 Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 15-15 H: 0-150 N: 0-10 O: 0-10 Na: 0-1 69Ga: 0-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

226.1226 226.1232 -0.6 -2.7 8.5 426.1 C15 H16 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)

100.0125 1.013e0

100.0507 5.063e0

100.0794 3.199e1

100.1082 3.785e0

100.1255 1.938e0

100.1628 2.025e0

100.1906 1.013e0

100.2012 1.013e0

100.2200 1.013e0

100.2784 1.013e0

100.2917 1.013e0

100.3370 1.013e0

100.3484 3.038e0

100.3929 1.013e0

100.4407 1.013e0

100.4623 1.013e0

100.4779 1.013e0

100.5353 4.051e0

100.5527 2.025e0

100.6086 1.013e0

100.6180 2.025e0

100.6353 1.013e0

100.6553 2.025e0

100.6831 1.013e0

100.8433 1.013e0

100.8780 2.025e0

100.9368 1.013e0

100.9609 1.013e0

100.9899 1.013e0

101.0061 3.038e0

101.0719 1.961e2

101.0977 3.932e0

101.1264 1.013e0

101.1425 1.013e0

101.1531 1.013e0

101.1808 5.063e0

101.2696 3.038e0

101.3350 1.013e0

101.3724 1.013e0

101.3937 1.013e0

101.4394 1.013e0

101.4553 2.025e0

101.5142 1.013e0

101.5463 2.025e0

101.5946 1.013e0

101.6105 1.013e0

101.6348 1.013e0

101.6533 1.013e0

101.6667 1.013e0

101.6883 1.013e0

101.7125 1.013e0

101.7472 1.013e0

101.7713 1.013e0

101.7819 1.013e0

101.8008 1.013e0

101.8170 1.013e0

101.8329 1.013e0

101.8596 1.013e0

101.8920 1.013e0

101.9026 2.025e0

101.9376 2.025e0

102.0075 4.051e0

102.0341 1.013e0

102.0750 2.410e1

102.0944 5.158e0

102.1307 2.022e1

102.1550 1.013e0

102.1791 1.013e0

102.1953 1.013e0

102.2167 1.013e0

102.2329 1.013e0

102.2491 2.025e0

102.2693 2.025e0

102.2920 2.025e0

102.3323 1.013e0

102.3701 1.013e0

102.4239 1.013e0

102.4466 2.025e0

102.4856 1.013e0

102.4990 1.013e0

102.5153 1.013e0

102.5677 2.025e0

102.6084 3.038e0

102.6875 1.013e0

102.7036 1.013e0

102.8543 1.013e0

102.8745 2.025e0

102.9487 1.013e0

103.0109 1.013e0

103.0430 4.051e0

103.0666 1.424e0

103.0889 3.039e0

103.1375 1.013e0

103.1701 1.013e0

103.2375 1.013e0

103.2995 1.013e0

103.3805 1.013e0

103.4183 1.013e0

103.4481 2.025e0

103.4751 1.013e0

103.5103 1.013e0

103.5347 1.013e0

103.5697 1.013e0

103.5980 3.038e0

103.7292 1.013e0

103.8052 1.013e0

103.8403 2.025e0

103.8687 2.025e0

103.8986 2.025e0

103.9229 2.025e0

103.9812 1.013e0

104.0177 2.025e0

104.0496 7.977e0

104.0733 9.937e0

104.1009 2.773e0

104.1194 3.899e0

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104.1994 2.025e0

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104.2765 1.013e0

104.3120 1.013e0

104.3428 3.038e0

104.3707 3.038e0

104.4043 1.013e0

104.4640 3.038e0

104.5128 1.013e0

104.5509 1.013e0

104.5671 1.013e0

104.5999 2.025e0

104.6570 2.025e0

104.6895 2.025e0

104.7042 3.038e0

104.7328 1.013e0

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104.8256 1.013e0

104.8500 1.013e0

104.8715 1.013e0

104.8922 2.025e0

104.9452 1.013e0

104.9560 1.013e0

104.9831 1.013e0

105.0432 3.689e2

105.1178 4.836e0

105.1433 3.038e0

105.1729 3.085e0

105.1929 1.013e0

105.2149 1.013e0

105.2422 3.129e0

105.2831 4.051e0

105.3198 2.025e0

105.3403 1.013e0

105.3630 3.038e0

105.3894 4.051e0

105.4057 1.013e0

105.4385 1.013e0

105.4715 1.013e0

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105.5053 2.025e0

105.5340 1.013e0

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105.5833 2.025e0

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105.7879 2.025e0

105.8291 4.051e0

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105.9767 1.013e0

105.9931 1.013e0

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106.0465 1.930e1

106.0666 5.456e1

106.0893 4.712e0

106.1408 1.013e0

106.1642 2.025e0

