 

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

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

Elements Used:

C: 14-14 H: 0-100 N: 0-10 O: 0-14 Na: 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

314.0747 314.0756 -0.9 -2.9 4.5 243.4 0.0 C14 H21 N O2 Br

152.2639 1.013e0

152.2723 2.025e0

152.2790 2.025e0

152.2890 2.025e0

152.3031 1.013e0

152.3048 2.025e0

152.3082 2.025e0

152.3098 1.013e0

152.3265 1.013e0

152.3299 2.025e0

152.3429 2.025e0

152.3457 2.025e0

152.3524 1.013e0

152.3647 2.025e0

152.3691 3.038e0

152.3949 1.013e0

152.3982 3.038e0

152.3999 2.025e0

152.4056 1.013e0

152.4150 1.013e0

152.4218 1.013e0

152.4240 3.038e0

152.4357 3.038e0

152.4476 1.013e0

152.4610 1.013e0

152.4643 1.013e0

152.4711 2.037e0

152.4757 3.038e0

152.4801 4.051e0

152.4921 4.051e0

152.5045 3.038e0

152.5108 1.013e0

152.5204 1.013e0

152.5345 2.025e0

152.5445 1.151e1

152.5491 2.859e1

152.5563 4.051e0

152.5631 1.657e0

152.5652 3.038e0

152.5786 1.013e0

152.5888 2.025e0

152.6128 1.013e0

152.6142 4.051e0

152.6157 2.025e0

152.6280 1.031e0

152.6347 1.013e0

152.6448 2.025e0

152.6646 2.025e0

152.6794 3.038e0

152.6942 5.063e0

152.6960 3.038e0

152.6974 1.013e0

152.7047 1.013e0

152.7198 1.013e0

152.7233 1.013e0

152.7269 2.025e0

152.7467 1.013e0

152.7501 1.013e0

152.7596 1.013e0

152.7692 1.013e0

152.7776 2.025e0

152.7793 1.013e0

152.7979 2.025e0

152.7995 2.025e0

152.8088 2.025e0

152.8191 1.013e0

152.8353 2.025e0

152.8420 1.013e0

152.8506 2.025e0

152.8548 2.025e0

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152.9632 1.013e0

152.9666 1.013e0

152.9800 1.013e0

152.9962 1.013e0

153.0109 2.025e0

153.0126 1.013e0

153.0235 2.321e0

153.0407 7.545e0

153.0431 1.658e1

153.0453 2.978e1

153.0475 7.938e0

153.0725 2.978e0

153.0766 1.398e0

153.0868 7.431e0

153.1017 1.198e0

153.1320 6.479e0

153.1419 2.025e0

153.1837 1.013e0

153.1899 1.013e0

153.2070 2.025e0

153.2201 2.025e0

153.2283 2.025e0

153.2299 1.013e0

153.2494 3.216e0

153.2667 1.013e0

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153.2888 5.063e0

153.3092 4.051e0

153.3121 1.013e0

153.3284 1.013e0

153.3380 1.013e0

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153.3683 1.013e0

153.3874 1.013e0

153.3908 1.013e0

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153.4178 2.025e0

153.4239 2.025e0

153.4306 1.013e0

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153.8323 2.025e0

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153.9453 1.013e0

153.9673 1.013e0

153.9706 1.013e0

153.9841 1.013e0

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154.0437 1.100e1

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154.0984 7.288e0

154.1042 2.474e0

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154.1325 1.519e0

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154.1720 2.025e0

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154.2554 3.038e0

154.2710 2.025e0

154.2811 1.013e0

154.3070 1.013e0

154.3571 1.013e0

154.3717 2.025e0

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154.3869 1.013e0

154.3999 1.013e0

154.4020 2.025e0

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154.4730 1.013e0

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154.7141 1.013e0

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154.7371 1.013e0

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154.8757 2.025e0

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155.1203 3.719e0

155.1423 2.025e0

155.1473 3.038e0

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155.9296 1.013e0

155.9427 1.013e0

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155.9761 2.025e0

155.9952 2.025e0

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157.0102 1.013e0

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157.0668 1.013e0

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157.0958 1.559e1

157.0982 1.446e1

157.1009 5.738e0

157.1033 6.701e0

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157.1353 1.832e0

157.1582 2.025e0

157.1671 3.038e0

157.1730 2.025e0

157.1860 1.013e0

157.1894 3.038e0

157.2206 1.013e0

157.2265 3.038e0

157.2281 2.025e0

157.2392 1.013e0

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157.2830 1.013e0

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157.3163 1.013e0

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157.3873 1.013e0

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157.4595 2.025e0

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157.4986 2.025e0

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157.7599 1.013e0

157.7718 2.025e0

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157.9065 1.013e0

157.9091 5.063e0

157.9768 1.013e0

157.9802 1.013e0

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158.0784 3.782e0

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158.0989 1.839e0

158.1069 2.651e0

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158.8533 1.013e0

158.8881 2.025e0

158.9273 2.025e0

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158.9978 1.013e0

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159.0514 1.013e0

159.0570 3.691e0

159.0702 5.800e0

159.0759 1.918e0

159.0999 2.706e0

159.1086 3.499e0

159.1119 1.007e1

159.1146 1.186e1

159.1414 1.013e0

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159.1567 2.025e0

159.1727 1.013e0

159.1965 2.025e0

159.2154 1.013e0

159.2296 1.013e0

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159.2757 1.013e0

159.2809 2.025e0

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160.0629 4.051e0

160.0683 2.025e0

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160.0981 1.435e1

160.0995 2.000e1

160.1162 2.771e0

160.1339 1.519e0

160.1408 2.025e0

160.1430 1.013e0

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160.1790 1.013e0

160.1859 1.013e0

160.1933 1.013e0

160.1978 2.025e0

160.2030 1.013e0

160.2047 2.025e0

160.2065 3.038e0

160.2261 1.013e0

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160.2581 3.038e0

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160.3206 2.025e0

160.3561 2.025e0

160.3571 2.025e0

160.3709 1.013e0

160.3880 1.013e0

160.3989 1.013e0

160.4211 2.025e0

160.4246 1.013e0

160.4383 1.013e0

160.4554 1.013e0

160.4629 1.013e0

160.4689 1.013e0

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160.4886 1.013e0

160.4994 1.013e0

160.5228 1.013e0

160.5424 1.013e0

160.5526 1.013e0

160.5731 1.013e0

160.5903 2.025e0

160.5999 2.025e0

160.6183 2.025e0

160.6308 2.025e0

160.6405 1.013e0

160.6703 2.025e0

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160.7394 2.025e0

160.7514 1.013e0

160.7583 2.025e0

160.7755 2.025e0

160.7823 2.025e0

160.7855 1.013e0

160.7893 1.013e0

160.7981 2.025e0

160.8086 1.013e0

160.8191 3.038e0

160.8232 3.038e0

160.8291 3.038e0

160.8429 1.013e0

160.8564 4.051e0

160.8670 3.038e0

160.8726 2.025e0

160.8749 4.192e0

160.8864 2.025e0

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160.8966 3.038e0

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160.9142 2.025e0

160.9200 2.025e0

160.9407 2.025e0

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160.9670 5.063e0

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161.0452 2.025e0

161.0547 3.038e0

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161.0845 8.701e0

161.0856 1.100e1

161.0935 4.420e0

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161.1241 3.512e0

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