

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 = 7.0 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

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

Elements Used:

C: 22-22 H: 20-25 N: 0-7 O: 0-6 Na: 0-1 S: 1-1

Minimum: -1.5

Maximum: 5.0 7.0 100.0

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

366.1513 366.1528 -1.5 -4.1 11.5 786.9 0.0 C22 H24 N O2 S

100.0022 1.266e-2

100.0076 1.013e0

100.0103 1.013e0

100.0394 1.266e-2

100.0414 3.038e0

100.0567 2.116e0

100.0673 2.025e0

100.0695 3.038e0

100.1072 2.025e0

100.1165 1.266e-2

100.1325 1.013e0

100.1459 1.013e0

100.1699 1.266e-2

100.1776 1.013e0

100.2070 1.013e0

100.2148 1.013e0

100.2415 1.266e-2

100.2708 1.025e0

100.3214 1.013e0

100.3278 1.038e0

100.3773 1.013e0

100.3905 1.025e0

100.4120 1.013e0

100.4199 1.266e-2

100.4520 1.266e-2

100.4571 1.266e-2

100.4586 2.025e0

100.4626 2.532e-2

100.4919 1.266e-2

100.4944 2.038e0

100.4998 1.266e-2

100.5028 1.013e0

100.5183 1.013e0

100.5399 1.266e-2

100.5689 1.013e0

100.5850 2.025e0

100.5956 1.266e-2

100.6172 1.013e0

100.6251 2.025e0

100.6462 1.013e0

100.6652 1.266e-2

100.6946 1.266e-2

100.7159 1.013e0

100.7476 1.266e-2

100.7610 1.266e-2

100.7876 1.266e-2

100.7904 1.266e-2

100.7933 1.266e-2

100.8065 1.013e0

100.8094 1.266e-2

100.8171 1.013e0

100.8332 1.266e-2

100.8345 2.025e0

100.8573 1.266e-2

100.8705 1.013e0

100.9106 1.013e0

100.9280 2.025e0

100.9346 1.266e-2

100.9452 1.266e-2

100.9559 1.025e0

100.9615 2.025e0

100.9760 2.025e0

100.9798 1.266e-2

100.9932 1.013e0

101.0039 1.266e-2

101.0173 2.038e0

101.0200 2.025e0

101.0294 2.025e0

101.0961 2.859e0

101.1071 2.051e0

101.1136 4.047e0

101.1296 2.532e-2

101.1417 2.025e0

101.1431 1.266e-2

101.1510 1.266e-2

101.1588 1.266e-2

101.1643 1.266e-2

101.1750 1.266e-2

101.1816 4.051e0

101.1938 1.013e0

101.1954 1.243e0

101.2044 1.266e-2

101.2165 2.025e0

101.2179 2.038e0

101.2419 3.038e0

101.2560 1.038e0

101.2660 1.025e0

101.2714 1.013e0

101.2860 2.025e0

101.2881 1.038e0

101.3021 4.051e0

101.3134 2.038e0

101.3295 2.051e0

101.3394 2.038e0

101.3423 2.025e0

101.3596 2.025e0

101.3999 1.038e0

101.4076 2.532e-2

101.4211 1.266e-2

101.4333 2.025e0

101.4372 1.013e0

101.4586 6.076e0

101.4746 1.266e-2

101.4853 1.013e0

101.4976 2.051e0

101.5069 1.025e0

101.5444 1.266e-2

101.5523 1.266e-2

101.5629 1.025e0

101.5897 1.013e0

101.6032 3.038e0

101.6273 1.013e0

101.6367 4.051e0

101.6461 1.266e-2

101.6528 2.025e0

101.6623 1.266e-2

101.6914 1.266e-2

101.7104 1.025e0

101.7171 2.025e0

101.7238 3.038e0

101.7345 1.013e0

