 Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 18-18 H: 0-100 N: 0-10 O: 0-10 Na: 0-1 S: 0-1

Minimum: -15.0

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

349.1110 349.1110 0.0 0.0 8.5 18.0 C18 H21 O5 S

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)

144.0205 7.946e-1

144.0400 2.025e0

144.0527 4.301e0

144.0596 5.539e0

144.0619 5.513e0

144.0645 1.208e1

144.0672 2.034e1

144.0757 9.618e0

144.0781 1.588e1

144.1038 3.549e0

144.1368 6.192e-1

144.1389 1.013e0

144.1473 3.038e0

144.1535 2.025e0

144.1590 3.002e0

144.1628 2.532e-2

144.1776 3.038e0

144.1820 4.051e0

144.1877 5.124e0

144.2022 1.266e-2

144.2089 1.266e-2

144.2119 1.013e0

144.2185 2.025e0

144.2315 2.025e0

144.2335 2.025e0

144.2374 1.013e0

144.2567 1.266e-2

144.2642 2.038e0

144.2696 1.266e-2

144.2853 1.013e0

144.2886 1.013e0

144.2906 2.532e-2

144.3023 4.063e0

144.3069 3.038e0

144.3080 2.025e0

144.3142 1.013e0

144.3154 2.025e0

144.3287 3.038e0

144.3359 3.038e0

144.3372 1.013e0

144.3493 1.013e0

144.3543 5.063e0

144.3555 1.013e0

144.3746 2.927e0

144.3812 3.038e0

144.3825 2.025e0

144.3939 1.025e0

144.4080 3.063e0

144.4103 1.013e0

144.4258 2.025e0

144.4355 2.532e-2

144.4405 2.025e0

144.4517 1.013e0

144.4545 1.025e0

144.4642 4.051e0

144.4674 2.025e0

144.4690 2.532e-2

144.4865 1.013e0

144.4927 1.013e0

144.4962 2.532e-2

144.5011 3.336e0

144.5029 1.013e0

144.5060 2.532e-2

144.5127 2.025e0

144.5188 1.013e0

144.5247 2.025e0

144.5281 1.013e0

144.5298 3.038e0

144.5445 1.013e0

144.5478 1.013e0

144.5555 2.025e0

144.5573 1.013e0

144.5678 2.051e0

144.5797 1.013e0

144.5859 1.962e0

144.5894 2.025e0

144.5922 1.013e0

144.6017 1.013e0

144.6219 2.038e0

144.6414 2.025e0

144.6561 1.013e0

144.6682 4.051e0

144.6718 3.038e0

144.6737 2.025e0

144.6749 2.025e0

144.6782 1.013e0

144.6917 2.025e0

144.6979 1.013e0

144.7014 2.025e0

144.7038 7.774e0

144.7071 1.013e0

144.7235 1.025e0

144.7264 1.013e0

144.7297 2.532e-2

144.7313 2.025e0

144.7365 1.013e0

144.7420 1.266e-2

144.7467 2.025e0

144.7518 1.013e0

144.7615 2.025e0

144.7717 1.025e0

144.7753 2.832e0

144.7772 1.266e-2

144.7821 2.025e0

144.7869 1.053e0

144.7902 1.013e0

144.7968 3.038e0

144.8036 1.266e-2

144.8081 2.025e0

144.8123 2.025e0

144.8153 2.025e0

144.8187 1.025e0

144.8241 2.025e0

144.8270 2.025e0

144.8355 1.013e0

144.8507 1.013e0

144.8542 1.266e-2

144.8557 4.022e0

144.8572 1.266e-2

144.8609 1.266e-2

144.8736 2.025e0

144.8860 2.038e0

144.8907 2.025e0

144.8989 1.266e-2

144.9120 1.013e0

144.9225 2.025e0

144.9268 4.051e0

144.9292 2.025e0

144.9312 1.013e0

144.9374 2.025e0

144.9423 2.025e0

144.9593 2.025e0

144.9836 1.646e-1

144.9878 1.823e1

144.9918 3.038e0

145.0032 2.025e0

145.0044 1.013e0

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145.0159 3.038e0

145.0230 2.025e0

145.0241 2.865e0

145.0272 2.025e0

145.0420 2.608e0

145.0491 2.456e0

145.0567 5.298e0

145.0613 4.449e0

145.0631 1.026e1

145.0684 1.863e-2

145.0739 3.989e0

145.0953 1.076e1

145.0973 3.429e0

145.1264 1.147e0

145.1279 9.402e-1

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145.1599 2.025e0

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145.1967 1.266e-2

145.1983 2.051e0

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145.2254 4.063e0

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145.2740 1.013e0

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145.2863 2.532e-2

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145.3023 1.013e0

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145.3173 2.025e0

145.3217 1.013e0

145.3278 2.025e0

145.3375 1.013e0

