 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

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

Elements Used:

C: 12-12 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

192.1393 192.1388 0.5 2.6 4.5 315.4 0.0 C12 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.

99.6069 1.013e0

99.6337 5.063e0

99.6546 1.013e0

99.6760 1.013e0

99.6918 1.013e0

99.7159 1.013e0

99.7675 2.025e0

99.7874 1.013e0

99.7980 1.013e0

99.8312 2.025e0

99.8883 1.013e0

99.9041 2.025e0

99.9228 1.013e0

99.9333 1.013e0

99.9571 2.025e0

99.9958 2.025e0

100.0237 1.013e0

100.0476 1.013e0

100.0819 1.924e1

100.1187 6.076e0

100.1327 2.025e0

100.1832 1.013e0

100.2124 1.013e0

100.2271 2.025e0

100.2737 2.025e0

100.3269 1.013e0

100.3746 1.013e0

100.3908 1.013e0

100.4215 2.025e0

100.4413 1.013e0

100.4680 4.051e0

100.4919 1.013e0

100.5080 1.013e0

100.5280 2.025e0

100.5533 2.025e0

100.5798 1.013e0

100.5986 2.025e0

100.6170 1.013e0

100.6304 1.013e0

100.6451 2.025e0

100.6599 2.025e0

100.6758 3.038e0

100.6879 2.025e0

100.7146 2.025e0

100.7692 2.025e0

100.8412 1.013e0

100.8697 3.038e0

100.8840 1.013e0

100.9026 2.025e0

100.9265 1.013e0

100.9532 2.025e0

100.9680 4.051e0

101.0028 2.025e0

101.0173 1.013e0

101.0527 3.038e0

101.0761 2.620e2

101.1137 1.607e0

101.1349 2.025e0

101.1553 4.352e0

101.1778 2.025e0

101.2138 2.025e0

101.2327 3.038e0

101.2498 2.025e0

101.2751 3.038e0

101.3006 2.025e0

101.3195 1.013e0

101.3301 1.013e0

101.3608 2.025e0

101.3782 2.025e0

101.3887 1.013e0

101.4077 1.013e0

101.4331 2.025e0

101.4451 1.013e0

101.4732 2.025e0

101.4951 4.051e0

101.5241 2.025e0

101.5388 1.013e0

101.5696 2.025e0

101.5976 1.013e0

101.6191 2.025e0

101.6567 1.013e0

101.6741 2.025e0

101.6886 1.013e0

101.7049 3.038e0

101.7238 1.013e0

101.7437 2.025e0

101.7612 1.013e0

101.7848 4.051e0

101.8148 3.804e0

101.8283 1.013e0

101.8575 1.013e0

101.8829 3.038e0

101.9059 3.038e0

101.9247 2.025e0

101.9355 1.013e0

101.9878 2.025e0

102.0766 3.034e1

102.0944 8.107e0

102.1335 2.329e1

102.1622 2.025e0

102.1770 1.013e0

102.2106 2.025e0

102.2307 1.013e0

102.2521 1.013e0

102.2683 1.013e0

102.2859 2.025e0

102.3428 3.038e0

102.3934 2.131e0

102.4083 1.013e0

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102.4672 1.013e0

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102.7081 2.025e0

102.7392 2.025e0

102.8145 2.025e0

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102.8926 1.013e0

102.9144 1.013e0

102.9541 3.038e0

103.0111 1.013e0

103.0518 3.038e0

103.0984 4.661e0

103.1429 3.038e0

103.1712 3.038e0

103.2020 3.038e0

103.2433 1.013e0

103.2528 2.025e0

103.2731 1.013e0

103.3080 1.013e0

103.3569 1.013e0

103.4431 1.013e0

103.4650 1.013e0

103.5082 1.013e0

103.5377 1.013e0

103.5647 1.013e0

103.5782 1.013e0

103.6029 1.013e0

103.6188 1.013e0

103.6976 1.013e0

103.7230 2.025e0

103.7489 1.013e0

103.7704 1.013e0

103.7826 2.025e0

103.8003 1.013e0

103.8138 2.025e0

103.8721 2.025e0

103.8896 1.013e0

103.9193 1.013e0

103.9412 1.013e0

103.9519 1.013e0

103.9736 2.025e0

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104.2772 1.013e0

104.3071 1.013e0

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104.3791 2.025e0

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104.4783 1.013e0

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104.6602 2.025e0

104.6840 3.038e0

104.7035 1.013e0

104.7309 2.025e0

104.7622 4.051e0

104.7827 1.013e0

104.8234 1.013e0

104.8464 2.025e0

104.8671 1.013e0

104.9064 2.131e0

104.9497 2.235e0

105.0058 1.013e0

105.0478 3.443e2

105.1094 2.014e0

105.1291 7.089e0

105.1446 3.038e0

105.1619 5.063e0

105.1745 3.038e0

105.2061 4.051e0

105.2264 1.013e0

105.2654 5.063e0

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105.3067 2.025e0

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105.3409 1.013e0

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112.5505 2.025e0

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114.1021 4.680e0

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114.1991 3.038e0

114.2425 2.025e0

114.2596 1.013e0

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114.3304 2.025e0

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114.5238 2.025e0

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116.2477 1.013e0

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116.3450 1.013e0

116.3881 1.013e0

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116.9449 1.013e0

116.9981 2.025e0

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117.0340 2.025e0

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117.1120 2.268e0

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117.7422 2.025e0

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118.2227 2.025e0

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119.8938 1.013e0

119.9128 2.025e0

119.9581 1.013e0

119.9815 2.025e0

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120.0550 7.759e1

120.1618 1.013e0

120.1925 2.025e0

120.2200 1.013e0

120.2403 2.025e0

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120.2783 1.013e0

120.3061 2.025e0

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120.5932 1.013e0

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120.7015 1.013e0

120.7274 1.013e0

120.7539 1.013e0

120.7918 1.013e0

120.9350 1.013e0

121.0020 1.013e0

121.0262 5.063e0

121.0677 7.595e0

121.2713 1.013e0

121.2858 1.013e0

121.3268 1.013e0

121.3488 2.025e0

121.3708 2.025e0

121.4438 2.025e0

121.4849 1.013e0

121.5114 2.025e0

121.5730 2.025e0

121.5989 1.013e0

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121.7982 1.013e0

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121.8954 2.025e0

121.9322 2.025e0

121.9481 1.013e0

121.9686 1.013e0

121.9979 1.013e0

122.0273 1.013e0

122.0482 7.068e0

122.0714 1.013e0

122.1033 5.352e1

122.1506 1.013e0

122.1772 2.025e0

122.1918 1.013e0

122.2183 2.025e0

122.2535 1.013e0

122.2741 1.013e0

122.3092 1.013e0

122.3408 3.038e0

122.3739 1.013e0

122.3885 1.013e0

122.4443 1.013e0

122.4884 1.013e0

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122.5240 1.013e0

122.5532 2.025e0

122.5959 2.025e0

122.6768 1.013e0

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122.7311 2.025e0

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122.7669 3.038e0

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123.1717 1.013e0

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123.5021 2.025e0

123.5319 1.013e0

123.5480 2.025e0

123.5702 1.013e0

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