 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

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

Elements Used:

C: 17-17 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 I: 0-1

Minimum: -15.0

Maximum: 5.0 15.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

252.1396 252.1388 0.8 3.2 9.5 71.4 C17 H18 N O

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.

ANALYSIS RUN USING: WATERS LCT PREMIER (ESI POSITIVE/ESI NEGATIVE)

149.3578 2.025e0

149.3629 1.266e-2

149.3696 1.013e0

149.3951 3.038e0

149.4184 1.025e0

149.4344 2.532e-2

149.4474 1.013e0

149.4540 1.013e0

149.4573 1.013e0

149.4590 2.025e0

149.4781 2.025e0

149.4829 1.266e-2

149.5046 2.025e0

149.5062 1.266e-2

149.5128 1.013e0

149.5252 1.025e0

149.5341 5.063e0

149.5609 1.025e0

149.5936 3.629e0

149.6130 1.266e-2

149.6363 1.266e-2

149.6439 3.038e0

149.6552 2.025e0

149.6586 1.266e-2

149.6752 1.013e0

149.6768 2.025e0

149.6786 1.266e-2

149.6907 2.025e0

149.7141 1.013e0

149.7243 1.025e0

149.7364 2.532e-2

149.7388 3.038e0

149.7498 1.013e0

149.7663 1.013e0

149.7724 2.025e0

149.7920 1.013e0

149.8054 1.013e0

149.8147 1.013e0

149.8234 3.038e0

149.8277 1.013e0

149.8310 1.013e0

149.8524 2.025e0

149.8539 1.013e0

149.8561 3.798e-2

149.8666 1.013e0

149.8733 1.013e0

149.9074 3.038e0

149.9338 2.532e-2

149.9355 1.013e0

149.9386 2.025e0

149.9595 2.025e0

149.9745 2.025e0

149.9818 2.038e0

149.9968 1.013e0

150.0034 1.025e0

150.0117 2.025e0

150.0134 1.013e0

150.0232 1.013e0

150.0428 7.267e0

150.0504 1.037e1

150.0667 4.294e0

150.0903 1.177e1

150.0929 5.209e0

150.0944 2.509e1

150.1064 1.094e1

150.1267 1.705e1

150.1357 1.612e1

150.1610 2.025e0

150.1826 3.038e0

150.1893 1.036e0

150.2000 3.038e0

150.2031 2.025e0

150.2350 1.013e0

150.2381 1.013e0

150.2606 1.013e0

150.2706 2.532e-2

150.2851 2.766e0

150.3079 2.025e0

150.3129 1.266e-2

150.3146 2.025e0

150.3453 1.266e-2

150.3749 3.748e0

150.3843 2.532e-2

150.3876 1.013e0

150.3893 2.025e0

150.4059 2.025e0

150.4283 4.051e0

150.4333 1.013e0

150.4383 4.051e0

150.4500 2.025e0

150.4656 1.013e0

150.4889 3.038e0

150.4906 2.025e0

150.5069 4.076e0

150.5146 1.013e0

150.5476 1.593e1

150.5494 1.620e1

150.5528 7.165e0

150.5607 5.193e-1

150.5753 2.025e0

150.5786 2.025e0

150.6047 5.375e0

150.6093 1.013e0

150.6261 2.025e0

150.6352 1.013e0

150.6450 2.532e-2

150.6517 1.025e0

150.6583 1.013e0

150.6747 1.266e-2

150.6792 2.025e0

150.6806 1.025e0

150.6974 3.038e0

150.7108 1.013e0

150.7171 1.013e0

150.7322 3.038e0

150.7344 4.051e0

150.7359 1.496e0

150.7519 5.804e-1

150.7755 1.013e0

150.7805 2.025e0

150.7955 1.025e0

150.8022 1.013e0

150.8113 1.013e0

150.8246 3.038e0