101.7670 1.266e-2

101.7692 1.013e0

101.7854 2.025e0

101.8178 1.266e-2

101.8311 1.013e0

101.8391 1.013e0

101.8485 2.025e0

101.8929 2.532e-2

101.9330 3.051e0

101.9437 2.532e-2

101.9456 1.038e0

101.9761 1.013e0

101.9867 1.013e0

101.9933 2.532e-2

102.0002 2.025e0

102.0257 2.025e0

102.0270 1.266e-2

102.0349 1.266e-2

102.0642 2.732e0

102.0670 1.422e0

102.0814 8.380e0

102.0869 3.983e0

102.0961 3.670e0

102.1128 1.025e0

102.1200 3.038e0

102.1347 1.013e0

102.1502 1.013e0

102.1532 1.013e0

102.1961 1.013e0

102.2096 1.013e0

102.2149 1.266e-2

102.2338 1.025e0

102.2377 2.025e0

102.2551 1.013e0

102.2740 1.266e-2

102.2875 2.038e0

102.3038 1.025e0

102.3252 1.013e0

102.3306 2.532e-2

102.3373 2.025e0

102.3547 1.013e0

102.3576 1.013e0

102.3761 1.013e0

102.3910 2.025e0

102.4030 2.025e0

102.4137 1.266e-2

102.4271 1.266e-2

102.4434 1.266e-2

102.4596 1.266e-2

102.4676 1.013e0

102.4919 1.025e0

102.5029 1.266e-2

102.5404 2.038e0

102.5753 1.025e0

102.6480 1.266e-2

102.6587 1.013e0

102.6628 2.211e0

102.6763 2.025e0

102.6776 2.532e-2

102.6952 2.025e0

102.6991 1.013e0

102.7261 1.266e-2

102.7584 3.038e0

102.7666 1.013e0

102.7829 1.266e-2

102.8122 1.013e0

102.8178 1.266e-2

102.8483 3.038e0

102.8540 2.025e0

102.8553 1.013e0

102.8660 1.266e-2

102.8716 2.532e-2

102.8985 1.013e0

102.9013 1.013e0

102.9148 1.013e0

102.9470 1.013e0

102.9874 1.013e0

102.9984 1.266e-2

103.0037 1.266e-2

103.0120 1.266e-2

103.0172 1.013e0

103.0278 1.266e-2

103.0469 2.532e-2

103.0658 1.266e-2

103.0917 1.038e0

103.0953 1.013e0

103.1172 1.025e0

103.1183 2.025e0

103.1223 1.013e0

103.1373 2.532e-2

103.1493 1.266e-2

103.1791 1.266e-2

103.1926 1.013e0

103.2358 1.266e-2

103.2466 1.013e0

103.2546 1.266e-2

103.2816 2.025e0

103.2833 2.025e0

103.3411 1.013e0

103.3548 1.013e0

103.3710 1.266e-2

103.3789 1.013e0

103.4385 1.013e0

103.4898 1.266e-2

103.5116 1.025e0

103.5361 1.266e-2

103.5411 1.266e-2

103.5872 1.013e0

103.5980 1.266e-2

103.6007 1.013e0

103.6172 1.266e-2

103.6222 1.013e0

103.6407 3.038e0

103.6441 1.013e0

103.6738 1.013e0

103.7091 1.266e-2

103.7197 1.013e0

103.7469 1.025e0

103.7550 1.013e0

103.8117 2.532e-2

103.8905 1.266e-2

103.9176 1.013e0

103.9363 1.013e0

103.9470 1.266e-2

103.9797 1.266e-2

103.9933 1.013e0

104.0124 1.013e0

104.0339 1.013e0

104.0640 6.044e0

104.1001 3.142e0

104.1112 2.532e-2

104.1290 1.266e-2

104.1302 2.025e0

104.1395 1.266e-2

104.1451 1.013e0

104.1615 1.013e0

104.1803 1.013e0

104.1830 1.013e0

104.1966 1.013e0

104.2373 1.013e0

104.2401 1.013e0

104.2457 1.013e0

