

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

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

Elements Used:

C: 1-30 H: 0-100 O: 0-10 S: 1-2

Minimum: -1.5

Maximum: 5.0 5.0 100.0

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

303.1057 303.1055 0.2 0.7 8.5 75.7 0.0 C17 H19 O3 S

Elemental Composition Report for [M+NH4]+

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

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

Elements Used:

C: 1-30 H: 0-100 N: 0-1 O: 0-10 S: 1-2

Minimum: -1.5

Maximum: 5.0 5.0 100.0

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

320.1326 320.1320 0.6 1.9 7.5 72.0 0.0 C17 H22 N O3 S