

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 1000.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 27-27 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 S: 0-2

Minimum: -1.5

Maximum: 5.0 10.0 1000.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

478.2342 478.2342 0.0 0.0 13.5 268.1 C27 H32 N3 O5

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.

Peak list

100.0347 3.038e0

100.0564 4.051e0

100.0768 1.275e0

100.0949 2.163e0

100.1241 2.025e0

100.1427 1.013e0

100.1719 2.025e0

100.1920 2.025e0

100.2472 3.038e0

100.2611 2.025e0

100.2829 3.038e0

100.3010 2.025e0

100.3338 3.038e0

100.3680 3.038e0

100.3914 2.025e0

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101.9652 2.025e0

101.9763 2.346e0

101.9893 2.025e0

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102.1413 2.736e1

102.1745 2.025e0

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102.2243 2.025e0

102.2418 2.025e0

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