104.2780 1.013e0

104.2915 1.013e0

104.2943 1.013e0

104.3188 1.013e0

104.3297 1.013e0

104.3379 1.013e0

104.3977 1.013e0

104.4136 1.013e0

104.4206 2.025e0

104.4492 1.013e0

104.4707 1.013e0

104.4763 1.013e0

104.5280 2.532e-2

104.5634 1.266e-2

104.5715 1.013e0

104.5794 1.266e-2

104.5877 1.013e0

104.6013 1.266e-2

104.6340 1.266e-2

104.6449 1.013e0

104.6529 1.025e0

104.6858 1.013e0

104.6964 1.013e0

104.7128 1.013e0

104.7293 1.025e0

104.7453 1.013e0

104.7617 2.532e-2

104.7781 1.013e0

104.7808 1.266e-2

104.7836 2.532e-2

104.8216 1.013e0

104.8461 1.013e0

104.8568 1.266e-2

104.8732 1.013e0

104.9088 1.266e-2

104.9388 1.266e-2

104.9547 1.013e0

104.9576 1.013e0

104.9768 1.266e-2

104.9796 2.025e0

104.9876 1.013e0

105.0040 1.266e-2

105.0120 2.025e0

105.0796 2.269e-2

105.0884 1.266e-2

105.0911 1.025e0

105.1237 1.266e-2

105.1279 2.025e0

105.1308 2.025e0

105.1387 2.025e0

105.1483 1.025e0

105.1509 1.266e-2

105.1838 1.266e-2

105.1947 3.038e0

105.1988 2.025e0

105.2138 2.025e0

105.2151 2.532e-2

105.2231 3.038e0

105.2246 1.013e0

105.2329 1.266e-2

105.2574 1.013e0

105.2643 2.025e0

105.2766 1.025e0

105.3037 2.532e-2

105.3063 1.266e-2

105.3201 1.025e0

105.3311 1.266e-2

105.3501 1.025e0

105.3608 1.013e0

105.3761 2.025e0

105.3829 1.266e-2

105.3937 1.266e-2

105.4101 1.266e-2

105.4195 3.038e0

105.4454 1.013e0

105.4496 2.532e-2

105.4592 1.013e0

105.4667 3.038e0

105.4696 1.323e0

105.4865 2.532e-2

105.4961 2.025e0

105.5003 1.013e0

105.5300 1.025e0

105.5465 2.025e0

105.5576 1.266e-2

105.5630 1.038e0

105.5972 2.025e0

105.6039 1.025e0

105.6777 1.013e0

105.6819 2.025e0

105.6915 1.266e-2

105.7064 2.025e0

105.7214 1.266e-2

105.7598 1.266e-2

105.7652 1.013e0

105.8034 2.038e0

105.8048 2.025e0

105.8228 1.266e-2

105.8254 1.266e-2

105.8443 1.266e-2

105.8526 2.025e0

105.8554 1.266e-2

105.8773 1.266e-2

105.9319 1.266e-2

105.9700 1.266e-2

106.0168 1.025e0

106.1152 3.798e-2

106.1224 2.025e0

106.1237 1.013e0

106.1423 2.089e0

106.1571 3.038e0

106.1630 4.080e0

106.1755 2.123e0

106.1974 1.145e1

106.2054 1.620e1

106.2326 3.076e0

106.2512 3.203e0

106.2799 2.532e-2

106.3015 1.266e-2

106.3113 2.575e0

106.3123 1.266e-2

106.3346 1.266e-2

106.3359 2.025e0

106.3453 2.025e0

106.3591 3.798e-2

106.3618 2.532e-2

106.3755 1.076e0

106.3855 5.063e0

106.3878 1.038e0

106.4031 1.013e0

106.4319 4.051e0

106.4446 3.282e-1

106.4935 2.532e-2

106.5209 3.798e-2

106.5268 2.051e0

106.5392 5.063e-2

106.5564 1.266e-2

106.5741 3.798e-2

106.5758 3.798e-2

106.5894 1.013e0

106.6084 5.076e0

106.6224 3.038e0

