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

1319 formula(e) evaluated with 10 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-30 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 S: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 80.0

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

438.1381 438.1375 0.6 1.4 13.5 79.2 1.0 C24 H24 N O5 S

438.1389 -0.8 -1.8 18.5 80.7 2.5 C25 H20 N5 O S

438.1365 1.6 3.7 15.5 79.5 1.3 C23 H21 N5 O Na S

438.1400 -1.9 -4.3 9.5 85.2 7.0 C20 H24 N O10

438.1403 -2.2 -5.0 16.5 85.6 7.4 C20 H17 N9 O2 Na

438.1355 2.6 5.9 23.5 85.6 7.4 C28 H16 N5 O

438.1351 3.0 6.8 10.5 80.0 1.8 C22 H25 N O5 Na S

438.1414 -3.3 -7.5 14.5 86.0 7.8 C21 H20 N5 O6

438.1348 3.3 7.5 14.5 80.4 2.2 C20 H20 N7 O3 S

438.1341 4.0 9.1 18.5 85.8 7.5 C27 H20 N O5