 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

99 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

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

206.1549 206.1545 0.4 1.9 4.5 0.9 C13 H20 N O

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)

148.9992 1.013e0

149.0412 1.013e0

149.0739 1.013e0

149.1487 1.013e0

149.1806 1.013e0

149.2136 1.013e0

149.3236 2.025e0

149.3786 3.038e0

149.4017 2.025e0

149.4925 2.025e0

149.5250 2.025e0

149.5448 1.013e0

149.6417 1.013e0

149.6814 1.013e0

149.7133 1.013e0

149.7558 1.013e0

149.8209 1.013e0

149.8494 4.259e0

149.8664 2.025e0

149.9050 1.013e0

149.9281 2.025e0

149.9605 1.013e0

149.9800 1.013e0

150.0166 3.038e0

150.0615 1.013e0

150.1233 1.013e0

150.1398 1.013e0

150.1884 1.013e0

150.2320 2.025e0

150.3152 1.013e0

150.3615 2.025e0

150.4001 3.038e0

150.4553 1.013e0

150.4918 2.025e0

150.5106 1.013e0

150.6219 1.013e0

150.6739 1.013e0

150.6921 2.025e0

150.7816 1.013e0

150.8373 1.013e0

150.8549 2.025e0

150.9091 1.013e0

151.0031 1.013e0

151.0196 1.013e0

151.0428 1.013e0

151.0624 1.013e0

151.1420 2.025e0

151.1799 1.013e0

151.1981 2.025e0

151.2718 2.025e0

151.3037 2.025e0

151.3236 2.025e0

151.4036 3.038e0

151.4608 2.025e0

151.5236 3.038e0

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151.6503 1.013e0

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151.8405 2.025e0

151.8959 1.013e0

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151.9745 1.013e0

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152.0234 1.013e0

152.0565 1.013e0

152.0799 2.025e0

152.2039 1.013e0

152.2338 2.025e0

152.2925 3.038e0

152.3646 2.025e0

152.4201 1.013e0

152.5155 1.013e0

152.6378 2.025e0

152.6797 1.013e0

152.7025 1.013e0

152.7319 1.013e0

152.7973 1.013e0

152.8190 2.025e0

152.8895 1.013e0

152.9095 1.013e0

152.9389 1.013e0

152.9583 2.025e0

152.9792 3.038e0

153.0051 1.013e0

153.0461 4.051e0

153.0755 4.051e0

153.1177 4.051e0

153.1561 1.013e0

153.2166 2.025e0

153.2350 1.013e0

153.2922 2.025e0

153.4063 2.025e0

153.4751 1.013e0

153.6347 2.025e0

153.6920 1.013e0

153.7513 1.013e0

153.7710 1.013e0

153.8534 1.013e0

153.9098 1.013e0

153.9274 2.025e0

153.9474 2.025e0

154.0018 2.025e0

154.0541 3.038e0

154.0699 2.025e0

154.0843 1.013e0

154.1106 1.013e0

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154.1863 1.013e0

154.2314 2.141e0

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154.4403 2.025e0

154.4872 1.013e0

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155.0768 2.025e0

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155.5387 1.013e0

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155.6907 1.013e0

155.7479 1.013e0

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156.0899 2.315e0

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156.3152 3.038e0

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156.9946 2.356e0

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157.0463 1.013e0

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157.3625 1.013e0

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157.4776 2.025e0

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157.7731 1.013e0

157.8164 1.013e0

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157.9706 2.025e0

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162.7686 2.025e0

162.7993 2.025e0

162.8364 3.369e0

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162.9779 4.051e0

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163.2077 3.038e0

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163.4454 1.013e0

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163.7661 3.038e0

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165.9734 3.038e0

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166.1198 1.013e0

166.1469 1.013e0

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166.6781 2.025e0

166.7599 2.025e0

166.8427 1.013e0

166.9117 2.025e0

166.9538 3.038e0

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167.0396 2.025e0

167.0862 1.013e0

167.1293 2.025e0

167.2035 1.013e0

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167.2838 2.025e0

167.3643 1.013e0

167.3989 1.013e0

167.4472 1.013e0

167.5197 2.025e0

167.5498 3.038e0

167.5847 1.013e0

167.6703 2.025e0

167.7152 1.013e0

167.7583 2.025e0

167.7980 1.013e0

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167.9697 1.013e0

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168.0663 1.013e0

168.1319 1.013e0

168.2167 2.025e0

168.2870 1.013e0

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168.9875 3.038e0

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169.0894 2.025e0

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169.2009 2.025e0

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170.8681 1.013e0

170.9286 7.089e0

171.0050 2.025e0

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171.0668 3.038e0

171.1002 1.013e0

171.1348 2.025e0

171.1505 2.025e0

171.1972 2.025e0

171.2319 1.013e0

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171.7683 2.025e0

171.8136 2.025e0

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171.8938 2.025e0

171.9740 3.038e0

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172.1777 4.051e0

172.2147 2.025e0

172.2530 1.013e0

172.2845 3.038e0

172.3124 2.025e0

172.3383 2.025e0

172.3620 3.038e0

172.3821 1.013e0

172.4274 1.013e0

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172.9369 1.013e0

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173.0663 1.013e0

173.0947 4.051e0

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173.2062 2.025e0

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175.7902 2.025e0

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177.1440 1.013e0

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177.7980 1.013e0

177.8159 1.013e0

177.8480 3.038e0

177.9310 5.063e0

177.9756 2.025e0

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178.1972 2.025e0

178.2525 1.013e0

178.3152 3.038e0

178.3584 1.013e0

178.4255 1.013e0

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178.5557 4.051e0

178.6178 1.013e0

178.6755 4.051e0

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178.7661 2.025e0

178.8432 2.025e0

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178.9490 3.038e0

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179.2060 2.025e0

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179.5100 1.013e0

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180.6040 2.025e0

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180.8450 3.038e0

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180.9868 1.013e0

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