

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 = -15.0, max = 100.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 8-9 H: 5-13 N: 1-10 Na: 0-1 Br: 1-1

Minimum: -15.0

Maximum: 5.0 7.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

214.0233 214.0231 0.2 0.9 3.5 18.9 C9 H13 N Br

175.7818 1.013e0

175.7856 1.013e0

175.8282 3.038e0

175.8490 1.013e0

175.8627 1.013e0

175.8800 1.013e0

175.9263 1.013e0

175.9796 1.013e0

176.0044 1.013e0

176.0251 1.013e0

176.0707 1.013e0

176.0816 1.013e0

176.0885 2.025e0

176.0916 7.089e0

176.0941 8.101e0

176.1109 3.038e0

176.1153 4.379e0

176.1224 2.025e0

176.1311 1.013e0

176.1492 1.013e0

176.1872 2.025e0

176.2151 1.013e0

176.2260 2.025e0

176.2509 1.013e0

176.3668 1.013e0

176.3812 1.013e0

176.4079 2.025e0

176.4308 2.025e0

176.4346 1.013e0

176.4450 1.013e0

176.4735 1.013e0

176.4949 1.013e0

176.5018 1.013e0

176.5260 1.013e0

176.5399 1.013e0

176.5553 5.063e0

176.5572 5.063e0

176.5593 3.038e0

176.5790 1.013e0

176.6815 1.013e0

176.7273 1.013e0

176.7876 2.025e0

176.7950 1.013e0

176.8126 1.013e0

176.8685 1.013e0

176.8898 1.013e0

176.9218 2.025e0

176.9537 1.013e0

176.9931 3.038e0

177.0175 1.013e0

177.0247 1.013e0

177.0555 6.076e0

177.0577 3.038e0

177.0647 2.025e0

177.0860 2.025e0

177.1140 6.202e1

177.1221 5.063e0

177.1341 6.076e0

177.1380 6.952e0

177.1662 1.013e0

177.1840 1.013e0

177.2205 2.025e0

177.2224 1.013e0

177.2291 1.013e0

177.2469 1.013e0

177.2577 1.013e0

177.2718 1.013e0

177.2791 2.025e0

177.3040 1.013e0

177.3359 1.013e0

177.3538 1.013e0

177.4487 1.013e0

177.4736 1.013e0

177.4881 2.025e0

177.5237 1.013e0

177.5450 1.013e0

177.5593 1.013e0

177.5660 1.013e0

177.5764 1.013e0

177.6722 1.013e0

177.6827 1.013e0

177.7148 1.013e0

177.7186 1.013e0

177.7238 2.025e0

177.7436 4.051e0

177.7645 1.013e0

177.8026 1.013e0

177.8277 1.013e0

177.8741 2.025e0

177.9522 1.013e0

177.9783 2.025e0

178.0175 2.025e0

178.0191 1.013e0

178.0387 3.038e0

178.0423 3.038e0

178.0621 1.013e0

178.0655 2.025e0

178.1002 6.076e0

178.1014 1.013e0

178.1128 8.101e0

178.1153 1.316e1

178.1211 2.025e0

178.1227 2.025e0

178.1422 2.025e0

178.1475 2.025e0

178.1543 2.025e0

178.1647 1.013e0

178.1754 1.013e0

178.1858 1.013e0

178.1998 1.013e0

178.2179 1.013e0

178.2249 1.013e0

178.2820 1.013e0

178.2963 1.013e0

178.3144 1.013e0

178.3600 1.013e0

178.3949 1.013e0

178.4274 1.013e0

178.5309 2.025e0

178.5501 2.025e0

178.5627 1.013e0

178.5729 1.013e0

178.6080 1.013e0

178.6190 1.013e0

178.6369 1.013e0

178.6474 1.013e0

178.6655 2.025e0

178.6689 1.013e0

178.6833 1.013e0

178.6867 2.025e0

178.7404 1.013e0

178.7480 2.025e0

178.7618 3.038e0

178.8070 1.013e0

178.9926 1.013e0

178.9946 6.076e0

179.0143 1.519e1

179.0154 7.089e0

179.0171 1.418e1

179.0454 1.013e0

179.0596 1.013e0

179.0667 1.013e0

179.0795 2.025e0

179.0813 2.025e0

179.1077 7.529e0

179.1094 1.608e1

179.1117 2.025e0

179.1327 3.610e0

179.1474 2.025e0

179.1849 1.013e0

179.1870 2.025e0

179.2167 1.013e0

179.2183 2.025e0

179.2377 1.013e0

179.3018 1.013e0

179.3195 2.025e0

179.3269 1.013e0

179.3481 1.013e0

179.3731 1.013e0

179.3841 1.013e0

179.4548 1.013e0

179.4620 1.013e0

179.4901 1.013e0

179.5222 1.013e0

179.5366 1.013e0

179.5404 1.013e0

179.5598 2.025e0

179.5869 1.013e0

179.6084 1.013e0

179.6189 1.013e0

179.6299 1.013e0

179.6547 1.013e0

179.6655 1.013e0

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179.7681 1.013e0

179.7752 1.013e0

179.8077 1.013e0

179.8148 2.025e0

179.9097 2.025e0

179.9392 2.025e0

179.9500 1.013e0

179.9676 1.013e0

179.9902 3.038e0

180.0143 3.038e0

180.0187 3.038e0

180.0203 4.051e0

180.0257 6.076e0

180.0312 3.038e0

180.0429 3.038e0

180.0501 2.025e0

180.0534 1.013e0

180.0716 1.013e0

180.0749 1.013e0

180.0847 3.038e0

180.1065 4.051e0

180.1288 1.013e0

180.1361 7.227e0

180.1547 3.038e0

180.1645 1.013e0

180.1748 1.013e0

180.1960 1.013e0

