



Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 26-26 H: 0-200 N: 0-10 O: 0-10 Br: 1-1

Minimum: -1.5

Maximum: 5.0 7.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

526.1337 526.1341 -0.4 -0.8 13.5 1.5 C26 H29 N3 O4 Br

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.

100.0089 1.013e0

100.0898 2.025e0

100.1378 2.025e0

100.1656 1.013e0

100.2241 1.013e0

100.2401 1.013e0

100.2611 1.013e0

100.3119 3.038e0

100.3997 1.013e0

100.4158 1.013e0

100.4318 1.013e0

100.5197 1.013e0

100.5408 1.013e0

100.5687 2.025e0

100.5861 1.013e0

100.6713 1.013e0

100.7033 1.013e0

100.7273 1.013e0

100.7592 2.025e0

100.7725 1.013e0

100.7968 1.013e0

100.9034 2.025e0

100.9302 1.013e0

100.9435 3.038e0

101.0008 2.025e0

101.0503 1.013e0

101.0770 5.063e0

101.1036 1.013e0

101.1344 2.025e0

101.1624 1.013e0

101.1757 1.013e0

101.1973 2.025e0

101.2184 2.025e0

101.2933 1.013e0

101.3148 1.013e0

101.3415 1.013e0

101.3654 2.025e0

101.3787 1.013e0

101.4057 2.025e0

101.4739 2.025e0

101.5037 4.051e0

101.5180 1.013e0

101.5874 2.025e0

101.6813 1.013e0

101.7107 1.013e0

101.7724 1.013e0

101.7829 1.013e0

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101.8824 1.013e0

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102.0473 2.025e0

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102.1155 1.013e0

102.1267 1.013e0

102.1907 1.013e0

102.2138 2.025e0

102.2475 1.013e0

102.2687 1.013e0

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102.7775 4.051e0

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102.8687 2.025e0

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102.9334 1.013e0

102.9630 1.013e0

102.9859 2.025e0

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103.0709 2.025e0

103.1410 2.025e0

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103.1843 1.013e0

103.2084 1.013e0

103.2341 2.025e0

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103.3622 1.013e0

103.3812 1.013e0

103.4516 1.013e0

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103.5284 2.025e0

103.5486 1.013e0

103.5690 2.025e0

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103.9153 2.025e0

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105.9655 2.025e0

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120.9815 3.038e0

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