 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

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

Elements Used:

C: 17-17 H: 0-200 N: 0-10 O: 0-10

Minimum: -1.5

Maximum: 5.0 7.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

298.1550 298.1556 -0.6 -2.0 9.5 1.8 C17 H20 N3 O2

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.

100.0016 2.025e0

100.0334 1.013e0

100.0600 2.025e0

100.0891 1.013e0

100.1385 2.025e0

100.1637 1.013e0

100.1837 2.025e0

100.2144 1.013e0

100.2487 2.025e0

100.2701 1.013e0

100.3365 1.013e0

100.3525 2.025e0

100.3740 1.013e0

100.3898 2.025e0

100.4111 2.025e0

100.4298 2.025e0

100.4727 6.076e0

100.5044 1.013e0

100.5254 1.013e0

100.5790 1.013e0

100.6001 1.013e0

100.6134 2.025e0

100.6294 2.025e0

100.6534 2.025e0

100.6987 1.013e0

100.7342 3.038e0

100.7721 2.025e0

100.8002 1.013e0

100.8160 1.013e0

100.8429 1.013e0

100.9016 1.013e0

100.9787 1.013e0

100.9947 1.013e0

101.0190 1.013e0

101.0669 1.013e0

101.0778 2.025e0

101.0917 3.038e0

101.1099 2.025e0

101.1498 1.013e0

101.1953 1.013e0

101.2173 2.383e0

101.2540 1.013e0

101.2873 2.025e0

101.3062 2.025e0

101.3381 2.025e0

101.3583 1.013e0

101.3764 3.038e0

101.4199 1.013e0

101.4866 2.264e0

101.5054 2.025e0

101.5571 4.051e0

101.5857 2.025e0

101.6031 2.025e0

101.6204 1.013e0

101.6512 2.025e0

101.6820 1.013e0

101.6982 1.013e0

101.7122 3.038e0

101.7987 2.025e0

101.8132 1.013e0

101.8428 1.013e0

101.8651 3.038e0

101.8818 2.025e0

101.8993 1.013e0

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101.9850 1.013e0

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102.0843 2.025e0

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102.1435 1.013e0

102.1595 1.013e0

102.1898 4.051e0

102.2211 1.013e0

102.2827 1.013e0

102.3072 1.013e0

102.3284 1.013e0

102.3529 1.013e0

102.3651 3.038e0

102.4025 2.025e0

102.4175 1.013e0

102.5410 1.013e0

102.5843 1.013e0

102.6688 2.025e0

102.7039 2.025e0

102.7335 2.025e0

102.7672 1.013e0

102.7885 1.013e0

102.8214 3.038e0

102.8371 1.013e0

102.8777 2.025e0

102.9026 3.038e0

102.9233 3.038e0

102.9504 1.013e0

102.9731 2.476e0

103.0124 1.013e0

103.0258 3.038e0

103.0392 2.025e0

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103.1578 1.013e0

103.1943 2.025e0

103.2416 2.025e0

103.2712 3.038e0

103.3092 2.025e0

103.3322 5.063e0

103.3576 3.038e0

103.3764 1.013e0

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103.6874 2.025e0

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103.9960 1.013e0

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104.2564 1.013e0

104.2941 1.013e0

104.3213 1.013e0

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104.4625 2.025e0

104.5321 2.308e0

104.5766 1.013e0

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104.7370 2.025e0

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104.8891 1.013e0

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105.1577 5.568e0

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105.2342 6.076e0

105.2621 1.013e0

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105.2976 3.038e0

105.3345 2.025e0

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105.4107 2.062e0

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105.5281 3.038e0

105.5517 4.051e0

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105.6741 1.013e0

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105.7809 1.783e0

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105.8792 2.025e0

105.9007 2.025e0

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105.9284 1.013e0

105.9570 2.143e0

105.9692 1.013e0

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106.0771 4.051e0

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106.1457 2.025e0

106.1712 4.051e0

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106.2291 2.025e0

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114.1811 1.013e0

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114.5189 2.025e0

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116.6868 1.013e0

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116.7929 1.013e0

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116.8820 2.025e0

116.9133 1.013e0

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120.1643 1.013e0

120.1876 2.025e0

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120.2717 1.013e0

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120.5559 2.025e0

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120.7470 2.025e0

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120.8850 3.038e0

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121.3488 2.025e0

121.3873 1.013e0

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121.5714 1.013e0

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121.9407 1.013e0

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