Supplementary Material

SeO_2-Mediated Ritter reaction of aryl methyl ketones catalyzed by boron trifluoride etherate at room temperature

Mugada Sugunakara Rao,*[a] Maheswara Rao Addepalli,[b] Majji Pavani,[a] and K. Koteswara Rao[c]

[a]Department of Chemistry, Vignan's Institute of Information Technology, Duvvada, Visakhapatnam, Andhra Pradesh 530049, India
[b]Department of Chemistry, Aditya Institute of Technology and Management, Tekkali, Andhra Pradesh 532201, India
[c]Chemistry Division, Department Basic Science & Humanities (BS&H), GMR Institute of Technology, Rajam, 532127, Andhra Pradesh, India
Email: sugunakararao.iitp@gmail.com

Table of Contents

2. Copies of NMR spectra data

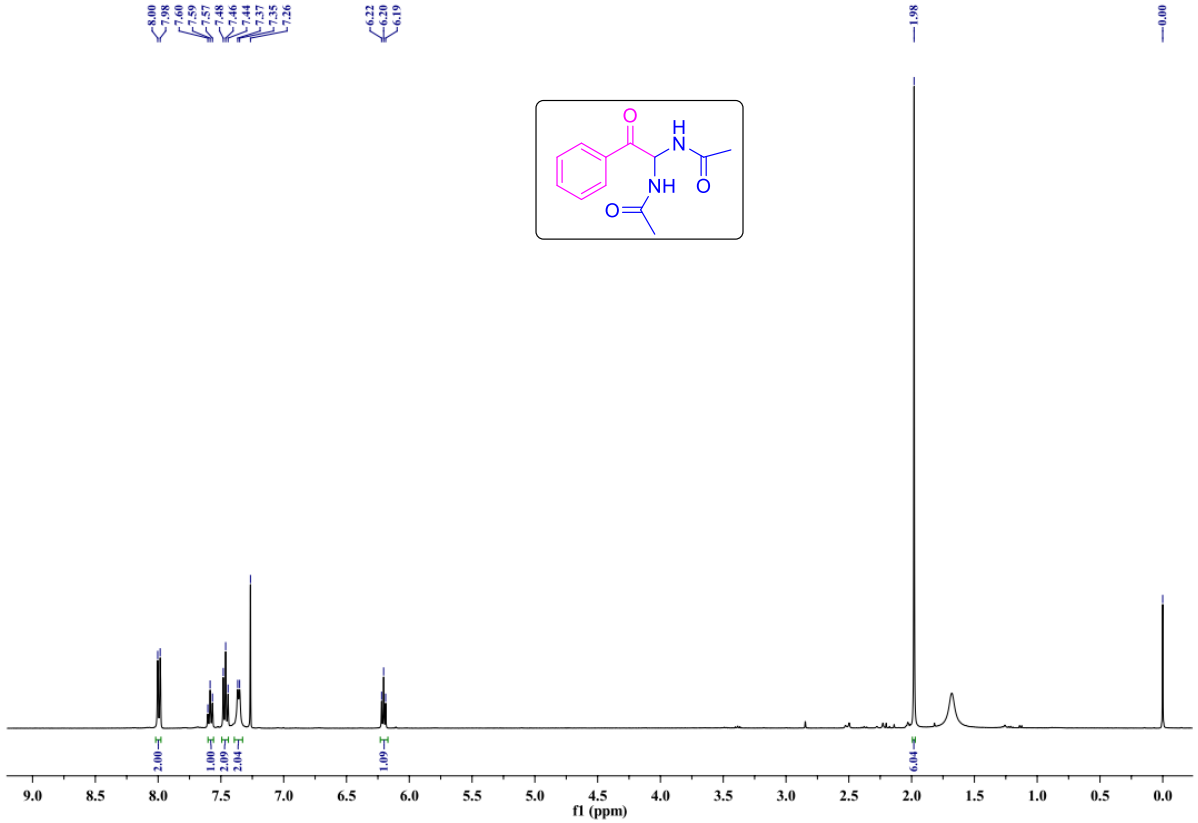

Figure S1. ^{1}H NMR spectrum of **2a**.

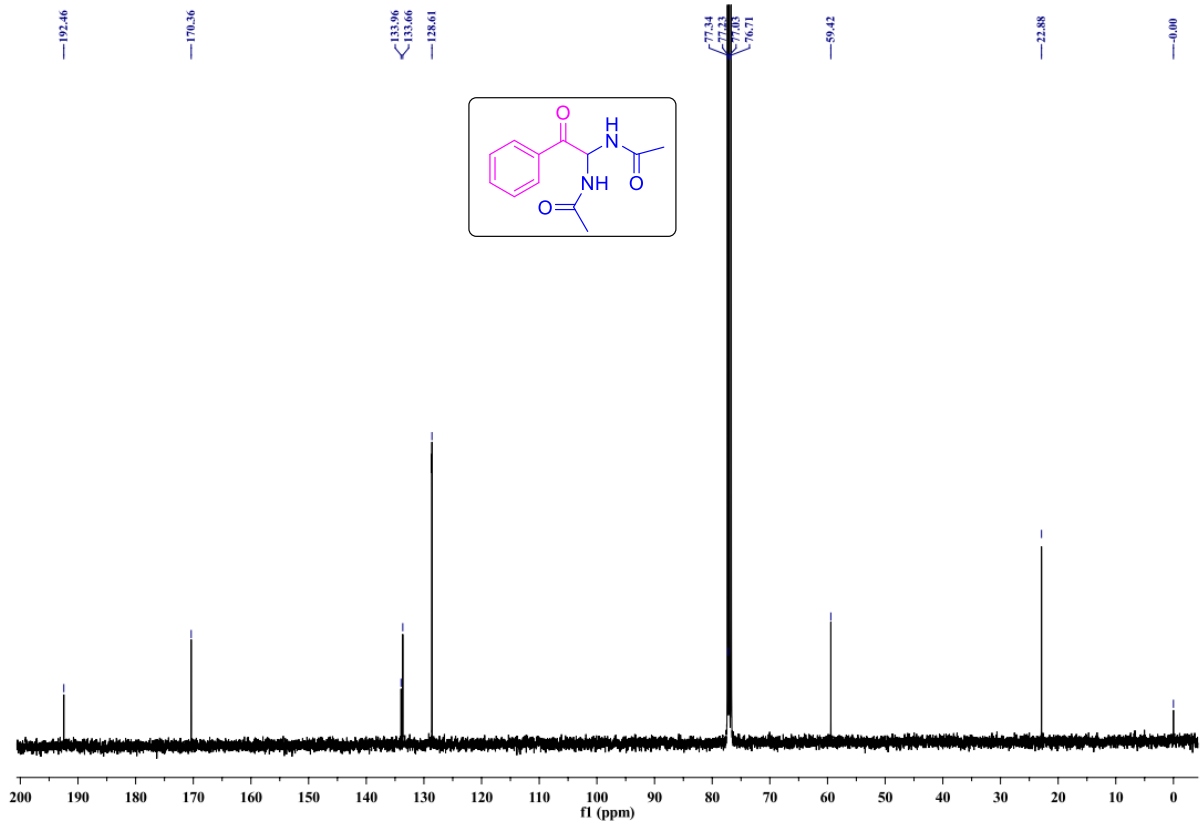

Figure S1. ^{13}C NMR spectrum of **2a**.

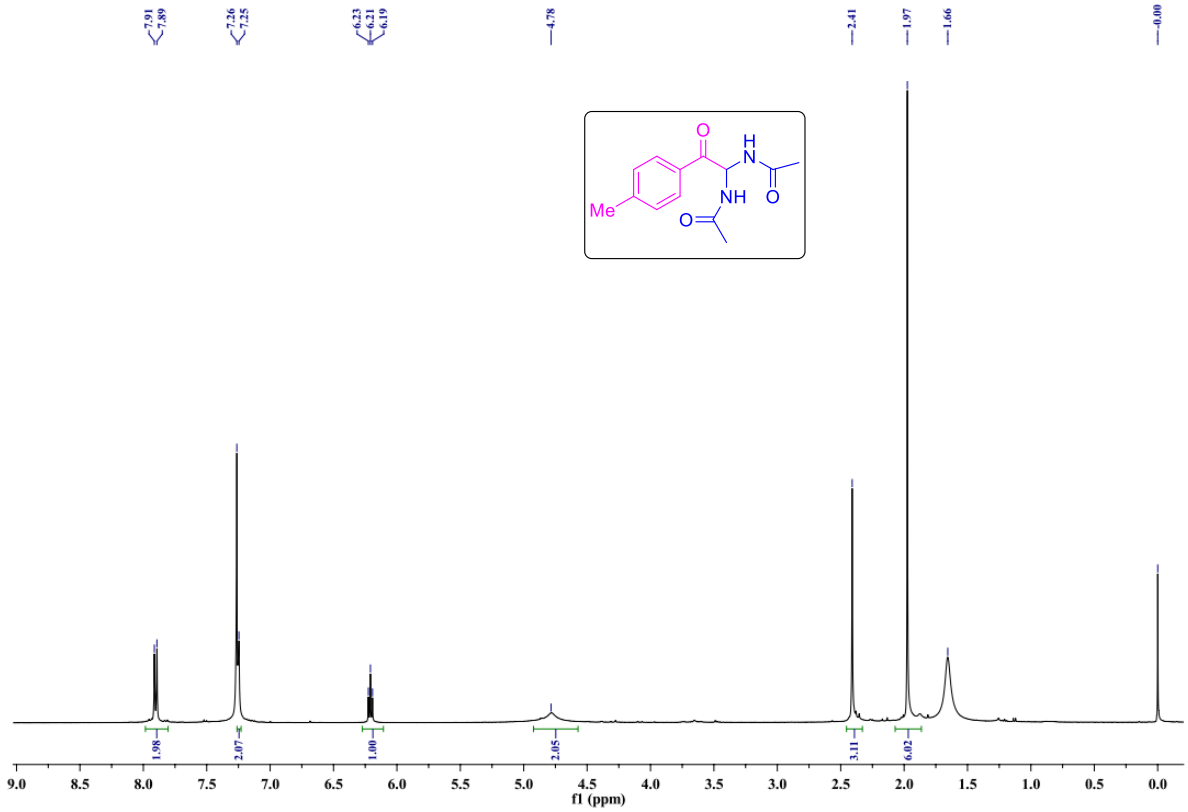

Figure S2. ^{1}H NMR spectrum of **2b**.

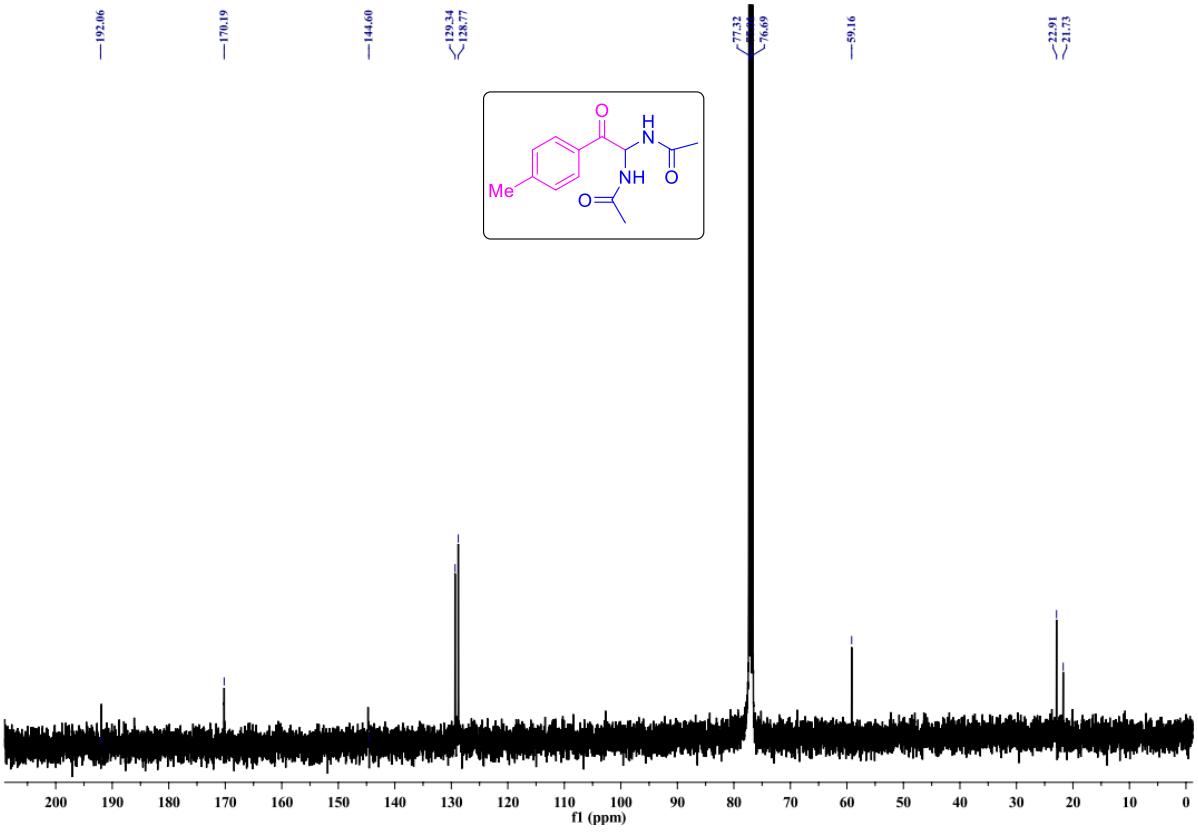

Figure S2. ^{13}C NMR spectrum of **2b**.