150.8329 4.051e0

150.8508 2.532e-2

150.8523 2.025e0

150.8786 2.025e0

150.8870 1.013e0

150.8933 1.013e0

150.9026 1.013e0

150.9160 1.266e-2

150.9226 1.013e0

150.9294 1.025e0

150.9501 6.076e0

150.9634 2.025e0

150.9650 1.266e-2

150.9866 4.051e0

151.0008 3.038e0

151.0461 2.137e2

151.0868 6.314e0

151.0951 3.106e0

151.1019 3.884e0

151.1110 8.801e-1

151.1153 2.429e0

151.1290 3.207e0

151.1396 2.704e0

151.1454 2.667e0

151.1546 3.038e0

151.1563 2.025e0

151.1704 1.013e0

151.1772 4.051e0

151.1820 3.038e0

151.1938 1.038e0

151.2047 4.877e0

151.2263 2.025e0

151.2279 2.025e0

151.2304 2.363e0

151.2315 3.038e0

151.2586 2.532e-2

151.2610 2.038e0

151.2770 2.025e0

151.2796 3.038e0

151.2837 2.025e0

151.2888 3.038e0

151.3010 1.013e0

151.3044 2.532e-2

151.3111 1.266e-2

151.3297 1.051e0

151.3360 2.025e0

151.3375 2.025e0

151.3502 1.013e0

151.3669 1.013e0

151.3736 1.025e0

151.3817 2.025e0

151.3960 2.025e0

151.4027 2.025e0

151.4038 2.051e0

151.4127 2.038e0

151.4335 2.025e0

151.4384 1.013e0

151.4418 2.025e0

151.4456 3.051e0

151.4585 1.013e0

151.4842 1.013e0

151.4876 2.025e0

151.4906 3.519e0

151.5100 2.051e0

151.5497 1.510e0

151.5529 4.152e1

151.5759 3.038e0

151.5787 4.501e0

151.5806 5.283e0

151.5993 2.025e0

151.6136 5.063e0

151.6227 6.513e0

151.6418 2.025e0

151.6526 4.051e0

151.6576 1.025e0

151.6742 1.013e0

151.6768 2.051e0

151.6809 2.025e0

151.6960 5.063e0

151.7034 1.013e0

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151.7608 4.051e0

151.7889 1.025e0

151.7982 2.532e-2

151.8005 4.054e0

151.8017 1.266e-2

151.8150 1.013e0

151.8332 2.025e0

151.8419 3.038e0

151.8708 3.038e0

151.8725 2.025e0

151.8805 1.266e-2

151.8848 2.025e0

151.9117 2.025e0

151.9211 2.038e0

151.9292 2.025e0

151.9392 1.013e0

151.9465 3.038e0

151.9719 3.051e0

151.9753 1.013e0

151.9884 2.025e0

151.9918 1.025e0

152.0180 1.013e0

152.0217 2.808e0

152.0500 3.890e1

152.0533 9.531e0

152.0694 1.522e1

152.1099 2.331e0

152.1192 3.361e0

152.1279 1.481e0

152.1468 1.415e0

152.1557 1.266e-2

152.1633 2.025e0

152.1752 2.025e0

152.1954 2.025e0

152.2035 2.815e0

152.2078 5.718e0

152.2144 1.013e0

152.2284 2.277e0

152.2413 1.013e0

152.2490 2.025e0

152.2536 1.266e-2

152.2637 1.266e-2

152.2704 1.013e0

152.2720 2.532e-2

152.2770 1.013e0

152.2934 1.013e0

152.2995 1.013e0

152.3028 2.025e0

152.3044 2.025e0

152.3263 1.013e0

152.3455 2.025e0

152.3487 1.013e0

152.3671 1.038e0

152.3688 1.013e0

152.3722 1.013e0

152.3947 6.076e0

152.3980 1.013e0

152.4114 3.038e0

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152.4202 4.051e0

152.4312 1.013e0

152.4473 2.025e0

152.4557 2.025e0

152.4573 1.266e-2

