 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 10-10 H: 0-100 N: 0-15 O: 0-20 S: 0-1

Minimum: -15.0

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

179.0536 179.0531 0.5 2.8 5.5 3.9 C10 H11 O S

M-OH

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)

108.6951 2.025e0

108.7132 4.051e0

108.7465 1.013e0

108.7767 3.038e0

108.7955 3.038e0

108.8213 1.013e0

108.8337 2.025e0

108.8737 1.013e0

108.8941 5.063e0

108.9209 1.013e0

108.9446 4.051e0

108.9598 2.025e0

108.9739 1.013e0

109.0044 2.025e0

109.0338 3.038e0

109.0513 1.013e0

109.1162 2.994e0

109.1541 2.025e0

109.1775 2.025e0

109.1985 1.013e0

109.2227 3.038e0

109.2471 2.025e0

109.2610 2.025e0

109.2901 3.038e0

109.3136 2.025e0

109.3374 1.013e0

109.3623 1.013e0

109.3847 1.013e0

109.4013 1.013e0

109.4305 2.025e0

109.4499 2.025e0

109.4735 2.025e0

109.4998 2.025e0

109.5399 1.790e0

109.5528 4.051e0

109.5708 3.038e0

109.5873 1.013e0

109.6236 3.038e0

109.6375 7.089e0

109.6738 3.038e0

109.7112 3.038e0

109.7294 3.255e0

109.7489 3.038e0

109.7656 1.013e0

109.7854 2.733e0

109.8018 3.038e0

109.8350 1.013e0

109.8523 4.875e0

109.8761 3.038e0

109.9132 3.038e0

109.9369 2.025e0

109.9590 2.025e0

110.0086 3.038e0

110.0413 1.013e0

110.0721 7.605e0

110.1277 1.013e0

110.1419 2.025e0

110.1752 3.038e0

110.1960 4.051e0

110.2162 3.038e0

110.2310 2.025e0

110.2866 1.013e0

110.3322 3.038e0

110.3566 1.013e0

110.3807 3.038e0

110.4069 2.025e0

110.4411 3.038e0

110.4749 3.038e0

110.4904 1.013e0

110.5101 1.013e0

110.5297 1.013e0

110.5465 1.013e0

110.5657 4.051e0

110.5845 5.063e0

110.6331 5.839e0

110.6735 2.025e0

110.6915 1.013e0

110.7140 1.013e0

110.7402 2.420e0

110.7847 5.063e0

110.8259 1.013e0

110.8427 1.013e0

110.8706 1.013e0

110.8816 1.013e0

110.8986 3.038e0

110.9400 7.089e0

110.9658 2.025e0

110.9874 3.038e0

111.0191 1.013e0

111.0908 1.411e1

111.1335 3.633e0

111.1492 2.025e0

111.1672 1.013e0

111.1922 3.038e0

111.2187 4.051e0

111.2552 3.038e0

111.2741 1.013e0

111.2977 2.025e0

111.3159 1.013e0

111.3337 4.051e0

111.3639 5.095e0

111.3804 2.025e0

111.4113 1.013e0

111.4281 3.038e0

111.4449 1.013e0

111.4779 3.038e0

111.5277 2.209e0

111.5459 4.051e0

111.6202 3.038e0

111.6386 2.025e0

111.6602 3.038e0

111.6919 2.025e0

111.7186 2.025e0

111.7407 3.038e0

111.7565 2.025e0

111.7904 5.063e0

111.8225 2.025e0

111.8493 1.013e0

111.8787 2.025e0

111.8987 3.269e0

111.9320 2.025e0

111.9530 2.025e0

111.9889 3.038e0

112.0066 2.025e0

112.0474 2.025e0

112.0622 3.366e0

112.0947 1.092e0

112.1191 1.340e0

112.1360 2.025e0

112.1593 3.038e0

112.1837 6.076e0

112.2345 1.013e0

112.3029 3.038e0

112.3147 2.039e0

112.3374 2.025e0

112.3471 1.013e0

112.3698 2.025e0

112.3868 2.025e0

112.4109 4.051e0

112.4472 2.025e0

112.4737 1.013e0

112.4878 1.013e0

112.5057 2.766e0

112.5260 2.025e0

112.5398 3.038e0

112.5598 2.025e0

112.5807 4.051e0

112.6113 3.038e0

112.6345 1.013e0

112.6648 6.076e0

112.7083 5.063e0

112.7278 2.025e0

112.7485 3.038e0

112.7926 2.025e0

112.8405 1.013e0

112.8632 1.013e0

112.9105 3.038e0

112.9298 3.569e0

112.9613 1.013e1

