



Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 26-26 H: 0-200 N: 0-10 O: 0-10 Br: 1-1

Minimum: -1.5

Maximum: 5.0 7.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

510.1412 510.1392 2.0 3.9 13.5 0.3 C26 H29 N3 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.

150.1140 1.013e0

150.1317 2.025e0

150.1790 1.013e0

150.1985 1.013e0

150.2342 1.013e0

150.2574 1.013e0

150.3191 1.013e0

150.4130 1.013e0

150.4929 2.025e0

150.6247 1.013e0

150.6546 2.025e0

150.6932 1.013e0

150.7263 2.025e0

150.7649 1.013e0

150.7865 2.025e0

150.8534 1.013e0

150.9937 1.013e0

151.0458 1.423e1

151.0887 1.013e0

151.1115 6.076e0

151.1472 1.013e0

151.1638 1.013e0

151.1861 1.013e0

151.2677 1.013e0

151.2844 1.013e0

151.3563 2.025e0

151.4148 3.038e0

151.4414 1.013e0

151.4675 1.013e0

151.5456 2.025e0

151.5603 2.025e0

151.5945 3.165e0

151.6538 1.013e0

151.7457 1.013e0

151.8110 1.013e0

151.8277 1.013e0

151.8564 1.013e0

151.8797 1.013e0

151.9250 2.025e0

151.9683 1.013e0

152.0270 1.013e0

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152.3018 1.013e0

152.3384 1.013e0

152.3646 1.013e0

152.4005 1.013e0

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153.7277 2.025e0

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154.3246 1.013e0

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154.7182 2.025e0

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155.2002 1.013e0

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193.6226 1.013e0

193.6442 1.013e0

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193.9472 3.038e0

194.1123 2.025e0

194.1286 1.013e0

194.1885 1.013e0

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194.3658 1.013e0

194.4282 3.038e0

194.4771 1.013e0

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197.1871 1.013e0

197.3585 2.025e0

197.3804 1.013e0

197.4314 3.038e0

197.4845 1.013e0

197.5861 1.013e0

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