

Elemental Composition Report

Single Mass Analysis

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

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

279 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 13-13 H: 5-150 N: 0-12 O: 0-11 Na: 0-1 I: 0-2

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

236.1290 236.1287 0.3 1.3 5.5 108.2 0.0 C13 H18 N O3

REPORT MASSES AS +/-5mDa, referenced against

Leucine Enkelphalin @ 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.

147.9822 1.013e0

148.0272 1.013e0

148.0469 1.013e0

148.0598 1.013e0

148.0820 1.013e0

148.1196 2.025e0

148.2311 1.013e0

148.2976 2.025e0

148.3376 1.013e0

148.3573 1.013e0

148.3702 1.013e0

148.3991 1.013e0

148.4286 1.013e0

148.4506 1.013e0

148.6065 1.013e0

148.6842 3.038e0

148.7131 1.013e0

148.7779 1.013e0

148.8395 1.013e0

148.8876 2.025e0

148.9373 2.025e0

148.9559 1.013e0

149.0142 1.013e0

149.0537 1.013e0

149.0760 1.013e0

149.1604 1.013e0

149.1769 1.013e0

149.2902 1.013e0

149.3650 1.013e0

149.4655 1.013e0

149.5500 1.013e0

149.5830 1.013e0

149.6182 2.025e0

149.7581 1.013e0

149.7907 1.013e0

149.8031 1.013e0

149.9288 2.025e0

149.9955 1.013e0

150.0467 4.051e0

150.0914 2.025e0

150.1306 3.038e0

150.1647 1.013e0

150.2098 2.025e0

150.2281 2.025e0

150.2529 1.013e0

150.2940 3.038e0

150.3994 1.013e0

150.4118 1.013e0

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150.5332 1.013e0

150.6111 5.063e0

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150.9040 1.013e0

150.9207 1.013e0

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151.4664 1.013e0

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151.5188 1.013e0

151.5741 1.013e0

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151.7080 1.013e0

151.9239 1.013e0

151.9802 1.013e0

152.0059 1.013e0

152.0408 2.025e0

152.1309 1.013e0

152.1434 1.013e0

152.2652 1.013e0

152.4126 1.013e0

152.4452 1.013e0

152.5436 1.013e0

152.6223 2.025e0

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152.7965 1.013e0

152.8853 1.013e0

152.9943 3.038e0

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153.1252 1.013e0

153.1708 1.013e0

153.2396 1.013e0

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153.3059 1.013e0

153.3402 2.025e0

153.4175 1.013e0

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153.7235 1.013e0

153.9114 1.013e0

153.9314 1.013e0

154.0339 1.013e0

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154.0945 2.025e0

154.1519 1.013e0

154.1987 1.013e0

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188.6962 1.013e0

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189.0935 1.013e0

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190.1179 3.038e0

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190.4876 1.013e0

190.7406 1.013e0

190.7634 1.013e0

190.7923 1.013e0

190.8583 2.025e0

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191.7693 1.013e0

191.8022 1.013e0

191.8469 1.013e0

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192.0602 1.013e0

192.0802 2.025e0

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192.2971 2.025e0

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388.0887 2.025e0

388.1682 4.051e0

388.2442 3.038e0

388.3435 1.013e0

388.5357 2.025e0

388.7826 3.038e0

388.8228 1.013e0

388.9297 1.013e0

389.0351 1.013e0

389.1259 2.025e0

389.1864 1.013e0

389.2646 2.025e0

389.3515 2.025e0

389.4940 1.013e0

389.7359 1.013e0

389.8573 1.013e0

389.9836 1.013e0

390.1145 1.013e0

390.4076 1.013e0

390.4648 1.013e0

390.5292 1.013e0

390.6205 2.025e0

390.6584 1.013e0

390.7956 1.013e0

390.9080 2.025e0

390.9801 1.013e0

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391.1115 3.038e0

391.1676 3.038e0

391.2258 3.038e0

391.2830 1.052e1

391.5630 1.013e0

391.6794 1.013e0

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391.8476 1.013e0

391.8952 1.013e0

391.9534 1.013e0

391.9983 1.013e0

392.1049 3.038e0

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392.9406 1.013e0

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394.0058 2.025e0

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394.9339 2.025e0

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395.0601 1.013e0

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395.2094 3.038e0

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395.7948 2.025e0

395.8792 1.013e0

395.9566 2.025e0

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397.1183 1.013e0

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399.6638 2.025e0

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