

Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

5974 formula(e) evaluated with 33 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 30-70 H: 0-200 N: 0-15 O: 0-15 Na: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

962.4527 962.4573 -4.6 -4.8 41.5 365.4 C70 H60 N O3

962.4592 -6.5 -6.8 28.5 878.1 C58 H64 N3 O10

962.4581 -5.4 -5.6 30.5 901.3 C57 H61 N7 O6 Na

962.4578 -5.1 -5.3 34.5 927.5 C55 H56 N13 O4

962.4568 -4.1 -4.3 25.5 1010.9 C56 H65 N3 O10 Na

962.4565 -3.8 -3.9 29.5 1038.6 C54 H60 N9 O8

962.4549 -2.2 -2.3 38.5 1191.8 C68 H61 N O3 Na

962.4546 -1.9 -2.0 42.5 1214.2 C66 H56 N7 O

962.4533 -0.6 -0.6 37.5 1323.8 C65 H60 N3 O5

962.4522 0.5 0.5 39.5 1342.4 C64 H57 N7 O Na

962.4509 1.8 1.9 34.5 1457.5 C63 H61 N3 O5 Na

962.4506 2.1 2.2 38.5 1484.7 C61 H56 N9 O3

962.4493 3.4 3.5 33.5 1605.3 C60 H60 N5 O7

962.4482 4.5 4.7 35.5 1628.9 C59 H57 N9 O3 Na

962.4479 4.8 5.0 39.5 1658.1 C57 H52 N15 O

962.4479 4.8 5.0 28.5 1730.9 C59 H64 N O11

962.4469 5.8 6.0 30.5 1756.0 C58 H61 N5 O7 Na

962.4466 6.1 6.3 34.5 1787.0 C56 H56 N11 O5

962.4583 -5.6 -5.8 16.5 1870.6 C42 H64 N11 O15

962.4573 -4.6 -4.8 18.5 1911.0 C41 H61 N15 O11 Na

962.4554 -2.7 -2.8 31.5 1975.1 C53 H57 N13 O4 Na

962.4551 -2.4 -2.5 24.5 2083.1 C53 H64 N5 O12

962.4541 -1.4 -1.5 26.5 2111.9 C52 H61 N9 O8 Na

962.4538 -1.1 -1.1 30.5 2146.0 C50 H56 N15 O6

962.4527 0.0 0.0 21.5 2252.2 C51 H65 N5 O12 Na

962.4525 0.2 0.2 25.5 2286.8 C49 H60 N11 O10

962.4514 1.3 1.4 27.5 2319.6 C48 H57 N15 O6 Na

962.4511 1.6 1.7 20.5 2431.4 C48 H64 N7 O14

962.4501 2.6 2.7 22.5 2465.4 C47 H61 N11 O10 Na

962.4487 4.0 4.2 17.5 2612.4 C46 H65 N7 O14 Na

962.4484 4.3 4.5 21.5 2650.8 C44 H60 N13 O12

962.4460 6.7 7.0 18.5 2839.7 C42 H61 N13 O12 Na

962.4559 -3.2 -3.3 13.5 3030.8 C40 H65 N11 O15 Na

