



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

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

Elements Used:

C: 1-30 H: 0-120 N: 0-1 O: 0-8 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

345.1164 345.1161 0.3 0.9 9.5 79.2 0.0 C19 H21 O4 S

Elemental Composition Report for 362m/z

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

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

Elements Used:

C: 1-30 H: 0-120 N: 0-1 O: 0-8 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

362.1419 362.1426 -0.7 -1.9 8.5 106.2 0.0 C19 H24 N O4 S [M+NH4]+