 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

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

Elements Used:

C: 10-10 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 I: 0-2

Minimum: -1.5

Maximum: 5.0 10.0 100.0

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

180.1017 180.1025 -0.8 -4.4 4.5 303.5 0.0 C10 H14 N O2

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.

99.1471 2.041e0

99.1767 2.025e0

99.1948 3.921e0

99.2177 1.013e0

99.2414 1.013e0

99.2601 2.025e0

99.2752 3.038e0

99.3131 1.013e0

99.3421 1.013e0

99.3554 1.013e0

99.3874 1.013e0

99.4096 2.051e0

99.4826 2.025e0

99.5037 2.025e0

99.5280 2.265e0

99.5435 1.266e-2

99.5833 3.798e-2

99.6072 2.025e0

99.6292 3.038e0

99.6682 1.013e0

99.6787 1.013e0

99.7158 1.013e0

99.7373 1.013e0

99.7842 3.038e0

99.7992 4.051e0

99.8167 1.013e0

99.8532 3.038e0

99.8655 3.038e0

99.8804 2.025e0

99.9090 1.038e0

99.9403 2.025e0

99.9919 1.013e0

100.0173 1.962e0

100.0563 3.975e0

100.0796 2.528e1

100.1198 9.775e0

100.1396 2.025e0

100.1795 2.025e0

100.1994 1.025e0

100.2309 4.545e0

100.2619 2.025e0

100.2926 1.013e0

100.3231 2.025e0

100.3447 5.063e0

100.3639 2.038e0

100.3829 1.013e0

100.4103 1.276e0

100.4283 3.038e0

100.4574 4.051e0

100.5001 2.025e0

100.5456 1.013e0

100.5590 1.013e0

100.5788 5.063e0

100.5934 1.013e0

100.6441 1.013e0

100.6533 2.025e0

100.6961 2.025e0

100.7173 2.099e0

100.7615 1.013e0

100.7707 2.532e-2

100.7926 3.038e0

100.8190 1.038e0

100.8508 2.025e0

100.8665 2.564e0

100.8854 2.025e0

100.9042 2.025e0

100.9148 2.025e0

100.9430 3.038e0

101.0106 4.051e0

101.0400 9.001e0

101.1445 2.025e0

101.1606 2.025e0

101.1939 3.038e0

101.2126 2.025e0

101.2393 3.038e0

101.2699 4.170e0

101.2928 2.025e0

101.3383 1.013e0

101.3517 3.798e-2

101.3720 4.301e0

101.4134 7.089e0

101.4385 3.038e0

101.4533 1.013e0

101.4794 3.038e0

101.4953 4.051e0

101.5149 4.051e0

101.5524 1.013e0

101.5767 1.013e0

101.6168 1.013e0

101.6275 1.266e-2

101.6515 3.038e0

101.6963 3.517e0

101.7149 5.063e0

101.7516 5.144e0

101.7840 2.532e-2

101.8050 3.038e0

101.8176 1.266e-2

101.8351 2.025e0

101.8847 1.266e-2

101.9283 4.051e0

101.9490 1.013e0

101.9584 2.025e0

101.9793 3.038e0

102.0027 1.013e0

102.0209 3.038e0

102.0712 3.320e1

102.1319 4.179e1

102.1690 1.013e0

102.1880 1.013e0

102.2042 2.025e0

102.2411 6.076e0

102.2765 1.013e0

102.2914 2.025e0

102.3089 1.013e0

102.3559 2.025e0

102.4003 1.013e0

102.4191 1.013e0

102.4351 1.013e0

102.4587 2.038e0

102.4728 1.013e0

102.4984 2.025e0

102.5159 2.025e0

102.5669 1.013e0

102.6291 1.013e0

102.6425 1.013e0

102.6976 2.025e0

102.7219 2.025e0

102.7660 1.013e0

102.8418 1.013e0

102.8714 1.013e0

102.8929 1.013e0

102.9199 1.013e0

102.9455 2.532e-2

103.0028 3.038e0

103.0413 4.051e0

103.0579 4.385e0

103.1018 2.730e0

103.1235 1.570e0

103.1363 3.038e0

103.1492 1.013e0

103.1706 1.013e0

103.1963 2.025e0

103.2139 2.025e0

103.2409 1.013e0

103.2571 3.038e0

103.3139 4.051e0

103.3461 1.013e0

103.3652 1.013e0

103.3860 1.051e0

103.4071 2.025e0

103.4243 1.266e-2

103.4378 1.013e0

103.4570 1.013e0