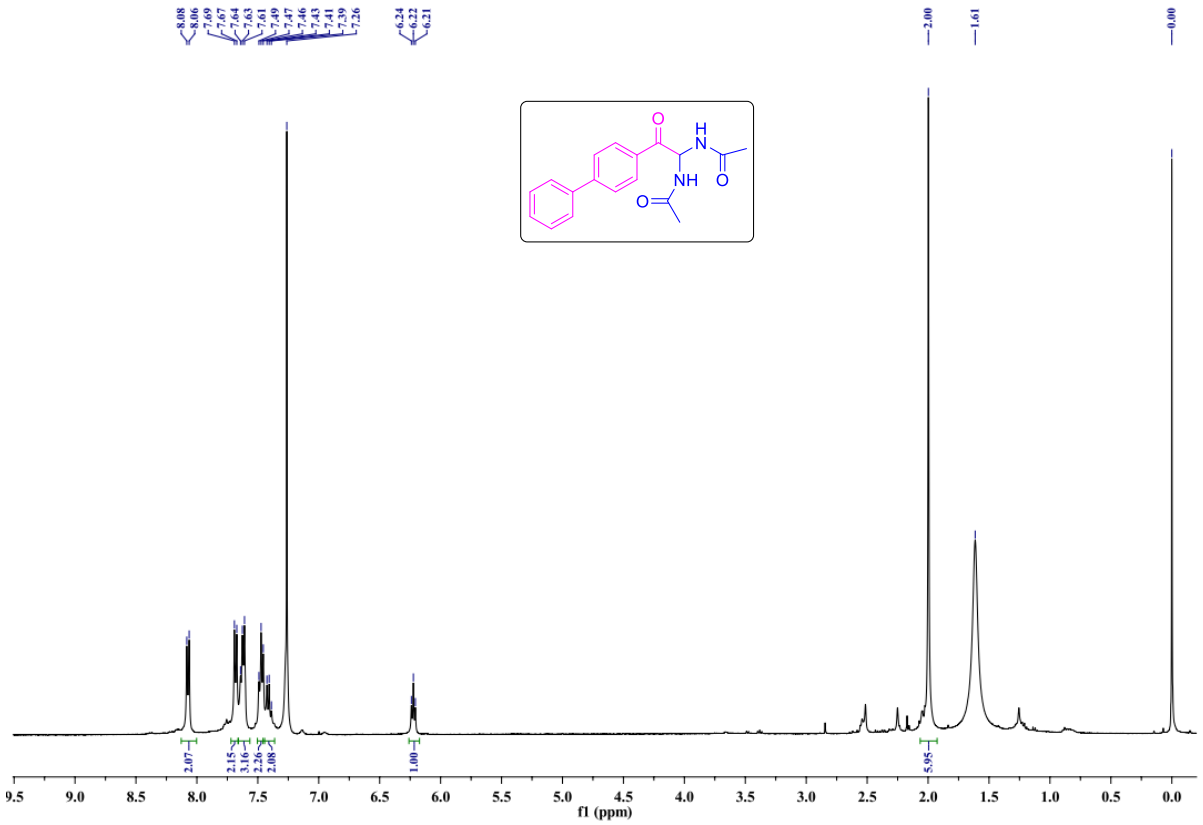

Figure S3. ^{1}H NMR spectrum of **2c**.

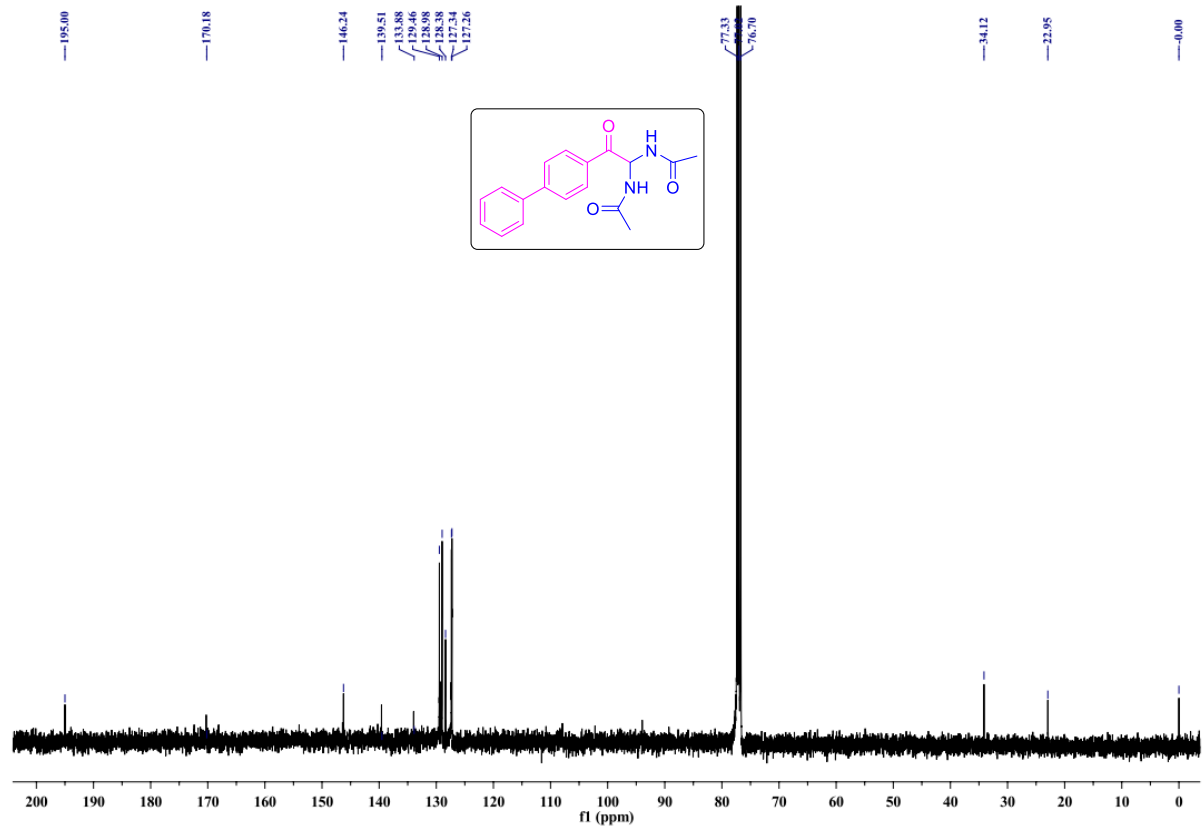

Figure S3. ^{13}C NMR spectrum of **2c**.

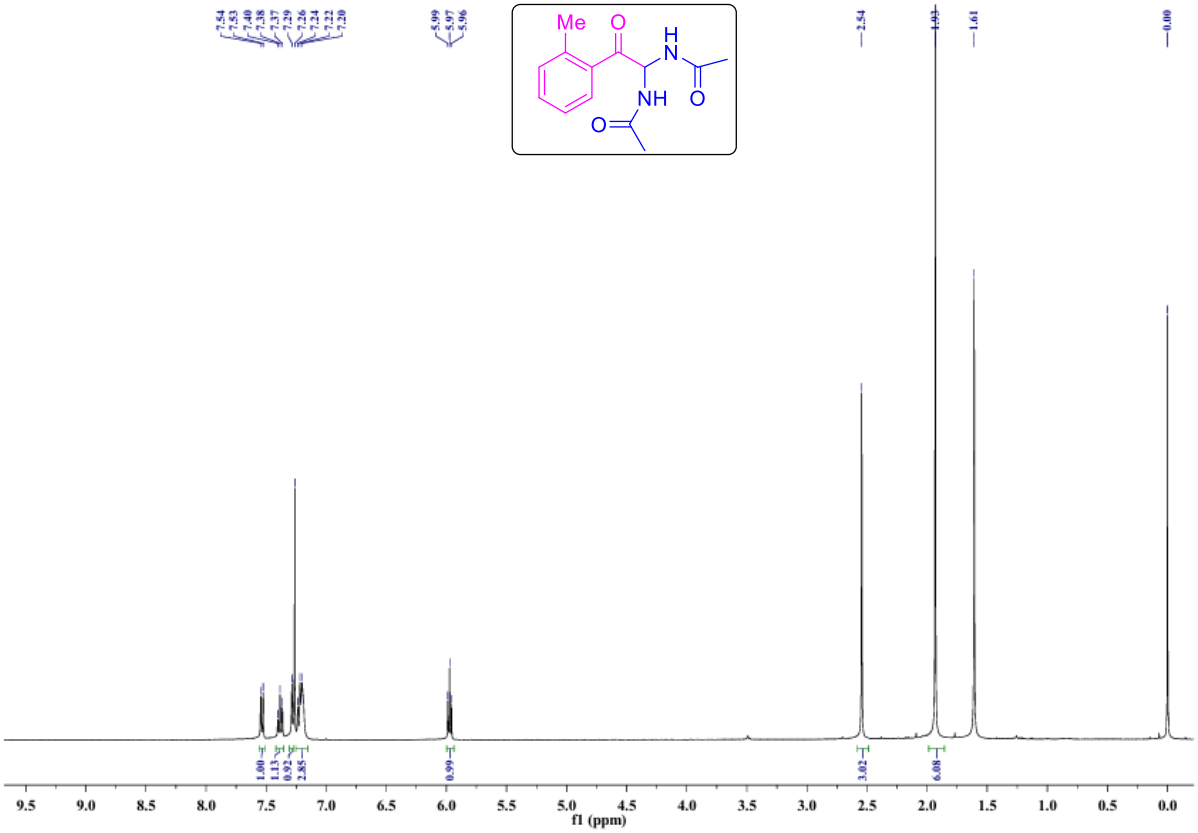

Figure S4. ^{1}H NMR spectrum of **2d**.

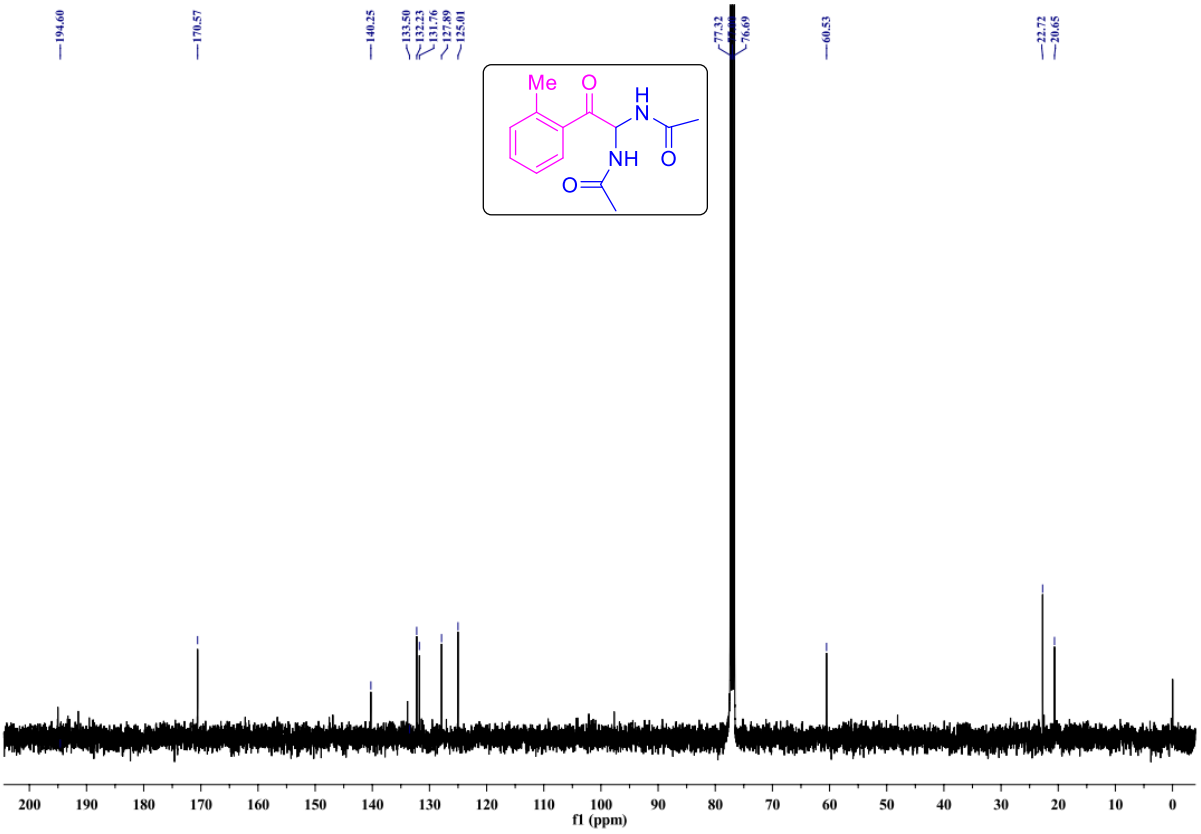

Figure S4. ^{13}C NMR spectrum of **2d**.

