

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 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: 13-13 H: 0-200 N: 0-10 O: 0-20

Minimum: 80.00 -1.5

Maximum: 100.00 5.0 5.0 50.0

Mass RA Calc. Mass mDa PPM DBE i-FIT Formula

235.1454 100.00 235.1447 0.7 3.0 5.5 158.0 C13 H19 N2 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.

131.8433 1.013e0

131.8857 1.013e0

131.9130 2.025e0

131.9318 1.013e0

132.0067 8.101e0

132.0388 1.013e0

132.1030 1.735e1

132.1669 1.013e0

132.1846 3.038e0

132.2167 2.025e0

132.2841 2.025e0

132.3224 1.013e0

132.3413 1.013e0

132.3592 1.013e0

132.3811 3.038e0

132.3990 1.013e0

132.4327 2.025e0

132.4694 2.025e0

132.5242 3.038e0

132.5546 1.013e0

132.5817 3.038e0

132.6039 1.013e0

132.6465 3.038e0

132.7200 1.013e0

132.7565 1.013e0

132.7997 1.013e0

132.8490 1.013e0

132.8779 2.025e0

132.8960 2.025e0

132.9532 1.013e0

132.9985 1.013e0

133.0250 2.025e0

133.0724 6.578e0

133.1020 6.693e0

133.1396 2.548e0

133.1733 2.025e0

133.1913 3.038e0

133.2133 1.013e0

133.2454 2.025e0

133.3709 3.038e0

133.3912 1.013e0

133.4137 2.025e0

133.4313 2.025e0

133.4744 1.013e0

133.4861 1.013e0

133.5168 1.013e0

133.5420 2.025e0

133.5594 1.505e0

133.5788 2.025e0

133.6094 1.013e0

133.6212 1.013e0

133.6463 1.013e0

133.6769 3.038e0

133.6949 1.013e0

133.7169 1.013e0

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133.7643 3.038e0

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133.8810 2.025e0

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133.9982 2.025e0

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134.0965 8.410e0

134.1194 9.619e0

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134.2120 2.025e0

134.2300 1.013e0

134.2764 1.013e0

134.3747 2.025e0

134.4344 4.051e0

134.4746 2.025e0

134.4919 1.013e0

134.5075 1.013e0

134.5289 1.013e0

134.5673 3.038e0

134.6077 2.025e0

134.6321 2.025e0

134.6593 3.038e0

134.6982 1.013e0

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135.0714 2.154e1

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136.3030 1.013e0

136.3189 1.013e0

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136.3965 1.013e0

136.4258 2.025e0

136.4614 1.013e0

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136.7687 1.013e0

136.8266 2.025e0

136.8686 1.013e0

136.8964 1.013e0

136.9495 1.013e0

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137.1604 1.013e0

137.1935 2.025e0

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146.5645 2.025e0

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150.9733 1.013e0

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151.2331 3.038e0

151.2788 3.038e0

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151.3380 3.038e0

151.3872 3.038e0

151.4174 4.051e0

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151.6657 2.025e0

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151.7725 2.025e0

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152.0101 1.013e0

152.0480 3.735e1

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152.2262 3.038e0

152.2583 1.013e0

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153.1453 1.224e0

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156.9857 1.013e0

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157.1264 3.967e0

157.1427 4.784e0

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157.2854 1.013e0

157.3165 3.038e0

157.3521 1.013e0

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157.4902 2.025e0

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157.6953 1.013e0

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157.7918 1.013e0

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158.7587 2.025e0

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158.9094 4.051e0

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