

Supplementary Information

Design and synthesis of novel triazole based small molecules mimicking HDACi as new modular drugs candidate against Omicron and future variants of Sars-Cov-2

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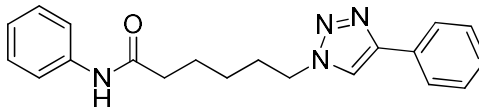
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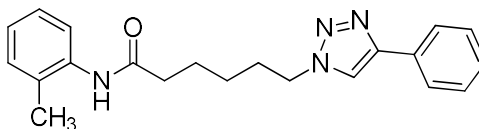
NMR Data

Compound 1c: *N*-phenyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)hexanamide



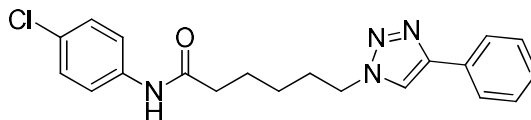
¹H NMR (400 MHz, (CD₃)₂SO), δ: 1.253-1.335 (m, 2H), 1.598-1.673 (m, 2H), 1.859-1.932 (m, 2H), 2.281-2.317 (t, 2H, *J* = 7.6 Hz), 4.390-4.425 (t, 2H, *J* = 7.2 Hz), 6.986-7.023 (d, 1H, *J* = 8 Hz), 7.241-7.280 (dd, 2H, *J* = 8 Hz), 7.304-7.344 (t, 1H, *J* = 8 Hz), 7.422-7.460 (dd, 2H), 7.554-7.576 (d, 2H, *J* = 8.76 Hz), 7.820-7.843 (d, 2H), 8.594 (s, 1H) and 9.869 (NH). ¹³C NMR (100 MHz, (CD₃)₂SO), δ: 24.96, 25.99, 29.95, 36.64, 49.84, 119.50, 121.80, 123.45, 125.58, 128.29, 129.15, 129.41, 131.37, 139.78, 146.75 and 171.56.

Compound 2c: 6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-(*o*-tolyl)hexanamide



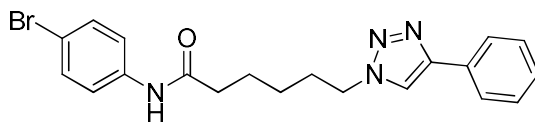
¹H NMR (400 MHz, (CD₃)₂SO), δ: 1.224-1.358 (m, 2H), 1.613-1.687 (m, 2H), 1.875-1.948 (m, 2H), 2.144(s, 3H), 2.307-2.344 (t, 2H, *J* = 7.6 Hz), 4.399-4.434 (t, 2H, *J* = 7.2 Hz), 7.027-7.045 (t, 1H, *J* = 8.76 Hz), 7.063 -7.087 (d, 1H, *J* = 8.7 Hz), 7.103 -7.124 (t, 2H, *J* = 8 Hz), 7.312 -7.348 (t, 2H), 7.830 -7.851 (d, 2H, *J* = 8.76 Hz), 8.597 (s, 1H) and 9.236 (NH). ¹³C NMR (100 MHz, (CD₃)₂SO), δ: 18.38, 25.22, 25.99, 29.94, 36.01, 49.90, 121.79, 125.59, 125.72, 126.34, 128.29, 129.40, 130.70, 131.38, 132.28, 136.90, 146.77 and 171.44.

Compound 3c: *N*-(4-chlorophenyl)-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)hexanamide



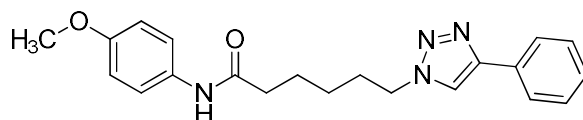
¹H NMR (400 MHz, (CD₃)₂SO), δ: 1.235-1.292 (m, 2H), 1.614-1.651 (m, 2H), 1.875-1.913(m, 2H), 2.285-2.336 (t, 2H, *J* = 7.6 Hz), 4.391-4.426 (t, 2H, *J* = 7.2 Hz), 7.331-7.350 (t, 1H, *J* = 8.76 Hz), 7.427 -7.465 (d, 4H), 7.536 -7.558 (d, 2H, *J* = 8 Hz), 7.820 -7.841 (d, 2H, *J* = 8.76Hz), 8.591 (s, 1H) and 10.014 (NH).

Compound 4c: *N*-(4-bromophenyl)-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)hexanamide