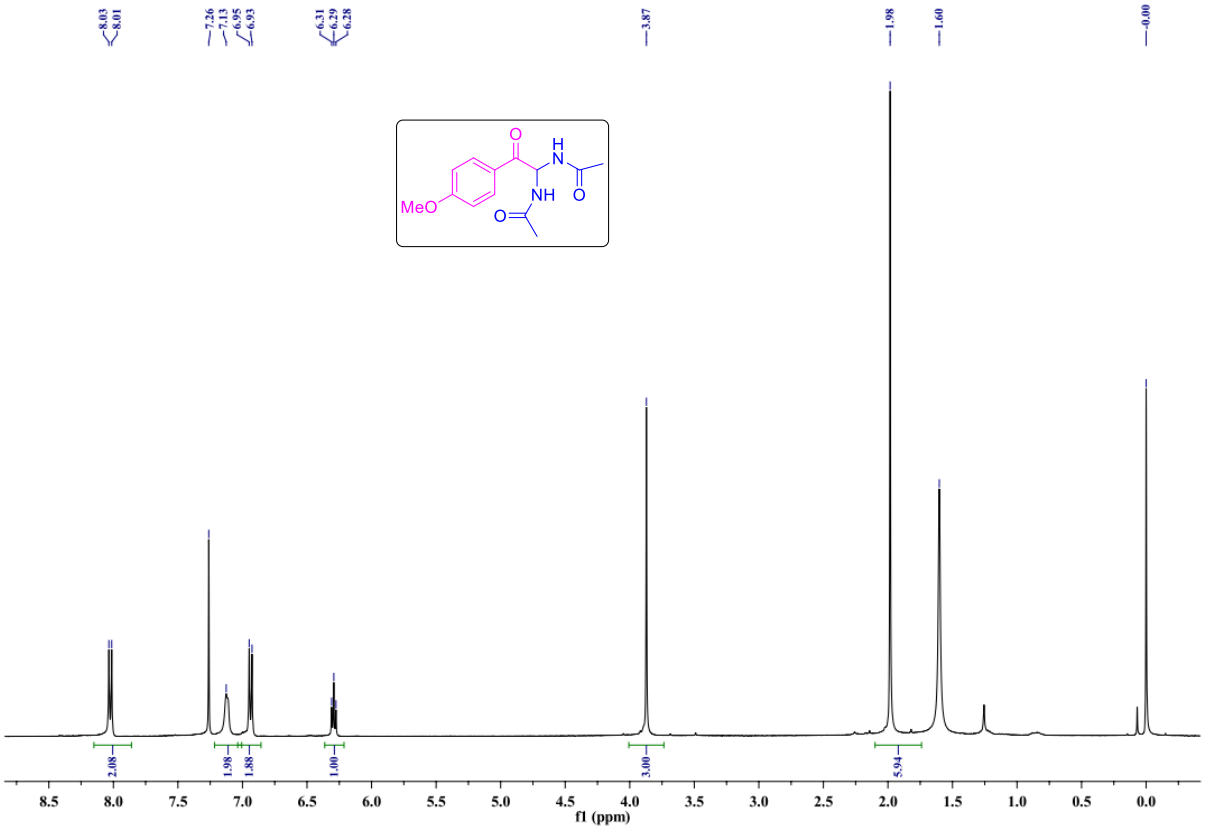

Figure S5. ^{1}H NMR spectrum of **2e**.

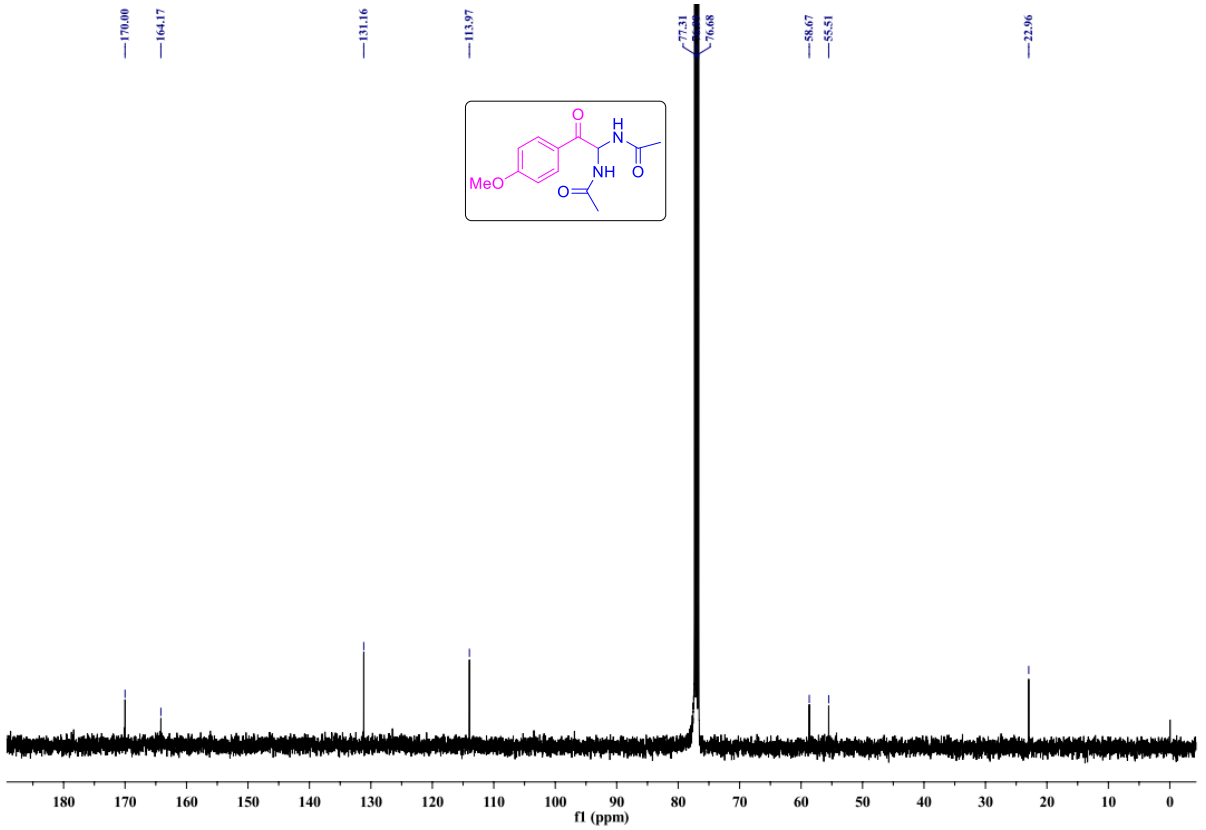

Figure S5. ^{13}C NMR spectrum of **2e**.

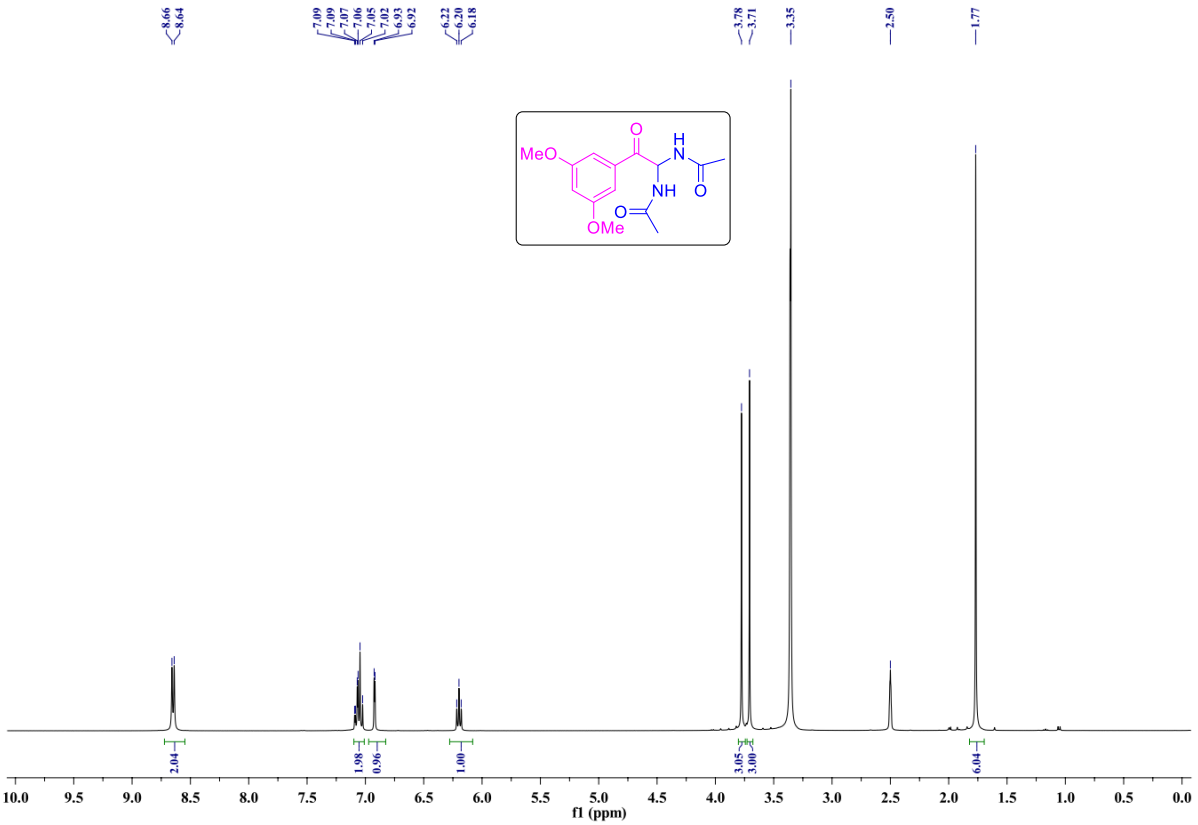

Figure S6. ^{1}H NMR spectrum of **2f**.

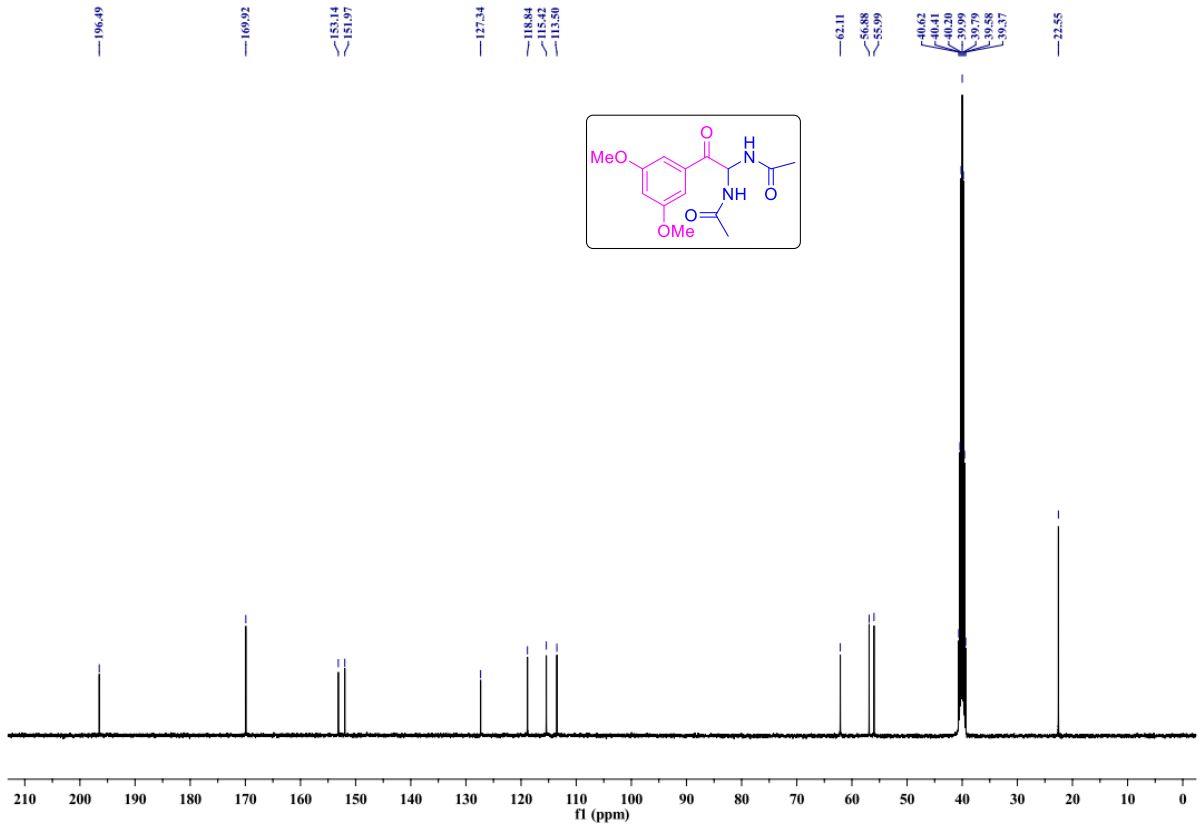

Figure S6. ^{13}C NMR spectrum of **2f**.

