

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

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

Elements Used:

C: 27-27 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

462.2396 462.2393 0.3 0.6 13.5 11.7 C27 H32 N3 O4

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.

158.2395 2.025e0

158.2648 1.013e0

158.3413 1.013e0

158.4022 1.013e0

158.4753 1.013e0

158.5159 1.013e0

158.5421 1.013e0

158.6624 1.013e0

158.7400 2.025e0

158.7664 1.013e0

158.7928 1.013e0

158.8658 2.025e0

158.8868 1.013e0

158.9168 2.025e0

158.9405 1.013e0

159.0209 3.038e0

159.0645 1.013e0

159.0814 1.013e0

159.1214 1.013e0

159.1581 1.013e0

159.1987 5.063e0

159.2257 1.013e0

159.2617 1.013e0

159.2991 1.013e0

159.4198 2.025e0

159.4966 1.013e0

159.5236 1.013e0

159.5507 1.013e0

159.5693 2.025e0

159.5928 2.851e0

159.6909 3.038e0

159.8262 1.013e0

159.8911 2.025e0

159.9539 1.013e0

159.9805 1.013e0

160.1380 1.013e0

160.1686 1.013e0

160.1855 1.013e0

160.2691 1.013e0

160.3541 1.013e0

160.3969 2.025e0

160.4546 1.013e0

160.6218 2.025e0

160.6627 1.013e0

160.7580 1.013e0

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160.9424 2.025e0

160.9663 3.038e0

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161.0874 1.013e0

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161.2222 1.013e0

161.3810 1.013e0

161.4957 1.013e0

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161.6263 2.025e0

161.7088 2.025e0

161.7764 1.013e0

161.7996 1.013e0

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161.9034 2.151e0

161.9252 1.013e0

161.9483 1.013e0

161.9857 1.013e0

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162.1515 1.013e0

162.1788 1.013e0

162.2382 3.038e0

162.2798 2.025e0

162.3326 3.038e0

162.3583 1.013e0

162.4901 1.013e0

162.5912 1.013e0

162.6425 1.013e0

162.7105 1.013e0

162.7641 1.013e0

162.7880 1.013e0

162.8563 1.013e0

162.9032 1.013e0

162.9627 2.025e0

163.0029 3.038e0

163.0293 1.013e0

163.0894 1.013e0

163.1237 1.013e0

163.1749 1.013e0

163.2292 1.013e0

163.2492 1.013e0

163.2796 2.025e0

163.3139 1.013e0

163.3412 1.013e0

163.3755 1.013e0

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163.5246 1.013e0

163.5975 2.025e0

163.6517 2.025e0

163.6705 2.025e0

163.7726 1.013e0

163.7960 1.013e0

163.8129 1.013e0

163.8507 1.013e0

163.8917 1.013e0

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163.9864 1.013e0

164.0034 2.025e0

164.0856 1.013e0

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165.9690 1.013e0

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167.4338 1.013e0

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167.8297 1.013e0

167.8745 1.013e0

167.9325 1.013e0

167.9802 1.013e0

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168.1566 2.025e0

168.1929 2.025e0

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168.3112 1.013e0

168.3801 1.013e0

168.4251 1.013e0

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168.4873 1.013e0

168.5323 1.013e0

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168.6015 1.013e0

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190.3430 1.013e0

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190.5327 2.025e0

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196.6501 1.013e0

196.6683 1.013e0

196.7303 2.025e0

196.8781 1.013e0

196.9463 2.025e0

196.9893 1.013e0

197.0278 3.038e0

197.0804 2.025e0

197.1047 1.013e0

197.1607 1.013e0

197.2023 1.013e0

197.2595 2.025e0

197.2804 1.013e0

197.3547 2.025e0

197.4216 1.013e0

197.4910 2.025e0

197.5971 1.013e0

197.6425 2.025e0

197.6989 1.013e0

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197.7552 2.356e0

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197.8142 1.013e0

197.8781 1.013e0

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199.6414 2.025e0

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