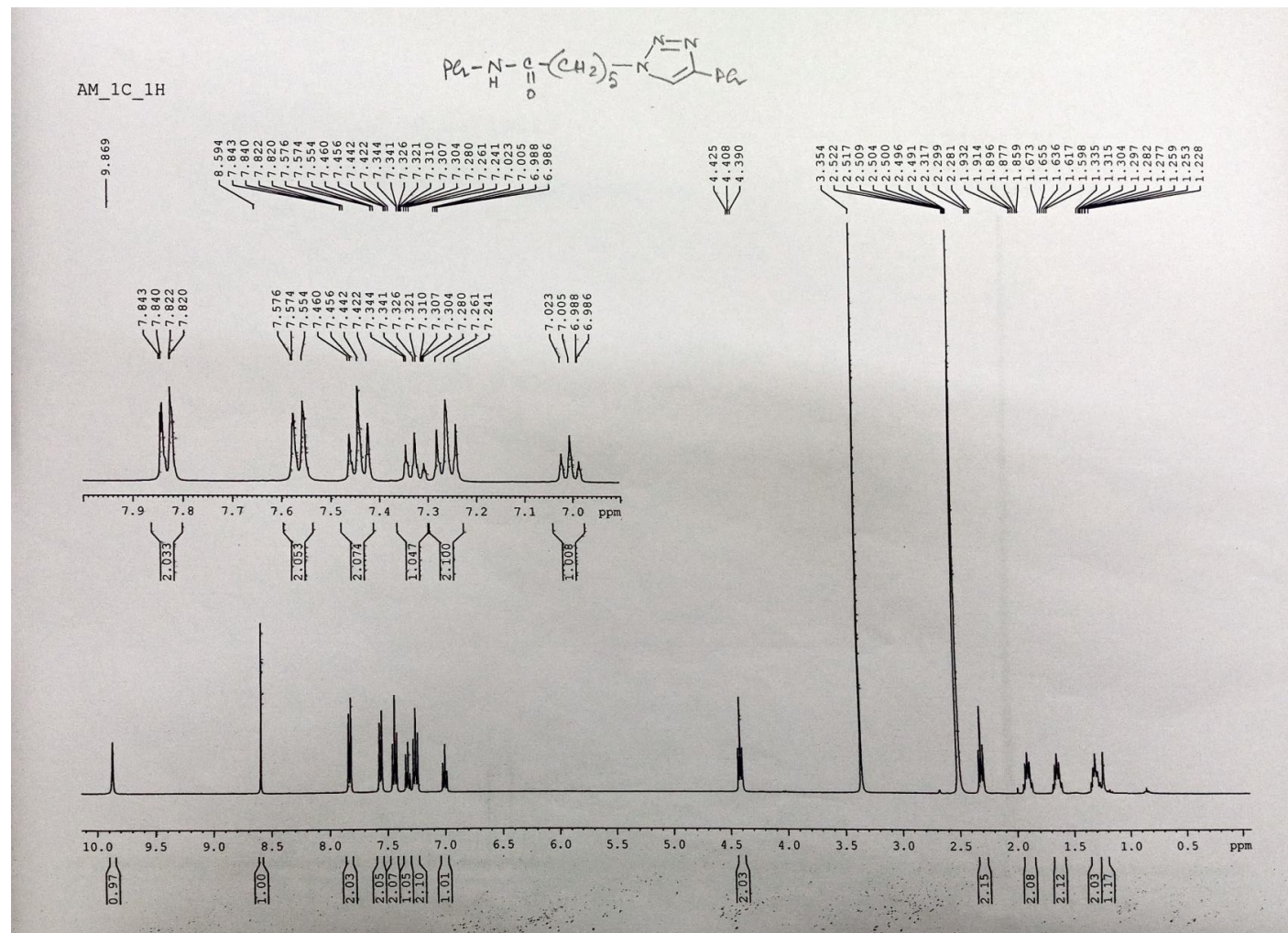


^1H NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$), δ : 1.226-1.329 (m, 2H), 1.594-1.669 (m, 2H), 1.855-1.928 (m, 2H), 2.284-2.321 (t, 2H, $J = 7.6$ Hz), 4.387-4.422 (t, 2H, $J = 7.2$ Hz), 7.304-7.344 (m, 3H, $J = 8.76$ Hz), 7.421 -7.459 (d, 2H, $J = 8.7$ Hz), 7.585-7.607 (d, 2H, $J = 8$ Hz), 7.817 - 7.836 (d, 2H, $J = 8.76$ Hz), 8.584 (s, 1H) and 10.010 (NH). ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$), δ : 24.87, 25.96, 29.93, 36.62, 49.83, 121.01, 121.79, 125.58, 126.95, 128.29, 129.06, 129.40, 131.35, 138.71, 146.74 and 171.73.