106.6520 3.798e-2

106.6555 1.013e0

106.6635 1.266e-2

106.6814 2.532e-2

106.6897 2.025e0

106.6925 2.532e-2

106.6938 1.051e0

106.7034 2.532e-2

106.7046 4.051e0

106.7156 1.013e0

106.7198 2.532e-2

106.7419 2.025e0

106.7624 1.013e0

106.7706 2.532e-2

106.7775 2.532e-2

106.7809 2.038e0

106.7858 2.025e0

106.7882 3.038e0

106.8119 2.025e0

106.8271 2.025e0

106.8337 3.797e-2

106.8365 1.266e-2

106.8449 1.266e-2

106.8697 1.013e0

106.8942 1.013e0

106.9050 1.266e-2

106.9107 1.266e-2

106.9188 1.013e0

106.9216 2.025e0

106.9396 2.025e0

106.9494 4.063e0

106.9686 1.266e-2

106.9725 2.025e0

106.9753 2.025e0

107.0206 2.025e0

107.0370 1.013e0

107.0399 3.038e0

107.0626 1.298e1

107.1156 1.051e0

107.1199 1.266e-2

107.1249 3.708e0

107.1294 2.025e0

107.1417 1.266e-2

107.1525 2.038e0

107.1554 1.013e0

107.1654 1.038e0

107.1724 5.063e0

107.1885 1.266e-2

107.1939 2.532e-2

107.1965 1.013e0

107.2242 2.038e0

107.2269 1.266e-2

107.2381 1.266e-2

107.2478 2.025e0

107.2795 1.266e-2

107.3040 2.025e0

107.3413 4.051e0

107.3757 2.025e0

107.3922 1.013e0

107.4116 1.013e0

107.4129 2.025e0

107.4197 2.025e0

107.4420 1.266e-2

107.4444 1.266e-2

107.4473 1.013e0

107.4722 1.025e0

107.4912 1.025e0

107.5272 1.266e-2

107.5341 2.025e0

107.5411 1.266e-2

107.5768 1.013e0

107.5823 1.013e0

107.5851 1.013e0

107.5880 1.025e0

107.6003 2.025e0

107.6031 2.025e0

107.6069 1.266e-2

107.6320 2.025e0

107.6373 1.013e0

107.6430 1.013e0

107.6638 1.025e0

107.6705 1.266e-2

107.6834 3.051e0

107.6954 2.038e0

107.7091 1.266e-2

107.7203 1.013e0

107.7340 1.266e-2

107.7464 2.025e0

107.7948 1.013e0

107.7982 3.038e0

107.8114 1.025e0

107.8167 1.025e0

107.8333 1.266e-2

107.8527 1.013e0

107.8694 1.266e-2

107.8732 2.025e0

107.8860 1.266e-2

107.9032 3.038e0

107.9187 1.266e-2

107.9382 1.266e-2

107.9439 2.532e-2

107.9686 1.266e-2

107.9881 1.025e0

108.0046 1.013e0

108.0210 1.266e-2

108.0265 3.798e-2

108.0322 1.266e-2

108.0730 1.225e1

108.0957 1.027e0

108.1179 3.034e0

108.1206 1.025e0

108.1398 1.013e0

108.1425 1.266e-2

108.1439 2.025e0

108.1454 1.013e0

108.1649 1.025e0

108.1815 1.013e0

108.1842 1.266e-2

108.1954 1.013e0

108.2395 1.025e0

108.2740 1.025e0

108.2866 1.266e-2

108.2890 1.266e-2

108.2932 2.025e0

108.3004 1.013e0

108.3056 1.266e-2

108.3085 1.266e-2

108.3193 1.266e-2

108.3210 2.532e-2

108.3613 2.025e0

108.3888 1.013e0

108.4053 2.038e0

108.4170 4.051e0

108.4304 1.038e0

108.4469 1.266e-2

108.4759 2.025e0

108.5050 1.266e-2

108.5246 2.025e0

108.5436 1.013e0

108.5492 1.025e0

108.5825 1.266e-2

108.5881 1.013e0

108.6075 1.266e-2

