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

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

Elements Used:

C: 16-16 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 S: 1-1 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

413.9820 413.9811 0.9 2.2 9.5 105.8 0.0 C16 H14 N O4 S Br F