106.1806 2.025e0

106.2146 1.013e0

106.2340 1.013e0

106.2641 1.013e0

106.2886 2.025e0

106.3160 1.013e0

106.3369 3.038e0

106.3572 2.025e0

106.3736 1.013e0

106.3929 1.013e0

106.4094 1.013e0

106.4462 2.132e0

106.4669 1.013e0

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106.5463 2.025e0

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106.6449 1.013e0

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106.6848 2.025e0

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106.7715 2.025e0

106.8920 2.025e0

106.9031 3.038e0

106.9994 2.025e0

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107.1368 2.025e0

107.1644 2.025e0

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107.3241 1.013e0

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107.6393 2.025e0

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107.8779 1.013e0

107.9139 1.013e0

107.9581 1.013e0

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111.7961 1.013e0

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111.8631 1.013e0

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111.9732 2.025e0

111.9996 2.025e0

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112.8462 1.013e0

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112.9847 2.025e0

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113.3711 3.038e0

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113.6110 2.025e0

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113.6852 3.321e0

113.7234 6.076e0

113.7485 1.013e0

113.7752 2.025e0

113.7907 1.013e0

113.8077 1.013e0

113.8321 2.025e0

113.8817 2.025e0

113.9209 4.051e0

113.9699 4.051e0

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114.0263 3.038e0

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114.0562 2.025e0

114.0718 1.987e0

114.0937 8.253e0

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114.1826 4.051e0

114.2335 1.013e0

114.2705 1.013e0

114.2919 2.025e0

114.3089 2.025e0

114.3260 2.025e0

114.3612 5.063e0

114.3771 2.025e0

114.3982 1.013e0

114.4210 1.013e0

114.4447 3.304e0

114.4863 1.013e0

114.5005 2.025e0

114.5135 2.025e0

114.5643 3.038e0

114.5974 1.013e0

114.6369 3.329e0

114.6478 3.038e0

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114.8677 1.013e0

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114.9077 1.013e0

114.9419 1.013e0

114.9560 1.013e0

114.9814 1.013e0

115.0157 2.025e0

115.0328 1.013e0

115.0578 3.038e0

115.0883 1.892e2

115.1276 3.938e0

115.1397 2.025e0

115.1671 1.013e0

115.1896 2.025e0

115.2125 2.025e0

115.2453 2.025e0

115.2580 1.013e0

115.2824 2.025e0

115.3039 1.013e0

115.3381 2.025e0

115.3494 1.013e0

115.3753 1.013e0

115.4104 3.038e0

115.4296 1.013e0

115.4492 1.013e0

115.4664 2.025e0

115.5265 2.025e0

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115.7119 1.013e0

115.7320 1.013e0

115.8193 2.025e0

115.8453 4.051e0

115.8721 1.013e0

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115.9065 2.025e0

115.9525 1.013e0

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115.9951 1.013e0

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116.0383 1.013e0

116.0672 7.089e0

116.0884 1.742e1

116.1168 1.836e0

116.1340 2.025e0

116.1457 2.025e0

116.1845 2.025e0

116.2413 1.013e0

116.2585 1.013e0

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116.3390 1.013e0

116.3734 2.025e0

116.4107 3.038e0

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116.4838 2.025e0

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116.6602 1.013e0

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116.7922 2.025e0

116.8068 1.013e0

116.8413 5.063e0