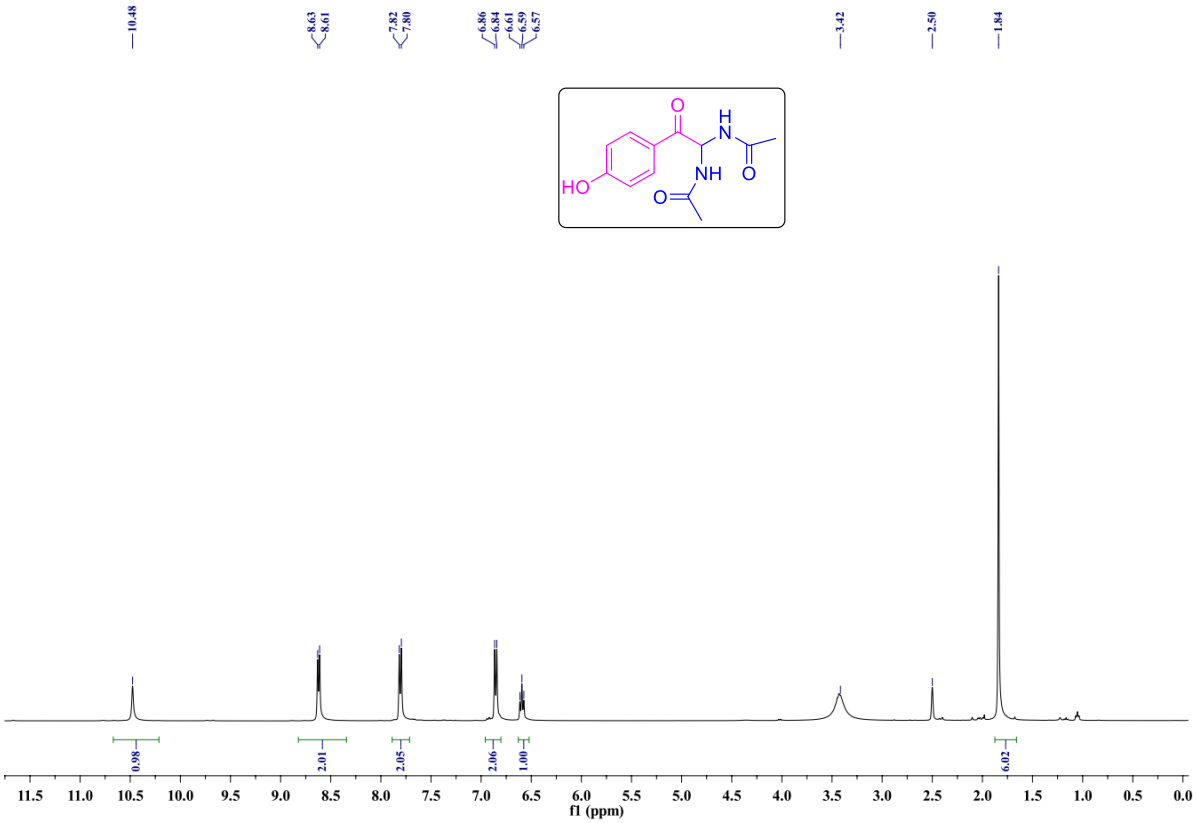

Figure S7. [1] H NMR spectrum of **2g**.

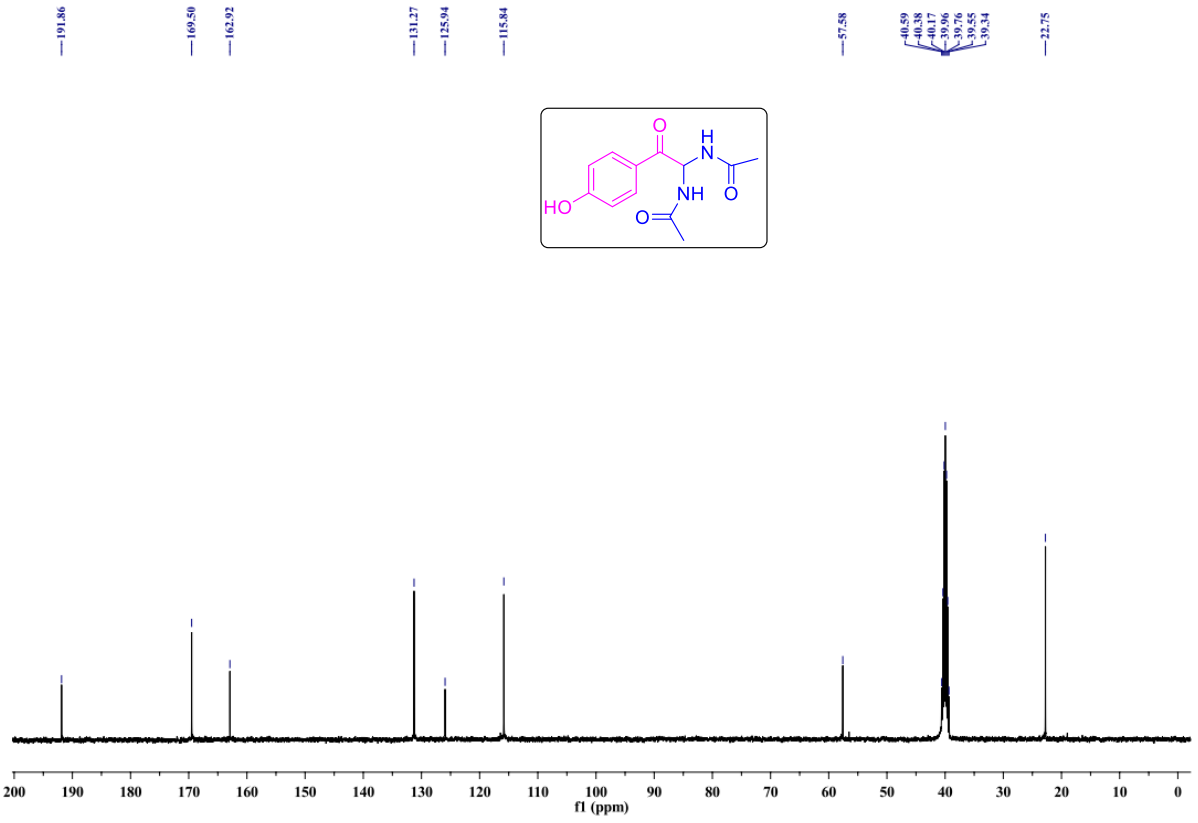

Figure S7. [13]C NMR spectrum of **2g**.

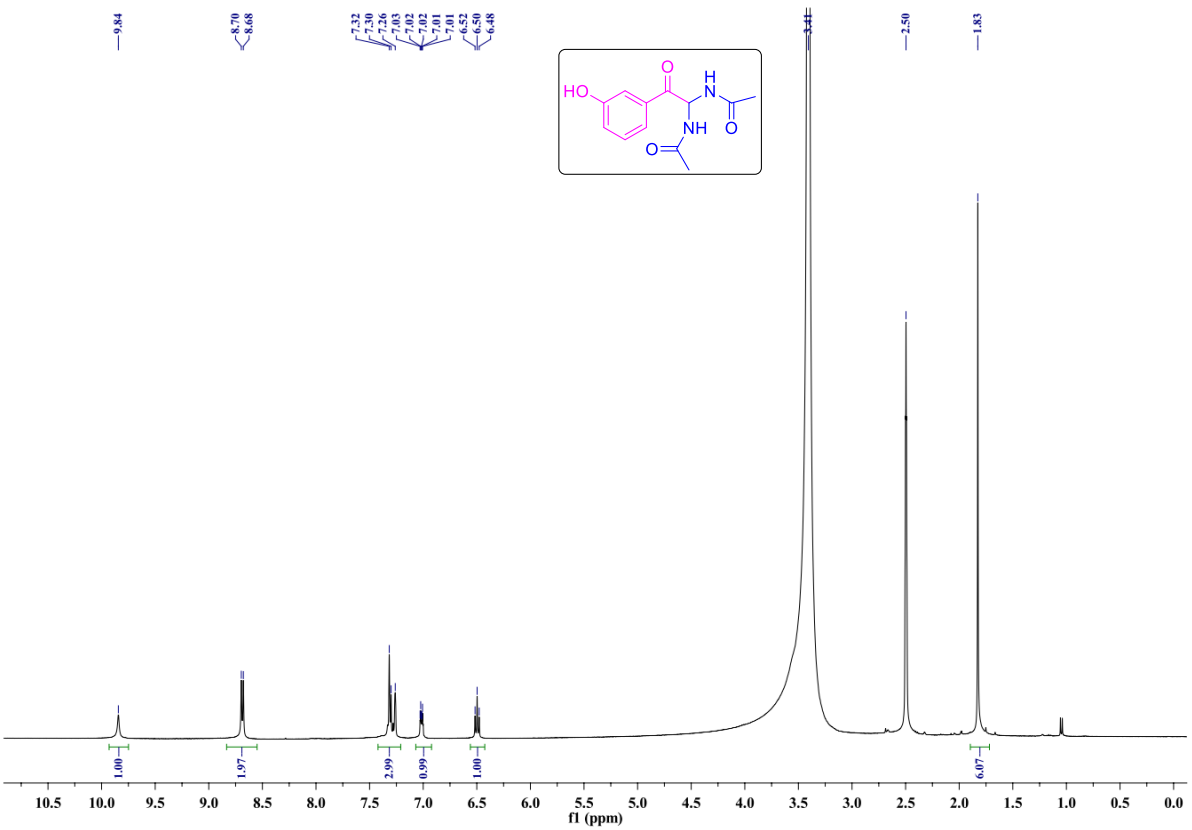

Figure S8. ^{1}H NMR spectrum of **2h**.

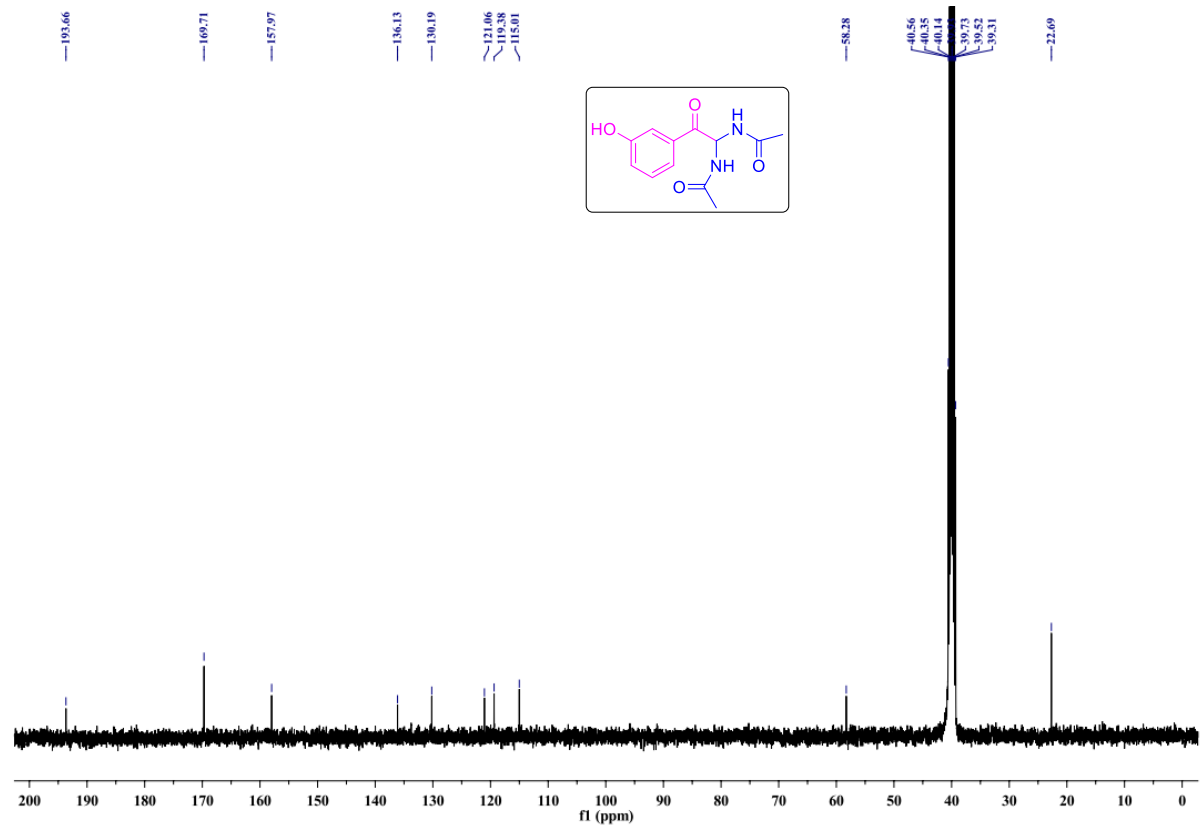

Figure S8. ^{13}C NMR spectrum of **2h**.

