 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

232 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 15-15 H: 0-200 N: 0-10 O: 0-15 Na: 0-1 S: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

276.1049 276.1058 -0.9 -3.3 7.5 374.6 0.0 C15 H18 N O2 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.

155.7133 1.266e-2

155.7164 1.013e0

155.7228 1.266e-2

155.7347 2.532e-2

155.7422 3.038e0

155.7499 1.266e-2

155.7583 2.025e0

155.7632 1.266e-2

155.7663 2.025e0

155.7729 3.038e0

155.7895 3.038e0

155.7962 4.051e0

155.7996 1.013e0

155.8194 2.532e-2

155.8207 2.025e0

155.8225 1.013e0

155.8451 5.063e0

155.8488 5.063e0

155.8632 3.038e0

155.8648 2.025e0

155.8821 1.025e0

155.8889 1.013e0

155.8923 2.532e-2

155.8990 1.025e0

155.9041 2.025e0

155.9058 2.025e0

155.9126 2.025e0

155.9160 1.266e-2

155.9180 2.025e0

155.9283 2.532e-2

155.9318 1.266e-2

155.9454 2.025e0

155.9555 2.532e-2

155.9589 1.025e0

155.9817 1.013e0

155.9849 1.266e-2

155.9917 1.013e0

156.0002 2.532e-2

156.0052 2.025e0

156.0069 2.025e0

156.0120 2.025e0

156.0210 5.011e0

156.0321 5.063e0

156.0495 4.127e0

156.0527 1.057e1

156.0545 6.480e0

156.0748 3.739e0

156.1129 3.311e0

156.1211 2.522e1

156.1258 2.025e0

156.1275 1.637e1

156.1301 1.963e1

156.1323 1.255e1

156.1470 4.350e0

156.1486 2.737e0

156.1536 8.225e-1

156.1748 3.002e0

156.1762 1.405e-2

156.1820 1.025e0

156.1859 3.038e0

156.1901 1.038e0

156.1939 2.025e0

156.1958 2.025e0

156.2110 3.038e0

156.2138 1.051e0

156.2262 2.025e0

156.2281 7.089e0

156.2441 2.038e0

156.2473 1.013e0

156.2540 1.025e0

156.2556 2.025e0

156.2574 1.013e0

156.2802 3.089e0

156.2878 4.051e0

156.2987 6.076e0

156.3004 1.025e0

156.3036 1.025e0

156.3071 1.038e0

156.3210 4.063e0

156.3308 3.038e0

156.3325 2.025e0

156.3395 2.025e0

156.3474 1.266e-2

156.3489 2.532e-2

156.3526 3.038e0

156.3568 2.038e0

156.3586 2.025e0

156.3806 1.266e-2

156.3866 1.038e0

156.4021 4.051e0

156.4100 1.038e0

156.4183 7.089e0

156.4253 2.025e0

156.4406 2.038e0

156.4538 1.266e-2

156.4568 1.025e0

156.4600 1.025e0

156.4644 3.038e0

156.4666 1.013e0

156.4903 2.038e0

156.4950 3.038e0

156.5038 1.266e-2

156.5131 5.063e0

156.5283 2.025e0

156.5385 2.025e0

156.5401 1.025e0

156.5419 2.532e-2

156.5453 1.182e0

156.5586 2.025e0

156.5634 1.013e0

156.5681 2.025e0

156.5696 1.013e0

156.5730 1.266e-2

156.5832 1.266e-2

156.5849 2.025e0

156.5883 2.025e0

156.5933 1.266e-2

156.6052 2.025e0

156.6209 3.089e0

156.6261 1.025e0

156.6272 3.038e0

156.6310 3.038e0

156.6398 1.266e-2

156.6432 2.025e0

156.6465 1.013e0

156.6516 2.025e0