145.3510 1.013e0

145.3571 1.013e0

145.3711 2.025e0

145.3747 2.025e0

145.3809 5.040e0

145.3858 1.013e0

145.3891 1.013e0

145.3983 1.266e-2

145.4096 2.025e0

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145.4181 1.013e0

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145.8592 4.051e0

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146.2107 1.266e-2

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146.2171 3.038e0

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146.2328 2.170e0

146.2493 1.013e0

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146.2585 3.038e0

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146.2651 1.013e0

146.2681 1.013e0

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146.3551 1.266e-2

146.3685 1.013e0

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146.3886 3.015e0

146.3941 1.266e-2

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146.4158 2.025e0

146.4233 3.798e-2

146.4294 2.532e-2

146.4356 1.266e-2

146.4367 3.405e0

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146.4842 1.266e-2

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146.5001 2.025e0

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146.5245 3.038e0

146.5257 1.266e-2

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146.6797 2.025e0

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146.6895 1.013e0

146.6932 1.266e-2

146.6994 1.025e0

146.7010 2.025e0

146.7030 1.266e-2

146.7094 2.038e0

146.7188 2.038e0

146.7218 1.013e0

146.7285 2.025e0

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146.7331 4.051e0

146.7430 2.025e0

146.7569 1.013e0

146.7585 2.025e0

146.7638 1.013e0

146.7668 1.266e-2

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146.8474 3.038e0

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146.8639 1.266e-2

146.8711 2.532e-2

146.8798 1.013e0

146.8812 5.046e0

146.8927 2.025e0

146.9055 1.025e0

146.9100 2.025e0

146.9115 1.266e-2

146.9184 1.013e0

146.9255 2.038e0

146.9448 5.076e0

146.9485 3.038e0

146.9702 1.013e0

146.9802 4.076e0

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146.9828 1.076e0

146.9858 2.532e-2

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146.9924 1.013e0

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147.0798 8.491e1

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147.1698 2.025e0

147.1736 1.266e-2

147.1763 1.266e-2

147.1891 1.013e0

147.1929 3.038e0

147.2036 4.051e0

147.2052 1.013e0

147.2119 1.266e-2

147.2184 1.013e0

147.2199 2.025e0

147.2240 1.025e0

147.2291 4.051e0

147.2308 1.266e-2

147.2410 1.013e0

147.2443 1.013e0

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147.2720 6.773e0

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147.2929 2.025e0

147.3014 2.025e0

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147.3213 1.266e-2

147.3316 1.266e-2

147.3372 1.025e0

147.3469 3.038e0

147.3496 4.051e0

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147.3642 3.038e0

147.3704 1.266e-2

147.3720 4.816e0

147.3790 1.013e0

147.3826 1.025e0

147.3855 1.013e0

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147.3954 2.999e0

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147.4276 9.929e-1

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147.4761 1.266e-2

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147.5536 1.025e0

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147.5738 4.695e0

147.5762 1.266e-2

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147.5806 2.025e0

147.5989 1.266e-2

147.6026 2.025e0

147.6056 1.013e0

147.6146 1.266e-2

147.6178 1.266e-2

