 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

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

Elements Used:

C: 14-14 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 69Ga: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

216.1393 216.1388 0.5 2.3 6.5 107.9 C14 H18 N O

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.

ANALYSIS RUN USING: WATERS LCT PREMIER (ESI POSITIVE/ESI NEGATIVE)

100.0041 1.013e0

100.0454 3.807e0

100.0781 3.026e1

100.1121 8.792e0

100.1423 1.013e0

100.1649 2.025e0

100.1957 1.013e0

100.3123 1.013e0

100.3857 4.051e0

100.4112 2.025e0

100.5135 2.025e0

100.5280 1.013e0

100.5496 1.013e0

100.5773 3.038e0

100.6030 1.013e0

100.6667 2.025e0

100.7094 1.013e0

100.7388 2.025e0

100.7641 2.025e0

100.7867 1.013e0

100.8067 2.025e0

100.8214 1.013e0

100.8347 1.013e0

100.8457 1.013e0

100.8668 1.013e0

100.9014 1.013e0

100.9264 3.715e0

100.9549 1.013e0

100.9772 3.038e0

101.0083 1.013e0

101.0296 1.855e0

101.0720 2.482e2

101.1146 2.429e0

101.1310 1.013e0

101.1472 1.013e0

101.1794 1.013e0

101.2020 3.038e0

101.2301 1.013e0

101.2514 1.013e0

101.2916 1.013e0

101.3317 2.025e0

101.3479 1.013e0

101.3664 2.025e0

101.3851 4.049e0

101.4079 2.025e0

101.4306 1.013e0

101.4494 3.038e0

101.4789 3.038e0

101.5137 1.013e0

101.5350 1.013e0

101.5752 2.025e0

101.5886 1.013e0

101.6315 1.013e0

101.6611 2.025e0

101.6796 1.013e0

101.7011 1.013e0

101.7278 2.025e0

101.7467 3.038e0

101.7601 1.013e0

101.7762 1.013e0

101.8031 1.013e0

101.8593 4.051e0

101.9129 2.025e0

101.9384 2.025e0

101.9748 1.013e0

102.0188 1.977e0

102.0401 2.867e0

102.0711 2.625e1

102.0929 1.018e1

102.1284 2.651e1

102.1741 3.038e0

102.2296 1.013e0

102.2565 1.013e0

102.2833 2.025e0

102.3184 1.013e0

102.3775 2.025e0

102.3988 1.013e0

102.4257 1.013e0

102.4475 1.013e0

102.4609 1.013e0

102.4831 3.038e0

102.5120 2.025e0

102.5496 1.013e0

102.5765 1.013e0

102.5886 2.025e0

102.6248 1.013e0

102.6494 1.013e0

102.6842 4.051e0

102.7111 1.013e0

102.7287 2.025e0

102.7813 1.013e0

102.8027 1.013e0

102.8181 3.038e0

102.8324 1.013e0

102.8782 2.025e0

102.9119 2.025e0

102.9942 1.013e0

103.0076 1.013e0

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103.2045 2.025e0

103.2491 2.025e0

103.2707 2.025e0

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103.6694 1.013e0

103.6829 1.013e0

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103.7532 2.025e0

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104.0706 9.542e0

104.1090 2.307e0

104.1405 1.013e0

104.1760 1.013e0

104.1921 1.013e0

104.2070 2.025e0

104.2342 2.025e0

104.2966 2.025e0

104.3088 1.020e0

104.3415 1.013e0

104.3551 1.013e0

104.4105 2.025e0

104.4392 1.013e0

104.4676 2.025e0

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104.8181 2.025e0

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104.9134 2.025e0

104.9690 2.025e0

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105.0701 2.872e2

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105.2200 5.466e0

105.2383 7.698e0

105.2621 2.025e0

105.2996 9.096e0

105.3180 3.038e0

105.3340 3.800e0

105.3530 4.025e0

105.3698 2.216e0

105.4009 8.101e0

105.4180 3.038e0

105.4428 3.038e0

105.4642 5.063e0

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105.9856 2.025e0

105.9993 2.025e0

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106.0484 3.569e1

106.0752 6.970e1

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106.2485 2.025e0

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108.2169 2.025e0

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111.8768 2.025e0

111.9080 1.013e0

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112.0788 2.110e1

112.1232 1.587e0

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115.9490 1.013e0

115.9721 1.013e0

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116.1893 1.013e0

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116.2982 1.013e0

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116.4244 1.013e0

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117.0667 2.819e1

117.1059 5.592e0

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120.3788 7.089e0

120.3951 7.089e0

120.4253 3.038e0

120.4426 5.063e0

120.4667 3.311e0

120.4875 2.025e0

120.5121 1.013e1

120.5301 4.713e0

120.5654 3.038e0

120.5922 2.607e0

120.6120 3.038e0

120.6323 5.797e0

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120.7497 2.025e0

120.7632 2.025e0

120.8070 4.051e0

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120.8660 3.038e0

120.8815 2.025e0

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120.9355 2.174e0

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120.9779 1.013e0

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121.0769 8.641e0

121.1401 2.025e0

121.1605 2.025e0

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121.2967 2.025e0

121.3227 1.013e0

121.3402 2.025e0

121.3637 1.013e0

121.3903 4.051e0

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122.7994 1.013e0

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