

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 1000.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

767 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 3-150 N: 0-20 O: 0-20 Na: 0-1 Br: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 1000.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

553.1794 553.1814 -2.0 -3.6 13.5 116.7 C28 H34 N4 O3 Br

REPORT MASSES AS +/-5mDa, referenced against

Leucine Enkephalin @ 557.2802 (M+H, C13 isotope) and 556.2771 (M+H, C12 isotope) positive mode, 555.2645 (M-H, C13) and 554.2615 (M-H, C12) negative mode.

or Sulfadimethoxine @312.0840 (M+H, C13) and 311.0814 (M+H, C12) positive mode, 310.0684 (M-H, C13) and 309.0658 (M-H, C12) negative mode.

This software version MassLynx 4.1 is calibrated ignoring the electron in all cases.

PEAK LIST

150.4943 1.013e0

150.5195 1.013e0

150.5499 4.051e0

150.5880 1.013e0

150.6631 1.013e0

150.8149 2.025e0

150.9149 1.013e0

150.9502 2.025e0

150.9717 2.025e0

151.0120 2.025e0

151.0473 6.481e1

151.1005 3.038e0

151.1265 8.093e0

151.1713 6.076e0

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