113.0006 5.063e0

113.0192 4.051e0

113.0498 8.101e0

113.0756 5.288e0

113.1090 3.110e1

113.1662 5.082e0

113.1909 2.025e0

113.2049 2.025e0

113.2288 2.025e0

113.2604 4.051e0

113.2972 5.063e0

113.3208 2.025e0

113.3364 2.025e0

113.3645 2.025e0

113.3944 3.038e0

113.4368 1.013e0

113.4621 3.487e0

113.4893 3.176e0

113.5189 1.013e0

113.5387 1.013e0

113.5558 2.025e0

113.5898 2.025e0

113.6532 3.038e0

113.6689 3.038e0

113.6830 2.025e0

113.7000 1.013e0

113.7340 2.025e0

113.7625 2.025e0

113.7938 2.025e0

113.8093 2.025e0

113.8404 2.025e0

113.8575 2.025e0

113.8930 1.013e0

113.9113 2.025e0

113.9397 2.025e0

113.9616 6.076e0

113.9921 4.051e0

114.0149 1.013e0

114.0262 1.013e0

114.0475 2.025e0

114.0952 1.752e0

114.1122 1.752e0

114.1240 2.025e0

114.1655 1.013e0

114.1980 2.025e0

114.2135 3.038e0

114.2404 2.025e0

114.2581 3.038e0

114.2788 3.145e0

114.3030 2.025e0

114.3300 1.042e0

114.3518 3.038e0

114.3724 1.013e0

114.3944 3.038e0

114.4278 3.038e0

114.4410 4.051e0

114.4723 1.013e0

114.4946 1.013e0

114.5190 2.145e0

114.5432 2.025e0

114.5607 2.721e0

114.5872 2.140e0

114.6058 2.025e0

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114.7308 1.013e0

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114.7765 1.013e0

114.7992 1.013e0

114.8390 3.038e0

114.8731 1.013e0

114.8961 2.025e0

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114.9302 1.013e0

114.9568 5.063e0

114.9874 1.013e0

114.9986 1.013e0

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115.0880 1.393e2

115.1283 1.437e1

115.1611 1.013e0

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115.2052 2.025e0

115.2415 4.051e0

115.2737 2.025e0

115.2893 2.025e0

115.3145 3.038e0

115.3250 2.025e0

115.3436 1.013e0

115.3636 2.025e0

115.3813 4.023e0

115.4051 3.467e0

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115.5832 2.025e0

115.5963 2.025e0

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115.6663 1.013e0

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115.7977 3.038e0

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116.0325 1.013e0

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116.0908 7.952e0

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116.1437 2.581e0

116.1560 2.482e0

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116.2698 1.013e0

116.2885 2.025e0

116.3057 2.025e0

116.3258 4.051e0

116.3572 2.025e0

116.3746 2.025e0

116.3960 1.013e0

116.4146 2.025e0

116.4271 5.063e0

116.4706 3.038e0

116.4977 4.051e0

116.5423 4.051e0

116.5580 2.025e0

116.5826 2.025e0

116.5959 4.051e0

116.6103 4.051e0

116.6426 2.025e0

116.6650 6.076e0

116.6872 2.025e0

116.7223 3.038e0

116.7479 5.063e0

116.7756 3.038e0

116.8020 6.076e0

116.8205 1.013e0

116.8537 2.025e0

116.8779 5.063e0

116.9041 1.013e0

116.9296 2.025e0

116.9579 3.038e0

116.9760 2.025e0

116.9981 3.038e0

117.0198 3.038e0

117.0375 2.025e0

117.0699 6.246e0

117.1051 1.035e1

117.1324 2.025e0

117.1482 1.013e0

117.1827 2.025e0

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117.4505 2.025e0

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117.6420 6.076e0

