

Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 30-30 H: 0-200 N: 0-15 O: 0-15 Na: 0-1

Minimum: -1.5

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

496.2231 496.2236 -0.5 -1.0 17.5 25.5 C30 H30 N3 O4

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)

148.1604 3.725e0

148.1805 4.306e0

148.2079 4.041e0

148.2385 3.020e0

148.2725 2.025e0

148.2920 5.063e0

148.3255 3.582e0

148.3608 1.861e0

148.3945 3.038e0

148.4124 1.906e0

148.4375 2.299e0

148.4577 2.848e0

148.4936 1.812e0

148.5175 3.038e0

148.5338 1.013e0

148.5699 1.013e0

148.6002 2.025e0

148.6357 3.038e0

148.6864 1.013e0

148.7156 2.025e0

148.7430 2.025e0

148.7724 5.063e0

148.8062 2.025e0

148.8333 6.076e0

148.8604 7.189e0

148.8974 1.013e0

148.9202 3.038e0

148.9672 5.757e0

148.9895 2.832e0

149.0355 3.038e0

149.0730 2.968e0

149.0907 6.358e0

149.1258 7.201e0

149.1457 5.319e0

149.1660 3.926e0

149.1987 1.984e0

149.2260 6.946e0

149.2792 3.038e0

149.3036 1.696e0

149.3257 3.570e0

149.3614 3.886e0

149.3775 1.071e1

149.4196 1.888e0

149.4435 1.888e0

149.4713 1.017e1

149.5052 2.674e0

149.5416 3.038e0

149.5726 4.673e0

149.5909 3.428e0

149.6161 2.025e0

149.6357 3.038e0

149.6676 5.011e0

149.6861 1.868e0

149.7314 4.051e0

149.7572 1.013e0

149.7799 1.013e0

149.8030 1.013e0

149.8193 2.025e0

149.8382 1.013e0

149.8647 1.013e0

149.8968 5.802e0

149.9283 5.477e0

149.9833 2.853e0

150.0240 1.013e0

150.0466 1.013e0

150.0699 1.278e0

150.1415 1.724e0

150.1652 2.788e0

150.2081 2.089e0

150.2357 5.933e0

150.2963 5.063e0

150.3230 2.899e0

150.3982 2.969e0

150.4312 1.865e0

150.4599 4.814e0

150.5286 1.013e0

150.5496 3.038e0

150.5888 4.051e0

150.6166 3.545e0

150.6837 3.998e0

150.7446 7.089e0

150.7839 3.038e0

150.8454 1.013e0

150.8709 1.013e0

150.9171 1.013e0

150.9559 1.956e0

150.9830 3.889e0

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151.0593 1.566e0

151.0796 1.661e0

151.1447 6.633e0

151.1749 2.405e0

151.2517 4.039e0

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151.3498 2.615e0

151.3929 3.038e0

151.4113 2.924e0

151.4492 1.878e0

151.4983 2.009e0

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151.5574 4.051e0

151.5844 4.051e0

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151.6605 4.051e0

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151.9463 1.013e0

151.9771 4.879e0

152.0047 2.946e0

152.0489 6.691e0

152.1184 1.724e0

152.1538 1.861e0

152.1900 4.022e0

152.2320 1.013e0

152.2576 3.104e0

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152.3624 4.169e0

152.3919 7.896e0

152.4230 2.141e0

152.4599 1.966e0

152.4846 3.018e0

152.5320 2.025e0

152.5528 1.013e0

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152.6087 3.038e0

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152.6663 2.025e0

152.6812 3.038e0

152.7024 2.025e0

152.7334 2.025e0

152.7634 2.025e0

152.8039 2.025e0

152.8367 5.215e0

152.8531 2.887e0

152.8827 2.025e0

152.9196 3.147e0

152.9372 2.929e0

152.9883 1.853e0

153.0049 1.922e0

153.0470 3.038e0

153.0848 2.683e0

153.1201 4.662e0

153.1452 2.787e0

153.1696 1.992e0

153.2015 2.002e0

153.2207 3.038e0

153.2415 4.051e0

153.2608 2.025e0

153.2754 1.013e0

153.3157 2.215e0

153.3318 1.202e0

153.3827 2.025e0

153.4404 3.907e0

153.4733 3.328e0

153.4979 1.799e0

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153.5556 3.038e0

153.5884 4.839e0

153.6218 3.418e0

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153.6735 2.025e0

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153.7959 1.013e0

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153.8966 4.117e0

153.9374 4.051e0

153.9917 4.857e0

154.0240 4.609e0

154.0422 3.038e0

154.0745 3.614e0

154.0970 3.296e0

154.1204 3.077e0

154.1514 4.813e0

154.2034 4.051e0

154.2280 1.013e0