156.6567 1.266e-2

156.6667 1.013e0

156.6862 3.038e0

156.6910 3.038e0

156.6930 2.532e-2

156.6947 2.025e0

156.6964 1.013e0

156.7168 2.025e0

156.7263 1.013e0

156.7343 2.025e0

156.7394 1.013e0

156.7428 3.051e0

156.7597 1.266e-2

156.7631 1.266e-2

156.7666 6.089e0

156.7873 2.025e0

156.7919 4.051e0

156.8028 1.013e0

156.8096 4.051e0

156.8222 3.038e0

156.8298 1.013e0

156.8359 1.025e0

156.8458 2.532e-2

156.8527 2.532e-2

156.8662 2.025e0

156.8674 2.063e0

156.8798 1.266e-2

156.8877 3.038e0

156.8949 5.802e0

156.9059 1.013e0

156.9093 5.063e0

156.9127 2.038e0

156.9271 3.798e-2

156.9296 1.266e-2

156.9396 1.013e0

156.9584 4.063e0

156.9625 1.025e0

156.9659 1.013e0

156.9710 2.025e0

156.9897 1.013e0

156.9932 2.025e0

156.9962 1.025e0

157.0106 2.532e-2

157.0124 1.013e0

157.0293 2.025e0

157.0344 2.025e0

157.0361 4.051e0

157.0656 6.559e0

157.0670 2.684e-1

157.0774 9.265e0

157.0823 3.429e0

157.0899 5.618e0

157.0925 1.273e0

157.1039 3.429e0

157.1346 5.058e0

157.1358 1.908e1

157.1503 5.192e-1

157.1657 1.977e0

157.1710 1.310e0

157.1780 4.908e0

157.1925 1.076e0

157.1953 3.798e-2

157.1976 2.025e0

157.2044 2.025e0

157.2222 2.532e-2

157.2254 1.266e-2

157.2383 4.051e0

157.2424 1.025e0

157.2441 2.025e0

157.2594 1.266e-2

157.2628 2.025e0

157.2694 2.025e0

157.2788 2.532e-2

157.2945 3.038e0

157.3008 2.025e0

157.3136 2.195e0

157.3161 1.013e0

157.3211 2.025e0

157.3244 2.025e0

157.3291 1.013e0

157.3323 2.532e-2

157.3339 2.532e-2

157.3575 4.051e0

157.3591 2.038e0

157.3625 3.038e0

157.3794 2.532e-2

157.3857 4.051e0

157.4023 2.051e0

157.4091 2.025e0

157.4176 2.025e0

157.4209 2.025e0

157.4329 1.266e-2

157.4455 1.013e0

157.4590 1.013e0

157.4680 3.038e0

157.4794 7.595e-2

157.4911 2.025e0

157.5022 2.025e0

157.5088 1.025e0

157.5157 2.025e0

157.5191 1.013e0

157.5275 3.038e0

157.5327 1.266e-2

157.5429 1.266e-2

157.5468 3.051e0

157.5525 1.013e0

157.5557 1.013e0

157.5588 2.025e0

157.5741 2.025e0

157.5792 1.038e0

157.5809 2.025e0

157.5860 1.013e0

157.5911 2.025e0

157.5997 1.013e0

157.6029 1.266e-2

157.6155 1.013e0

157.6173 2.025e0

157.6292 1.025e0

157.6478 4.051e0

157.6564 1.266e-2

157.6628 1.013e0

157.6649 4.888e0

157.6825 2.025e0

157.6927 3.798e-2

157.6944 2.025e0

157.7029 2.025e0

157.7063 1.013e0

157.7130 3.038e0

157.7163 1.013e0

157.7217 3.038e0

157.7289 1.266e-2

157.7341 2.025e0

157.7392 1.266e-2

157.7460 2.051e0

157.7494 2.051e0

157.7562 1.266e-2

157.7595 5.485e-1

157.7696 4.051e0

157.7762 2.025e0

157.7943 2.025e0

157.8095 1.266e-2

157.8107 3.038e0

157.8147 2.025e0