108.6212 2.025e0

108.6821 1.013e0

108.7045 1.013e0

108.7155 1.266e-2

108.7931 1.266e-2

108.8292 1.266e-2

108.8456 1.013e0

108.8541 1.025e0

108.8709 1.013e0

108.8927 1.025e0

108.8958 1.013e0

108.9486 1.025e0

108.9539 1.025e0

108.9791 1.013e0

109.0012 1.266e-2

109.0024 2.025e0

109.0059 3.038e0

109.0262 1.025e0

109.0454 1.013e0

109.0603 2.026e0

109.0635 2.025e0

109.0721 1.038e0

109.0816 2.025e0

109.0926 1.266e-2

109.0979 6.052e0

109.1151 1.025e0

109.1384 2.025e0

109.2148 1.013e0

109.2205 1.013e0

109.2287 1.266e-2

109.2552 1.025e0

109.3036 1.013e0

109.3150 1.266e-2

109.3204 2.532e-2

109.3481 1.266e-2

109.3761 1.266e-2

109.4010 1.266e-2

109.4150 2.038e0

109.4345 2.025e0

109.4553 2.025e0

109.4651 1.013e0

109.4820 2.025e0

109.4985 1.013e0

109.5040 1.013e0

109.5207 1.266e-2

109.5513 1.266e-2

109.5679 1.013e0

109.5903 1.013e0

109.6167 2.025e0

109.6209 1.266e-2

109.6348 1.013e0

109.7129 1.013e0

109.7348 1.266e-2

109.7406 1.013e0

109.8214 1.013e0

109.8353 1.266e-2

109.8462 1.013e0

109.8740 1.013e0

109.8827 1.266e-2

109.8879 1.013e0

109.8992 1.013e0

109.9158 1.013e0

109.9185 1.013e0

109.9465 2.532e-2

109.9521 2.532e-2

109.9798 1.013e0

110.0023 1.266e-2

110.0106 1.013e0

110.0232 2.025e0

110.0273 1.266e-2

110.0455 2.025e0

110.0651 2.025e0

110.0775 3.038e0

110.0796 3.798e-2

110.1166 1.013e0

110.1487 2.025e0

110.2004 1.013e0

110.2587 1.266e-2

110.3063 1.266e-2

110.3148 1.266e-2

110.3288 1.013e0

110.3624 1.266e-2

110.3792 1.266e-2

110.4683 1.266e-2

110.4880 1.266e-2

110.5160 2.025e0

110.5269 1.013e0

110.5409 1.266e-2

110.5547 1.013e0

110.6752 1.266e-2

110.6806 1.013e0

110.6922 1.266e-2

110.7089 1.013e0

110.7255 2.025e0

110.7645 2.025e0

110.7730 1.013e0

110.7953 1.013e0

110.8010 1.266e-2

110.8934 1.013e0

110.8962 1.013e0

110.9156 1.013e0

110.9520 1.013e0

110.9608 1.013e0

110.9632 1.013e0

111.0083 1.266e-2

111.0193 1.013e0

111.0305 1.266e-2

111.0375 2.025e0

111.0417 1.013e0

111.0488 2.025e0

111.0823 2.025e0

111.1018 2.233e0

111.1061 1.013e0

111.1215 2.025e0

111.1511 1.266e-2

111.1732 2.025e0

111.1958 1.013e0

111.1988 1.266e-2

111.2098 1.013e0

111.2546 1.013e0

111.2824 1.013e0

111.2966 1.013e0

111.3022 1.266e-2

111.3191 1.266e-2

111.3443 1.013e0

111.3836 1.266e-2

111.4230 1.266e-2

111.4254 1.266e-2

111.4314 1.013e0

111.4371 1.013e0

111.4621 1.013e0

111.4650 1.266e-2

111.4874 1.013e0

111.5604 1.013e0

111.5664 1.013e0

111.5830 1.266e-2

111.6164 1.266e-2

111.6279 1.266e-2

111.6618 1.266e-2

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