 Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

621 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 S: 0-1 56Fe: 0-1

Minimum: -15.0

Maximum: 5.0 15.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

236.1657 236.1651 0.6 2.5 4.5 27.8 C14 H22 N 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.

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

115.9386 2.437e0

115.9575 2.025e0

115.9747 2.025e0

115.9942 4.051e0

116.0291 2.025e0

116.0420 3.038e0

116.0853 1.114e1

116.1085 2.807e1

116.1466 1.235e1

116.1674 3.038e0

116.1923 1.013e1

116.2282 2.025e0

116.2439 1.013e0

116.2649 3.038e0

116.2925 1.013e0

116.3206 1.215e1

116.3740 3.038e0

116.4102 3.038e0

116.4299 3.753e0

116.4443 3.336e0

116.4702 1.013e0

116.4971 4.051e0

116.5190 3.496e0

116.5449 1.013e0

116.5642 5.063e0

116.5979 4.051e0

116.6317 3.038e0

116.6480 2.025e0

116.6681 2.025e0

116.6884 1.013e0

116.7115 2.967e0

116.7295 3.038e0

116.7619 5.063e0

116.8106 4.051e0

116.8357 5.063e0

116.8558 3.038e0

116.8899 4.051e0

116.9230 3.038e0

116.9416 5.063e0

116.9755 3.038e0

117.0121 3.038e0

117.0272 1.013e0

117.0658 6.014e0

117.1029 3.218e0

117.1217 4.051e0

117.1553 6.098e0

117.1750 5.041e0

117.1955 2.025e0

117.2143 2.025e0

117.2401 2.025e0

117.2724 4.051e0

117.2898 2.449e0

117.3064 2.025e0

117.3198 3.038e0

117.3480 2.025e0

117.3694 1.013e0

117.3937 5.063e0

117.4154 2.285e0

117.4330 2.025e0

117.4487 3.038e0

117.4616 2.025e0

117.4862 2.025e0

117.5035 2.025e0

117.5193 2.025e0

117.5395 2.025e0

117.5553 4.051e0

117.6075 3.038e0

117.6390 2.025e0

117.6553 3.530e0

117.6749 3.038e0

117.7138 2.025e0

117.7457 2.025e0

117.7838 4.051e0

117.8219 7.089e0

117.8595 3.038e0

117.8815 5.063e0

117.9141 4.051e0

117.9379 5.063e0

117.9828 3.038e0

118.0000 4.051e0

118.0212 5.063e0

118.0460 6.137e0

118.0657 1.132e1

118.0879 6.909e0

118.1251 1.722e1

118.1499 6.937e0

118.1812 4.008e0

118.2178 4.051e0

118.2704 7.196e0

118.3013 2.025e0

118.3205 6.629e0

118.3489 2.025e0

118.3782 5.063e0

118.4083 2.025e0

118.4256 2.025e0

118.4610 5.063e0

118.4832 3.299e0

118.5047 5.063e0

118.5309 2.025e0

118.5643 6.076e0

118.5840 2.799e0

118.6080 4.051e0

118.6570 1.013e0

118.6728 4.051e0

118.6988 2.025e0

118.7161 2.025e0

118.7349 2.025e0

118.7552 1.013e0

118.7988 2.025e0

118.8228 4.051e0

118.8478 1.013e0

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118.9703 6.076e0

118.9916 2.025e0

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119.0443 3.038e0

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119.1279 3.038e0

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119.2375 3.038e0

119.2555 2.025e0

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119.3816 3.038e0

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119.4687 2.025e0

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119.5152 2.183e0

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119.5589 1.013e0

119.5882 3.038e0

119.6125 3.038e0

119.6305 4.051e0

119.6488 1.013e0

119.6896 1.013e0

119.7128 5.800e0

119.7477 3.038e0

119.7820 4.051e0

119.7969 1.013e0

119.8339 5.063e0

119.8633 3.038e0

119.8884 5.063e0

119.9250 2.843e0

119.9427 2.025e0

119.9586 2.025e0

119.9775 1.063e0

119.9904 2.025e0

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120.1054 2.062e0

120.1385 1.072e1

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120.3330 2.025e0

120.3475 2.025e0

120.3649 2.025e0

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120.4335 4.051e0

120.4860 2.025e0

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120.5763 2.025e0

120.5902 3.038e0

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120.6483 4.693e0

120.6712 4.051e0

120.6885 2.025e0

120.7339 2.025e0

120.7744 4.051e0

120.8026 2.025e0

120.8322 4.051e0

120.8712 2.025e0

120.8871 6.076e0

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122.2319 3.038e0

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126.7464 2.025e0

126.7827 1.013e0

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126.8392 2.025e0

126.8664 1.013e0

126.8811 1.013e0

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126.9739 2.025e0

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127.0970 1.694e0

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127.1960 1.013e0

127.2333 4.051e0

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127.3232 2.025e0

127.3562 2.025e0