103.4936 2.025e0

103.5218 1.013e0

103.5381 2.025e0

103.5626 6.076e0

103.6084 3.051e0

103.6840 1.013e0

103.6948 1.266e-2

103.7111 2.025e0

103.7626 2.025e0

103.8086 1.013e0

103.8384 1.013e0

103.8534 3.038e0

103.8716 3.038e0

103.9388 1.266e-2

103.9692 1.038e0

103.9981 1.013e0

104.0236 3.251e0

104.0429 2.025e0

104.0571 3.038e0

104.0737 5.615e0

104.1100 6.130e0

104.1364 2.025e0

104.1758 2.025e0

104.2069 1.013e0

104.2233 1.013e0

104.2612 1.013e0

104.2926 3.038e0

104.3101 1.266e-2

104.3290 1.013e0

104.3535 2.025e0

104.3745 1.060e0

104.4049 2.038e0

104.4254 2.071e0

104.4553 2.025e0

104.5165 1.013e0

104.5639 2.025e0

104.5796 3.038e0

104.6182 9.715e0

104.6659 1.013e0

104.6781 2.025e0

104.7195 6.042e0

104.7392 1.013e0

104.7569 2.025e0

104.7774 3.038e0

104.8064 2.379e0

104.8460 5.800e0

104.8834 1.013e0

104.9052 4.051e0

104.9290 3.038e0

104.9503 6.076e0

105.0184 5.250e0

105.1006 1.434e0

105.1364 8.797e0

105.1623 9.114e0

105.1870 1.316e1

105.2219 3.071e0

105.2401 5.063e0

105.2791 5.839e0

105.3028 3.038e0

105.3206 5.916e0

105.3547 1.038e0

105.3709 1.013e0

105.3915 2.532e-2

105.4409 4.051e0

105.4561 7.361e0

105.4699 1.038e0

105.4876 3.038e0

105.5034 2.025e0

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105.5448 4.051e0

105.5668 3.038e0

105.5810 3.038e0

105.6071 2.025e0

105.6342 2.256e0

105.6468 1.025e0

105.6590 2.025e0

105.6795 2.025e0

105.7014 1.013e0

105.7253 8.101e0

105.7504 1.025e0

105.7724 2.025e0

105.7906 3.038e0

105.8134 1.013e0

105.8319 3.038e0

105.8651 2.025e0

105.9009 1.013e0

105.9104 2.025e0

105.9403 3.038e0

105.9527 2.025e0

105.9884 2.025e0

106.0287 5.063e0

106.0503 2.092e1

106.0708 4.180e1

106.1421 3.038e0

106.1834 3.798e-2

106.2019 1.013e0

106.2211 3.798e-2

106.2347 2.038e0

106.2812 1.013e0

106.3198 1.013e0

106.3376 2.253e0

106.3580 1.013e0

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106.4331 3.038e0

106.4623 1.266e-2

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106.5539 2.025e0

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106.8023 1.266e-2

106.8421 2.025e0

106.8599 2.532e-2

106.8737 1.266e-2

106.9177 1.013e0

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106.9906 4.051e0

107.0302 1.013e0

107.0533 4.051e0

107.0673 9.516e0

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107.1962 3.038e0

107.2697 1.013e0

107.3123 2.025e0

107.3302 2.025e0

107.3686 1.013e0

107.3852 1.013e0

107.3990 1.013e0

107.4155 2.025e0

107.4404 1.025e0

107.4567 1.266e-2

107.4680 1.013e0

107.5231 1.013e0

107.5478 1.013e0

107.5685 2.025e0

107.5947 1.013e0

107.6305 2.025e0

107.6597 5.063e0

107.6941 4.051e0

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107.9822 2.025e0

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108.2240 1.013e0

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108.4672 1.013e0

108.4811 2.025e0

108.5172 2.025e0

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108.6695 1.266e-2

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109.7802 2.025e0

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109.9333 1.013e0