157.8232 1.013e0

157.8249 2.025e0

157.8345 4.051e0

157.8373 2.025e0

157.8390 1.025e0

157.8424 1.013e0

157.8440 2.025e0

157.8493 1.266e-2

157.8528 1.025e0

157.8629 2.532e-2

157.8651 2.297e0

157.8714 1.051e0

157.8819 2.025e0

157.8879 5.063e0

157.8960 1.013e0

157.8992 2.532e-2

157.9168 2.051e0

157.9180 2.532e-2

157.9282 2.025e0

157.9316 2.025e0

157.9367 1.013e0

157.9437 3.038e0

157.9495 1.025e0

157.9560 1.266e-2

157.9576 2.532e-2

157.9646 2.025e0

157.9663 2.025e0

157.9706 3.798e-2

157.9777 6.076e0

157.9867 1.013e0

157.9884 2.025e0

157.9901 2.532e-2

158.0020 2.025e0

158.0033 1.013e0

158.0128 1.266e-2

158.0162 1.266e-2

158.0197 2.025e0

158.0333 1.025e0

158.0538 2.025e0

158.0612 4.051e0

158.0647 2.870e0

158.0821 4.725e0

158.0901 6.667e0

158.0925 3.447e0

158.0998 1.437e0

158.1129 3.155e0

158.1184 3.465e-1

158.1331 6.388e0

158.1537 2.898e0

158.1554 3.454e0

158.1570 7.685e0

158.1832 5.063e0

158.1882 2.063e0

158.2051 4.051e0

158.2088 2.051e0

158.2104 4.051e0

158.2120 3.038e0

158.2258 2.532e-2

158.2274 3.038e0

158.2338 1.013e0

158.2401 2.025e0

158.2537 1.178e0

158.2571 1.013e0

158.2648 1.038e0

158.2673 1.025e0

158.2707 1.013e0

158.2773 5.104e0

158.2938 1.038e0

158.2983 2.532e-2

158.3053 2.025e0

158.3105 3.038e0

158.3139 1.025e0

158.3194 3.330e0

158.3309 1.013e0

158.3343 1.013e0

158.3475 1.013e0

158.3758 4.051e0

158.3775 3.051e0

158.3826 2.025e0

158.3844 2.025e0

158.3909 1.063e0

158.3968 3.798e-2

158.4032 5.063e0

158.4063 3.798e-2

158.4157 2.532e-2

158.4310 3.076e0

158.4344 2.025e0

158.4412 1.013e0

158.4516 3.798e-2

158.4530 2.051e0

158.4549 1.266e-2

158.4565 2.025e0

158.4845 1.266e-2

158.4895 2.025e0

158.4914 4.451e0

158.5183 1.266e-2

158.5215 1.025e0

158.5328 2.532e-2

158.5379 1.266e-2

158.5396 2.025e0

158.5464 2.025e0

158.5549 2.025e0

158.5651 1.025e0

158.5747 4.051e0

158.5816 2.025e0

158.5848 1.025e0

158.5892 2.735e0

158.5947 2.025e0

158.6050 1.013e0

158.6118 1.266e-2

158.6386 1.266e-2

158.6418 1.013e0

158.6499 3.038e0

158.6516 1.266e-2

158.6532 2.025e0

158.6550 1.013e0

158.6619 1.013e0

158.6687 1.266e-2

158.6720 1.266e-2

158.6857 2.025e0

158.6874 2.025e0

158.6988 4.051e0

158.7144 3.798e-2

158.7163 5.063e0

158.7187 1.013e0

158.7255 1.266e-2

158.7392 1.266e-2

158.7441 3.038e0

158.7495 3.038e0

158.7558 1.013e0

158.7687 1.266e-2

158.7841 2.025e0

158.7960 1.025e0

158.7995 1.013e0

158.8064 1.266e-2

158.8099 2.532e-2

158.8128 1.266e-2

158.8160 1.013e0

158.8256 1.266e-2

158.8409 3.038e0

158.8496 3.038e0

158.8545 2.051e0

