 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

262 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 I: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

332.0512 332.0511 0.1 0.3 4.5 0.1 C13 H19 N O I

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.

ANALYSIS RUN USING: WATERS LCT PREMIER (ESI POSITIVE/ESI NEGATIVE)

149.0026 2.025e0

149.0790 1.013e0

149.1015 1.013e0

149.1340 1.013e0

149.1663 2.025e0

149.2312 1.013e0

149.2522 2.025e0

149.3221 1.013e0

149.4387 1.013e0

149.4784 1.013e0

149.4972 1.013e0

149.5769 2.025e0

149.6699 1.013e0

149.7382 1.013e0

149.7650 2.025e0

149.8032 1.013e0

149.8782 1.013e0

149.9785 1.013e0

150.0180 1.013e0

150.0766 1.013e0

150.0910 2.025e0

150.1137 3.038e0

150.1736 1.013e0

150.2261 1.013e0

150.2945 1.013e0

150.3587 2.025e0

150.3754 1.013e0

150.4085 1.013e0

150.4282 1.013e0

150.4471 1.013e0

150.4753 2.025e0

150.5060 1.013e0

150.6171 1.013e0

150.6823 1.013e0

150.7739 1.013e0

150.8060 1.013e0

150.8645 2.025e0

150.9595 1.013e0

150.9985 1.013e0

151.0513 1.013e0

151.0883 2.025e0

151.1065 1.013e0

151.1452 1.013e0

151.2171 1.013e0

151.3741 1.013e0

151.4326 2.025e0

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151.5246 1.013e0

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151.6264 1.013e0

151.7404 1.013e0

151.8224 1.013e0

151.9563 1.013e0

151.9730 1.013e0

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152.1054 2.025e0

152.1386 2.025e0

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152.1857 1.013e0

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152.4385 1.013e0

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152.5290 2.025e0

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152.8125 1.013e0

152.8617 1.013e0

152.8796 2.025e0

152.9534 1.013e0

152.9951 2.025e0

153.0757 1.013e0

153.2068 1.013e0

153.3613 1.013e0

153.4174 1.013e0

153.5060 1.013e0

153.6516 1.013e0

153.6706 1.013e0

153.7322 2.025e0

153.8096 2.025e0

153.8290 2.025e0

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154.0367 1.013e0

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154.1621 1.013e0

154.3174 1.013e0

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154.6997 1.013e0

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154.8325 1.013e0

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175.3058 2.025e0

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175.4999 4.051e0

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175.6918 1.013e0

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179.4083 1.013e0

179.4444 1.013e0

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184.4855 2.025e0

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185.9648 1.013e0

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187.3369 3.038e0

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187.7766 1.013e0

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190.6709 1.013e0

190.6972 1.013e0

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190.7809 1.013e0

190.8506 1.013e0

190.8873 1.013e0

191.0963 1.013e0

191.1447 1.013e0

191.1881 1.013e0

191.3169 1.013e0

191.4311 1.013e0

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191.8693 1.013e0

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195.8674 1.013e0

195.9190 1.013e0

195.9712 1.013e0

195.9929 1.013e0

196.0421 1.013e0

196.1716 1.013e0

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196.5923 1.013e0

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197.6968 1.013e0

197.8841 1.013e0

197.9809 1.013e0

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198.0413 1.013e0

198.0705 1.013e0

198.1344 2.025e0

198.1636 1.013e0

198.2611 1.013e0

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198.3542 2.025e0

198.4067 1.013e0

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