154.2519 5.063e0

154.2982 5.277e0

154.3439 3.373e0

154.3787 3.038e0

154.4187 5.760e0

154.4434 5.909e0

154.4860 3.356e0

154.5176 2.025e0

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154.5973 6.042e0

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154.6431 3.038e0

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155.1410 4.051e0

155.1627 1.013e0

155.2126 2.025e0

155.2427 4.051e0

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155.3163 3.038e0

155.3389 3.038e0

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155.5676 7.638e0

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155.6990 2.025e0

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155.8947 3.269e0

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156.0570 1.939e0

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156.1743 3.038e0

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156.7909 5.063e0

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158.7453 5.063e0

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161.4516 1.906e0

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161.5508 1.770e0

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162.6604 2.025e0

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163.0806 2.840e0

163.1007 2.840e0

163.1203 5.024e0

163.1488 8.503e0

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163.3046 2.025e0

163.3387 3.038e0

163.3592 3.038e0

163.3851 2.780e0

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163.6766 2.025e0

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165.1606 1.970e0

165.1843 1.749e0

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165.3481 3.038e0

165.3944 2.025e0

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165.5756 2.988e0

165.6099 2.006e0

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165.7693 2.936e0

165.8027 1.013e0

165.8285 2.025e0

165.8578 2.025e0

165.8798 4.051e0

165.9119 1.963e0

165.9279 3.038e0

165.9442 2.025e0

165.9817 3.866e0

166.0018 2.900e0

166.0483 6.004e0

166.0906 1.723e0

166.1415 3.038e0

166.1666 1.859e0

166.1989 4.445e0

166.2415 3.022e0

166.3205 6.076e0

166.3681 9.114e0

166.3965 6.076e0

166.4255 2.025e0

166.4630 3.038e0

166.4819 3.038e0

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166.5526 2.025e0

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166.6608 2.025e0

166.7100 2.025e0

166.7289 3.038e0

166.7623 3.038e0

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168.1473 4.051e0

168.1870 4.964e0

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168.5593 4.051e0

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168.6642 5.063e0

168.7039 2.025e0

168.7278 1.925e0

168.7506 4.051e0

168.7802 1.205e1

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168.8363 4.696e0

168.8889 5.590e0

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170.2223 2.021e0

170.2412 2.025e0

170.2807 9.035e0

170.3067 2.104e0

170.3352 5.099e0

170.3812 3.942e0

170.4378 2.748e0

170.4656 6.076e0

170.5045 5.414e0

170.5560 1.204e1

170.5862 1.679e0

170.6297 3.038e0

170.6887 7.478e0

170.7185 3.038e0

170.7617 1.013e0

170.7809 4.051e0

170.8234 5.063e0

170.8667 4.051e0

170.8940 2.025e0

170.9234 4.051e0

170.9516 5.063e0

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171.0560 4.654e0

171.0724 2.970e0

171.1035 2.072e0

171.1225 1.013e0

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171.2167 4.018e0

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171.5069 2.025e0

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171.8587 2.025e0

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172.0319 1.929e0

172.0923 2.025e0

172.1219 1.013e0

172.1747 4.043e0

172.2171 3.227e0

172.2498 3.022e0

172.2678 3.030e0

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