158.8633 2.532e-2

158.8699 1.038e0

158.8730 1.013e0

158.8826 1.013e0

158.8856 5.063e0

158.8912 5.063e0

158.9201 1.013e0

158.9236 1.266e-2

158.9334 2.025e0

158.9480 2.025e0

158.9515 2.025e0

158.9532 3.797e-2

158.9571 4.051e0

158.9634 1.266e-2

158.9668 2.532e-2

158.9839 1.266e-2

158.9872 4.051e0

158.9904 1.013e0

158.9999 1.038e0

159.0101 1.025e0

159.0169 1.013e0

159.0203 1.013e0

159.0271 5.063e0

159.0425 2.532e-2

159.0443 3.038e0

159.0566 4.051e0

159.0694 7.012e0

159.0794 4.907e0

159.1115 1.477e1

159.1352 2.323e0

159.1471 4.051e0

159.1500 5.063e-2

159.1536 4.301e0

159.1581 3.757e0

159.1607 1.203e0

159.1645 2.987e-1

159.1842 1.266e-2

159.1877 3.038e0

159.2048 1.025e0

159.2082 2.038e0

159.2150 1.266e-2

159.2184 1.013e0

159.2285 3.797e-2

159.2481 1.266e-2

159.2549 2.532e-2

159.2617 3.038e0

159.2685 1.013e0

159.2707 6.076e0

159.2730 3.798e-2

159.2828 3.038e0

159.2839 2.025e0

159.2919 1.266e-2

159.3051 2.038e0

159.3085 1.025e0

159.3221 1.013e0

159.3272 2.025e0

159.3323 1.013e0

159.3339 3.038e0

159.3391 2.038e0

159.3539 2.025e0

159.3555 1.266e-2

159.3613 6.076e0

159.3774 2.025e0

159.3893 1.038e0

159.3956 5.089e0

159.3996 1.013e0

159.4141 2.532e-2

159.4214 1.038e0

159.4309 2.025e0

159.4395 1.013e0

159.4566 1.266e-2

159.4591 3.038e0

159.4669 2.038e0

159.4703 8.101e0

159.4845 4.051e0

159.4896 4.051e0

159.4931 1.013e0

159.4965 3.797e-2

159.5152 2.025e0

159.5603 2.025e0

159.5622 8.101e0

159.5654 4.051e0

159.6001 1.025e0

159.6016 3.038e0

159.6035 1.266e-2

159.6139 1.013e0

159.6173 1.266e-2

159.6253 1.038e0

159.6528 3.798e-2

159.6640 1.266e-2

159.6743 1.013e0

159.6760 2.532e-2

159.6846 1.025e0

159.6911 3.076e0

159.6948 1.013e0

159.7017 1.266e-2

159.7117 2.532e-2

159.7141 1.038e0

159.7382 1.025e0

159.7497 4.051e0

159.7570 2.025e0

159.7626 2.063e0

159.7672 4.074e-2

159.7690 1.013e0

159.7832 8.101e0

159.8055 2.038e0

159.8123 2.532e-2

159.8226 1.013e0

159.8330 1.025e0

159.8455 1.266e-2

159.8488 1.063e0

159.8504 2.025e0

159.8591 1.025e0

159.8660 1.013e0

159.8693 2.025e0

159.8864 1.266e-2

159.8883 4.051e0

159.8998 1.025e0

159.9041 2.025e0

159.9126 1.025e0

159.9186 3.038e0

159.9230 6.076e0

159.9400 1.013e0

159.9418 2.025e0

159.9452 2.051e0

159.9472 2.038e0

159.9556 5.063e0

159.9602 1.025e0

159.9731 2.025e0

159.9800 3.076e0

159.9852 2.025e0

159.9869 1.013e0

160.0074 1.013e0

160.0108 1.266e-2

160.0123 3.038e0

160.0143 1.266e-2

160.0208 2.025e0

160.0256 2.025e0

160.0335 2.025e0

160.0354 2.025e0

160.0381 1.038e0

160.0429 4.051e0

160.0455 5.063e0

