

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

201 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: 0-15 Na: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

222.1503 222.1494 0.9 4.1 4.5 2.7 C13 H20 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.

139.2353 2.025e0

139.2596 1.013e0

139.3626 1.013e0

139.3881 2.025e0

139.4225 2.025e0

139.4552 2.025e0

139.4854 1.013e0

139.5104 1.013e0

139.5447 1.013e0

139.5639 1.013e0

139.5887 1.013e0

139.6294 1.013e0

139.6894 1.013e0

139.7333 1.013e0

139.7645 1.013e0

139.7805 1.013e0

139.7988 1.013e0

139.8181 1.013e0

139.8428 1.013e0

139.8747 4.051e0

139.9139 3.038e0

139.9501 1.013e0

139.9715 2.025e0

139.9877 2.025e0

140.0317 1.013e0

140.0546 4.051e0

140.0757 1.013e0

140.1036 1.013e0

140.1443 2.025e0

140.1669 1.013e0

140.1898 2.025e0

140.2142 1.013e0

140.2559 3.038e0

140.3031 3.038e0

140.3237 1.013e0

140.3482 3.038e0

140.3807 2.025e0

140.4151 1.013e0

140.4784 1.013e0

140.5414 1.013e0

140.5899 2.025e0

140.6270 2.025e0

140.6516 1.013e0

140.6709 1.013e0

140.6989 1.013e0

140.7318 5.063e0

140.7652 2.025e0

140.8048 2.025e0

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140.9949 2.025e0

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141.0851 4.051e0

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141.2052 2.025e0

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141.3613 1.013e0

141.4084 2.025e0

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141.5950 1.013e0

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141.8201 1.013e0

141.8417 1.013e0

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141.9085 2.025e0

141.9378 5.063e0

141.9742 2.025e0

142.0101 2.025e0

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142.0952 1.013e0

142.1079 1.013e0

142.1362 1.013e0

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142.1805 1.013e0

142.1967 1.013e0

142.2183 1.013e0

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142.3425 1.013e0

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143.7461 4.051e0

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158.9190 2.025e0

158.9647 1.013e0

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162.0389 2.025e0

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164.0312 1.013e0

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164.0825 1.013e0

164.1336 1.013e0

164.1908 1.013e0

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164.2628 1.013e0

164.2861 4.718e0

164.3310 1.013e0

164.3612 1.013e0

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164.5928 1.013e0

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164.7095 1.013e0

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164.8780 2.025e0

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166.1304 2.025e0

166.1642 1.013e0

166.2002 2.025e0

166.2329 2.025e0

166.2604 2.025e0

166.3397 1.013e0

166.3704 1.013e0

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