

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.

Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 20-24 H: 0-26 N: 1-2 O: 1-5 Na: 0-1 S: 1-5

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

424.1582 424.1583 -0.1 -0.2 12.5 6.1 C24 H26 N O4 S

100.0368 3.038e0

100.0487 2.025e0

100.0513 3.038e0

100.0621 1.013e0

100.0699 2.025e0

100.0759 5.063e0

100.0832 1.013e0

100.0859 1.013e0

100.0910 1.013e0

100.1097 4.051e0

100.1126 1.013e0

100.1204 1.013e0

100.1337 1.013e0

100.1604 2.025e0

100.2003 1.013e0

100.2348 1.013e0

100.2481 1.013e0

100.2748 1.013e0

100.3065 1.013e0

100.3253 1.013e0

100.3466 1.013e0

100.3704 1.013e0

100.4744 1.013e0

100.4850 1.013e0

100.5384 1.013e0

100.5572 2.025e0

100.5706 1.013e0

100.5917 1.013e0

100.6157 2.025e0

100.6557 2.025e0

100.6718 1.013e0

100.7008 1.013e0

100.7250 1.013e0

100.7437 1.013e0

100.7464 1.013e0

100.7891 1.013e0

100.7916 1.013e0

100.8077 1.013e0

100.8399 1.013e0

100.8505 1.013e0

100.8878 1.013e0

100.9012 1.013e0

100.9063 1.013e0

100.9280 1.013e0

100.9386 1.013e0

100.9439 2.025e0

100.9465 1.013e0

100.9946 2.025e0

101.0079 1.013e0

101.0188 1.013e0

101.0428 1.013e0

101.0710 1.066e2

101.0725 3.821e2

101.1148 1.013e0

101.1203 1.013e0

101.1254 1.013e0

101.1337 1.013e0

101.1483 2.025e0

101.1536 2.025e0

101.1710 1.013e0

101.1761 1.013e0

101.1923 1.013e0

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101.2164 2.025e0

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101.2352 1.013e0

101.2458 1.013e0

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101.3529 1.013e0

101.3636 2.025e0

101.3742 1.013e0

101.3848 1.013e0

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101.4192 3.038e0

101.4305 1.013e0

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101.4439 2.025e0

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101.4707 1.013e0

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101.5082 1.013e0

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101.5429 2.025e0

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101.8889 1.013e0

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102.1262 2.025e0

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111.1026 4.051e0

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112.2930 1.013e0

112.4226 2.025e0

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