

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

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

Elements Used:

C: 16-17 H: 20-22 N: 0-3 O: 0-2 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

304.1360 304.1371 -1.1 -3.6 7.5 128.6 0.0 C17 H22 N O2 S

100.0454 2.025e0

100.0572 1.013e0

100.0785 6.076e0

100.1104 1.013e0

100.1210 1.013e0

100.2115 1.013e0

100.2408 1.013e0

100.3340 2.025e0

100.3712 1.013e0

100.4350 1.013e0

100.5150 1.013e0

100.5363 1.013e0

100.5496 1.013e0

100.5978 1.013e0

100.6484 1.013e0

100.6857 1.013e0

100.7041 1.013e0

100.7297 2.025e0

100.7576 1.013e0

100.7870 1.013e0

100.8589 1.013e0

100.8778 1.013e0

100.9071 1.013e0

100.9418 1.013e0

100.9765 1.013e0

100.9979 3.038e0

101.0718 7.969e1

101.1074 1.013e0

101.1448 1.013e0

101.1582 1.013e0

101.1862 2.025e0

101.2424 4.051e0

101.2625 1.013e0

101.3734 2.025e0

101.4204 1.013e0

101.4338 1.013e0

101.5059 1.013e0

101.5220 1.013e0

101.5461 1.013e0

101.5702 2.025e0

101.5970 1.013e0

101.6561 1.013e0

101.6908 1.013e0

101.7149 2.025e0

101.7338 1.013e0

101.8787 1.013e0

101.8893 1.013e0

101.9174 2.025e0

101.9778 1.013e0

102.0259 1.013e0

102.0661 1.013e1

102.0838 2.025e0

102.1248 4.051e0

102.1389 1.013e0

102.2006 1.013e0

102.2113 1.013e0

102.3081 1.013e0

102.3782 1.013e0

102.4882 1.013e0

102.5314 1.013e0

102.5852 1.013e0

102.6363 1.013e0

102.6604 1.013e0

102.7496 1.013e0

102.9704 1.013e0

103.0784 1.013e0

103.1244 1.013e0

103.1784 1.013e0

103.1919 1.013e0

103.2836 1.013e0

103.3294 1.013e0

103.3429 1.013e0

103.6133 1.013e0

103.8609 2.025e0

103.8865 1.013e0

103.9271 1.013e0

104.0304 1.013e0

104.0706 1.418e1

104.0954 2.025e0

104.1089 2.025e0

104.2174 1.013e0

104.3614 1.013e0

104.4129 1.013e0

104.4564 1.013e0

104.4700 1.013e0

104.4890 1.013e0

104.5894 1.013e0

104.6165 1.013e0

104.6929 1.013e0

105.0057 2.025e0

105.0412 1.632e2

105.1188 2.025e0

105.1309 1.013e0

105.1445 1.013e0

105.1581 1.013e0

105.2046 1.013e0

105.2591 2.025e0

105.2836 1.013e0

105.3220 1.013e0

105.4460 2.025e0

105.4719 1.013e0

105.5198 2.025e0

105.5443 2.025e0

105.5702 1.013e0

105.6083 1.013e0

105.6644 2.025e0

105.6906 1.013e0

105.7396 1.013e0

105.8708 2.025e0

105.8982 2.025e0

105.9297 2.025e0

105.9475 1.013e0

105.9697 4.051e0

106.0483 1.318e1

106.0843 3.557e2

106.1663 3.038e0

106.1917 5.063e0

106.2075 3.038e0

106.2238 4.051e0

106.2512 1.013e0

106.2719 2.025e0

106.3224 1.013e0

106.3431 2.025e0

106.3606 5.063e0

106.4021 1.013e0

106.4246 3.038e0

106.4649 2.358e0

106.4828 2.025e0

106.5026 3.151e0

106.5240 2.025e0

106.5583 2.025e0

106.5786 3.038e0

106.5994 1.013e0

106.6214 1.013e0

106.6491 1.013e0

106.6953 1.013e0

106.7161 2.025e0

106.7558 2.025e0

106.7752 1.013e0

106.8163 1.013e0

106.8357 1.013e0

106.8589 2.025e0

106.8848 1.013e0

106.9236 1.013e0

106.9522 2.025e0

107.0362 2.025e0

107.0553 3.038e0

107.0906 2.170e1

107.1134 1.013e0

107.1929 1.013e0

107.2109 2.025e0

107.2644 1.013e0

107.2756 1.013e0

107.3032 1.013e0

107.3278 1.013e0

107.3645 3.481e0

107.4492 1.013e0

107.4696 2.025e0

107.4876 1.013e0

107.5041 1.013e0

107.5620 3.038e0

107.5814 1.013e0

107.6421 1.013e0

107.6748 1.013e0

107.6886 1.013e0

107.7000 1.013e0

107.7247 1.013e0

107.7579 1.013e0

107.7922 2.025e0

107.8986 3.038e0

107.9758 1.013e0

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108.0891 4.744e0

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108.1858 1.013e0

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108.6341 1.013e0

108.8835 1.013e0

108.9529 1.013e0

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109.9789 1.013e0

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110.5120 1.013e0

110.6041 1.013e0

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110.8669 1.013e0

110.9649 1.013e0

110.9899 1.013e0

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111.6909 1.013e0

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111.7247 1.013e0