116.8928 1.013e0

116.9071 1.013e0

116.9359 1.013e0

116.9474 1.013e0

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117.0663 1.235e1

117.1105 3.087e0

117.1630 1.013e0

117.1915 1.013e0

117.2176 1.013e0

117.2608 1.013e0

117.3644 1.013e0

117.4049 1.013e0

117.4738 1.013e0

117.4997 3.038e0

117.5371 3.038e0

117.6036 1.013e0

117.6322 1.013e0

117.6696 1.013e0

117.7071 1.013e0

117.7259 2.051e0

117.7678 1.013e0

117.7965 1.013e0

117.8196 1.013e0

117.8917 1.013e0

117.9394 3.038e0

117.9954 1.013e0

118.0073 1.013e0

118.0301 1.013e0

118.0659 7.812e1

118.1284 1.912e0

118.1456 2.025e0

118.1659 1.013e0

118.2237 3.038e0

118.2484 2.025e0

118.2713 2.025e0

118.3262 2.025e0

118.3523 2.025e0

118.4695 1.013e0

118.5245 1.013e0

118.5576 4.051e0

118.6228 1.013e0

118.6661 1.013e0

118.8109 2.025e0

118.8325 2.025e0

118.8716 1.013e0

118.9091 5.063e0

118.9266 1.013e0

119.0019 2.025e0

119.0223 2.025e0

119.0659 1.013e0

119.0983 2.318e0

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119.1904 2.025e0

119.2430 1.013e0

119.2808 2.025e0

119.3066 1.013e0

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119.8412 2.025e0

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120.2401 2.025e0

120.2586 3.038e0

120.2829 4.394e0

120.3056 2.025e0

120.3305 4.051e0

120.3430 5.063e0

120.3706 6.263e0

120.3909 5.063e0

120.4097 6.351e0

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120.4565 5.063e0

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120.6587 3.106e0

120.6715 2.025e0

120.6934 2.025e0

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120.7476 1.013e0

120.7742 3.038e0

120.7943 1.013e0

120.8329 6.076e0

120.8743 5.063e0

120.8950 2.235e0

120.9111 1.013e0

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120.9610 2.025e0

120.9930 3.038e0

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121.1918 2.025e0

121.2025 3.038e0

121.2253 2.025e0

121.2422 3.038e0

121.2679 1.013e0

121.2823 1.013e0

121.3323 6.076e0

121.3749 4.051e0

121.4129 2.025e0

121.4289 2.025e0

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121.4829 2.025e0

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121.5224 1.013e0

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121.5976 2.614e0

121.6206 4.663e0

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121.6794 2.025e0

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121.8053 2.025e0

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121.8479 1.013e0

121.8896 4.051e0

121.9331 2.025e0

121.9594 1.013e0

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122.0468 1.143e2

122.0988 8.102e1

122.1891 3.038e0

122.2089 1.013e0

122.2797 1.013e0

122.3087 1.013e0

122.3308 2.025e0

122.3529 3.038e0

122.3851 1.013e0

122.4146 1.013e0

122.4497 2.025e0

122.4764 1.013e0

122.5031 4.051e0

122.5382 3.038e0

122.5558 2.025e0

122.5908 1.013e0

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122.6679 1.013e0

122.6939 1.013e0

122.7060 1.013e0

122.7472 1.013e0

122.8085 3.401e0

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122.8794 1.013e0

122.9046 2.025e0

122.9206 1.013e0

122.9489 2.025e0

122.9796 1.013e0

122.9947 1.013e0

123.0153 1.013e0

123.0328 4.523e0

123.0493 7.016e0

123.0937 1.689e1

123.1081 6.361e0

123.1391 1.013e0

123.1663 3.038e0

123.2125 2.025e0

123.2317 2.025e0

123.2867 1.013e0

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123.7205 1.013e0

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123.8179 2.025e0

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123.8940 3.038e0

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