

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 25-25 H: 0-200 N: 0-10 O: 0-20 S: 3-3 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

585.1632 585.1627 0.5 0.9 6.5 16.2 C25 H38 O8 S3 Na

M+NH4 ADDUCT ALSO SEEN

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.

100.0323 2.025e0

100.0470 1.013e0

100.0755 9.426e0

100.0910 5.063e0

100.1212 4.051e0

100.1614 1.013e0

100.2263 2.025e0

100.2491 1.013e0

100.2795 2.025e0

100.2941 1.013e0

100.3221 2.025e0

100.3503 2.025e0

100.4212 3.038e0

100.4392 2.025e0

100.4857 1.013e0

100.5210 4.051e0

100.5749 5.063e0

100.6138 1.013e0

100.6296 1.013e0

100.6551 2.025e0

100.6922 2.025e0

100.7029 2.025e0

100.7123 1.013e0

100.7445 1.013e0

100.7709 4.051e0

100.8242 1.013e0

100.8469 2.025e0

100.8723 1.013e0

100.8843 2.025e0

100.9003 2.025e0

100.9406 2.259e0

100.9659 2.025e0

100.9884 2.025e0

101.0164 1.013e0

101.0731 2.705e2

101.1113 6.076e0

101.1311 1.013e0

101.1421 1.013e0

101.1839 4.051e0

101.2128 2.025e0

101.2353 1.013e0

101.2703 1.013e0

101.2930 2.025e0

101.3250 2.025e0

101.3436 3.038e0

101.3834 3.038e0

101.4053 2.025e0

101.4239 6.076e0

101.4415 1.013e0

101.4600 1.013e0

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101.5300 1.013e0

101.5483 1.013e0

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101.6261 1.013e0

101.6449 2.025e0

101.6596 2.202e0

101.7132 4.051e0

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101.7816 1.013e0

101.7922 1.013e0

101.8483 1.013e0

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101.9049 2.025e0

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101.9529 1.013e0

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102.1043 3.038e0

102.1281 7.089e0

102.1438 2.025e0

102.1599 1.013e0

102.1980 3.038e0

102.2364 2.025e0

102.3029 3.038e0

102.3292 1.013e0

102.3451 2.025e0

102.4016 1.013e0

102.4418 1.013e0

102.4607 2.025e0

102.4769 1.013e0

102.5616 2.025e0

102.5870 5.063e0

102.6087 3.038e0

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102.8160 1.013e0

102.8563 2.025e0

102.8834 2.025e0

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102.9669 1.013e0

102.9937 1.013e0

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103.0990 1.013e0

103.1248 2.025e0

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103.2447 1.013e0

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103.8483 3.038e0

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103.9802 1.013e0

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104.0452 1.013e0

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104.1564 1.013e0

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104.2173 2.025e0

104.2620 2.025e0

104.2771 2.025e0

104.3136 1.013e0

104.3327 1.013e0

104.3462 1.013e0

104.3667 2.025e0

104.3872 1.013e0

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104.4496 4.051e0

104.4738 1.013e0

104.4901 1.013e0

104.5213 4.051e0

104.5446 1.013e0

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105.2928 3.038e0

105.3221 4.051e0

105.3453 3.038e0

105.3650 2.025e0

105.3814 2.025e0

105.4069 4.051e0

105.4360 2.025e0

105.4590 1.013e0

105.4782 2.025e0

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105.5246 3.038e0

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112.0866 5.063e0

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112.1756 1.013e0

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113.8673 1.013e0

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114.1679 2.025e0

114.2223 2.025e0

114.2518 2.025e0

114.2790 2.025e0

114.3071 2.025e0

114.3555 2.025e0

114.3842 1.013e0

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114.4529 5.063e0

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116.2208 1.013e0

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116.3243 2.025e0

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116.5190 2.025e0

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116.9440 1.013e0

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119.1721 1.013e0

119.2022 3.038e0

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121.0976 3.038e0

121.1219 2.025e0

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121.2751 1.013e0

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121.3497 2.025e0

121.3965 2.025e0

121.4131 1.013e0

121.4533 4.051e0

121.4890 2.025e0

121.5083 2.025e0

121.5360 1.013e0

121.5534 1.013e0

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121.7958 4.051e0

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121.9666 1.013e0

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122.0709 2.025e0

122.0981 4.224e1

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122.3469 2.025e0

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122.8839 3.038e0

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122.9396 1.013e0

122.9660 1.013e0

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