 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

98 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

204.1388 204.1388 0.0 0.0 5.5 4.7 C13 H18 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)

133.7021 2.025e0

133.7712 2.025e0

133.7986 1.013e0

133.8176 2.025e0

133.9004 1.013e0

134.0107 1.013e0

134.0477 1.013e0

134.0730 1.013e0

134.0941 1.013e0

134.1068 1.013e0

134.1311 2.025e0

134.1523 1.013e0

134.1775 1.013e0

134.2066 2.025e0

134.2710 2.025e0

134.3096 1.013e0

134.3403 1.013e0

134.3898 1.013e0

134.4495 3.038e0

134.4699 1.013e0

134.5040 1.013e0

134.5188 2.025e0

134.5387 3.038e0

134.5716 1.013e0

134.5835 1.013e0

134.6393 1.013e0

134.7425 2.025e0

134.8276 1.013e0

134.8533 3.038e0

134.8811 2.025e0

134.8953 2.025e0

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135.0557 1.013e0

135.0899 1.013e0

135.1356 1.013e0

135.1610 2.025e0

135.2238 4.051e0

135.2438 1.013e0

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137.4091 1.013e0

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137.8079 1.013e0

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288.2227 9.114e0

288.3293 2.025e0

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