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

199 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 Na: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

221.1182 221.1178 0.4 1.8 5.5 1.5 C13 H17 O3

M-OH

148.1313 1.013e0

148.1574 1.013e0

148.1993 3.038e0

148.2344 1.013e0

148.2542 2.025e0

148.2803 1.013e0

148.2926 1.013e0

148.3358 6.669e0

148.3672 1.013e0

148.4320 1.013e0

148.4550 1.013e0

148.5297 2.025e0

148.5747 2.025e0

148.6681 1.013e0

148.7494 2.025e0

148.7758 2.025e0

148.8241 2.025e0

148.8438 1.013e0

148.9086 1.013e0

148.9240 1.013e0

148.9570 1.013e0

148.9765 1.013e0

148.9889 1.013e0

149.0285 1.013e0

149.0475 3.038e0

149.1033 2.025e0

149.1352 1.013e0

149.1588 3.664e0

149.2034 1.013e0

149.2215 2.025e0

149.3055 2.025e0

149.3250 2.025e0

149.4015 1.013e0

149.4265 3.038e0

149.4499 1.013e0

149.4730 1.013e0

149.5764 2.025e0

149.6095 1.013e0

149.6695 2.025e0

149.6950 3.038e0

149.7097 2.094e0

149.7345 2.025e0

149.7591 1.013e0

149.7715 1.013e0

149.8257 2.025e0

149.8563 4.051e0

149.8986 1.013e0

149.9677 3.038e0

149.9913 2.025e0

150.0973 1.013e0

150.1197 1.013e0

150.1528 1.013e0

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150.2145 2.025e0

150.2579 3.038e0

150.2849 1.605e0

150.3148 2.025e0

150.3331 2.025e0

150.3709 2.025e0

150.4164 2.025e0

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150.6399 2.025e0

150.7354 1.013e0

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150.8535 1.013e0

150.9377 1.013e0

150.9861 3.127e0

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151.0798 9.114e0

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151.1846 2.025e0

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177.3770 2.025e0

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179.7026 2.025e0

179.7280 1.013e0

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