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109.9932 2.025e0

110.0113 2.025e0

110.0365 2.025e0

110.0726 4.922e0

110.1368 2.025e0

110.1478 1.013e0

110.2091 1.013e0

110.2232 1.013e0

110.2346 1.013e0

110.2539 1.013e0

110.2944 4.051e0

110.3237 1.013e0

110.3770 1.013e0

110.4215 1.013e0

110.4410 1.013e0

110.4662 5.063e0

110.4849 2.368e0

110.4997 1.013e0

110.5334 1.013e0

110.5554 1.266e-2

110.5722 1.013e0

110.5947 1.013e0

110.6197 1.013e0

110.6475 1.266e-2

110.6632 2.025e0

110.6782 1.013e0

110.6950 1.013e0

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110.8481 3.038e0

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111.0596 8.980e0

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111.1848 1.013e0

111.2339 2.025e0

111.2522 1.266e-2

111.2728 5.063e0

111.2918 2.526e0

111.3539 2.051e0

111.3869 1.013e0

111.4169 3.038e0

111.4386 2.532e-2

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111.4905 1.013e0

111.5117 2.113e0

111.5621 2.025e0

111.6393 1.013e0

111.7208 2.038e0

111.7403 3.038e0

111.7609 3.038e0

111.7961 2.051e0

111.8246 2.038e0

111.8555 1.013e0

111.9721 2.025e0

111.9835 3.038e0

112.0117 2.025e0

112.0459 3.038e0

112.0677 1.528e0

112.1158 2.079e0

112.1594 1.013e0

112.1762 3.038e0

112.2101 1.013e0

112.2221 3.798e-2

112.2338 3.038e0

112.2749 2.025e0

112.2889 2.025e0

112.3140 1.013e0

112.3456 3.038e0

112.3802 2.025e0

112.3986 2.025e0

112.4295 2.025e0

112.4698 3.038e0

112.5047 5.063e0

112.5325 2.025e0

112.5827 3.038e0

112.5945 2.025e0

112.6192 2.038e0

112.6495 2.025e0

112.6913 4.051e0

112.7132 1.326e0

112.7367 1.013e0

112.7484 1.013e0

112.7750 2.025e0

112.7919 2.025e0

112.8338 3.038e0

112.8611 3.038e0

112.8781 5.063e0

112.9033 1.013e0

112.9449 3.038e0

112.9599 2.532e-2

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113.1548 2.025e0

113.1887 1.013e0

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113.2607 2.025e0

113.3046 1.266e-2

113.3216 1.266e-2

113.3881 2.025e0

113.4123 1.013e0

113.4487 1.013e0

113.4701 2.025e0

113.4871 2.025e0

113.4997 1.013e0

113.5226 1.013e0

113.5454 1.266e-2

113.5595 1.025e0

113.5905 1.013e0

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113.6275 1.013e0

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113.6746 2.063e0

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113.7519 3.038e0

113.7718 1.013e0

113.8510 1.013e0

113.8796 2.025e0

113.8979 2.025e0

113.9278 1.013e0

113.9449 2.025e0

113.9645 5.063e0

114.0129 1.013e0

114.0426 2.025e0

114.1028 1.180e1

114.1230 2.559e0

114.1492 2.025e0

114.1641 3.038e0

114.1786 4.244e0

114.2056 1.013e0

114.2371 1.025e0

114.2571 3.051e0

114.2987 4.051e0

114.3215 3.038e0

114.3628 1.038e0

114.3790 1.013e0

114.4117 2.025e0

114.4431 4.051e0

114.4596 3.038e0

114.4955 2.025e0

114.5184 1.013e0

114.5384 1.013e0

114.5637 1.266e-2

114.5781 1.013e0

114.5993 2.025e0

114.6237 1.013e0

114.6478 2.025e0

114.6777 3.038e0

114.7014 4.051e0

114.7232 1.013e0

114.7488 2.025e0

114.7715 1.013e0

114.7886 1.013e0

114.8046 4.051e0

114.8333 3.038e0

114.8798 1.013e0

114.8990 3.798e-2