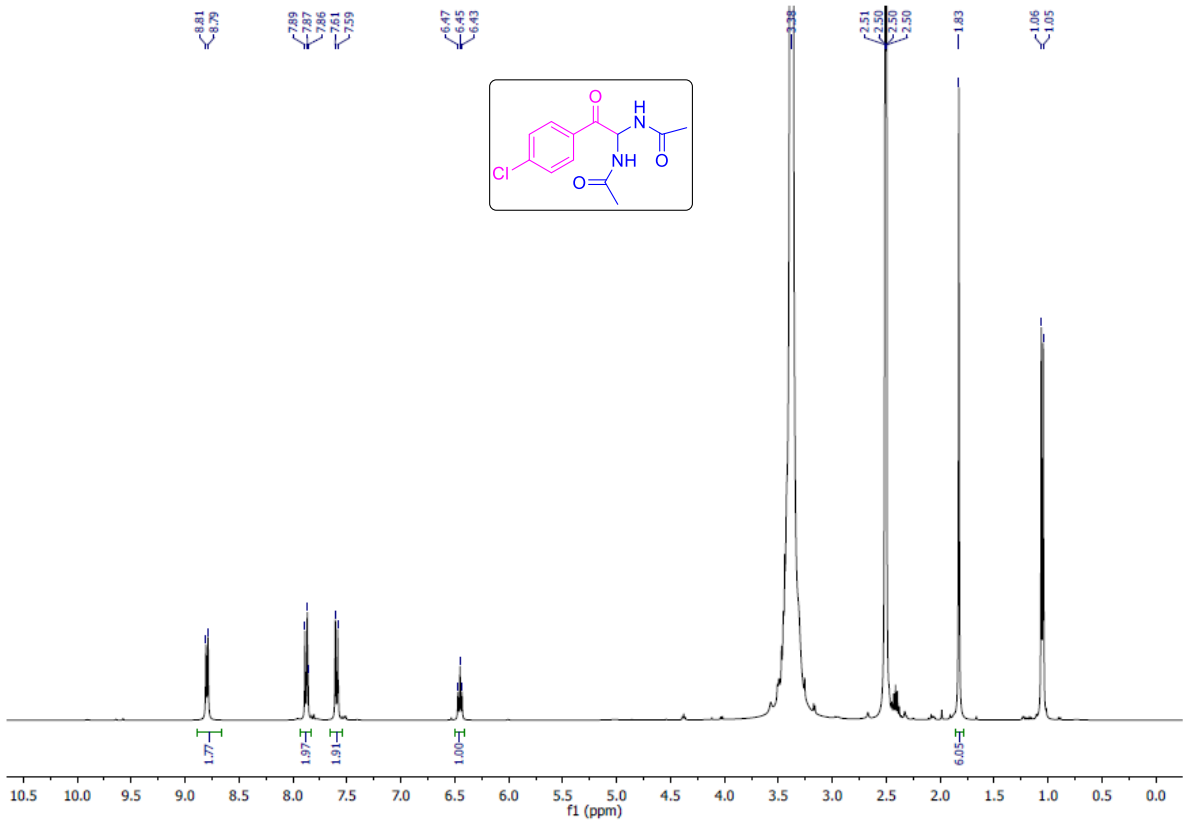

Figure S9. [1] H NMR spectrum of **2i**.

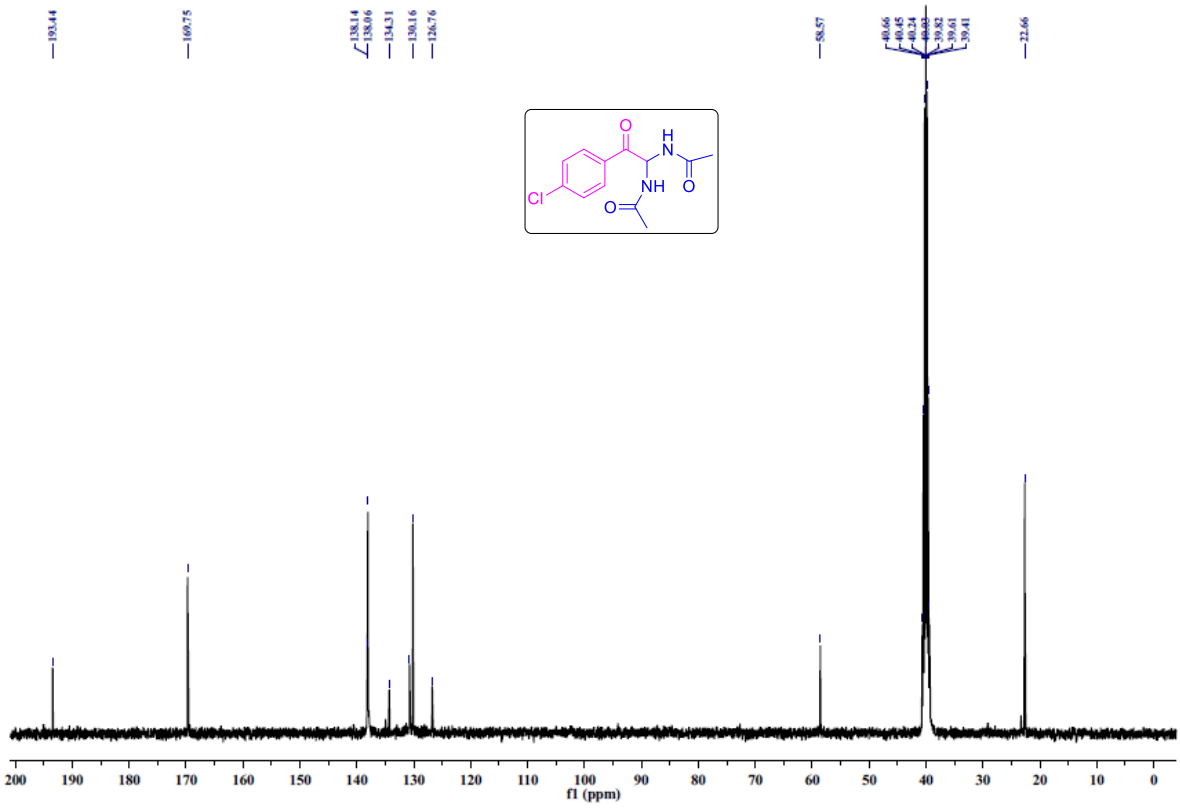

Figure S9. [13] C NMR spectrum of **2i**.

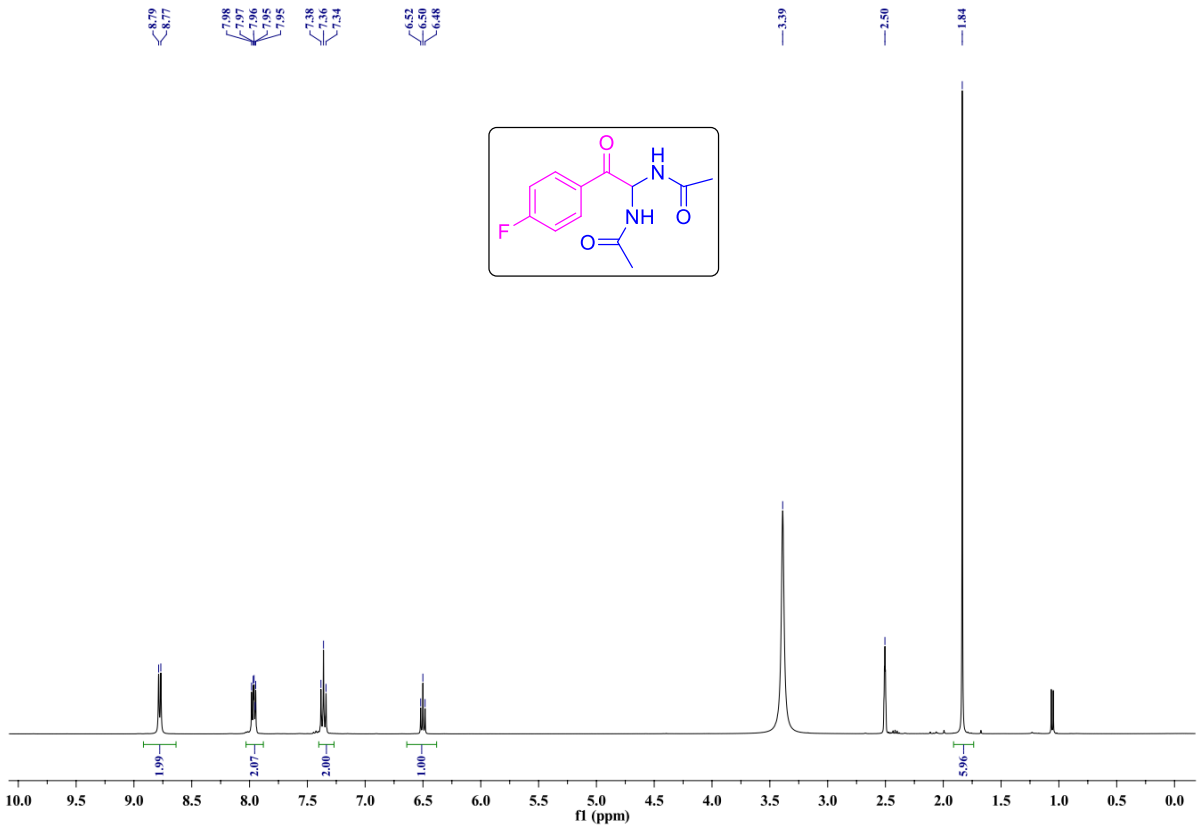

Figure S10. ^{1}H NMR spectrum of **2j**.

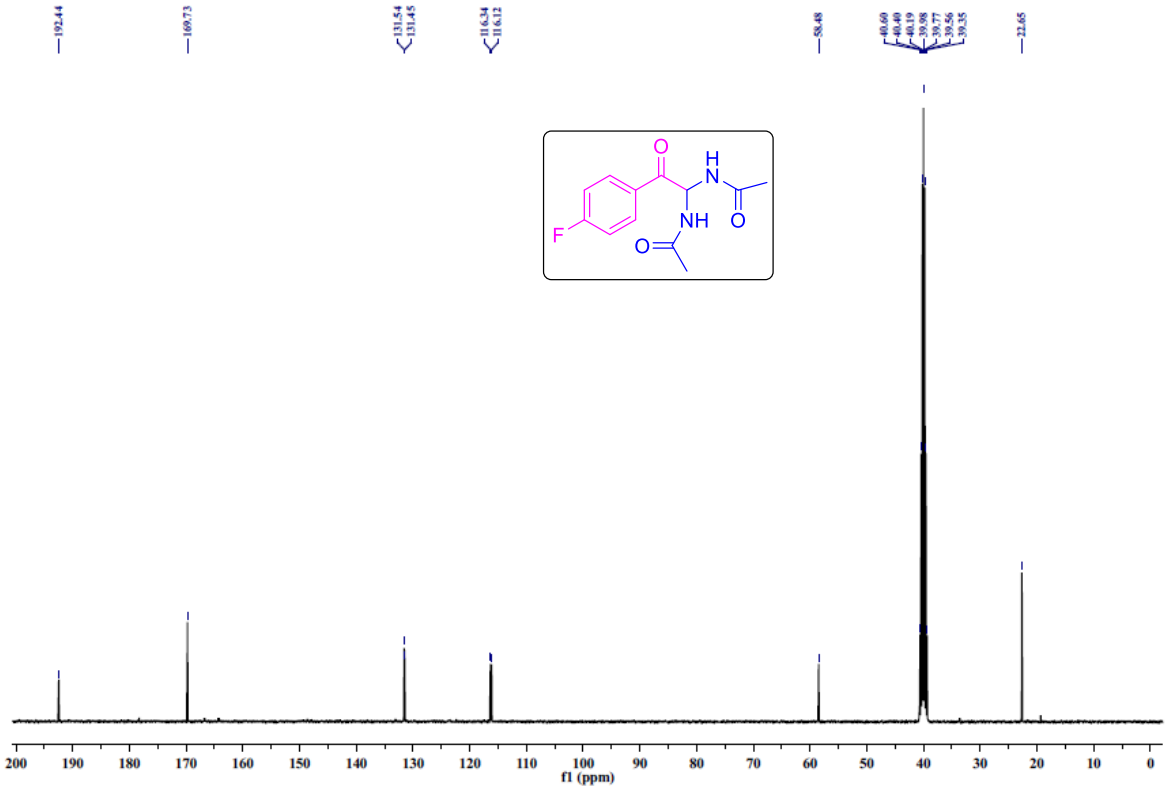

Figure S10. ^{1} ^{3}C NMR spectrum of **2j**.

