

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

3027 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 23-23 H: 0-200 N: 0-10 O: 0-20 Na: 0-1 S: 0-10

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

440.1637 440.1644 -0.7 -1.6 12.5 0.2 C23 H26 N3 O4 S

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.

150.8313 1.013e0

150.8897 1.013e0

150.9217 2.025e0

150.9872 2.025e0

151.0317 2.025e0

151.0498 2.025e0

151.1036 2.025e0

151.1671 2.025e0

151.2091 1.013e0

151.2257 2.025e0

151.2423 1.013e0

151.3075 1.013e0

151.3371 1.013e0

151.3695 1.013e0

151.4563 2.025e0

151.5067 1.013e0

151.5282 2.025e0

151.5466 1.013e0

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152.1487 1.013e0

152.1677 2.025e0

152.2094 2.025e0

152.2272 1.013e0

152.3152 1.013e0

152.3584 1.013e0

152.4289 2.025e0

152.5354 1.013e0

152.5981 1.013e0

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152.7653 1.013e0

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189.9493 1.013e0

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192.5007 2.025e0

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