 Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 11-13 H: 0-200 N: 0-15 O: 0-10 S: 0-1

Minimum: -15.0

Maximum: 5.0 5.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

177.0912 177.0916 -0.4 -2.3 5.5 103.0 C11 H13 O2

M-OH ION FOUND

REPORT MASSES AS +/-5mDa, referenced against

Leucine Enkelphalin @ 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.

108.3513 3.063e0

108.3596 1.013e0

108.3626 3.797e-2

108.3734 1.013e0

108.3762 1.266e-2

108.3815 1.266e-2

108.3981 1.266e-2

108.4077 2.271e0

108.4095 1.013e0

108.4118 1.266e-2

108.4177 2.038e0

108.4304 2.293e0

108.4399 1.013e0

108.4412 2.051e0

108.4424 1.013e0

108.4538 1.025e0

108.4562 1.013e0

108.4600 1.038e0

108.4676 1.266e-2

108.4702 2.025e0

108.4716 2.025e0

108.4842 1.038e0

108.5006 2.038e0

108.5159 2.532e-2

108.5228 1.025e0

108.5244 2.025e0

108.5256 1.266e-2

108.5325 2.025e0

108.5395 1.013e0

108.5450 1.266e-2

108.5700 2.025e0

108.5837 1.013e0

108.5896 1.013e0

108.5933 2.025e0

108.5947 1.266e-2

108.6018 2.025e0

108.6295 2.025e0

108.6339 1.013e0

108.6447 1.266e-2

108.6477 1.013e0

108.6516 1.025e0

108.6557 1.013e0

108.6781 3.038e0

108.7057 2.038e0

108.7086 1.266e-2

108.7138 2.532e-2

108.7485 1.025e0

108.7556 1.013e0

108.7611 1.266e-2

108.7720 1.013e0

108.7915 1.013e0

108.7928 2.025e0

108.8081 2.532e-2

108.8096 2.025e0

108.8165 1.013e0

108.8304 3.038e0

108.8470 1.013e0

108.8525 1.013e0

108.8611 1.266e-2

108.8705 1.025e0

108.8939 1.013e0

108.8982 5.063e-2

108.9135 1.013e0

108.9325 3.038e0

108.9371 2.038e0

108.9551 1.013e0

108.9665 1.266e-2

108.9717 1.013e0

108.9870 2.025e0

108.9883 2.025e0

108.9956 2.025e0

109.0355 1.025e0

109.0738 2.375e0

109.0760 1.077e0

109.0965 2.213e-4

109.0978 1.781e0

109.1043 1.813e0

109.1077 3.038e0

109.1133 1.013e0

109.1191 1.013e0

109.1201 4.449e0

109.1259 2.025e0

109.1469 1.266e-2

109.1548 1.025e0

109.1715 1.266e-2

109.1745 2.025e0

109.1759 2.025e0

109.1854 1.025e0

109.1939 3.038e0

109.2023 1.013e0

109.2119 2.025e0

109.2131 2.532e-2

109.2218 1.266e-2

109.2356 1.038e0

109.2384 2.038e0

109.2508 2.532e-2

109.2578 1.266e-2

109.2730 2.025e0

109.2742 2.025e0

109.2828 2.532e-2

109.2938 1.266e-2

109.3163 1.013e0

109.3215 2.038e0

109.3382 3.051e0

109.3426 2.025e0

109.3521 1.266e-2

109.3535 2.025e0

109.3647 2.025e0

109.3814 2.025e0

109.3841 2.532e-2

109.3912 1.013e0

109.4022 1.013e0

109.4036 2.025e0

109.4051 1.266e-2

109.4188 1.013e0

109.4300 1.013e0

109.4654 3.038e0

109.4691 2.038e0

109.4758 2.025e0

109.5070 3.063e0

109.5121 2.532e-2

109.5217 1.266e-2

109.5368 3.798e-2

109.5441 1.013e0

109.5456 2.025e0

109.5610 1.013e0

109.5720 1.266e-2

109.5776 1.013e0

109.5843 2.025e0

109.5967 1.013e0

109.5982 2.025e0

109.6084 1.266e-2

109.6105 1.013e0

109.6135 1.266e-2

109.6221 1.013e0

109.6302 1.013e0

109.6317 1.025e0

109.6441 2.038e0

109.6527 1.013e0

109.6554 1.013e0

109.6578 1.013e0

109.6637 3.038e0

109.6719 1.025e0

109.6872 1.025e0

109.7025 2.025e0

109.7110 1.013e0

109.7220 2.025e0

109.7249 1.013e0

109.7333 1.266e-2

109.7499 1.013e0

109.7527 1.013e0

109.7555 1.013e0

109.7639 1.266e-2

109.7652 2.025e0

109.7694 1.013e0

109.7765 2.532e-2

109.7895 9.827e-1

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109.8077 3.038e0

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109.8393 1.013e0

109.8473 1.266e-2

109.8670 1.266e-2

109.8711 2.532e-2

109.8723 2.025e0

109.8864 2.532e-2

109.9004 3.051e0

109.9115 1.013e0