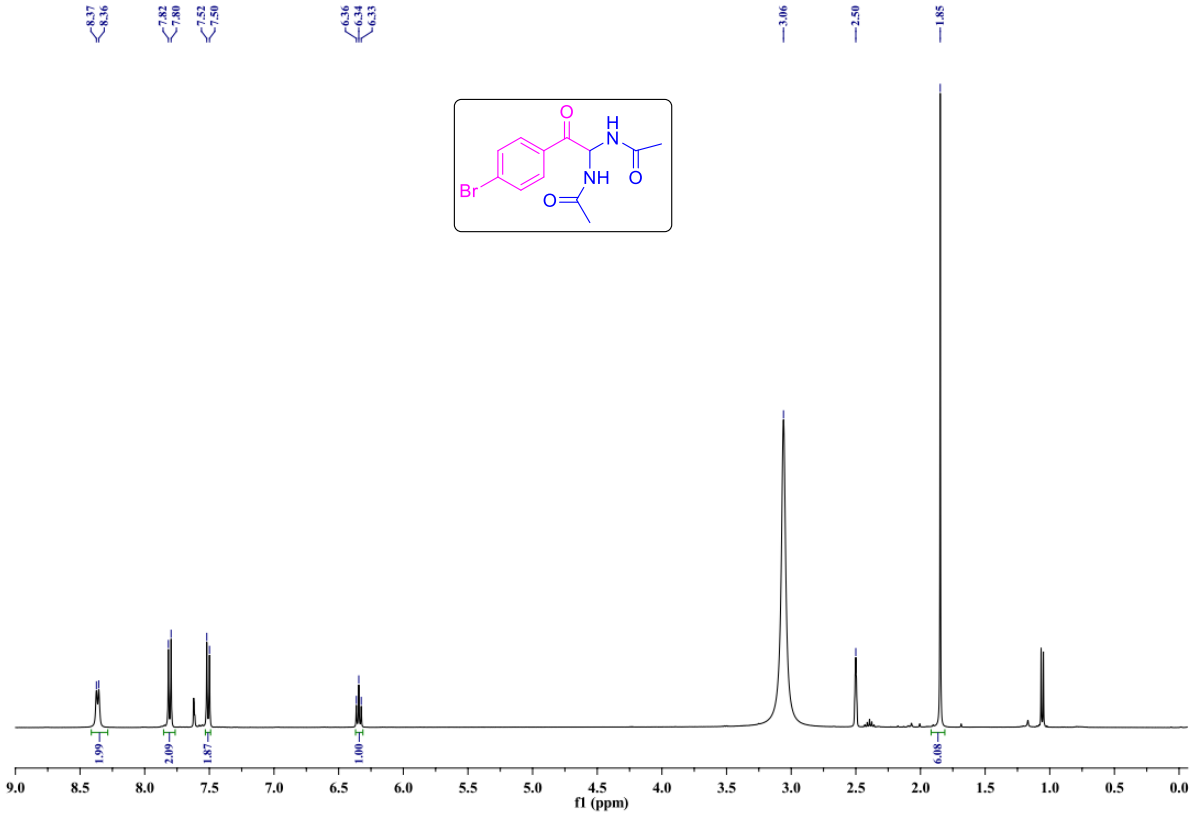

Figure S11. ^{1}H NMR spectrum of **2k**.

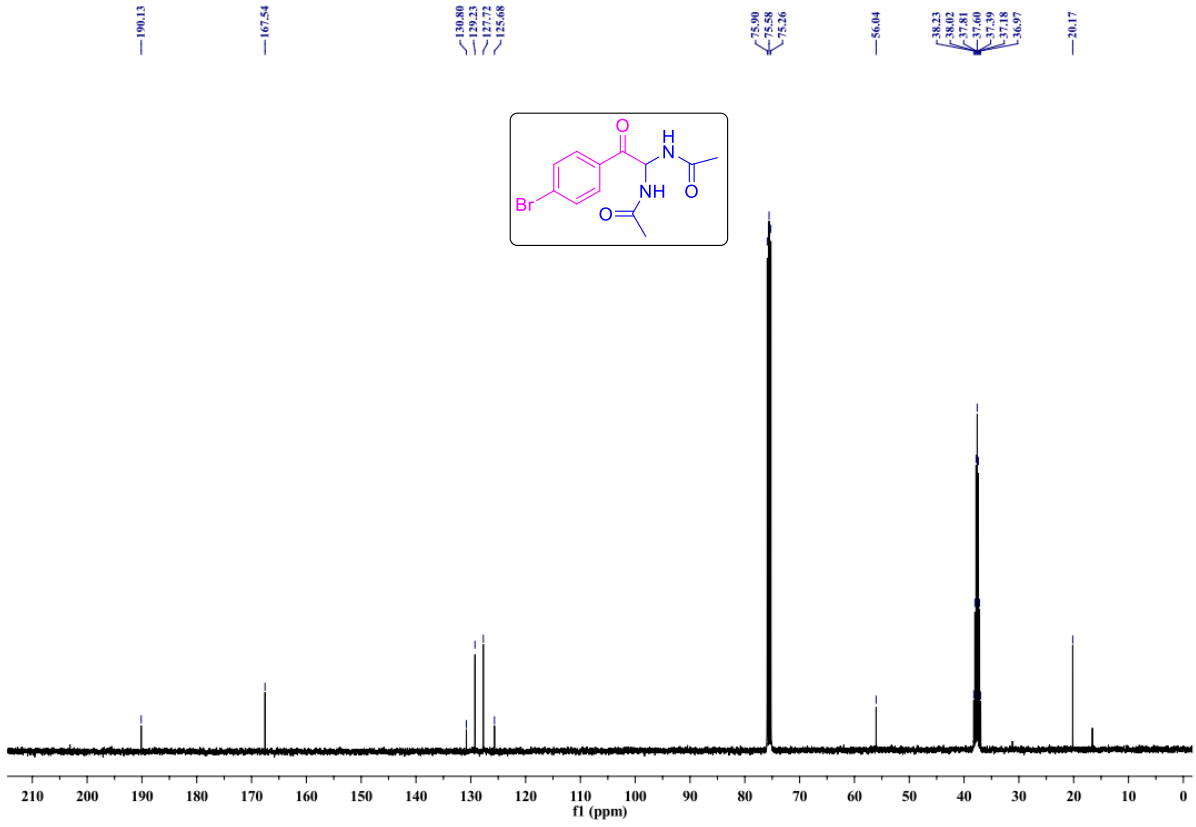

Figure S11. ^{13}C NMR spectrum of **2k**.

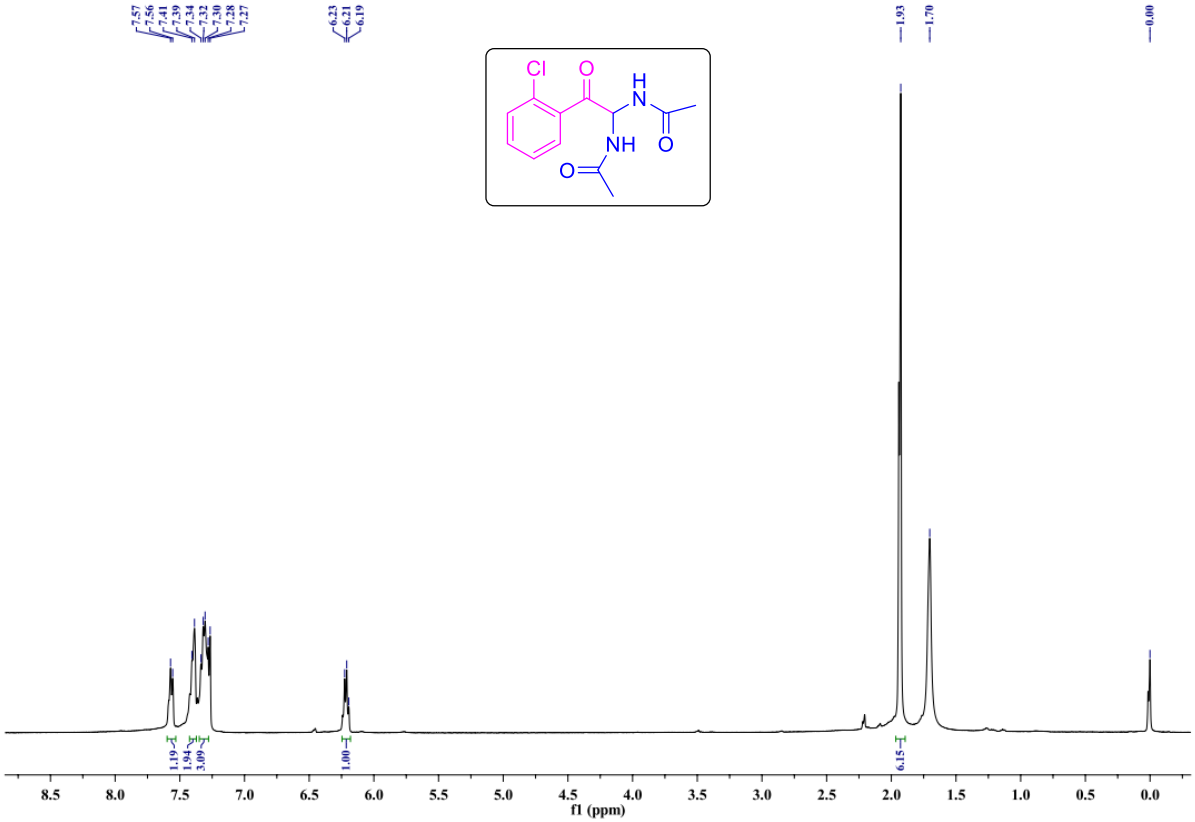

Figure S12. ^{1}H NMR spectrum of **2l**.

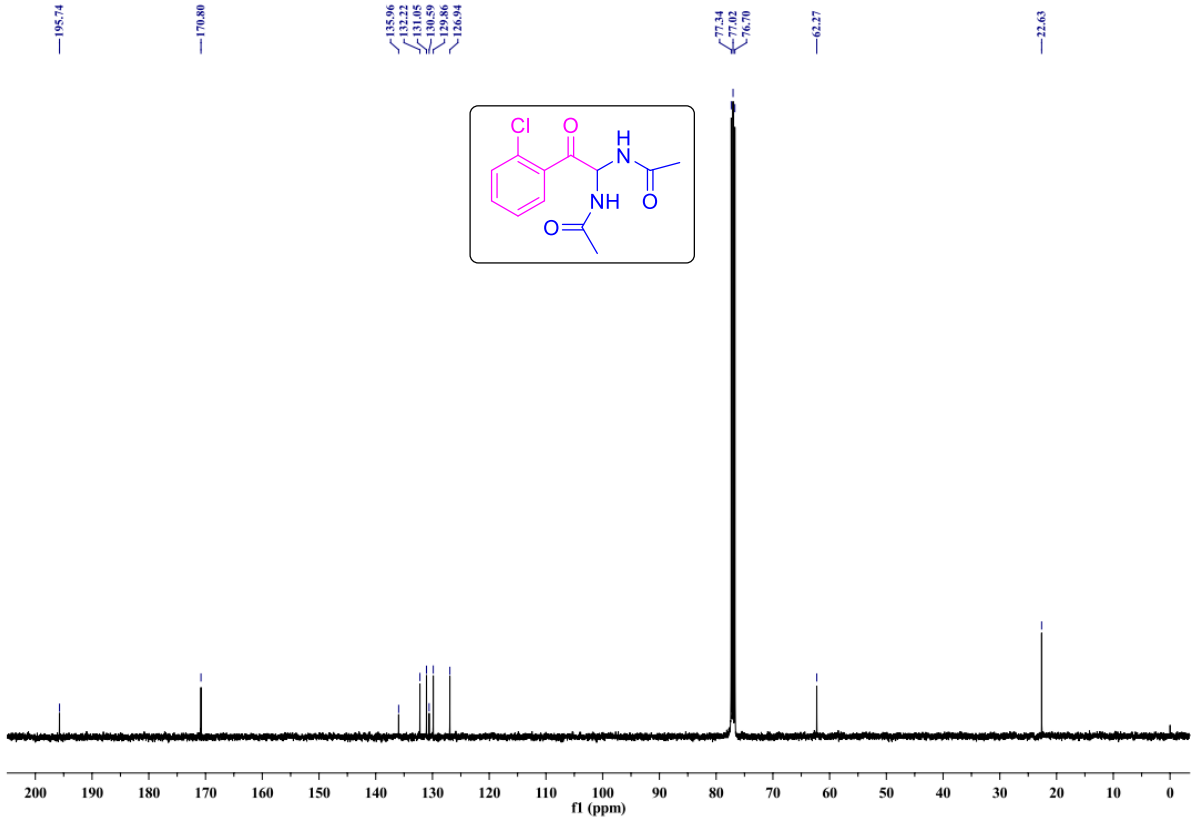

Figure S12. ^{13}C NMR spectrum of **2l**.