180.2064 4.079e0

180.2241 1.013e0

180.2387 1.013e0

180.2566 2.025e0

180.2995 1.013e0

180.3246 1.013e0

180.3392 1.013e0

180.3605 1.013e0

180.3967 1.013e0

180.4037 1.013e0

180.4494 1.013e0

180.4814 1.013e0

180.5423 2.025e0

180.5458 1.013e0

180.5639 1.013e0

180.5906 2.025e0

180.6177 1.013e0

180.6283 1.013e0

180.6411 2.025e0

180.6535 1.013e0

180.6929 1.013e0

180.7527 2.025e0

180.7705 1.013e0

180.8031 2.025e0

180.8173 1.013e0

180.8388 1.013e0

180.8783 1.013e0

180.8854 2.025e0

180.9144 1.013e0

180.9821 1.013e0

180.9856 2.025e0

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181.0853 1.013e0

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181.1158 2.025e0

181.1286 1.013e0

181.1573 1.013e0

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181.1661 3.038e0

181.1715 2.025e0

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181.1969 1.013e0

181.2825 1.013e0

181.2862 1.013e0

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181.3178 1.013e0

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181.3788 1.013e0

181.4526 2.025e0

181.4867 1.013e0

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181.7045 1.013e0

181.7192 1.013e0

181.7369 1.013e0

181.7408 1.013e0

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181.9412 2.025e0

181.9646 2.025e0

181.9803 1.013e0

181.9948 2.025e0

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182.0487 1.013e0

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182.1244 2.025e0

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182.1551 2.025e0

182.1767 2.025e0

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182.1893 1.013e0

182.2074 1.013e0

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182.2681 1.013e0

182.2749 1.013e0

182.2963 1.013e0

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182.3391 1.013e0

182.3822 1.013e0

182.4020 2.025e0

182.4725 2.025e0

182.4831 1.013e0

182.5155 1.013e0

182.5374 1.013e0

182.5390 2.025e0

182.5663 1.740e1

182.5692 9.114e0

182.5715 1.898e1

182.6253 2.025e0

182.6376 1.013e0

182.6447 1.013e0

182.6981 1.013e0

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182.7231 1.013e0

182.7306 1.013e0

182.7412 1.013e0

182.7737 1.013e0

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182.8064 1.013e0

182.8350 1.013e0

182.8604 1.013e0

182.8638 2.025e0

182.8676 1.013e0

182.8962 1.013e0

182.9251 1.013e0

182.9649 2.025e0

182.9847 3.051e1

182.9906 3.051e1

182.9926 2.037e1

182.9948 1.397e1

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183.0669 2.025e0

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183.1775 3.038e0

183.2088 1.013e0

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184.1562 1.013e0

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184.7590 1.013e0

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184.7807 2.025e0

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184.8278 1.013e0

184.8640 1.013e0

184.9434 1.013e0

184.9747 5.480e0

184.9796 1.013e0

184.9832 5.063e0

184.9941 2.025e0

184.9970 6.076e0

185.0087 2.025e0

185.0342 3.038e0

185.0376 1.013e0

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185.1030 2.025e0

185.1120 3.038e0

185.1192 3.038e0

185.1302 2.025e0

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185.1717 1.013e0

185.2149 1.013e0

185.2260 1.013e0

185.2437 1.013e0

185.2529 4.051e0

185.2563 2.025e0

185.3266 1.013e0

185.3518 2.025e0

185.3914 1.013e0

185.4025 1.013e0

185.4313 1.013e0

185.4693 2.025e0

185.4891 1.013e0

185.5145 1.013e0

185.5183 2.025e0

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185.7069 1.013e0

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185.9861 4.756e0

185.9897 1.013e0

186.0223 1.013e0

186.0335 1.013e0

186.0587 1.013e0

186.0732 1.013e0

186.1134 2.025e0

186.1243 1.013e0

186.1511 2.025e0

186.1569 1.013e0

186.1675 1.013e0

186.1856 1.013e0

186.1895 2.025e0