160.0596 1.161e1

160.0610 2.025e0

160.0624 1.694e0

160.0914 2.703e0

160.1003 2.476e0

160.1056 2.163e0

160.1196 8.674e0

160.1309 1.501e0

160.1462 1.880e0

160.1608 1.266e0

160.1799 2.886e0

160.1837 2.025e0

160.1889 2.025e0

160.1973 3.038e0

160.2060 3.797e-2

160.2107 2.025e0

160.2236 2.025e0

160.2254 2.532e-2

160.2289 3.797e-2

160.2323 1.025e0

160.2340 2.025e0

160.2426 1.266e-2

160.2460 1.013e0

160.2494 1.266e-2

160.2528 2.025e0

160.2563 2.025e0

160.2632 2.532e-2

160.2665 1.013e0

160.2790 2.532e-2

160.2894 1.266e-2

160.2928 1.025e0

160.2997 3.038e0

160.3116 2.025e0

160.3237 1.266e-2

160.3281 2.038e0

160.3304 1.266e-2

160.3368 1.013e0

160.3448 2.025e0

160.3464 3.797e-2

160.3481 2.025e0

160.3602 1.025e0

160.3645 2.441e0

160.3671 2.532e-2

160.3773 3.038e0

160.3808 4.051e0

160.3876 1.025e0

160.4070 1.266e-2

160.4156 2.025e0

160.4208 1.013e0

160.4259 4.051e0

160.4293 4.051e0

160.4310 1.266e-2

160.4378 1.266e-2

160.4413 2.025e0

160.4447 1.266e-2

160.4516 1.013e0

160.4630 2.025e0

160.4646 1.013e0

160.4950 1.013e0

160.4975 1.038e0

160.5001 2.025e0

160.5018 2.532e-2

160.5139 4.051e0

160.5221 1.266e-2

160.5253 2.532e-2

160.5285 1.013e0

160.5297 2.025e0

160.5327 3.063e0

160.5401 9.709e-2

160.5453 1.013e0

160.5590 3.797e-2

160.5658 2.025e0

160.5812 2.532e-2

160.5879 3.038e0

160.5956 1.266e-2

160.6059 1.013e0

160.6083 3.038e0

160.6127 5.063e-2

160.6315 2.025e0

160.6332 2.025e0

160.6532 3.038e0

160.6548 2.025e0

160.6596 1.013e0

160.6699 2.038e0

160.6811 2.038e0

160.6853 2.532e-2

160.6904 5.063e0

160.7076 1.013e0

160.7196 6.076e0

160.7269 1.013e0

160.7304 2.532e-2

160.7373 1.266e-2

160.7407 1.266e-2

160.7442 2.532e-2

160.7459 2.025e0

160.7471 3.402e0

160.7613 2.025e0

160.7650 1.038e0

160.7716 2.025e0

160.7748 3.051e0

160.7780 1.266e-2

160.7944 1.025e0

160.8030 2.532e-2

160.8048 2.025e0

160.8116 3.038e0

160.8219 1.013e0

160.8236 2.025e0

160.8437 2.025e0

160.8452 3.038e0

160.8550 1.025e0

160.8756 1.266e-2

160.8859 6.076e0

160.8876 2.025e0

160.8949 1.038e0

160.9029 1.025e0

160.9125 2.532e-2

160.9174 2.025e0

160.9397 1.025e0

160.9431 2.038e0

160.9446 3.038e0

160.9465 1.013e0

160.9517 2.532e-2

160.9534 1.266e-2

160.9638 1.025e0

160.9703 2.038e0

160.9866 1.013e0

160.9883 2.025e0

160.9897 8.101e0

161.0003 2.532e-2

161.0089 2.025e0

161.0153 5.063e0

161.0200 3.038e0

161.0228 4.634e0

161.0278 1.013e0

161.0340 2.051e0

161.0437 1.025e0

161.0541 1.013e0

161.0591 3.798e-2

161.0836 7.497e0

161.0854 1.964e1

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