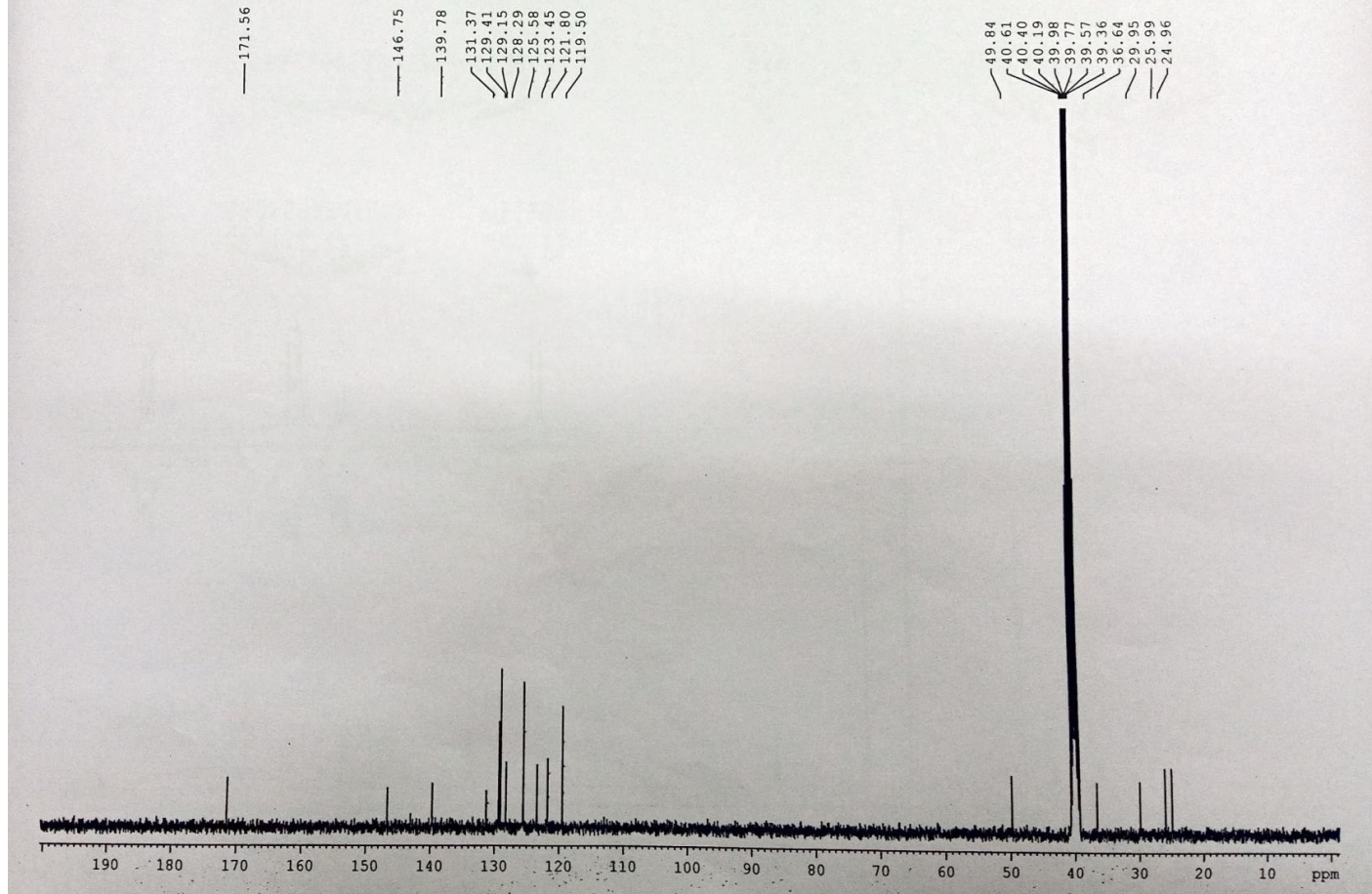
Compound 5c: *N*-(4-methoxyphenyl)-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)hexanamide



^1H NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$), δ : 1.227-1.287 (m, 2H), 1.606-1.644 (m, 2H), 1.872-1.909 (m, 2H), 2.240-2.277 (t, 2H, $J = 7.6$ Hz), 3.694 (s, 3H), 4.387-4.422 (t, 2H, $J = 7.2$ Hz), 6.817- 6.848 (d, 2H, $J = 8.76$ Hz), 7.308 -7.347 (m, 1H, $J = 8.7$ Hz), 7.422 -7.471 (m, 4H, $J = 8$ Hz), 7.821 -7.842 (d, 2H, $J = 8.76$ Hz), 8.588 (s, 1H) and 9.722 (NH). ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$), δ : 25.03, 25.98, 29.55, 36.49, 49.84, 55.60, 114.23, 121.07, 121.79, 125.58, 128.29, 129.41, 131.36, 132.94, 146.74, 155.46 and 171.02.

