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

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

Elements Used:

C: 14-14 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 S: 2-2 Br: 1-1 F: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

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

419.9368 419.9375 -0.7 -1.7 8.5 110.2 0.0 C14 H12 N O4 S2 Br F