

Elemental Composition Report for [M+H]+

Single Mass Analysis

Tolerance = 5.0 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

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

Elements Used:

C: 1-40 H: 1-80 N: 1-6 O: 1-6 F: 6-6 S: 1-1

Minimum: -1.5

Maximum: 5.0 5.0 100.0

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

412.0798 412.0806 -0.8 -1.9 7.5 114.1 0.0 C17 H16 N O2 F6 S

[M+H+ACN]+ 453m/z