 Elemental Composition Report

[M-H]-

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

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

Elements Used:

C: 19-19 H: 0-100 N: 0-10 O: 0-10 Na: 0-1 S: 1-1 Br: 1-1 56Fe: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 80.0

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

452.0161 452.0167 -0.6 -1.3 10.5 50.5 0.0 C19 H19 N O5 S Br