

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

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

Elements Used:

C: 23-23 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

390.1830 390.1818 1.2 3.1 13.5 0.9 C23 H24 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.

154.9571 2.025e0

154.9923 1.013e0

155.0282 1.013e0

155.1153 3.038e0

155.1609 4.051e0

155.2251 2.025e0

155.5251 1.013e0

155.7308 1.013e0

155.7440 1.013e0

155.7934 2.025e0

155.8694 1.013e0

155.8929 1.013e0

155.9164 1.013e0

155.9490 1.013e0

156.0585 1.013e0

156.0796 3.038e0

156.1615 1.013e0

156.1850 1.013e0

156.2102 2.025e0

156.2313 1.013e0

156.3642 1.013e0

156.6363 1.013e0

156.7000 4.051e0

156.7263 1.013e0

156.7582 3.038e0

156.8001 1.013e0

156.9492 1.013e0

156.9795 1.013e0

157.0152 3.038e0

157.0490 1.013e0

157.0693 3.038e0

157.1162 1.013e0

157.1893 1.013e0

157.2825 1.013e0

157.3129 1.013e0

157.3638 2.025e0

157.4325 1.013e0

157.4553 1.013e0

157.5126 1.013e0

157.5521 1.013e0

157.5924 1.013e0

157.6721 1.013e0

157.7330 2.025e0

157.7958 1.013e0

157.8329 1.013e0

157.8497 1.013e0

157.9160 1.013e0

157.9992 1.013e0

158.0732 1.013e0

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158.2094 1.013e0

158.4368 1.013e0

158.5011 1.013e0

158.5308 1.013e0

158.8119 1.013e0

158.8355 1.013e0

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159.0192 1.013e0

159.0970 1.013e0

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159.6702 1.013e0

159.7605 1.013e0

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159.8745 1.013e0

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160.5557 2.025e0

160.6184 1.013e0

160.6382 1.013e0

160.6751 2.025e0

160.7057 1.013e0

160.7484 6.076e0

160.7827 1.013e0

160.8642 1.013e0

160.9615 1.013e0

160.9853 2.025e0

161.0412 2.025e0

161.0558 1.019e0

161.0946 2.025e0

161.1474 2.025e0

161.2584 1.013e0

161.4035 2.025e0

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161.8049 1.013e0

161.8526 1.013e0

161.8782 2.025e0

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162.2887 1.013e0

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162.9937 1.013e0

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163.0846 1.013e0

163.2476 1.013e0

163.6383 1.013e0

163.7307 1.013e0

163.9581 1.013e0

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164.0636 2.025e0

164.1721 1.013e0

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168.4598 2.025e0

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168.5307 1.013e0

168.5653 1.013e0

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168.8651 1.013e0

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169.0487 1.013e0

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169.1258 2.025e0

169.1859 1.013e0

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169.6530 1.013e0

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206.8680 1.013e0

206.8919 1.013e0

206.9408 1.013e0

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207.5952 1.013e0

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208.3233 2.025e0

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208.6958 3.038e0

208.8103 2.025e0

208.8449 1.013e0

208.8717 1.013e0

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209.0790 3.038e0

209.1060 1.013e0

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209.2363 1.013e0

209.3737 3.038e0

209.4596 1.013e0

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210.2105 1.013e0

210.2756 1.013e0

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211.0777 1.013e0

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211.2400 1.013e0

211.3477 1.013e0

211.6380 1.013e0

211.8807 1.013e0

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212.1338 2.025e0

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212.2321 1.013e0

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213.8722 1.013e0

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214.1649 1.013e0

214.2380 1.013e0

214.2997 1.013e0

214.3337 2.025e0

214.3626 1.013e0

214.4988 1.013e0

214.5643 1.013e0

214.6546 1.013e0

214.7709 1.013e0

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