

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

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

Elements Used:

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

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

257.1294 257.1290 0.4 1.6 8.5 11.6 C15 H17 N2 O2

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.

156.1685 1.013e0

156.2445 1.013e0

156.2682 2.025e0

156.2916 1.013e0

156.3375 1.013e0

156.4179 1.013e0

156.5303 1.013e0

156.5436 1.013e0

156.6091 2.025e0

156.6552 2.025e0

156.6837 1.013e0

156.8530 1.013e0

156.9133 1.013e0

156.9495 1.013e0

156.9831 1.013e0

157.0134 2.025e0

157.0425 1.013e0

157.0628 1.013e0

157.0897 1.013e0

157.2164 1.013e0

157.4062 1.013e0

157.4589 1.013e0

157.5095 1.013e0

157.5265 1.013e0

157.5656 1.013e0

157.6558 1.013e0

157.7070 3.038e0

157.8129 2.025e0

157.9331 2.025e0

157.9795 1.013e0

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158.0231 1.013e0

158.0637 1.013e0

158.0962 1.013e0

158.1333 1.013e0

158.1535 1.013e0

158.2130 3.038e0

158.3234 1.013e0

158.3860 2.025e0

158.5047 1.013e0

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158.6883 1.013e0

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161.9272 1.013e0

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202.6610 2.025e0

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