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

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

Elements Used:

C: 13-13 H: 0-150 11B: 0-1 N: 0-10 O: 0-10 Na: 0-1 S: 1-1 Br: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

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

328.9854 328.9847 0.7 2.1 6.5 63.6 0.0 C13 H14 O3 S Br