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127.4156 4.051e0

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127.6335 2.025e0

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127.7389 2.025e0

127.7598 2.025e0

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127.8289 3.038e0

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127.9446 2.025e0

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128.0233 3.038e0

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128.1450 5.063e0

128.1839 1.013e0

128.2320 1.013e0

128.2453 2.025e0

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128.2771 1.013e0

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128.3339 1.013e0

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130.0466 1.013e0

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130.2221 3.038e0

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130.5483 2.025e0

130.5695 2.025e0

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130.6403 4.051e0

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130.7567 1.013e0

130.7778 1.013e0

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130.8538 1.013e0

130.8741 3.150e0

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130.9691 2.025e0

130.9917 2.025e0

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131.0869 2.576e0

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131.1735 4.051e0

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131.2279 1.013e0

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131.2944 4.261e0

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131.4399 6.076e0

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131.5537 1.013e0

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132.5687 2.025e0

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132.9822 2.025e0

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134.4291 4.051e0

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134.6139 4.051e0

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134.6741 2.025e0

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134.7501 2.025e0

134.7785 5.063e0

134.8319 1.013e0

134.8438 1.013e0

134.8788 3.038e0

134.9025 2.025e0

134.9183 2.025e0

134.9536 3.038e0

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135.0672 8.101e0

135.0940 7.678e0

135.1172 1.961e0

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135.9973 1.013e0

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136.0545 3.038e0

136.0932 1.313e1

136.1431 2.025e0

136.1637 3.038e0

136.2201 3.038e0

136.2688 3.038e0

136.2962 3.038e0

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301.7739 1.855e0

301.8018 4.435e0

301.8372 3.880e0

301.8689 4.426e0

301.9109 1.471e0

301.9605 5.758e0

302.0069 1.011e1

302.0870 2.657e0

302.1251 3.164e0

302.1734 7.982e0

302.3424 3.227e0

302.3863 3.255e0

302.4503 3.932e0

302.5039 2.025e0

302.5790 6.076e0

302.6490 4.460e0

302.7430 1.013e0

302.7738 2.604e0

302.8541 4.751e0

302.9053 8.826e0

302.9527 2.025e0

303.0125 3.027e0

303.0514 2.025e0

303.0887 4.796e0

303.1527 6.699e0

303.2832 9.228e0

303.3698 2.432e0

303.4456 7.966e0

303.5027 3.959e0

303.5495 1.387e0

303.6398 1.770e0

303.6650 2.924e0

303.7518 2.025e0

303.7774 1.685e0

303.8402 6.242e0

303.8737 1.467e0

303.9486 6.076e0

304.0086 3.027e0

304.0542 3.038e0

304.1037 5.227e0

304.1445 1.893e1

304.1916 2.962e0

304.3082 2.520e1

304.4042 6.076e0

304.4326 4.461e0

304.4758 3.918e0

304.5117 2.859e0

304.5450 2.248e0

304.5898 2.737e0

304.6417 6.944e0

304.6946 6.699e0

304.7773 1.796e0

304.8036 4.472e0

304.8669 4.051e0

304.9673 1.005e1

305.1463 1.468e3

305.2628 5.555e0

305.3118 1.740e1

305.3622 1.453e1

305.4145 2.973e0

305.4514 4.753e0

305.4873 6.209e0

305.5211 2.679e0

305.5663 1.993e0

305.6016 4.051e0

305.6635 4.564e0

305.7629 7.009e0

305.8487 6.727e0

305.9176 3.353e0

305.9473 8.385e0

306.0156 3.893e0

306.0788 2.111e0

306.1511 3.516e2

306.2372 7.889e0

306.3246 6.180e0

306.3872 4.769e0

306.4688 3.678e0

306.5023 4.039e0

306.5580 3.947e0

306.6158 5.063e0

306.6628 1.426e1

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306.8690 1.339e0

306.9360 4.997e0

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307.0573 6.521e0

307.1595 5.213e1

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307.4593 1.585e0

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307.6609 6.245e0

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