117.6853 2.025e0

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117.9751 1.013e0

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118.3057 2.025e0

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118.8353 2.025e0

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118.8925 3.038e0

118.9265 3.038e0

118.9744 5.063e0

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119.1961 2.025e0

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119.2772 1.013e0

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119.3657 4.051e0

119.3884 4.757e0

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119.5994 1.013e0

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119.6651 4.051e0

119.7093 3.038e0

119.7260 3.447e0

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119.8321 2.025e0

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119.9954 2.025e0

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120.1033 3.944e0

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120.1610 1.013e0

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120.2268 2.025e0

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120.2676 2.025e0

120.2965 2.025e0

120.3133 3.038e0

120.3358 2.025e0

120.3680 3.038e0

120.3864 5.063e0

120.4146 6.076e0

120.4524 4.051e0

120.4874 3.038e0

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120.5312 2.025e0

120.5605 2.025e0

120.5751 2.025e0

120.5956 2.025e0

120.6244 2.025e0

120.6365 1.013e0

120.6596 2.025e0

120.6774 1.013e0

120.7005 3.038e0

120.7457 4.051e0

120.8056 2.025e0

120.8305 4.051e0

120.8553 1.013e0

120.8786 3.038e0

120.9019 1.013e0

120.9224 1.013e0

120.9413 2.025e0

120.9545 1.013e0

120.9749 2.025e0

121.0207 5.063e0

121.0655 8.972e0

121.0835 2.126e0

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121.1605 3.038e0

121.1797 1.062e0

121.2132 2.025e0

121.2275 3.038e0

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121.3522 2.025e0

121.3656 2.025e0

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121.4227 1.013e0

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121.6372 3.038e0

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121.8427 5.063e0

121.8653 1.013e0

121.8896 5.063e0

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121.9803 5.086e0

122.0041 5.063e0

122.0267 2.025e0

122.0482 4.051e0

122.0969 1.728e1

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122.1923 2.025e0

122.2087 1.013e0

122.2347 1.013e0

122.2489 3.038e0

122.2733 4.051e0

122.2937 2.025e0

122.3125 2.597e0

122.3481 2.025e0

122.3627 2.025e0

122.3855 6.051e0

122.4229 2.025e0

122.4496 2.025e0

122.4693 3.038e0

122.4992 1.013e0

122.5144 1.013e0

122.5431 4.051e0

122.5804 2.025e0

122.5998 2.717e0

122.6228 5.063e0

122.6599 2.025e0

122.6818 2.025e0

122.6975 3.038e0

122.7230 2.025e0

122.7399 3.038e0

122.7525 2.128e0

122.7822 2.025e0

122.8288 1.013e0

122.8570 2.025e0

122.8852 1.013e0

122.9113 1.013e0

122.9380 2.025e0

122.9540 2.025e0

122.9702 1.013e0

122.9883 1.013e0

123.0130 2.025e0

123.0336 2.025e0

123.0550 6.076e0

123.0952 2.488e0

123.1381 5.279e0