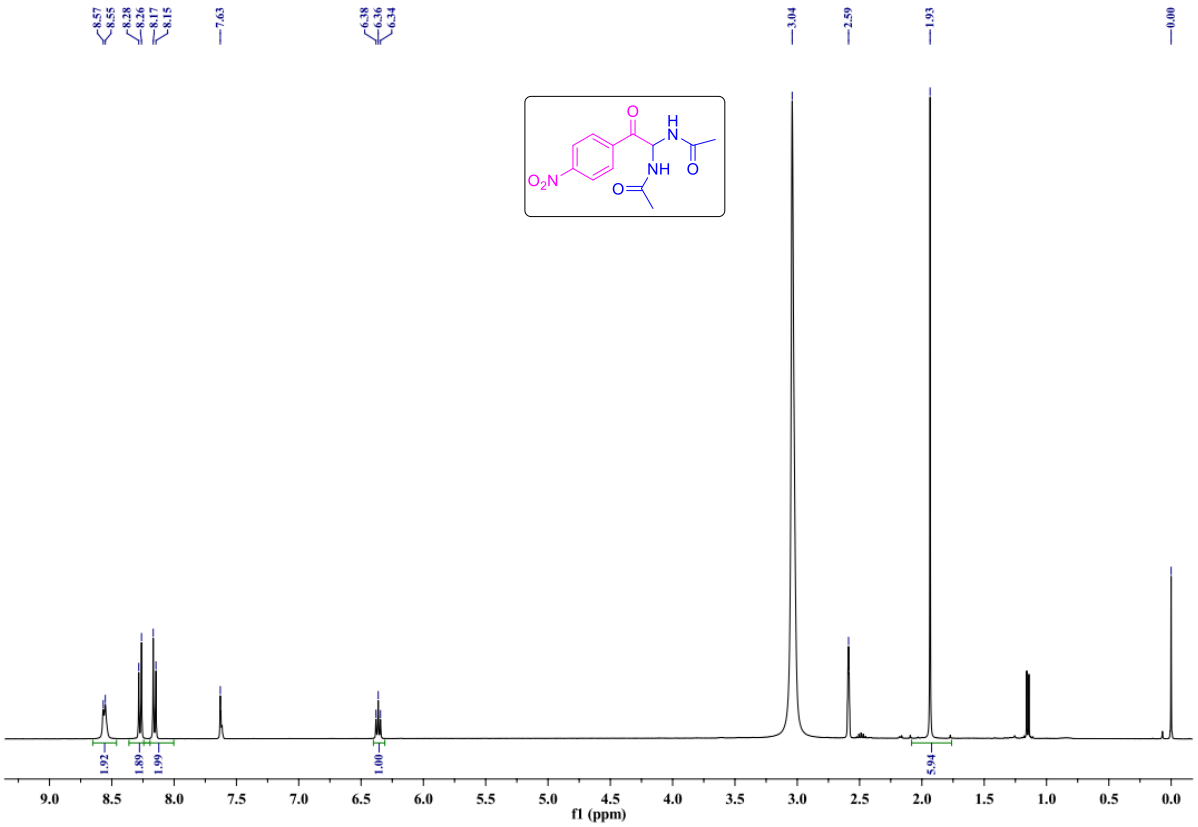

Figure S13. ^{1}H NMR spectrum of **2m**.

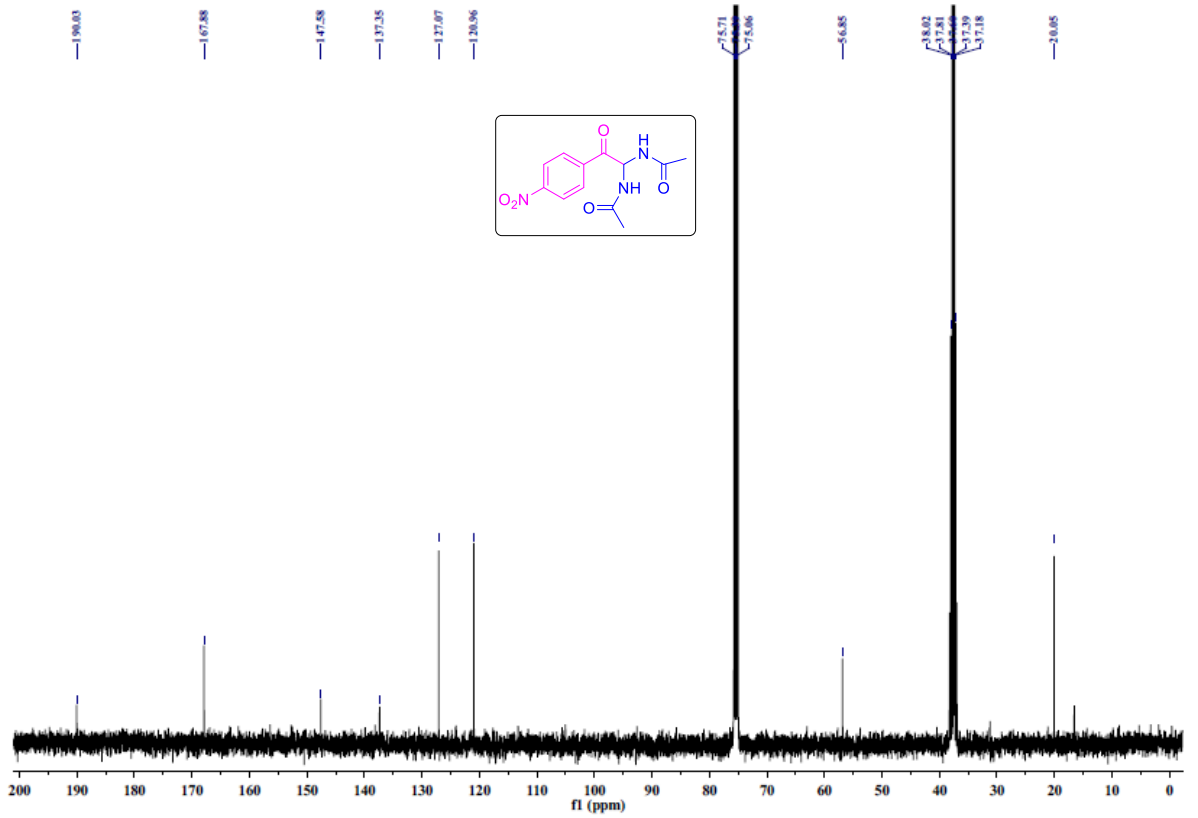

Figure S13. ^{13}C NMR spectrum of **2m**.

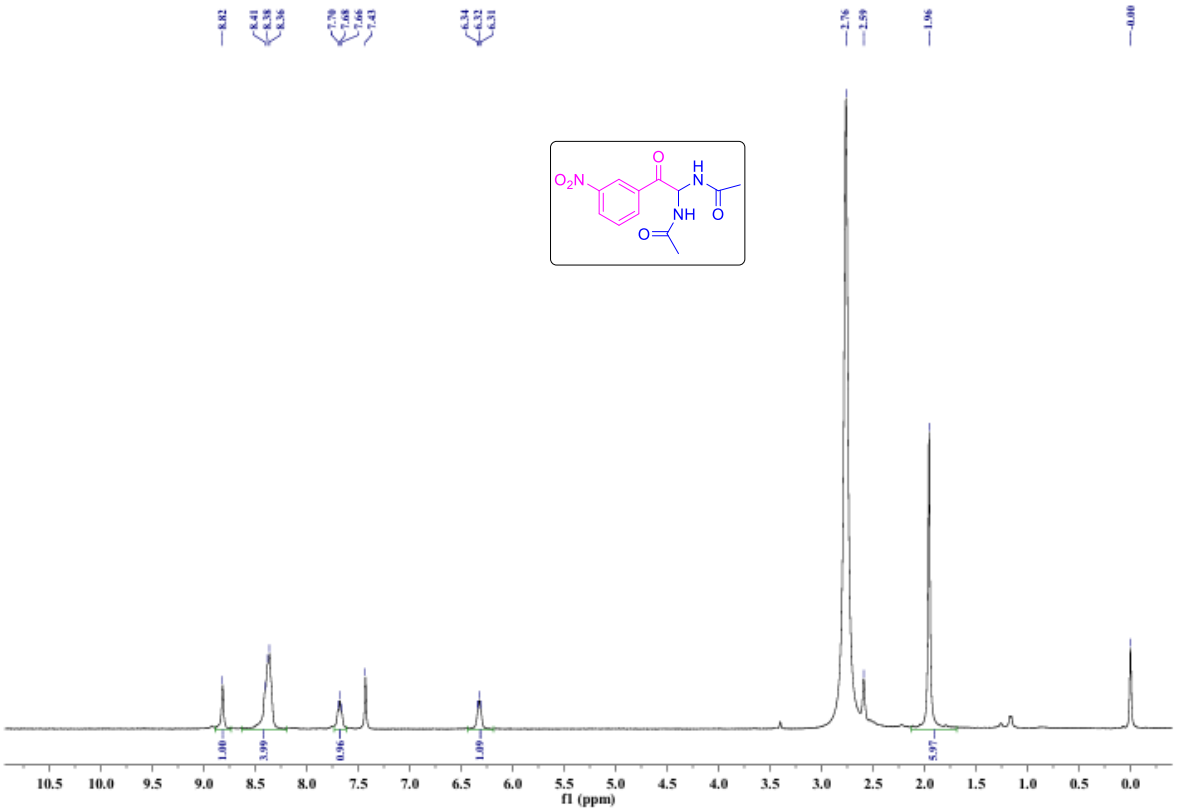

Figure S14. ^{1}H NMR spectrum of **2n**.

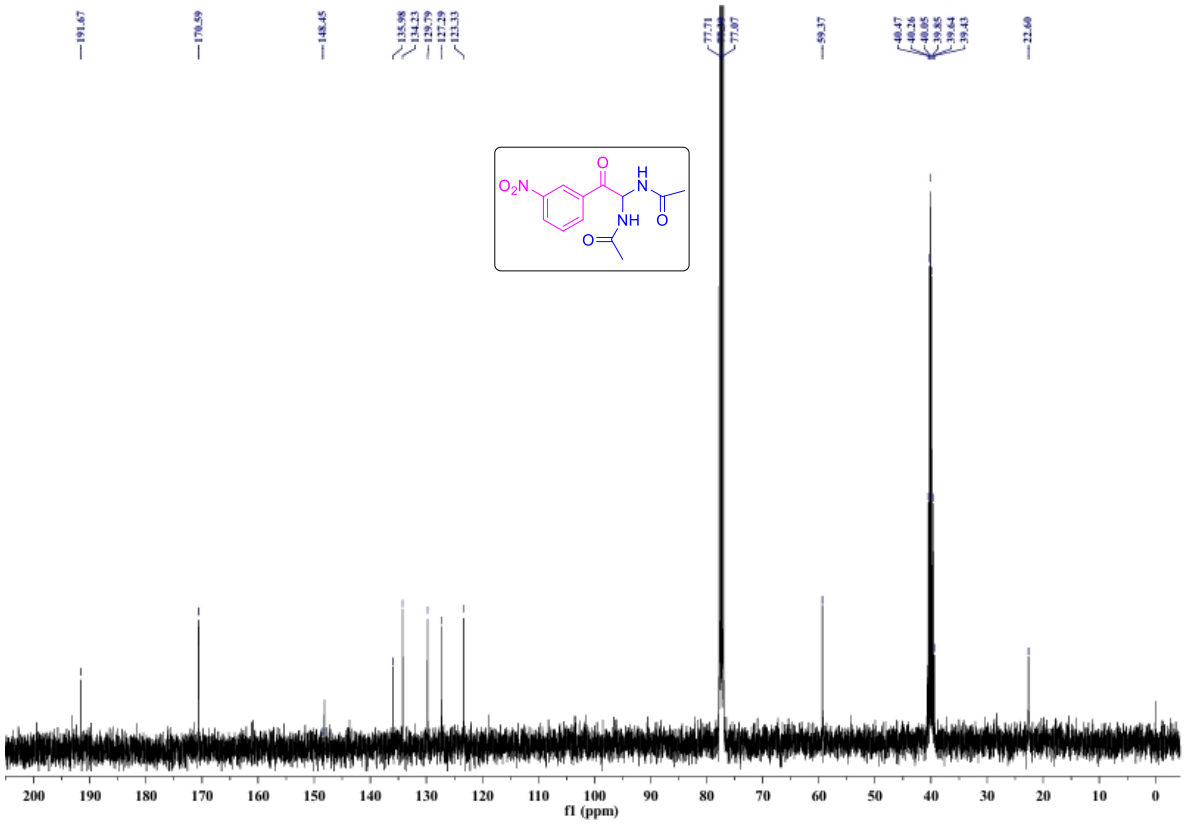

Figure S14. ^{13}C NMR spectrum of **2n**.

