 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

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

Elements Used:

C: 14-14 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

224.2020 224.2014 0.6 2.7 2.5 4.9 C14 H26 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)

148.1320 1.013e0

148.1452 1.013e0

148.1754 2.025e0

148.2191 1.013e0

148.2384 2.025e0

148.2933 1.013e0

148.3098 1.013e0

148.4327 1.013e0

148.4525 1.013e0

148.5672 2.025e0

148.6303 1.013e0

148.6688 1.013e0

148.7084 1.013e0

148.7208 1.013e0

148.7468 1.013e0

148.7699 1.013e0

149.1046 2.025e0

149.1992 2.025e0

149.3273 1.013e0

149.4342 1.013e0

149.4959 2.025e0

149.5453 1.013e0

149.5705 2.025e0

149.5871 1.013e0

149.7738 2.025e0

149.7887 1.013e0

149.8245 1.013e0

149.8471 1.013e0

149.8669 1.013e0

149.9641 1.013e0

150.0120 3.038e0

150.0521 1.013e0

150.0685 1.013e0

150.1138 1.013e0

150.1402 1.013e0

150.1566 1.013e0

150.3071 2.025e0

150.3648 1.013e0

150.3973 1.013e0

150.5702 1.013e0

150.6403 2.025e0

150.6593 2.025e0

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150.9747 1.013e0

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151.0819 1.013e0

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151.9783 1.013e0

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152.0866 1.013e0

152.1588 1.013e0

152.3883 1.013e0

152.4040 1.013e0

152.4606 1.013e0

152.4926 1.013e0

152.5292 1.013e0

152.6735 1.013e0

152.7030 1.013e0

152.7978 1.013e0

152.8637 1.013e0

152.9426 1.013e0

152.9621 1.013e0

153.0088 1.013e0

153.0810 1.013e0

153.1003 1.013e0

153.2354 1.013e0

153.2910 1.013e0

153.3633 1.013e0

153.3932 1.013e0

153.5245 1.013e0

153.5478 1.013e0

153.6051 2.025e0

153.6694 1.013e0

153.7292 1.013e0

153.8705 1.013e0

153.9261 1.013e0

154.1672 1.013e0

154.2498 1.013e0

154.2759 2.025e0

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154.6628 1.013e0

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154.7486 1.013e0

154.7747 1.013e0

154.8576 2.025e0

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155.1599 1.823e1

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177.0916 1.013e0

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179.9897 2.025e0

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180.9008 1.013e0

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181.6314 1.013e0

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181.7565 3.038e0

181.8355 1.013e0

181.9563 1.013e0

182.0214 2.025e0

182.0824 2.025e0

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182.2796 1.013e0

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182.3632 2.025e0

182.4912 1.013e0

182.6565 2.025e0

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182.7313 1.013e0

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186.6637 1.013e0

186.7910 1.013e0

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187.1679 1.013e0

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193.3234 1.013e0

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193.4402 2.025e0

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193.9527 1.013e0

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194.1486 1.013e0

194.2076 2.025e0

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194.4336 1.013e0

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194.6821 1.013e0

194.7298 1.013e0

194.8932 1.013e0

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195.0548 2.025e0

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195.2623 2.025e0

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397.2093 1.013e0

397.3006 3.038e0

397.3670 1.013e0

397.6429 1.013e0

397.8323 2.025e0

397.9301 1.013e0

398.2047 1.013e0

398.2762 1.013e0

398.3271 1.013e0

398.4760 1.013e0

398.6089 3.038e0

398.7901 2.025e0

398.8261 1.013e0

398.9840 1.013e0

399.0380 2.025e0

399.0973 1.013e0

399.1511 1.013e0

399.1803 1.013e0

399.2679 1.013e0

399.3926 1.013e0

399.5818 1.013e0

399.6111 1.013e0

399.7569 1.013e0

400.0143 1.013e0

400.0936 2.025e0

400.2247 1.114e1

400.3407 1.013e0

400.3936 1.013e0

400.5840 1.013e0

400.6326 1.013e0

400.6645 1.013e0