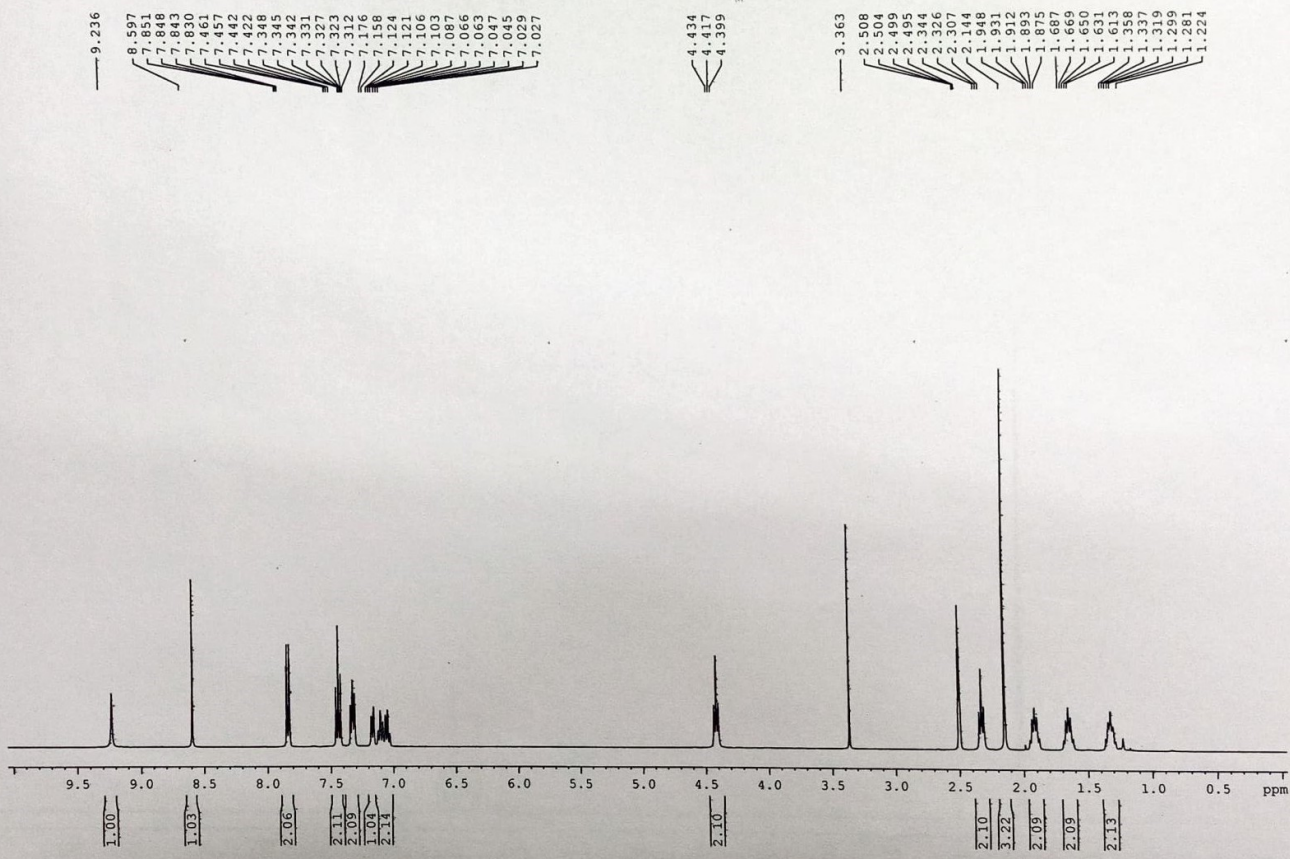
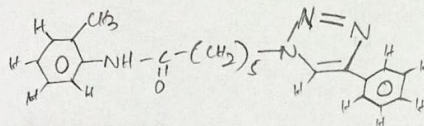


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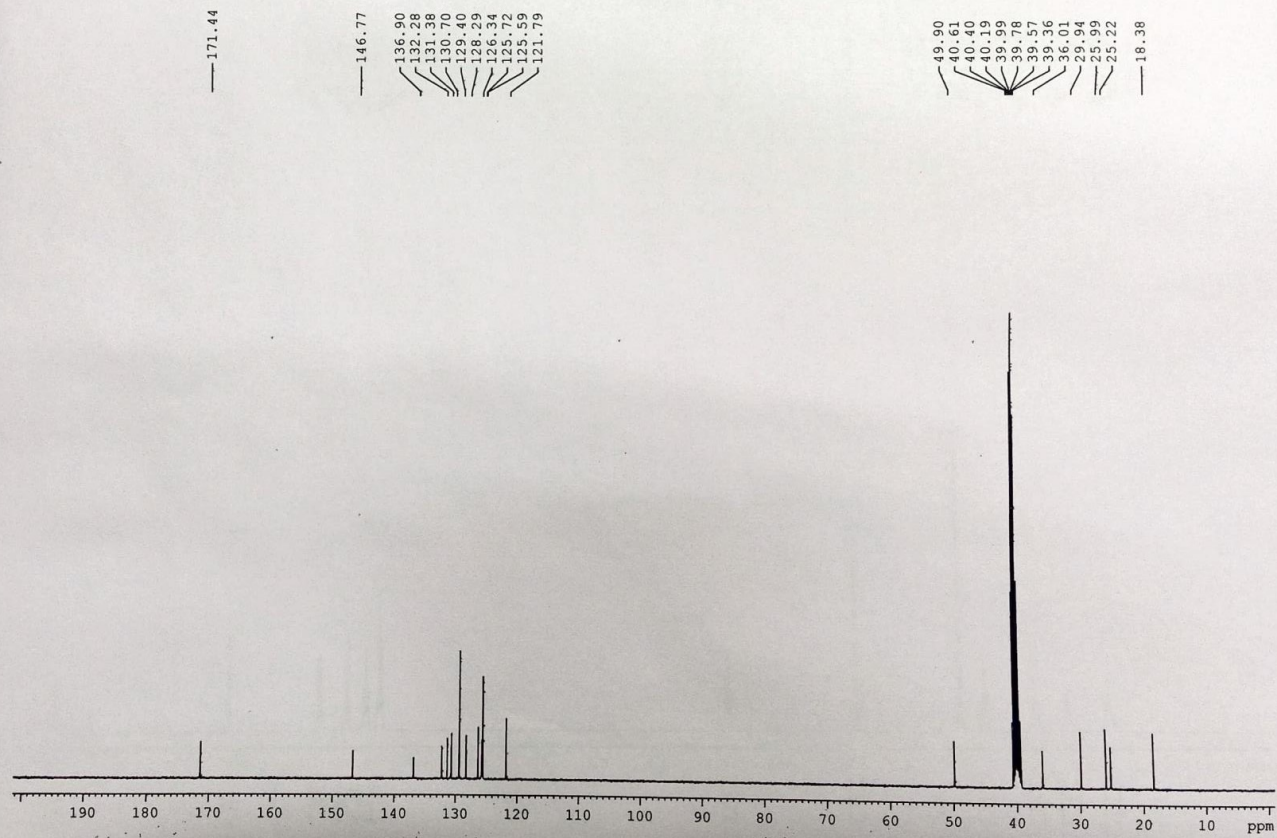


