

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

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

Elements Used:

C: 21-21 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

333.1610 333.1603 0.7 2.1 12.5 0.8 C21 H21 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.

148.6841 4.051e0

148.7276 1.013e0

148.7506 1.013e0

148.7858 1.013e0

148.8962 1.013e0

148.9088 1.013e0

148.9641 1.013e0

149.0133 1.013e0

149.0289 1.013e0

149.0633 2.025e0

149.0938 1.013e0

149.1782 4.051e0

149.2365 1.013e0

149.3534 1.013e0

149.4043 2.025e0

149.4929 1.013e0

149.5292 1.013e0

149.5569 3.038e0

149.6009 1.013e0

149.6209 2.025e0

149.6460 1.013e0

149.6977 1.013e0

149.8009 2.025e0

149.8442 1.013e0

149.9191 2.025e0

149.9513 1.013e0

149.9710 1.013e0

150.0196 1.013e0

150.0426 1.013e0

150.1594 1.013e0

150.1760 1.013e0

150.2034 3.038e0

150.2378 1.013e0

150.2675 1.013e0

150.6847 1.013e0

150.7315 3.038e0

150.7885 1.013e0

150.8603 1.013e0

150.9354 1.013e0

150.9907 1.013e0

151.0594 1.013e0

151.0807 3.038e0

151.1234 4.051e0

151.1542 1.013e0

151.2360 1.013e0

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151.3632 1.013e0

151.4164 3.038e0

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151.7788 1.013e0

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152.1490 1.013e0

152.1680 1.013e0

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152.6372 1.013e0

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152.7326 1.013e0

152.8539 1.013e0

152.8969 1.013e0

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153.0149 3.038e0

153.0513 3.038e0

153.1235 1.013e0

153.1725 1.013e0

153.1891 1.013e0

153.2157 1.013e0

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153.3114 1.013e0

153.3569 1.013e0

153.4190 1.013e0

153.4592 2.025e0

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153.5481 1.013e0

153.6271 1.013e0

153.6595 1.013e0

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153.9265 1.013e0

153.9531 1.013e0

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154.0746 2.025e0

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154.2205 1.013e0

154.2462 1.013e0

154.2762 1.013e0

154.3096 1.013e0

154.3385 1.013e0

154.3753 1.013e0

154.4444 1.013e0

154.4910 1.013e0

154.5037 1.013e0

154.5604 1.013e0

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155.2411 1.013e0

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172.2214 1.013e0

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173.2374 1.013e0

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184.9740 1.013e0

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185.0398 1.013e0

185.0684 1.013e0

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185.2453 1.013e0

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185.8531 2.025e0

185.9425 2.025e0

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186.1179 2.025e0

186.1718 1.013e0

186.2270 1.013e0

186.2485 1.013e0

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186.3169 1.013e0

186.3756 1.013e0

186.4222 1.013e0

186.4472 1.013e0

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186.5637 2.025e0

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186.6478 1.013e0

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186.7600 2.025e0

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186.8704 2.025e0

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187.0510 1.013e0

187.0868 2.025e0

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187.3504 2.025e0

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188.8280 1.013e0

188.8678 1.013e0

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