114.9252 2.025e0

114.9423 2.025e0

114.9667 2.025e0

114.9965 1.013e0

115.0165 2.025e0

115.0395 1.013e0

115.0684 4.076e0

115.1525 6.098e0

115.1763 1.266e-2

115.1974 3.468e0

115.2113 3.798e-2

115.2287 1.420e0

115.2477 1.013e0

115.2701 2.025e0

115.2988 2.038e0

115.3244 1.013e0

115.3688 2.025e0

115.3816 1.013e0

115.4100 2.025e0

115.4230 2.025e0

115.4628 2.025e0

115.4887 2.025e0

115.5114 5.063e0

115.5670 1.013e0

115.5944 2.025e0

115.6164 3.038e0

115.6355 4.051e0

115.6742 2.025e0

115.7168 3.038e0

115.7531 1.013e0

115.7742 2.025e0

115.7900 2.532e-2

115.8015 1.013e0

115.8286 2.025e0

115.8530 1.013e0

115.8642 1.266e-2

115.8815 3.038e0

115.9216 2.025e0

115.9402 2.025e0

115.9859 3.038e0

116.0245 1.266e-2

116.0715 7.640e0

116.1164 4.209e0

116.1477 5.063e0

116.1744 3.038e0

116.1990 1.266e-2

116.2222 1.013e0

116.2452 1.013e0

116.2852 1.013e0

116.3040 1.038e0

116.3370 1.266e-2

116.3568 1.013e0

116.3684 1.013e0

116.4057 1.013e0

116.4558 2.025e0

116.4827 1.013e0

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116.5692 2.025e0

116.5977 2.025e0

116.6149 4.051e0

116.6409 1.013e0

116.6606 1.266e-2

116.6779 1.013e0

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116.7249 3.038e0

116.7958 1.025e0

116.8273 1.013e0

116.8848 2.025e0

116.9093 2.025e0

116.9380 2.025e0

116.9566 1.013e0

116.9890 3.038e0

117.0226 2.025e0

117.0457 1.013e0

117.1041 1.330e0

117.1250 2.162e0

117.1521 1.013e0

117.1737 2.025e0

117.1924 1.013e0

117.2225 2.025e0

117.2355 1.013e0

117.2720 6.076e0

117.3290 2.025e0

117.3448 1.013e0

117.3737 2.025e0

117.3925 3.038e0

117.4368 1.013e0

117.4515 2.025e0

117.4674 2.025e0

117.4831 1.013e0

117.5147 2.025e0

117.5437 1.013e0

117.5611 1.013e0

117.5739 2.025e0

117.6128 1.013e0

117.6383 4.051e0

117.6895 3.038e0

117.7381 2.025e0

117.7495 2.025e0

117.8664 1.013e0

117.8897 2.025e0

117.9083 2.025e0

117.9430 2.025e0

117.9805 2.025e0

117.9934 1.025e0

118.0690 5.599e0

118.1290 6.092e0

118.1426 4.051e0

118.1653 2.025e0

118.1782 3.038e0

118.2056 2.025e0

118.2352 3.038e0

118.3082 1.025e0

118.3225 1.266e-2

118.3601 2.025e0

118.3920 2.025e0

118.4095 1.013e0

118.4254 2.025e0

118.4510 3.038e0

118.4845 2.025e0

118.5063 4.051e0

118.5278 1.013e0

118.5828 1.013e0

118.6175 2.025e0

118.6437 1.013e0

118.6610 1.013e0

118.6783 1.013e0

118.6926 1.013e0

118.7076 1.013e0

118.7261 2.025e0

118.7581 2.025e0

118.7972 2.025e0

118.8130 4.051e0

118.8319 1.266e-2

118.8552 1.013e0

118.8725 1.025e0

118.8869 1.013e0

118.9158 1.013e0

118.9593 1.013e0

118.9710 1.025e0

118.9969 1.013e0

119.0232 4.051e0

119.0639 1.013e0

119.1402 4.304e0

119.1608 2.025e0

119.1823 1.013e0

119.2043 2.025e0

119.2350 1.013e0

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119.3293 3.038e0

119.3725 2.025e0

119.4034 2.025e0

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119.5776 1.013e0

119.6328 1.266e-2

119.6457 2.025e0

119.6616 1.266e-2

119.7036 1.038e0

119.7605 2.025e0

119.7953 1.013e0

119.8142 2.025e0

119.8274 1.013e0

119.8748 3.223e0

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