S5

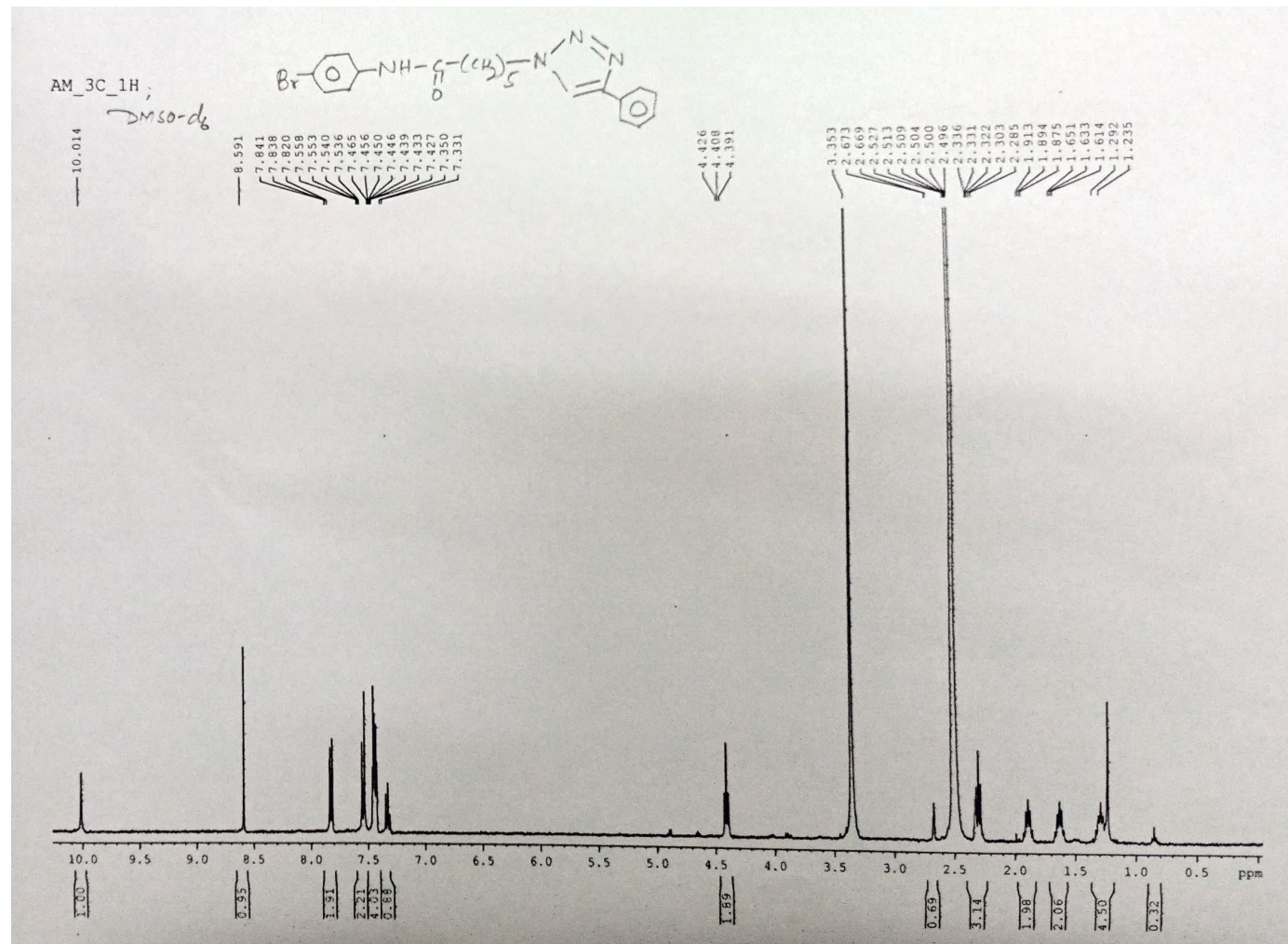
