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

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

Elements Used:

C: 14-17 H: 0-150 N: 0-10 O: 0-12 Na: 0-1 S: 0-1 I: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

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

267.1054 267.1055 -0.1 -0.4 5.5 64.6 0.0 C14 H19 O3 S

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

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

Elements Used:

C: 14-17 H: 0-150 N: 0-10 O: 0-12 Na: 0-1 S: 0-1 I: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

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

309.1501 309.1500 0.1 0.3 2.5 73.3 0.4 C15 H26 O3 Na S

309.1524 -2.3 -7.4 5.5 74.1 1.1 C17 H25 O3 S