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, Odd and Even Electron Ions

1122 formula(e) evaluated with 17 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 10-30 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

319.1474 319.1478 -0.4 -1.3 -1.0 140.5 6.5 C10 H25 N O10

319.1480 -0.6 -1.9 7.5 142.5 8.5 C17 H23 N2 O2 S

319.1467 0.7 2.2 8.0 142.9 8.9 C15 H21 N5 O S

319.1481 -0.7 -2.2 6.0 141.2 7.2 C10 H18 N9 O2 Na

319.1481 -0.7 -2.2 0.5 140.2 6.2 C11 H24 N2 O7 Na

319.1463 1.1 3.4 13.5 134.5 0.4 C23 H20 Na

319.1487 -1.3 -4.1 16.5 135.2 1.2 C25 H19

319.1456 1.8 5.6 4.5 143.5 9.4 C15 H24 N2 O2 Na S

319.1492 -1.8 -5.6 4.0 140.9 6.9 C11 H21 N5 O6

319.1453 2.1 6.6 8.5 143.7 9.7 C13 H19 N8 S

319.1453 2.1 6.6 3.0 144.1 10.1 C14 H25 N O5 S

319.1495 -2.1 -6.6 5.5 141.0 7.0 C12 H20 N6 O3 Na

319.1496 -2.2 -6.9 8.5 142.2 8.2 C20 H24 Na S

319.1447 2.7 8.5 12.5 137.2 3.2 C20 H19 N2 O2

319.1505 -3.1 -9.7 3.5 142.1 8.0 C13 H23 N2 O7

319.1443 3.1 9.7 5.0 144.4 10.4 C13 H22 N5 O Na S

319.1505 -3.1 -9.7 9.0 142.2 8.2 C12 H17 N9 O2