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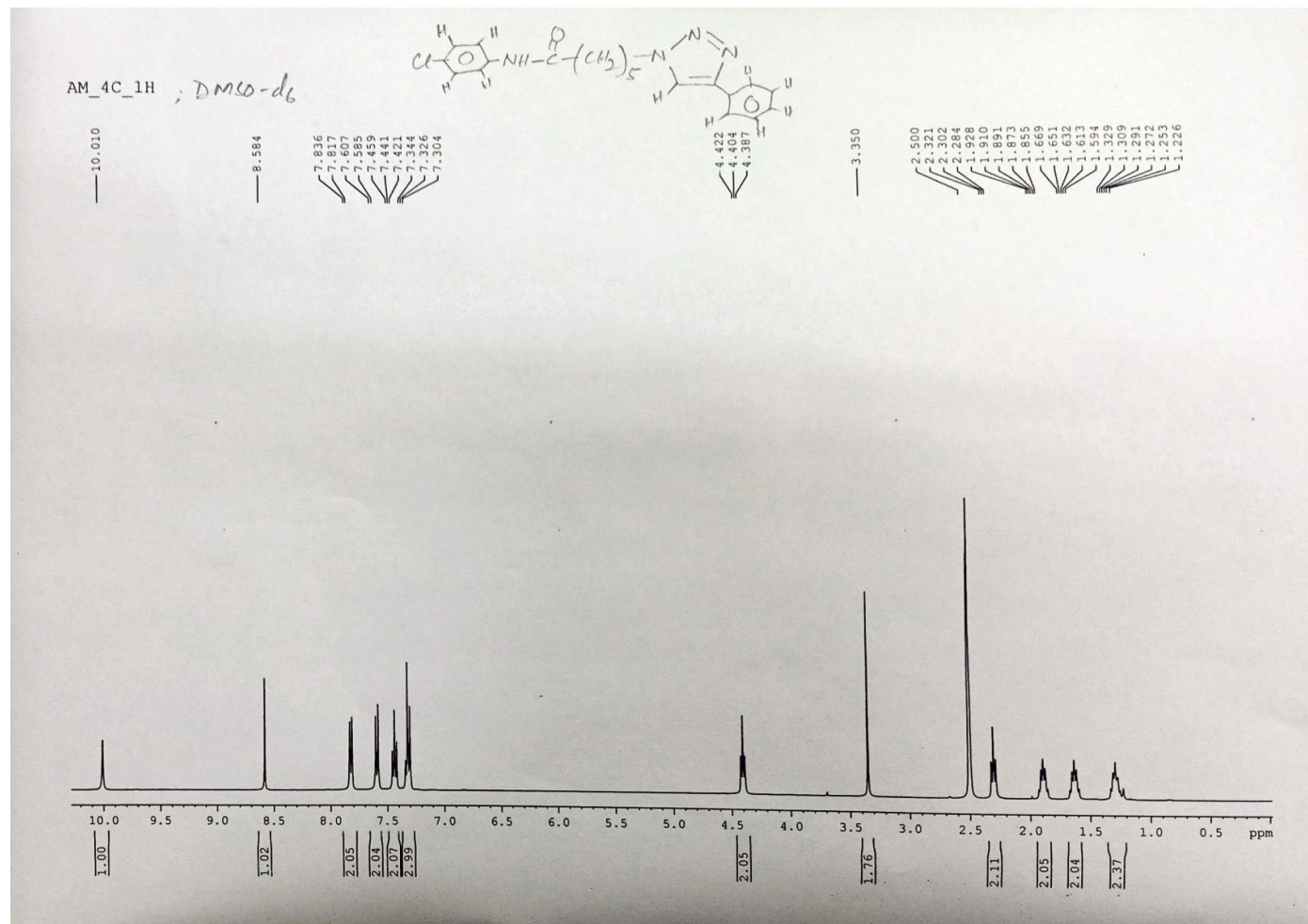