111.7643 1.013e0

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112.5522 1.013e0

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115.9741 2.025e0

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116.0153 1.013e0

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116.1144 2.025e0

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116.2244 2.025e0

116.2474 1.013e0

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116.3132 1.013e0

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116.4766 2.025e0

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116.6432 1.013e0

116.7754 1.013e0

116.8527 1.013e0

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116.9305 1.013e0

116.9807 2.025e0

116.9964 1.013e0

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117.6183 1.013e0

117.6731 1.013e0

117.8329 2.025e0

117.8720 1.013e0

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120.5006 1.013e0

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120.6741 2.025e0

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120.9124 1.013e0

120.9768 1.013e0

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121.3216 1.013e0

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122.0458 2.350e1

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122.1974 2.025e0

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122.3660 1.013e0

122.3945 3.038e0

122.4387 3.883e0

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122.5132 3.038e0

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123.2350 1.013e0

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123.4416 1.013e0

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123.8229 1.013e0

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128.0429 1.013e0

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128.7774 1.013e0

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129.0726 1.193e0

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129.2014 2.025e0

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129.5025 1.013e0

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130.0391 3.038e0

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130.5174 2.025e0

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133.9615 1.013e0

133.9823 3.038e0

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134.0318 3.038e0

134.0793 6.347e2

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134.1738 4.051e0

134.2065 7.089e0

134.2275 3.623e0

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134.3814 3.038e0

134.3941 4.051e0

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134.4297 3.038e0

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134.4886 5.063e0

134.5113 2.025e0

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134.5590 4.051e0

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134.6438 3.038e0

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134.8830 4.491e0

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135.0437 2.025e0

135.0822 6.220e1

135.1424 2.025e0

135.1863 3.038e0

135.2195 1.013e0

135.2520 2.025e0

135.2830 2.025e0

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135.4699 1.013e0

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135.6250 1.013e0

135.7022 5.063e0

135.7332 1.013e0

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135.7730 2.025e0

135.7907 3.038e0

135.8226 3.038e0

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135.9155 2.025e0

135.9406 1.013e0

135.9825 2.025e0

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136.2877 1.013e0

136.3096 1.013e0

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136.6234 1.013e0

136.6515 2.025e0

136.7600 2.025e0

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137.3450 1.013e0

137.3851 1.013e0

137.4009 1.013e0

137.5851 1.013e0

137.6034 1.013e0

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137.8561 1.013e0

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