400.5154 1.013e0

400.5739 1.013e0

400.6362 2.025e0

400.6786 1.013e0

400.7536 3.038e0

400.8083 1.013e0

400.8742 2.025e0

400.9291 2.025e0

401.0839 3.038e0

401.2089 4.051e0

401.2568 5.063e0

401.3059 1.418e1

401.4137 1.013e0