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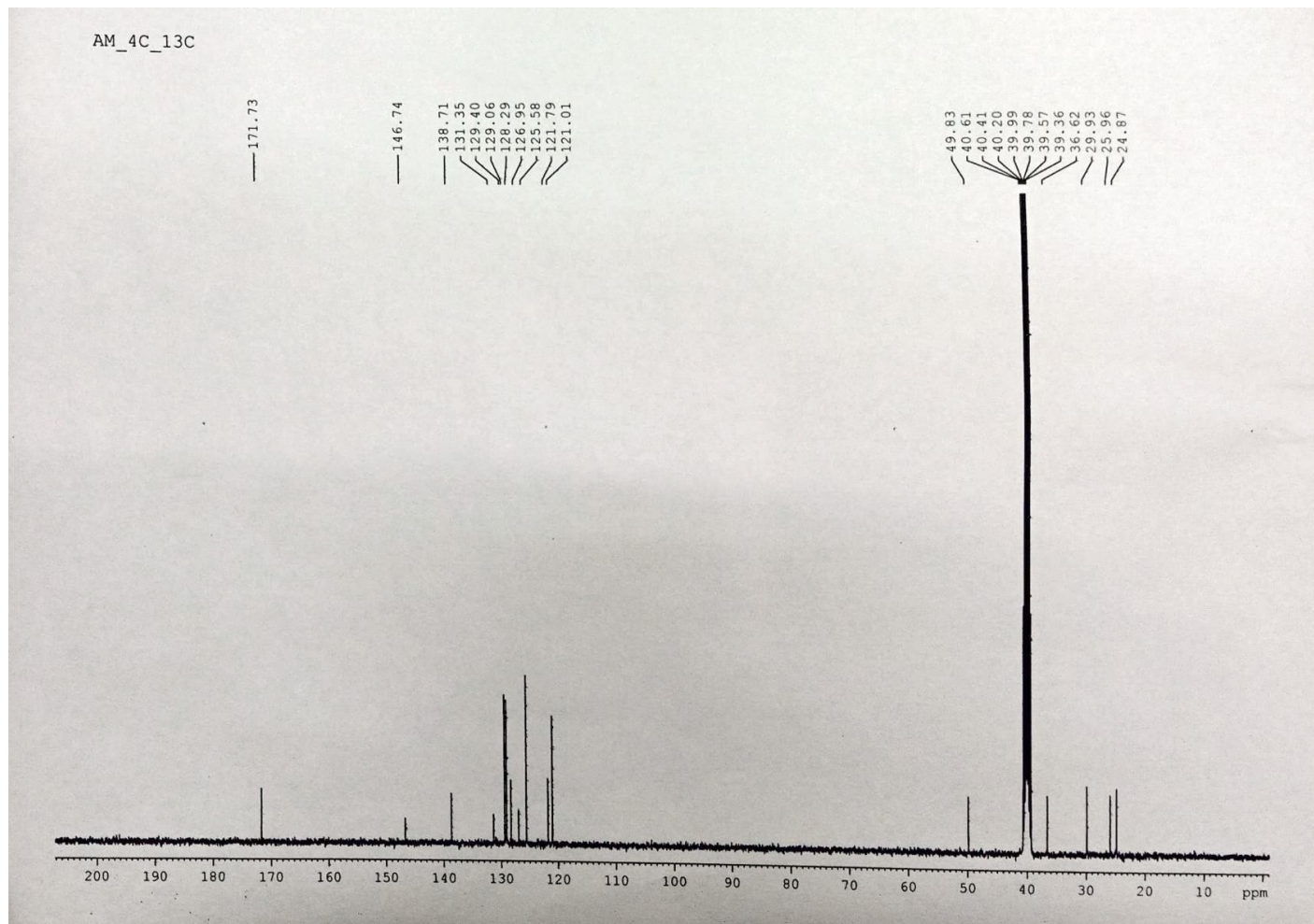


