

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

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

Elements Used:

C: 1-90 H: 0-120 N: 0-4 O: 1-10 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

444.1689 444.1692 -0.3 -0.7 6.5 102.0 0.0 C20 H30 N O8 S

[M+NH4]+ 461m/z