

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.

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 13-20 H: 15-27 O: 1-5 Na: 0-1 S: 1-1 Cl: 1-1

Minimum: -15.0

Maximum: 5.0 15.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

287.0520 287.0509 1.1 3.8 5.5 5.1 C13 H16 O3 S Cl

237.3848 1.013e0

237.3926 1.013e0

237.4054 2.025e0

237.4251 2.025e0

237.4348 1.013e0

237.4391 1.013e0

237.4793 1.013e0

237.4912 1.013e0

237.4999 1.013e0

237.5317 1.013e0

237.5492 1.013e0

237.5521 1.013e0

237.5600 3.038e0

237.5717 1.013e0

237.5728 1.013e0

237.5953 2.025e0

237.6170 1.013e0

237.6180 1.013e0

237.6585 1.013e0

237.6841 1.013e0

237.6875 1.013e0

237.7048 1.013e0

237.7232 1.013e0

237.7331 1.013e0

237.7569 1.013e0

237.7619 1.013e0

237.7659 2.025e0

237.7896 2.025e0

237.7995 1.013e0

237.8062 1.013e0

237.8345 1.013e0

237.8489 2.025e0

237.8555 1.013e0

237.8761 1.013e0

237.9165 2.025e0

237.9176 1.013e0

237.9269 2.025e0

237.9292 1.013e0

237.9469 1.013e0

237.9698 1.013e0

237.9798 2.025e0

238.0103 2.025e0

238.0120 2.604e0

238.0135 3.038e0

238.0156 5.063e0

238.0249 8.022e0

238.0293 3.038e0

238.0384 5.497e0

238.0540 6.067e0

238.0635 2.025e0

238.0934 4.376e0

238.0970 4.051e0

238.1030 2.025e0

238.1069 1.013e0

238.1168 3.038e0

238.1256 4.051e0

238.1284 2.025e0

238.1303 1.013e0

238.1431 1.013e0

238.1466 1.013e0

238.1494 3.038e0

238.1688 3.038e0

238.1744 5.063e0

238.1912 1.013e0

238.2011 1.013e0

238.2122 1.013e0

238.2413 1.013e0

238.2492 1.013e0

238.2626 1.013e0

238.2655 2.025e0

238.3276 1.013e0

238.3613 1.013e0

238.3769 1.013e0

238.3985 2.025e0

238.4054 1.013e0

238.4262 1.013e0

238.4456 1.013e0

238.4589 1.013e0

238.4845 2.025e0

238.4992 1.013e0

238.5198 1.013e0

238.5287 2.025e0

238.5449 1.013e0

238.5484 2.025e0

238.5702 3.038e0

238.6146 1.013e0

238.6156 1.013e0

238.6806 1.013e0

238.6835 1.013e0

238.7300 1.013e0

238.7464 2.025e0

238.7539 1.013e0

238.7583 1.013e0

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238.7714 1.013e0

238.8041 1.013e0

238.8076 4.051e0

238.8354 1.013e0

238.8578 1.013e0

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238.8730 1.013e0

238.8752 1.687e0

238.8809 2.025e0

238.8897 1.013e0

238.9056 2.025e0

238.9223 1.013e0

238.9352 2.025e0

238.9418 1.013e0

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238.9835 2.025e0

239.0042 2.025e0

239.0072 4.051e0

239.0094 3.038e0

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239.0190 8.101e0

239.0308 2.025e0

239.0400 4.051e0

239.0416 9.114e0

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239.1702 2.025e0

239.1935 1.013e0

239.1968 1.013e0

239.2068 1.013e0

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239.2605 1.013e0

239.3022 2.025e0

239.3172 2.025e0

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242.0223 9.215e1

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242.1718 7.089e0

242.1760 2.025e0

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242.3954 1.013e0

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242.6809 1.013e0

242.6878 2.025e0

242.7026 2.025e0

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242.7614 2.025e0

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242.9066 1.013e0

242.9408 4.051e0

242.9436 1.013e0

242.9474 1.013e0

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242.9865 1.013e0

242.9904 1.013e0

243.0061 3.038e0

243.0083 3.409e0

243.0223 1.532e1

243.0326 8.743e0

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243.0529 5.063e0

243.0620 1.013e0

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243.0927 2.025e0

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243.1174 3.038e0

243.1264 1.013e0

243.1274 2.025e0

243.1381 4.051e0

243.1483 2.025e0

243.1540 5.063e0

243.1552 4.051e0

243.1566 3.038e0

243.1770 2.025e0

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243.2028 1.013e0

243.2060 1.013e0

243.2187 1.013e0

243.2235 2.025e0

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243.2555 1.013e0

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243.2723 1.013e0

243.2787 3.038e0

243.2836 5.063e0

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243.2870 3.038e0

243.2938 2.025e0

243.2949 2.025e0

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244.1186 2.025e0

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244.1275 4.051e0

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244.1526 3.038e0

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244.1585 2.025e0

244.1780 2.025e0

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244.1884 7.089e0

244.1919 5.245e0

244.1935 3.038e0

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244.2179 1.013e0

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245.0499 5.063e0

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245.5592 4.051e0

245.5723 3.038e0

245.5746 4.051e0

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245.9882 1.519e1

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245.9987 9.254e0

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246.0417 1.013e0

246.0494 6.076e0

246.0511 5.063e0

246.0551 6.076e0

246.0574 8.942e0

246.0592 7.089e0

246.0634 4.051e0

246.0904 1.013e0

246.1002 2.025e0

246.1033 2.025e0

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246.1372 5.063e0

246.1618 2.025e0

246.1652 3.038e0

246.1684 2.025e0

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246.1891 3.038e0

246.2072 5.063e0

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