S7

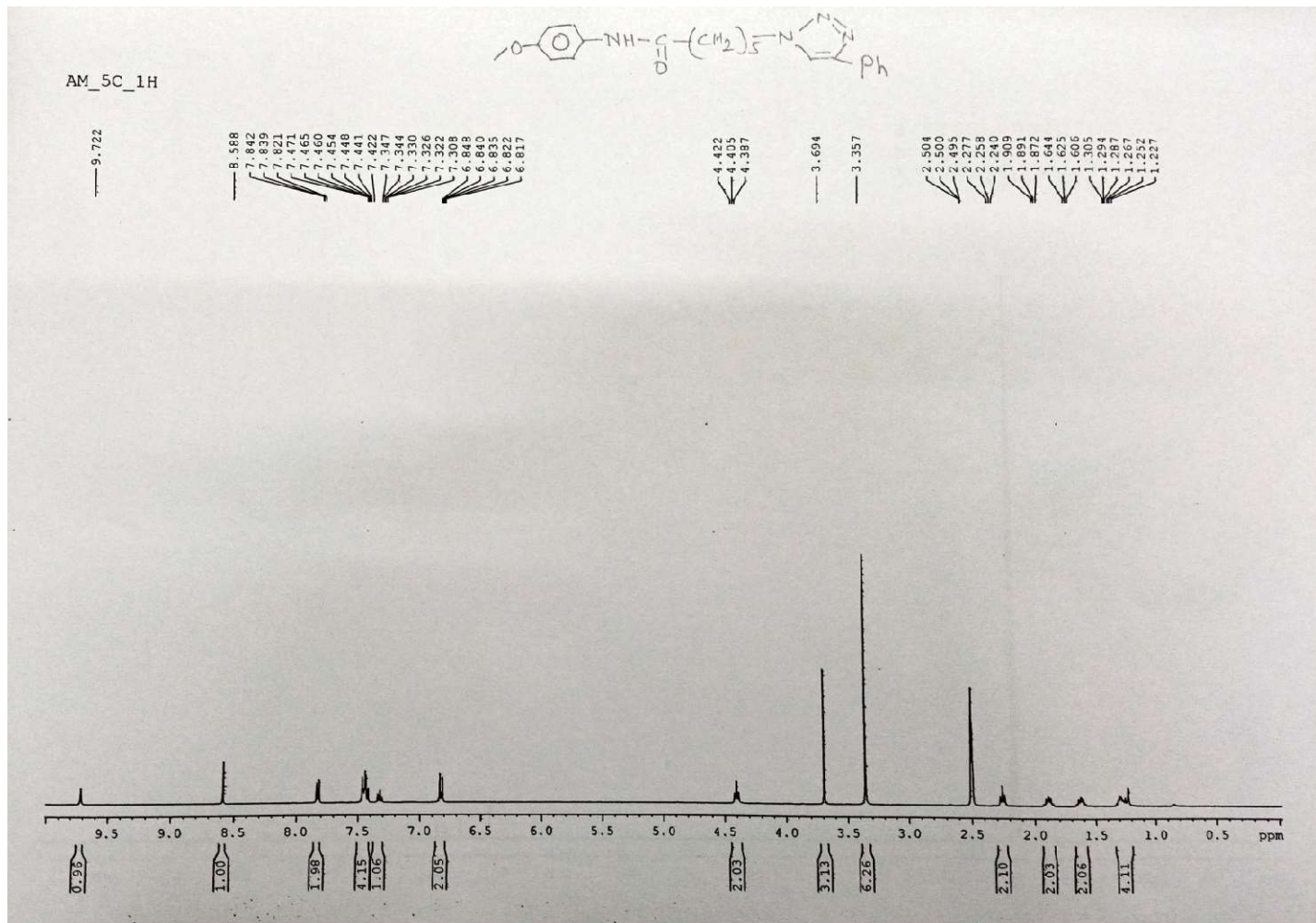




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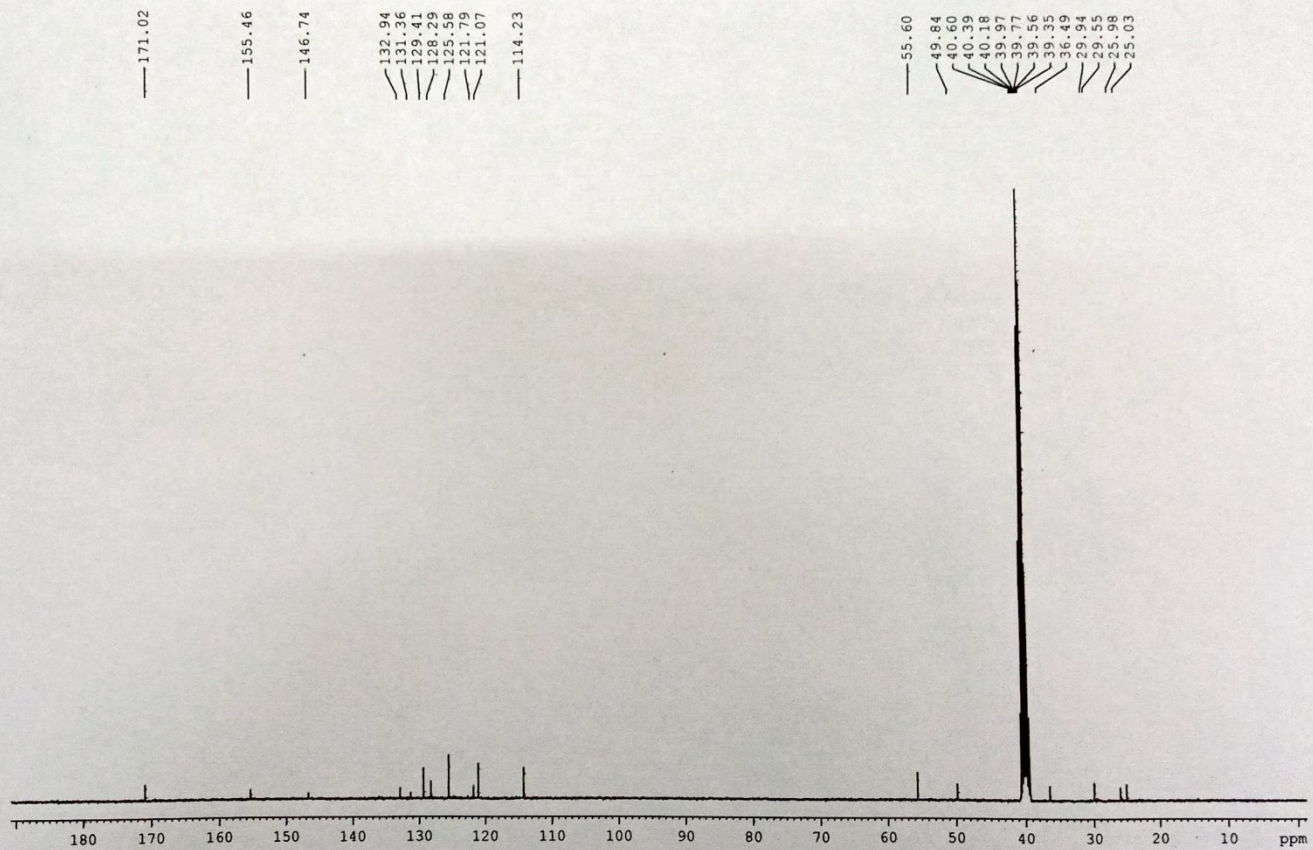


S10



S11

AM_5C_13C



S12