152.4623 2.532e-2

152.4864 2.025e0

152.5017 3.038e0

152.5167 1.013e0

152.5201 1.013e0

152.5250 2.025e0

152.5399 7.089e0

152.5436 7.182e0

152.5692 1.038e0

152.5851 1.013e0

152.5867 2.025e0

152.6068 2.025e0

152.6182 1.013e0

152.6344 1.013e0

152.6487 1.038e0

152.6536 3.038e0

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152.6819 2.025e0

152.6937 1.013e0

152.7195 1.013e0

152.7313 2.025e0

152.7404 3.038e0

152.7507 3.038e0

152.7549 4.051e0

152.7772 2.025e0

152.7789 1.013e0

152.8054 1.013e0

152.8190 1.038e0

152.8349 2.532e-2

152.8366 2.025e0

152.8469 2.025e0

152.8576 1.013e0

152.8657 2.025e0

152.8708 1.013e0

152.8943 1.013e0

152.9006 2.025e0

152.9202 1.266e-2

152.9259 5.063e0

152.9302 1.266e-2

152.9369 1.266e-2

152.9644 2.025e0

152.9728 1.013e0

152.9795 1.025e0

152.9863 1.013e0

153.0087 1.013e0

153.0101 3.038e0

153.0171 2.025e0

153.0188 1.013e0

153.0677 4.169e0

153.0769 1.486e0

153.0895 3.913e0

153.0961 3.194e0

153.1074 5.258e0

153.1168 3.860e0

153.1422 2.378e1

153.1770 4.051e0

153.1837 1.025e0

153.2028 1.013e0

153.2141 5.063e0

153.2404 2.025e0

153.2454 2.025e0

153.2574 1.038e0

153.2589 2.025e0

153.2914 1.013e0

153.3250 1.013e0

153.3281 1.266e-2

153.3374 1.013e0

153.3408 1.013e0

153.3509 1.025e0

153.3543 1.013e0

153.3758 2.025e0

153.3773 2.025e0

153.3965 6.076e0

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153.4297 1.013e0

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153.4676 4.051e0

153.4698 1.013e0

153.4730 2.025e0

153.4957 1.266e-2

153.5002 3.038e0

153.5283 2.025e0

153.5316 1.013e0

153.5462 2.304e0

153.5518 4.051e0

153.5535 2.025e0

153.5662 3.798e-2

153.5828 2.069e0

153.5945 1.013e0

153.5962 4.051e0

153.6046 1.013e0

153.6239 1.266e-2

153.6330 3.038e0

153.6473 2.025e0

153.6540 1.266e-2

153.6593 2.025e0

153.6640 1.013e0

153.6765 1.266e-2

153.6799 1.013e0

153.7069 1.013e0

153.7103 1.013e0

153.7260 1.266e-2

153.7328 1.013e0

153.7395 1.266e-2

153.7428 1.013e0

153.7582 2.025e0

153.7628 3.038e0

153.7658 1.013e0

153.7990 2.025e0

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153.8249 2.025e0

153.8484 1.013e0

153.8552 1.266e-2

153.8693 2.025e0

153.8743 1.013e0

153.8811 1.013e0

153.9013 1.266e-2

153.9155 2.025e0

153.9324 3.038e0

153.9355 2.025e0

153.9665 1.013e0

153.9766 1.013e0

154.0021 2.025e0

154.0066 1.013e0

154.0250 3.038e0

154.0306 4.051e0

154.0361 1.858e0

154.0473 2.526e0

154.0613 1.728e0

154.0972 2.055e1

154.1283 7.150e0

154.1351 9.028e0

154.1402 3.247e0

154.1583 5.114e0

154.1962 3.038e0

154.2107 1.266e-2

154.2173 3.038e0

154.2206 1.266e-2

154.2341 2.025e0

154.2408 1.013e0

154.2701 2.025e0

154.2745 3.038e0

