 Elemental Composition Report

Single Mass Analysis

Tolerance = 25.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 21-21 H: 0-200 N: 0-22 O: 0-15 Na: 0-1 Cl: 1-1

Minimum: -1.5

Maximum: 5.0 25.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

367.1220 367.1213 0.7 1.9 12.5 2.8 C21 H20 N2 O2 Cl

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.

152.0586 2.025e0

152.0956 2.025e0

152.1189 4.051e0

152.1470 1.013e0

152.1760 2.025e0

152.2059 2.025e0

152.2563 2.025e0

152.2813 1.013e0

152.3401 1.013e0

152.3764 3.038e0

152.3921 1.013e0

152.4188 1.013e0

152.4683 4.051e0

152.5108 1.013e0

152.5368 1.013e0

152.6012 3.038e0

152.6351 1.013e0

152.6634 2.025e0

152.6848 1.013e0

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152.7759 2.025e0

152.8252 3.038e0

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153.0459 2.025e0

153.0938 4.051e0

153.1314 1.013e0

153.1685 2.025e0

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153.2399 1.013e0

153.2858 1.013e0

153.3059 1.013e0

153.3498 2.025e0

153.3781 1.013e0

153.4043 1.013e0

153.4897 1.013e0

153.5427 2.025e0

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155.0905 1.013e0

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155.1546 2.025e0

155.1730 1.013e0

155.2323 1.013e0

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