 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 15-15 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 F: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

227.0862 227.0872 -1.0 -4.4 9.5 2773144.8 C15 H12 O F

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.

115.5360 7.127e0

115.5868 1.103e1

115.6154 2.122e0

115.6616 3.423e0

115.6990 2.273e0

115.7533 6.449e0

115.7883 2.877e0

115.8058 7.375e0

115.9111 4.063e0

115.9789 7.335e0

116.1012 1.580e1

116.1398 5.288e0

116.1760 4.567e0

116.2064 2.730e0

116.3045 1.527e0

116.3621 3.316e0

116.4011 3.206e0

116.4843 2.492e0

116.5152 3.213e0

116.5461 3.539e0

116.7297 3.106e0

116.8081 4.965e0

116.8495 2.915e0

116.8811 9.463e0

116.9165 5.401e0

116.9737 7.922e0

117.0118 3.585e0

117.0380 4.108e0

117.1144 4.515e0

117.1742 2.935e0

117.2144 8.004e0

117.2689 4.269e0

117.3080 4.620e0

117.3787 2.169e0

117.4066 6.002e0

117.4353 8.690e0

117.5084 6.644e0

117.6159 2.791e0

117.6447 1.930e0

117.7312 7.363e0

117.8212 3.255e0

117.9011 2.878e0

117.9481 6.431e0

117.9847 7.844e0

118.0329 3.050e0

118.0908 5.664e0

118.1375 1.598e0

118.1951 3.543e0

118.2621 9.772e0

118.3013 1.473e1

118.3451 1.517e0

118.4063 4.768e0

118.4605 6.151e0

118.5133 1.573e0

118.5747 3.928e0

118.6244 4.609e0

118.6960 4.669e0

118.7329 8.806e0

118.8128 9.682e0

118.8530 2.498e0

118.8806 2.120e0

118.9635 7.035e0

118.9941 4.973e0

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119.1489 6.938e0

119.2203 1.361e0

119.2387 6.018e0

119.2795 1.454e0

119.3048 2.924e0

119.3422 6.247e0

119.3770 4.186e0

119.4119 5.226e0

119.4596 3.668e0

119.4903 3.490e0

119.5499 3.906e0

119.5817 1.636e0

119.6545 3.539e0

119.7325 9.769e0

119.8868 5.008e0

119.9325 8.503e0

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120.1697 1.693e0

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120.3572 9.232e0

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120.8421 4.209e0

120.9703 9.021e0

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121.1998 6.236e0

121.2604 5.340e0

121.3032 2.482e0

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121.5623 1.064e0

121.6058 4.484e0

121.7413 5.353e0

121.7854 1.161e1

121.8646 5.979e0

121.9138 2.260e0

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123.5832 1.347e1

123.6580 3.840e0

123.6909 1.928e0

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123.8090 1.054e1

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123.9197 4.989e0

123.9579 2.613e0

124.0119 6.417e0

124.1237 2.000e0

124.1797 5.318e0

124.2859 4.604e0

124.3134 2.671e0

124.3596 4.178e0

124.4067 5.930e0

124.4829 2.329e0

124.5262 2.137e0

124.5642 4.689e0

124.6828 6.913e0

124.7297 9.729e0

124.7876 8.452e0

124.8244 3.540e0

124.8516 2.617e0

124.8852 1.479e0

124.9183 7.367e0

124.9853 1.068e1

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125.9759 4.479e0

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126.5217 6.655e0

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126.6424 9.805e0

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126.7658 4.570e0

126.8061 4.243e0

126.9661 1.688e1

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147.9527 6.086e0

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155.4473 1.118e0

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157.0533 3.570e0

157.0935 1.301e1

157.1431 4.607e0

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157.2450 1.437e0

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