

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

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

Elements Used:

C: 14-14 H: 0-150 N: 0-10 O: 0-15 Na: 0-1 S: 1-2 Br: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 80.0

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

401.9472 401.9469 0.3 0.7 8.5 106.4 0.0 C14 H13 N O4 S2 Br