147.6212 4.051e0

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147.6476 3.038e0

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147.6713 3.038e0

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147.6976 3.038e0

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147.7189 3.051e0

147.7221 1.266e-2

147.7234 2.025e0

147.7255 1.013e0

147.7283 1.025e0

147.7311 1.013e0

147.7390 2.025e0

147.7423 2.532e-2

147.7505 1.013e0

147.7638 1.013e0

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147.7959 2.025e0

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147.8103 2.025e0

147.8121 1.013e0

147.8148 1.013e0

147.8215 2.116e0

147.8248 1.013e0

147.8350 1.013e0

147.8396 2.025e0

147.8414 2.025e0

147.8501 9.114e0

147.8706 6.076e0

147.8801 2.085e0

147.8838 1.013e0

147.8882 1.839e0

147.8993 1.013e0

147.9155 1.013e0

147.9225 1.266e-2

147.9265 5.063e0

147.9285 2.025e0

147.9347 2.025e0

147.9456 3.066e0

147.9609 1.013e0

147.9646 1.013e0

147.9732 1.013e0

147.9745 3.038e0

147.9768 1.266e-2

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147.9864 1.013e0

147.9967 1.013e0

148.0095 2.025e0

148.0143 1.038e0

148.0204 2.652e0

148.0225 3.956e0

148.0388 1.013e0

148.0555 5.029e0

148.0570 3.916e0

148.0588 6.076e0

148.0599 6.216e0

148.0820 2.244e0

148.0848 2.841e1

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148.0970 8.929e-1

148.1060 5.450e0

148.1119 4.093e0

148.1140 2.217e0

148.1182 1.283e0

148.1419 1.013e0

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148.4106 2.025e0

148.4313 2.025e0

148.4330 1.013e0

148.4483 5.063e0

148.4498 3.038e0

148.4524 1.025e0

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148.4944 1.013e0

148.4971 6.725e0

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148.5239 2.025e0

148.5273 1.266e-2

148.5462 1.266e-2

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148.5754 1.013e0

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148.6052 1.266e-2

148.6190 2.025e0

148.6271 2.025e0

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148.6440 1.013e0

148.6508 1.266e-2

148.6548 5.063e0

148.6565 1.013e0

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148.6759 2.025e0

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148.6858 1.025e0

148.6985 2.025e0

148.7154 5.076e0

148.7220 1.404e0

148.7421 2.025e0

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148.8085 3.038e0

148.8124 2.025e0

148.8187 1.266e-2

148.8317 1.013e0

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148.8380 1.266e-2

148.8412 1.013e0

148.8479 1.266e-2

148.8516 1.266e-2

148.8546 1.013e0

148.8768 5.462e0

148.8867 1.013e0

148.8970 2.025e0

148.9043 2.025e0

148.9157 1.013e0

148.9256 1.013e0

148.9335 6.076e0

148.9453 1.266e-2

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148.9496 2.025e0

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148.9782 1.013e0

148.9840 2.025e0

148.9967 1.013e0

149.0079 2.038e0

149.0109 3.038e0

149.0167 2.025e0

149.0218 2.025e0

149.0276 1.770e0

149.0295 2.025e0

149.0318 7.135e0

149.0509 2.025e0

149.0671 2.025e0

149.0683 2.387e0

149.0769 1.612e0

149.0896 2.171e0

149.0945 5.414e0

149.1020 3.626e0

149.1175 1.524e0

149.1188 4.919e0

149.1206 2.364e0

149.1437 7.006e0

149.1559 1.013e0

149.1591 2.025e0

149.1601 7.089e0

149.1725 1.013e0

149.1808 6.076e0

149.1859 1.013e0

149.2011 1.266e-2

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149.2061 2.025e0

149.2214 1.013e0

149.2277 1.266e-2

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149.2717 2.025e0

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