

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

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

Elements Used:

C: 20-20 H: 0-200 N: 0-10 O: 0-15 Na: 0-1 S: 1-1

Minimum: -1.5

Maximum: 5.0 10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

340.1374 340.1371 0.3 0.9 10.5 880.7 0.0 C20 H22 N O2 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.

148.2444 2.025e0

148.2462 2.025e0

148.2493 2.025e0

148.2505 1.505e0

148.2677 1.013e0

148.2710 3.038e0

148.2797 2.025e0

148.2832 3.038e0

148.2866 1.013e0

148.2998 1.013e0

148.3015 2.025e0

148.3146 2.025e0

148.3204 2.025e0

148.3221 1.013e0

148.3253 2.025e0

148.3452 1.013e0

148.3504 2.025e0

148.3641 1.013e0

148.3708 2.025e0

148.3861 4.051e0

148.3872 2.025e0

148.3940 2.025e0

148.4000 1.013e0

148.4094 1.013e0

148.4227 1.013e0

148.4245 2.025e0

148.4262 1.013e0

148.4388 1.013e0

148.4418 1.013e0

148.4551 1.013e0

148.4716 2.025e0

148.4756 4.051e0

148.4840 2.025e0

148.4971 2.025e0

148.5088 2.025e0

148.5205 4.051e0

148.5287 5.063e0

148.5360 6.076e0

148.5459 1.013e0

148.5495 3.038e0

148.5560 1.013e0

148.5619 2.025e0

148.5675 4.051e0

148.5747 1.013e0

148.5848 1.013e0

148.5978 2.025e0

148.6040 4.051e0

148.6050 4.051e0

148.6268 2.025e0

148.6319 2.025e0

148.6429 2.025e0

148.6555 1.539e0

148.6573 5.063e0

148.6623 2.025e0

148.6658 2.025e0

148.6742 2.025e0

148.6788 1.013e0

148.6799 4.051e0

148.6849 1.013e0

148.6913 1.013e0

148.6980 2.025e0

148.7096 2.025e0

148.7179 1.013e0

148.7209 1.013e0

148.7224 2.025e0

148.7361 4.051e0

148.7434 2.025e0

148.7567 1.013e0

148.7600 3.038e0

148.7757 1.013e0

148.7789 2.025e0

148.7821 1.013e0

148.7934 4.051e0

148.7954 2.025e0

148.8112 1.013e0

148.8143 2.025e0

148.8162 2.025e0

148.8311 2.025e0

148.8357 7.089e0

148.8502 2.025e0

148.8532 2.025e0

148.8600 1.013e0

148.8633 2.025e0

148.8731 3.038e0

148.8818 2.025e0

148.8834 4.051e0

148.8953 1.013e0

148.9020 1.013e0

148.9055 1.013e0

148.9255 3.038e0

148.9313 2.025e0

148.9356 2.025e0

148.9375 3.038e0

148.9444 3.038e0

148.9628 2.025e0

148.9706 3.038e0

148.9783 2.025e0

148.9813 2.025e0

148.9882 2.025e0

148.9899 2.025e0

148.9932 1.013e0

148.9998 1.013e0

149.0048 2.025e0

149.0253 3.886e0

149.0287 2.188e0

149.0304 2.025e0

149.0443 5.146e0

149.0533 1.185e0

149.0561 1.688e0

149.0624 3.509e0

149.0930 2.823e0

149.1223 1.654e0

149.1249 3.166e0

149.1380 3.038e0

149.1601 2.025e0

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149.1782 3.038e0

149.1810 2.025e0

149.1874 1.013e0

149.1943 2.025e0

149.1990 2.025e0

149.2092 2.025e0

149.2231 1.013e0

149.2262 1.013e0

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149.2390 4.051e0

149.2429 4.051e0

149.2464 2.025e0

149.2481 2.025e0

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149.2785 1.013e0

149.2820 2.025e0

149.2953 1.013e0

149.2986 2.025e0

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149.3307 3.038e0

149.3349 4.051e0

149.3499 1.013e0

149.3545 2.025e0

149.3663 1.013e0

149.3741 3.038e0

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149.3799 2.025e0

149.3889 2.025e0

149.3952 1.013e0

149.3987 1.013e0

149.4085 1.013e0

149.4153 4.051e0

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149.6653 1.013e0

149.6688 1.013e0

149.6722 1.013e0

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149.7334 1.013e0

149.7399 1.013e0

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149.8985 4.051e0

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149.9109 2.025e0

149.9209 2.025e0

149.9225 2.025e0

149.9293 2.025e0

149.9414 3.038e0

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149.9580 1.013e0

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150.0071 2.025e0

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150.0506 2.767e1

150.0553 1.917e1

150.0631 6.568e0

150.0656 3.957e0

150.1115 4.398e1

150.1133 1.996e2

150.1149 1.314e2

150.1647 2.025e0

150.1700 3.834e0

150.1723 1.769e0

150.1764 1.887e0

150.1829 1.013e0

150.1972 4.051e0

150.1985 1.013e0

150.1996 6.076e0

150.2035 4.051e0

150.2052 1.013e0

150.2187 1.013e0

150.2288 1.013e0

150.2363 2.025e0

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150.5183 1.013e0

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150.9344 2.025e0

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151.2452 5.758e0

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151.6573 3.038e0

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151.9884 3.038e0

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152.0667 2.620e1

152.0681 2.690e1

152.0709 1.948e1

152.0997 4.307e0

152.1071 2.222e0

152.1085 1.910e0

152.1104 1.660e0

152.1241 3.133e0

152.1267 2.025e0

152.1336 3.501e0

152.1346 4.345e0

152.1479 5.063e0

152.1623 3.602e0

152.1661 6.390e0

152.1695 2.025e0

152.1743 2.025e0

152.1953 3.038e0

152.2004 5.063e0

152.2029 3.038e0

152.2077 3.038e0

152.2119 3.038e0

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152.2221 2.025e0

152.2284 3.038e0

152.2397 2.025e0

152.2443 2.025e0

152.2529 5.584e0

152.2574 5.382e0

152.2614 3.647e0

152.2738 3.038e0

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152.3020 2.025e0

152.3105 5.063e0

152.3156 2.025e0

152.3187 2.025e0

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152.6090 1.013e0

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152.6198 4.051e0

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152.6254 2.025e0

152.6290 5.063e0

152.6493 6.072e0

152.6522 2.025e0

152.6532 4.051e0

152.6661 3.042e0

152.6675 4.051e0

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152.6745 4.254e0

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152.9361 2.025e0

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152.9572 2.025e0

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152.9648 3.038e0

152.9706 2.025e0

152.9740 1.013e0

152.9863 7.089e0

152.9899 1.013e0

152.9960 3.038e0

153.0054 7.089e0

153.0092 2.348e0

153.0150 1.845e0

153.0259 2.273e0

153.0431 1.994e1

153.0443 1.172e2

153.0777 1.608e0

153.0911 4.563e0

153.0943 2.025e0

153.0969 1.798e0

153.1000 1.833e0

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153.1223 1.730e0

153.1240 4.822e0

153.1337 4.622e0

153.1350 6.652e0

153.1379 6.447e0

153.1416 1.019e1

153.1561 4.051e0

153.1581 2.589e0

153.1676 2.291e0

153.1714 2.025e0

153.1805 4.723e0

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