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

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

Elements Used:

C: 16-16 H: 0-200 N: 0-10 O: 0-11 Na: 0-1 S: 0-1 Br: 2-2

Minimum: -1.5

Maximum: 5.0 10.0 80.0

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

473.9025 473.9010 1.5 3.2 9.5 103.6 1.7 C16 H14 N O4 S Br2

473.9065 -4.0 -8.4 11.5 102.0 0.2 C16 H11 N3 O3 Na Br2