154.2836 1.013e0

154.3066 2.025e0

154.3331 1.266e-2

154.3466 1.013e0

154.3675 2.025e0

154.3742 2.025e0

154.3776 4.051e0

154.3876 2.025e0

154.3932 4.078e0

154.4088 1.013e0

154.4118 1.266e-2

154.4170 2.025e0

154.4456 1.266e-2

154.4583 1.025e0

154.4850 1.013e0

154.5101 3.038e0

154.5143 1.013e0

154.5177 1.266e-2

154.5513 1.013e0

154.5672 1.013e0

154.5740 1.013e0

154.6063 4.051e0

154.6472 2.642e-2

154.6491 2.025e0

154.6610 2.025e0

154.6623 4.051e0

154.6832 1.013e0

154.7032 1.266e-2

154.7094 1.013e0

154.7159 1.013e0

154.7260 2.532e-2

154.7670 2.025e0

154.7789 2.025e0

154.7890 1.266e-2

154.7907 2.532e-2

154.8117 2.025e0

154.8251 1.013e0

154.8352 1.266e-2

154.8420 1.013e0

154.8582 2.025e0

154.8614 1.266e-2

154.8645 1.013e0

154.8781 3.051e0

154.9080 1.013e0

154.9265 3.038e0

154.9277 1.266e-2

154.9344 1.013e0

154.9411 2.025e0

154.9608 3.038e0

154.9857 2.025e0

154.9924 2.025e0

155.0143 3.038e0

155.0269 1.013e0

155.0302 1.013e0

155.0336 1.013e0

155.0631 1.161e0

155.0834 5.747e0

155.0848 1.785e0

155.1161 3.116e0

155.1184 1.155e0

155.1225 2.819e0

155.1303 7.125e0

155.1513 2.071e0

155.1612 2.025e0

155.1627 3.038e0

155.1709 5.063e0

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155.2094 1.013e0

155.2140 2.025e0

155.2354 1.013e0

155.2388 2.025e0

155.2464 3.038e0

155.2669 2.025e0

155.2935 2.025e0

155.3087 1.266e-2

155.3151 1.038e0

155.3414 1.013e0

155.3448 1.013e0

155.3583 1.266e-2

155.3643 4.051e0

155.3774 2.025e0

155.3843 3.038e0

155.4079 1.025e0

155.4336 4.051e0

155.4407 1.013e0

155.4610 1.025e0

155.4644 2.038e0

155.4768 3.038e0

155.4836 1.013e0

155.5038 1.013e0

155.5072 1.025e0

155.5237 1.266e-2

155.5313 2.025e0

155.5451 2.025e0

155.5468 2.025e0

155.5673 3.038e0

155.5766 2.025e0

155.5782 2.025e0

155.5931 1.013e0

155.5985 1.287e0

155.6065 1.266e-2

155.6201 2.025e0

155.6359 2.025e0

155.6427 1.013e0

155.6461 2.038e0

155.6664 1.013e0

155.6732 1.013e0

155.6924 3.051e0

155.6958 1.013e0

155.6992 2.025e0

155.7194 1.025e0

155.7294 1.013e0

155.7341 2.025e0

155.7590 2.532e-2

155.7691 1.013e0

155.7725 1.013e0

155.7902 2.025e0

155.8002 2.025e0

155.8151 3.441e0

155.8205 2.025e0

155.8414 2.025e0

155.8482 1.266e-2

155.8618 1.013e0

155.8651 1.266e-2

155.8770 2.025e0

155.9165 2.025e0

155.9250 1.013e0

155.9309 3.038e0

155.9612 1.013e0

155.9646 4.051e0

155.9679 1.266e-2

155.9977 1.013e0

156.0075 1.013e0

156.0109 1.013e0

156.0143 2.025e0

156.0414 4.782e0

156.0540 3.696e0

156.0761 3.470e1

156.1113 5.249e0

156.1145 3.382e0

156.1226 2.483e0

156.1465 6.701e0

156.1500 3.428e0

156.1770 1.013e0

156.1905 2.025e0

156.1962 4.051e0

156.2086 2.025e0

