

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 18-18 H: 0-200 N: 0-10 O: 0-15 Na: 0-1 S: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

351.1750 351.1742 0.8 2.3 6.5 1.1 C18 H27 N2 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.

144.5832 1.013e0

144.6556 2.025e0

144.6886 1.013e0

144.7299 1.013e0

144.8104 2.025e0

144.8260 2.025e0

144.9390 2.025e0

144.9604 1.013e0

145.0297 2.025e0

145.0692 1.013e0

145.0916 1.013e0

145.1107 2.025e0

145.1667 2.025e0

145.2772 1.013e0

145.3512 1.013e0

145.4057 1.013e0

145.4634 1.013e0

145.5095 3.038e0

145.5462 1.013e0

145.5808 3.038e0

145.6391 1.013e0

145.6864 2.025e0

145.7276 2.025e0

145.7805 2.025e0

145.8781 2.025e0

145.8993 1.013e0

145.9440 1.013e0

145.9623 2.025e0

146.0034 2.025e0

146.0712 3.884e1

146.1207 1.013e0

146.2812 1.013e0

146.3097 2.025e0

146.3616 1.013e0

146.3805 1.013e0

146.4224 1.013e0

146.4515 1.013e0

146.5411 1.013e0

146.5672 1.013e0

146.6071 2.025e0

146.6757 3.038e0

146.8372 1.013e0

146.9115 1.013e0

146.9374 1.013e0

146.9702 3.038e0

147.0177 1.013e0

147.0748 6.076e0

147.0952 2.025e0

147.1159 2.025e0

147.1467 1.013e0

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147.2824 1.013e0

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147.4433 1.013e0

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147.7950 1.013e0

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147.9889 1.013e0

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148.0954 2.025e0

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148.1847 2.025e0

148.2355 3.038e0

148.3092 1.013e0

148.3444 2.025e0

148.3707 1.013e0

148.3897 1.013e0

148.4288 1.013e0

148.5453 1.013e0

148.6002 2.025e0

148.6848 2.025e0

148.7117 2.025e0

148.8078 1.013e0

148.8529 1.013e0

148.9078 1.013e0

148.9891 1.013e0

149.0754 2.025e0

149.1057 1.013e0

149.1440 2.025e0

149.2019 2.025e0

149.2388 1.013e0

149.2552 1.013e0

149.2779 1.013e0

149.2987 2.025e0

149.3966 2.025e0

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149.5084 2.025e0

149.5502 1.013e0

149.6449 1.013e0

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149.8167 1.013e0

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150.0497 2.025e0

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153.9878 1.013e0

154.0240 4.051e0

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154.2385 1.013e0

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181.6781 1.013e0

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181.7674 1.013e0

181.8183 1.013e0

181.9107 1.013e0

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181.9715 1.013e0

182.0261 1.013e0

182.0509 2.025e0

182.0829 2.025e0

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182.3841 1.013e0

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182.5486 1.013e0

182.6427 1.013e0

182.7211 1.013e0

182.7482 2.025e0

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184.9291 1.013e0

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185.0809 1.013e0

185.1239 2.025e0

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