 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

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

Elements Used:

C: 24-24 H: 0-200 N: 0-10 O: 0-20 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

404.1971 404.1974 -0.3 -0.7 13.5 2.3 C24 H26 N3 O3

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.

145.4283 2.025e0

145.4554 1.013e0

145.5246 2.025e0

145.5709 1.013e0

145.6385 1.013e0

145.8402 2.025e0

145.8691 1.013e0

145.8979 1.013e0

145.9297 1.013e0

145.9525 1.013e0

145.9906 2.025e0

146.0779 7.089e0

146.1030 1.053e0

146.1514 1.013e0

146.2608 1.013e0

146.3109 2.025e0

146.3344 2.025e0

146.3794 1.013e0

146.4054 1.013e0

146.4781 2.025e0

146.5162 2.025e0

146.5922 1.013e0

146.6337 2.025e0

146.6851 1.013e0

146.7298 2.025e0

146.8009 1.013e0

146.8363 1.013e0

146.8654 1.013e0

146.8852 2.025e0

146.9332 2.025e0

146.9748 1.013e0

147.0011 1.013e0

147.0683 1.013e0

147.2329 1.013e0

147.3243 2.025e0

147.5329 1.013e0

147.5481 2.025e0

147.5647 1.013e0

147.6128 1.013e0

147.6457 1.013e0

147.6841 2.025e0

147.8846 1.013e0

148.0017 3.038e0

148.0788 1.013e0

148.1171 1.013e0

148.1654 1.013e0

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148.5522 2.025e0

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148.6835 1.013e0

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148.8862 2.025e0

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148.9717 2.025e0

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149.0462 1.013e0

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149.3707 1.013e0

149.5105 2.025e0

149.5721 1.013e0

149.5919 1.013e0

149.6371 1.013e0

149.6830 1.013e0

149.7836 1.013e0

149.8067 1.013e0

150.0273 1.013e0

150.0862 1.013e0

150.1546 1.013e0

150.1754 2.025e0

150.2035 1.013e0

150.2851 1.013e0

150.3105 2.025e0

150.3822 2.025e0

150.4406 1.013e0

150.5651 1.013e0

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150.9497 1.013e0

150.9663 1.013e0

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151.2076 1.013e0

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151.4727 1.013e0

151.5148 1.013e0

151.5642 1.013e0

151.6199 1.013e0

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151.7472 1.013e0

151.7803 1.013e0

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153.3382 2.025e0

153.4250 2.025e0

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153.9477 1.013e0

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154.2874 1.013e0

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155.9579 2.025e0

155.9914 1.013e0

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156.1328 2.025e0

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175.9852 2.025e0

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182.7649 2.025e0

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184.6767 1.013e0

184.7078 2.025e0

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184.8474 3.038e0

184.9404 1.013e0

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185.1101 2.025e0

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185.7982 1.013e0

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186.2069 2.025e0

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186.5732 1.013e0

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186.8311 1.013e0

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