123.1856 1.013e0

123.2023 3.038e0

123.2239 2.025e0

123.2400 2.025e0

123.2622 3.038e0

123.2965 5.063e0

123.3392 2.025e0

123.3653 1.013e0

123.3859 1.013e0

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123.4466 2.025e0

123.4673 2.025e0

123.4939 2.025e0

123.5160 3.038e0

123.5307 1.013e0

123.5892 3.038e0

123.6193 2.025e0

123.6389 3.038e0

123.6713 2.025e0

123.6860 5.063e0

123.7021 3.038e0

123.7335 4.330e0

123.7943 5.179e0

123.8168 3.038e0

123.8440 1.013e0

123.8590 2.025e0

123.9145 4.051e0

123.9387 1.013e0

123.9665 5.063e0

124.0054 6.076e0

124.0321 2.025e0

124.0500 7.089e0

124.0874 7.950e0

124.1413 1.620e0

124.1827 2.025e0

124.1978 2.025e0

124.2201 1.013e0

124.2465 2.025e0

124.3259 3.450e0

124.3636 2.025e0

124.3868 5.063e0

124.4141 2.025e0

124.4419 2.025e0

124.4778 2.025e0

124.4956 1.013e0

124.5323 3.038e0

124.5473 6.076e0

124.5713 5.063e0

124.5931 2.025e0

124.6274 4.051e0

124.6567 3.038e0

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124.7593 2.025e0

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124.8692 3.038e0

124.8959 2.025e0

124.9136 2.025e0

124.9318 2.688e0

124.9550 8.101e0

124.9942 3.566e0

125.0205 1.013e0

125.0386 1.013e0

125.0728 1.228e0

125.1053 1.658e0

125.1280 1.066e0

125.1443 1.823e0

125.1614 2.795e0

125.1874 1.013e0

125.2218 4.051e0

125.2555 1.013e0

125.2714 3.038e0

125.2852 2.284e0

125.3060 2.025e0

125.3445 1.013e0

125.3775 2.025e0

125.3968 2.025e0

125.4176 4.051e0

125.4384 2.025e0

125.4668 2.025e0

125.4876 1.013e0

125.5100 2.025e0

125.5254 3.038e0

125.5755 2.025e0

125.6064 1.013e0

125.6261 2.025e0

125.6459 8.101e0

125.6924 2.721e0

125.7095 2.025e0

125.7376 2.025e0

125.7652 3.038e0

125.7957 1.386e0

125.8137 2.025e0

125.8452 2.025e0

125.8674 3.038e0

125.9047 1.013e0

125.9286 1.013e0

125.9448 2.025e0

125.9604 2.904e0

125.9804 5.234e0

126.0160 5.063e0

126.0477 3.038e0

126.0692 3.253e0

126.0896 1.044e0

126.1080 1.044e0

126.1288 3.409e0

126.1590 3.808e0

126.1748 1.985e0

126.2054 4.051e0

126.2312 2.025e0

126.2845 3.038e0

126.3051 3.314e0

126.3358 2.025e0

126.3741 3.038e0

126.3971 3.038e0

126.4097 3.038e0

126.4450 1.013e0

126.4776 2.025e0

126.5016 2.025e0

126.5334 5.063e0

126.5525 1.013e0

126.6054 3.038e0

126.6269 2.025e0

126.6500 6.076e0

126.6718 1.013e0

126.7040 3.038e0

126.7181 2.025e0

126.7451 2.025e0

126.7745 3.038e0

126.7957 5.063e0

126.8186 2.237e0

126.8395 4.051e0

126.8542 1.990e0

126.8817 3.204e0

126.9022 1.013e0

126.9293 1.013e0

126.9665 2.025e0

126.9888 1.013e0

127.0191 2.025e0

127.0452 3.038e0

127.0670 1.013e0

127.0867 4.322e0

127.1824 3.038e0

127.2111 1.013e0

127.2437 3.038e0

127.2661 4.051e0

127.3065 2.025e0

127.3367 1.013e0

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127.3813 4.051e0

127.4025 1.013e0

127.4205 1.013e0

127.4593 9.663e0

127.4746 5.173e0

127.4986 1.013e0

127.5304 2.025e0

127.5543 2.025e0

127.5784 2.025e0

127.5987 3.038e0

127.6188 1.013e0

127.6413 5.008e0

127.6638 1.013e0

127.6801 2.025e0

127.7168 5.063e0

127.7523 2.025e0

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