 Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 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

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

Elements Used:

C: 16-16 H: 0-100 N: 0-10 O: 0-10 S: 0-1 Br: 1-1

Minimum: -1.5

Maximum: 5.0 7.0 100.0

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

368.0327 368.0320 0.7 1.9 7.5 875.0 0.0 C16 H19 N O2 S Br

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.

147.3868 2.025e0

147.4050 1.013e0

147.4174 1.013e0

147.4214 4.051e0

147.4273 1.013e0

147.4404 1.013e0

147.4437 1.013e0

147.4532 2.025e0

147.4547 2.025e0

147.4693 1.013e0

147.4725 1.013e0

147.4843 2.025e0

147.4920 1.013e0

147.4971 3.038e0

147.5080 2.025e0

147.5212 1.013e0

147.5336 3.038e0

147.5433 3.038e0

147.5516 2.025e0

147.5533 1.013e0

147.5583 2.025e0

147.5726 1.013e0

147.5755 3.038e0

147.5951 6.261e0

147.6084 1.013e0

147.6340 1.013e0

147.6357 2.025e0

147.6390 2.025e0

147.6502 1.013e0

147.6662 3.038e0

147.6678 2.025e0

147.6794 1.013e0

147.6860 1.013e0

147.7033 2.025e0

147.7049 1.013e0

147.7181 1.013e0

147.7215 1.013e0

147.7470 1.013e0

147.7503 1.013e0

147.7602 1.013e0

147.7618 2.025e0

147.7696 1.013e0

147.7757 1.013e0

147.7791 2.025e0

147.7890 1.013e0

147.7923 1.013e0

147.7940 2.025e0

147.7956 1.013e0

147.8085 1.013e0

147.8195 2.025e0

147.8377 1.013e0

147.8410 2.025e0

147.8639 4.051e0

147.8831 1.013e0

147.8935 2.025e0

147.8987 1.013e0

147.9053 2.025e0

147.9119 1.013e0

147.9152 1.013e0

147.9251 1.013e0

147.9374 1.013e0

147.9506 3.038e0

147.9556 2.025e0

147.9620 3.038e0

147.9714 2.025e0

147.9762 2.025e0

147.9861 1.013e0

147.9894 1.013e0

147.9993 1.013e0

148.0027 1.013e0

148.0061 2.025e0

148.0166 2.025e0

148.0232 1.899e0

148.0310 6.650e0

148.0374 2.617e0

148.0561 7.089e0

148.0580 1.054e1

148.0735 5.316e0

148.0750 1.159e1

148.0805 3.654e0

148.0901 5.084e0

148.1006 2.182e0

148.1108 1.502e0

148.1346 3.666e0

148.1412 2.025e0

148.1674 1.013e0

148.1767 1.013e0

148.1965 1.013e0

148.2124 1.013e0

148.2320 1.013e0

148.2453 1.013e0

148.2514 6.076e0

148.2576 1.013e0

148.2609 1.013e0

148.2708 1.013e0

148.2841 1.013e0

148.2998 3.038e0

148.3064 2.025e0

148.3262 1.013e0

148.3296 4.051e0

148.3322 1.013e0

148.3567 2.025e0

148.3806 2.025e0

148.3889 2.025e0

148.3939 1.013e0

148.3972 1.013e0

148.4160 4.051e0

148.4461 2.025e0

148.4506 2.025e0

148.4582 1.013e0

148.4864 2.025e0

148.4909 4.924e0

148.5070 1.152e0

148.5103 2.025e0

148.5269 1.013e0

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148.5979 1.013e0

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148.6516 2.025e0

148.6723 1.013e0

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148.6889 2.025e0

148.6923 2.025e0

148.6981 2.025e0

148.7211 1.013e0

148.7311 1.013e0

148.7342 1.013e0

148.7466 1.013e0

148.7566 1.013e0

148.7583 2.025e0

148.7763 1.013e0

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148.8104 2.025e0

148.8574 1.013e0

148.8604 1.013e0

148.8632 2.025e0

148.8715 2.025e0

148.8897 1.013e0

148.8965 2.025e0

148.9087 1.013e0

148.9253 1.013e0

148.9386 1.013e0

148.9445 2.025e0

148.9493 2.025e0

148.9609 2.025e0

148.9675 1.013e0

148.9708 1.013e0

148.9775 1.013e0

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149.1196 1.267e0

149.1334 2.133e0

149.1552 3.038e0

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149.1974 1.013e0

149.2041 1.013e0

149.2075 1.013e0

149.2274 1.013e0

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149.2396 1.013e0

149.2629 1.013e0

149.2869 2.025e0

149.2891 3.038e0

149.3068 2.025e0

149.3179 1.013e0

149.3407 1.013e0

149.3440 1.013e0

149.3540 1.013e0

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149.3764 1.013e0

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149.4575 1.013e0

149.4674 1.013e0

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150.0758 1.936e0

150.1122 5.743e1

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152.0685 2.023e1

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152.1930 1.013e0

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152.2681 1.013e0

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152.2865 2.025e0

152.2931 2.025e0

152.3008 3.038e0

152.3102 4.051e0

152.3174 1.013e0

152.3207 2.025e0

152.3240 2.025e0

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153.0212 4.051e0

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153.0462 1.994e1

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153.0694 1.302e0

153.1038 3.020e0

153.1085 1.212e0

153.1416 4.570e0

153.1759 4.051e0

153.1783 1.013e0

153.1879 1.013e0

153.2075 2.025e0

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153.3760 2.025e0

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153.8793 1.013e0

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153.9849 1.013e0

154.0053 2.025e0

154.0097 4.051e0

154.0111 2.025e0

154.0277 2.676e0

154.0311 1.013e0

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154.0510 2.170e0

154.0602 4.051e0

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154.0677 2.818e0

154.0980 6.939e0

154.0998 7.260e0

154.1024 1.541e0

154.1312 3.544e0

154.1401 1.715e0

154.1568 1.596e1

154.1793 5.063e0

154.1998 1.013e0

154.2032 2.025e0

154.2136 2.025e0

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154.4372 1.013e0

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154.4599 1.013e0

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154.5001 1.013e0

154.5034 3.038e0

154.5174 3.038e0

154.5329 1.013e0

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154.5517 2.025e0

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155.1686 3.038e0

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155.2340 1.013e0

155.2408 1.013e0

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