109.9172 1.013e0

109.9226 1.013e0

109.9270 2.025e0

109.9517 2.025e0

109.9700 1.013e0

109.9867 3.038e0

110.0063 1.013e0

110.0153 4.076e0

110.0231 1.013e0

110.0386 3.038e0

110.0489 2.538e0

110.0688 5.565e0

110.0872 1.725e0

110.1071 5.255e-1

110.1095 3.051e0

110.1122 1.013e0

110.1164 1.025e0

110.1318 1.025e0

110.1346 1.013e0

110.1414 2.025e0

110.1539 1.013e0

110.1595 1.266e-2

110.1626 1.266e-2

110.1694 2.532e-2

110.1846 1.266e-2

110.1875 1.266e-2

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110.2071 1.266e-2

110.2100 1.013e0

110.2167 2.532e-2

110.2377 1.266e-2

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110.2474 2.025e0

110.2656 1.013e0

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110.3159 1.013e0

110.3215 1.013e0

110.3369 1.025e0

110.3409 1.266e-2

110.3452 1.025e0

110.3495 1.266e-2

110.3619 2.055e0

110.3730 2.532e-2

110.3744 1.266e-2

110.3883 1.013e0

110.3912 1.013e0

110.4022 1.013e0

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110.4247 2.025e0

110.4264 2.025e0

110.4305 4.063e0

110.4329 1.266e-2

110.4401 2.025e0

110.4507 3.038e0

110.4518 3.038e0

110.4564 3.038e0

110.4636 1.013e0

110.4708 2.532e-2

110.4738 3.038e0

110.4892 1.266e-2

110.4920 1.025e0

110.5030 1.266e-2

110.5173 3.798e-2

110.5376 2.675e-1

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110.5586 1.013e0

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110.5952 1.013e0

110.6162 1.025e0

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110.6231 1.266e-2

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110.6497 2.025e0

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110.7656 1.266e-2

110.7714 2.532e-2

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110.8861 1.266e-2

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110.9450 1.266e-2

110.9588 1.025e0

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110.9978 1.013e0

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111.0174 1.266e-2

111.0204 2.532e-2

111.0261 1.266e-2

111.0414 2.532e-2

111.0514 3.160e0

111.0597 1.959e-1

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111.2374 2.532e-2

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111.8845 3.038e0

111.8916 1.025e0

111.9213 1.038e0

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111.9435 3.038e0

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111.9955 2.025e0

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112.0615 6.049e-1

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112.2685 2.025e0

112.2728 1.013e0

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112.3037 1.266e-2

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112.3404 1.013e0

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112.3798 1.266e-2

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112.4758 1.013e0

112.4883 2.025e0

112.5156 4.076e0

112.5319 1.266e-2

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112.5517 1.025e0

112.5744 2.532e-2

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112.8451 1.266e-2

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112.8874 1.266e-2

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112.9410 2.025e0

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112.9807 1.266e-2

112.9948 1.013e0

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113.1005 1.446e0

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113.1557 1.038e0

113.1619 4.051e0

113.1644 2.532e-2