186.1931 1.013e0

186.2365 1.013e0

186.2654 1.013e0

186.3776 1.013e0

186.3918 1.013e0

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186.4483 2.025e0

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186.5113 1.013e0

186.5331 1.013e0

186.5693 1.013e0

186.5768 2.025e0

186.5876 1.013e0

186.6200 1.013e0

186.6999 1.013e0

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186.7763 1.013e0

186.8017 1.013e0

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186.8672 1.013e0

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186.9110 3.038e0

186.9509 2.025e0

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187.0927 1.013e0

187.1038 1.013e0

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187.1399 1.013e0

187.1547 2.025e0

187.1763 1.013e0

187.1909 1.013e0

187.2020 1.013e0

187.2782 1.013e0

187.3036 1.013e0

187.3075 1.013e0

187.3437 1.013e0

187.3730 1.013e0

187.4164 1.013e0

187.4565 1.013e0

187.5186 1.013e0

187.5256 1.013e0

187.5295 1.013e0

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187.6314 1.013e0

187.6749 1.013e0

187.6860 1.013e0

187.7261 1.013e0

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187.7698 1.013e0

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187.9227 1.013e0

187.9920 1.013e0

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188.0357 1.013e0

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188.0828 2.025e0

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188.1213 2.025e0

188.1257 5.465e0

188.1287 7.089e0

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188.6080 1.013e0

188.7538 1.013e0

188.7685 2.025e0

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189.4052 1.013e0

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189.4856 1.013e0

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189.5036 1.013e0

189.5475 1.013e0

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189.5770 4.051e0

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189.8219 1.013e0

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189.8803 2.025e0

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189.9751 1.013e0

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189.9864 1.013e0

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189.9972 1.013e0

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190.0340 1.013e0

190.0487 2.025e0

190.0637 2.025e0

190.0726 5.063e0

190.0761 5.063e0

190.0829 4.051e0

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190.1409 1.013e0

190.1464 2.025e0

190.1704 1.013e0

190.2072 1.013e0

190.2146 1.013e0

190.2330 1.013e0

190.2403 1.013e0

190.2951 2.025e0

190.3035 3.038e0

190.3498 1.013e0

190.3718 1.013e0

190.3830 2.025e0

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190.4376 1.013e0

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190.5075 1.013e0

190.5524 5.833e1

190.5545 2.835e1

190.5566 2.734e1

190.5924 3.038e0

190.6063 1.013e0

190.6427 1.013e0

190.6757 2.025e0

190.6868 2.025e0

190.6884 2.025e0

190.6941 2.025e0

190.7098 4.051e0

190.7195 2.025e0

190.7710 1.013e0

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190.8448 1.013e0

190.8524 2.025e0

190.8818 1.013e0

190.9133 2.025e0

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190.9337 1.013e0

190.9409 1.013e0

190.9742 1.013e0

190.9759 2.025e0

190.9822 3.038e0

190.9922 2.025e0

190.9949 3.038e0

190.9972 4.051e0

191.0270 2.025e0

191.0529 8.101e0

191.0547 5.063e0

191.0606 7.089e0

191.0676 4.051e0

191.1022 2.025e0

191.1170 1.013e0

191.1277 5.063e0

191.1295 7.659e0

191.1426 4.051e0

191.1500 3.038e0

191.1589 2.025e0

191.1665 2.025e0

191.1687 4.051e0

191.1791 1.013e0

191.2011 1.013e0

191.2160 1.013e0

191.2341 1.013e0

191.2380 1.013e0

191.2450 1.013e0

191.2489 2.025e0

191.2634 1.013e0

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278.0438 3.648e0

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