156.2267 3.038e0

156.2313 5.063e0

156.2436 1.013e0

156.2679 3.038e0

156.2731 1.013e0

156.2833 1.013e0

156.2867 1.013e0

156.2968 1.013e0

156.3103 1.266e-2

156.3165 1.266e-2

156.3296 1.266e-2

156.3330 1.013e0

156.3499 1.013e0

156.3602 1.013e0

156.3726 2.025e0

156.3759 1.266e-2

156.3793 2.025e0

156.4031 2.038e0

156.4048 2.025e0

156.4260 2.025e0

156.4376 2.025e0

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156.4665 1.013e0

156.4857 1.013e0

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156.5196 1.266e-2

156.5353 4.051e0

156.5423 2.025e0

156.5456 2.532e-2

156.5474 4.051e0

156.5626 1.266e-2

156.5778 2.025e0

156.5826 1.013e0

156.5900 3.038e0

156.5954 1.266e-2

156.5988 1.013e0

156.6107 2.025e0

156.6260 1.025e0

156.6310 2.025e0

156.6327 2.025e0

156.6537 2.025e0

156.6588 1.013e0

156.6656 2.532e-2

156.6985 1.013e0

156.6996 3.038e0

156.7137 2.025e0

156.7424 1.013e0

156.7618 1.013e0

156.7635 2.025e0

156.7787 1.013e0

156.7821 2.025e0

156.7924 1.013e0

156.7988 1.013e0

156.8133 2.025e0

156.8269 2.025e0

156.8319 1.013e0

156.8370 2.025e0

156.8553 1.266e-2

156.8582 1.025e0

156.8615 1.013e0

156.8852 1.013e0

156.8885 1.013e0

156.8988 1.013e0

156.9088 2.038e0

156.9180 2.025e0

156.9350 2.025e0

156.9418 1.013e0

156.9619 1.013e0

156.9651 2.025e0

156.9682 1.013e0

156.9764 2.025e0

156.9950 1.013e0

157.0169 4.051e0

157.0184 1.013e0

157.0352 5.865e-1

157.0426 1.795e0

157.0457 1.221e0

157.0483 2.287e0

157.0688 3.075e0

157.0766 6.598e0

157.0836 2.168e0

157.0974 6.498e0

157.1024 1.435e1

157.1283 1.147e0

157.1326 4.959e0

157.1536 3.038e0

157.1572 2.354e0

157.1649 2.025e0

157.1786 1.013e0

157.1864 2.025e0

157.2080 2.025e0

157.2114 2.051e0

157.2284 2.025e0

157.2415 1.013e0

157.2446 1.013e0

157.2545 1.025e0

157.2603 3.038e0

157.2766 2.025e0

157.2885 1.013e0

157.3042 2.025e0

157.3134 4.051e0

157.3281 1.013e0

157.3315 1.013e0

157.3452 1.013e0

157.3644 1.013e0

157.3781 1.013e0

157.3848 2.025e0

157.3865 2.025e0

157.3882 1.013e0

157.4018 1.013e0

157.4331 3.038e0

157.4364 2.025e0

157.4415 1.025e0

157.4552 1.025e0

157.4679 1.013e0

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157.5151 1.025e0

157.5464 2.025e0

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157.5651 1.013e0

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157.5981 2.038e0

157.6150 1.013e0

157.6254 2.025e0

157.6347 1.266e-2

157.6514 1.266e-2

157.6535 5.063e0

157.6582 1.013e0

157.6805 2.025e0

157.6868 3.038e0

157.7115 2.025e0

157.7216 1.013e0

157.7268 2.025e0

157.7387 1.013e0

157.7563 2.025e0

157.7580 1.013e0

157.7721 3.051e0

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