

reference

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1340 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 15-15 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 S: 0-2 79Br: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 80.0

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

365.9771 365.9756 1.5 4.1 16.5 94.2 1.1 C15 H4 N5 O3 S2

 365.9800 -2.9 -7.9 9.5 93.6 0.4 C15 H13 N O3 S 79Br