113.1727 1.266e-2

113.1785 1.013e0

113.1976 4.051e0

113.2207 1.266e-2

113.2349 1.013e0

113.2620 4.051e0

113.2858 1.013e0

113.2945 1.266e-2

113.2973 1.013e0

113.3002 2.532e-2

113.3171 2.532e-2

113.3255 1.266e-2

113.3314 1.266e-2

113.3342 1.266e-2

113.3425 1.266e-2

113.3537 1.013e0

113.3624 1.266e-2

113.3651 2.038e0

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113.3825 1.013e0

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113.4755 4.051e0

113.4954 1.266e-2

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113.5123 1.013e0

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113.5804 2.025e0

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113.6057 1.013e0

113.6146 1.266e-2

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113.6341 1.025e0

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113.6538 2.025e0

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113.7248 1.266e-2

113.7474 5.063e-2

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113.8327 1.266e-2

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113.8720 2.025e0

113.8865 2.038e0

113.9049 4.051e0

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114.1087 2.776e0

114.1113 3.798e-2

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114.1533 1.013e0

114.1704 1.013e0

114.1732 1.025e0

114.1914 2.025e0

114.1987 1.266e-2

114.2098 2.025e0

114.2132 3.038e0

114.2142 2.025e0

114.2193 3.798e-2

114.2370 2.025e0

114.2385 1.266e-2

114.2498 1.013e0

114.2546 3.038e0

114.2696 1.025e0

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114.2979 1.266e-2

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114.3179 1.266e-2

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114.3579 1.013e0

114.3663 1.013e0

114.3791 2.532e-2

114.3919 1.013e0

114.3946 1.266e-2

114.4033 1.266e-2

114.4061 2.025e0

114.4886 1.051e0

114.4969 1.013e0

114.5055 2.025e0

114.5070 2.025e0

114.5196 2.025e0

114.5285 1.266e-2

114.5456 1.013e0

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114.5674 5.089e0

114.5908 2.532e-2

114.5968 1.266e-2

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114.6250 1.266e-2

114.6279 1.266e-2

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114.6362 1.013e0

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114.6532 2.025e0

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114.7360 2.025e0

114.7374 2.025e0

114.7504 1.025e0

114.7531 1.013e0

114.7617 1.266e-2

114.7674 1.013e0

114.7881 2.038e0

114.7914 2.025e0

114.7957 1.266e-2

114.8114 2.025e0

114.8157 1.013e0

114.8285 2.025e0

114.8299 1.013e0

114.8411 1.013e0

114.8499 1.266e-2

114.8529 1.013e0

114.8583 1.013e0

114.8641 1.266e-2

114.8669 1.266e-2

114.8812 1.266e-2

114.9094 1.266e-2

114.9241 1.013e0

114.9281 2.025e0

114.9296 1.013e0

114.9495 2.025e0

114.9666 2.051e0

114.9753 4.063e0

114.9967 2.025e0

115.0008 1.013e0

115.0023 2.025e0

115.0208 2.038e0

115.0269 1.266e-2

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115.0378 1.013e0

115.0544 2.554e-2

115.1149 1.051e0

115.1315 1.553e0

115.1492 1.025e0

115.1576 1.266e-2

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115.1854 3.038e0

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115.2201 1.013e0

115.2348 1.266e-2

115.2461 1.266e-2

115.2490 1.266e-2

115.2745 1.013e0

115.2916 1.013e0

115.2974 1.266e-2

115.3018 2.025e0

115.3074 2.025e0

115.3258 1.013e0

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