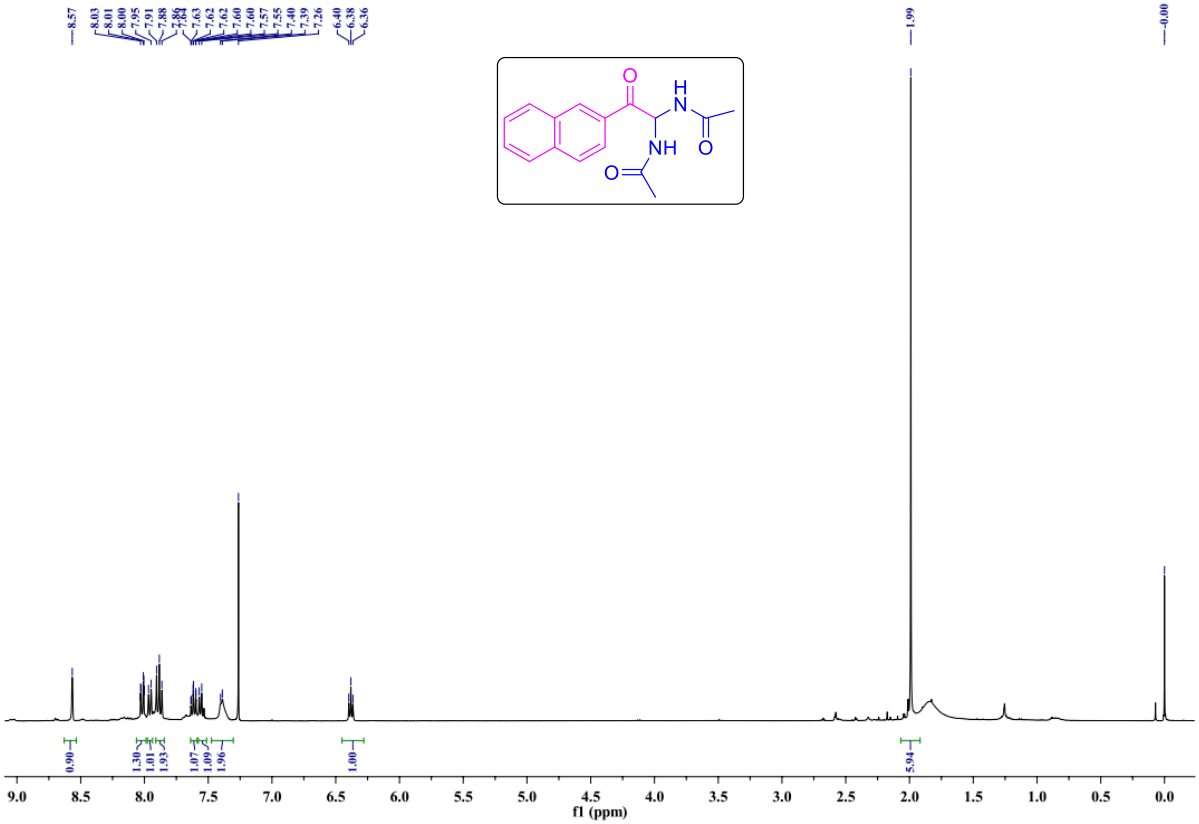

Figure S15. [1] H NMR spectrum of **2o.**

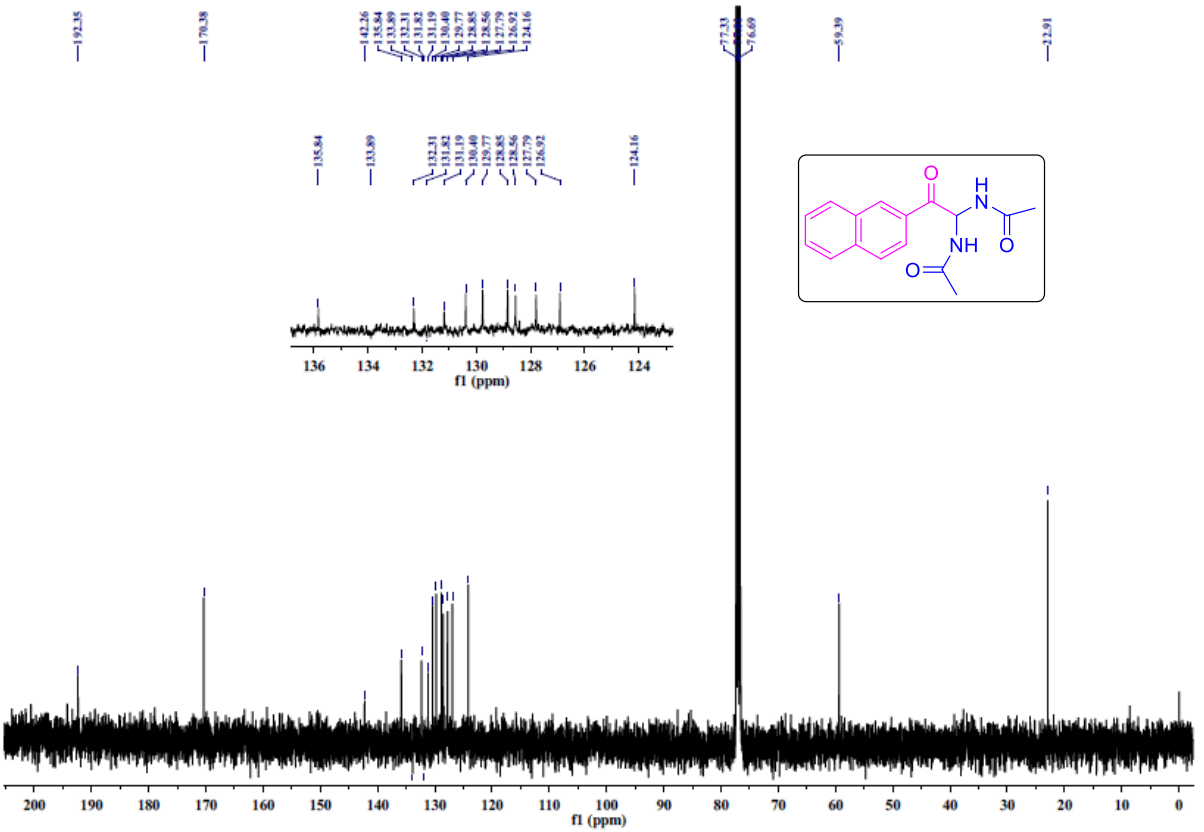

Figure S15. [13] C NMR spectrum of **2o.**

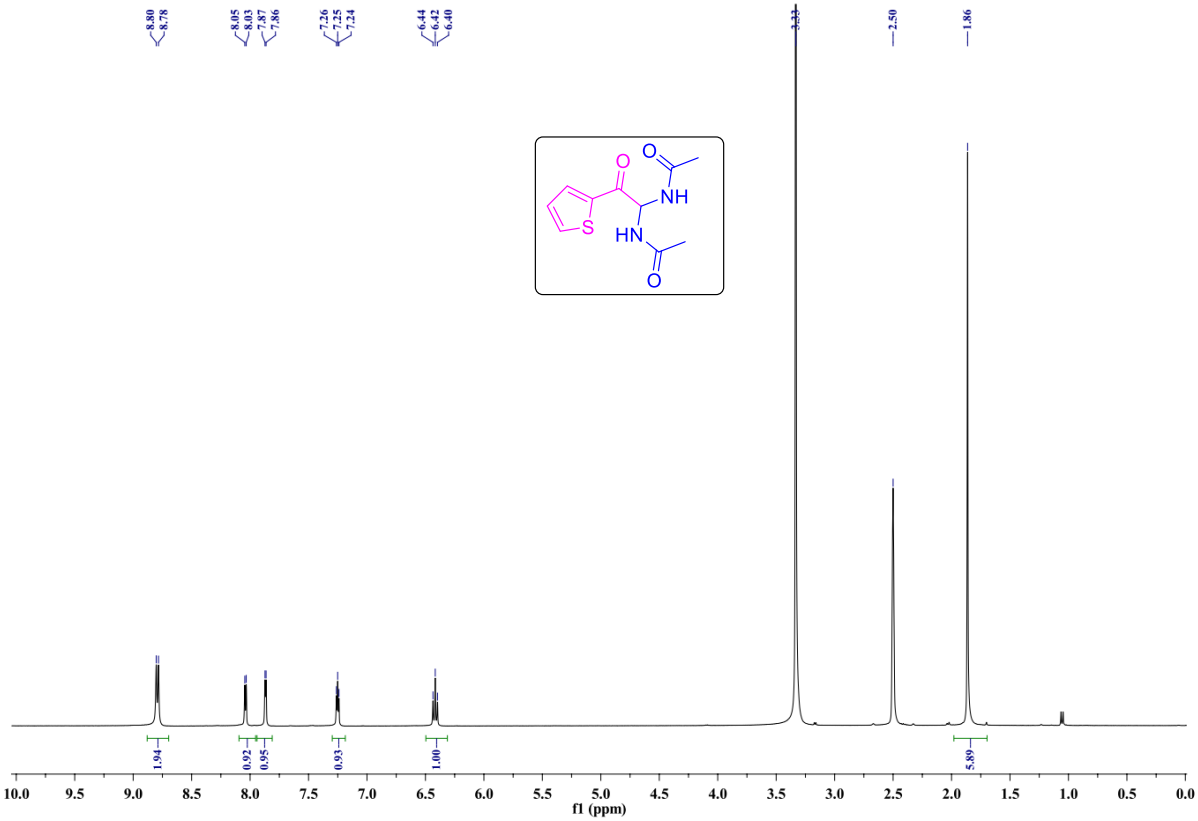

Figure S16. ^{1}H NMR spectrum of **2p**.

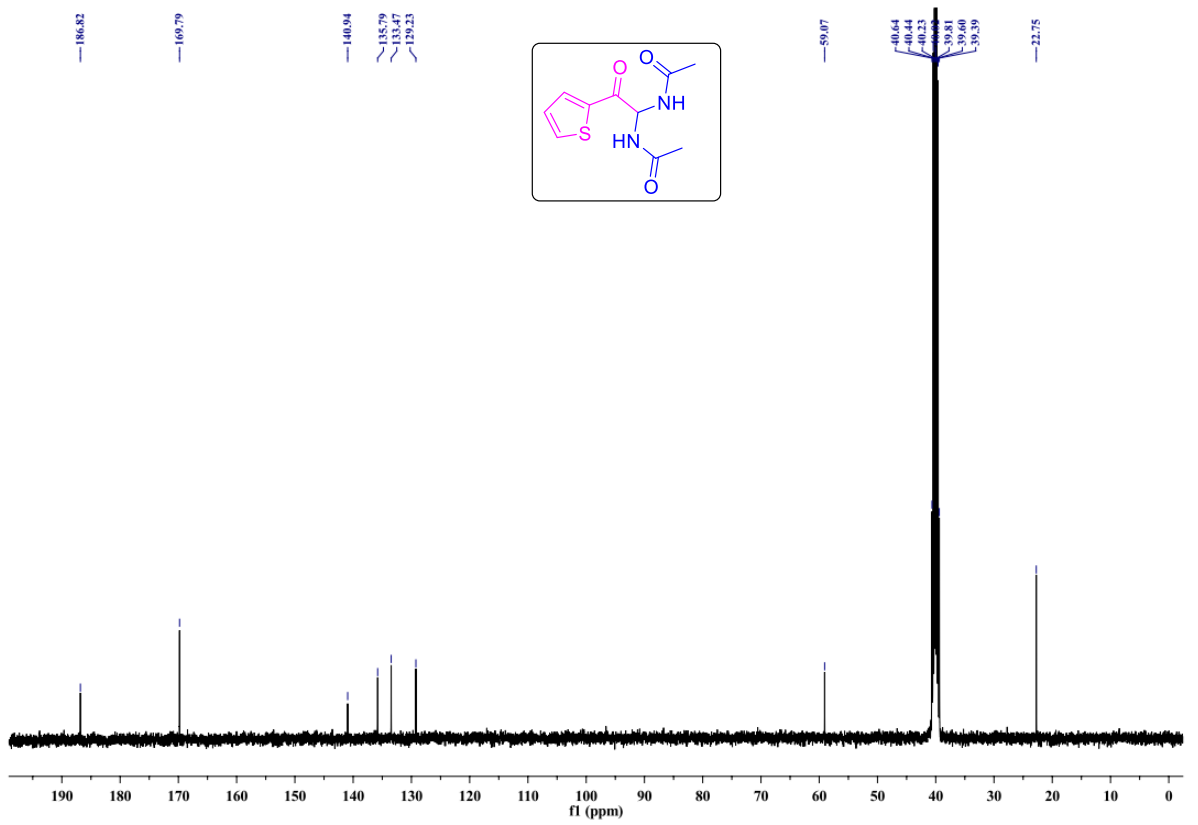

Figure S16. ^{13}C NMR spectrum of **2p**.

1.3. Crystallization Experiments.

N,N'-(2-(2-chlorophenyl)-2-oxoethane-1,1-diyl)diacetamide was crystallized in a methanol solution at room temperature and slow evaporation to afford crystal **2l**.

1.4. Crystallographic Analysis of Compounds 2l.

The single crystal X-ray diffraction (XRD) data were collected at 273 K with Mo Kα radiation (λ = 0.71073 Å) using a Bruker Smart Apex II CCD diffractometer equipped with an Oxford Cryostream low-temperature device and a finefocus sealed-tube X-ray source (graphite monochromated) operating at 50 kV and 30 mA. APEX3 software[1] was used for preliminary determination of the unit cell. Using Olex[2,3] the structure was solved with the Superflip[4] structure solution program using Charge Flipping solution method and refined with the ShelXL[5]refinement package using Least Squares minimization. All the non-hydrogen atoms were refined anisotropically and the hydrogen atoms were placed based on the Fourier difference maps. The ORTEP image of 2l is shown in Fig S17. The details of the crystallographic data are listed in Table S1.

Table S1. Crystallographic data and structure refinement parameters of molecules **2l**.

	Molecule 2l
Name of the compound	N,N'-(2-(2-chlorophenyl)-2-oxoethane-1,1-diyl)diacetamide (2l)
CCDC	2386688
Formula	$C_{12}H_{13}Cl\ N_2O_3$
Formula weight	268.69
Crystal System	Monoclinic
Space group	P 21
a [Å]	8.9965 (9)
b [Å]	7.9812 (10)
c [Å]	9.3003 (9)
α [^{0}]	90
β [^{0}]	106.255
γ [^{0}]	90
V [Å ^{3}]	641.09(12)
Z	2
λ [Å]	0.71073

ρ_{calcd} [gcm^{-3}]	1.392
F[000]	280.0
μ [mm^{-1}]	0.300
θ [^{0}]	2.75 to 26.37
index ranges	− 11≤ h ≤11 − 9≤ k ≤9 − 11≤ l ≤11
T [K]	273 K
R1	0.0497
wR2	0.1227
Parameters	175

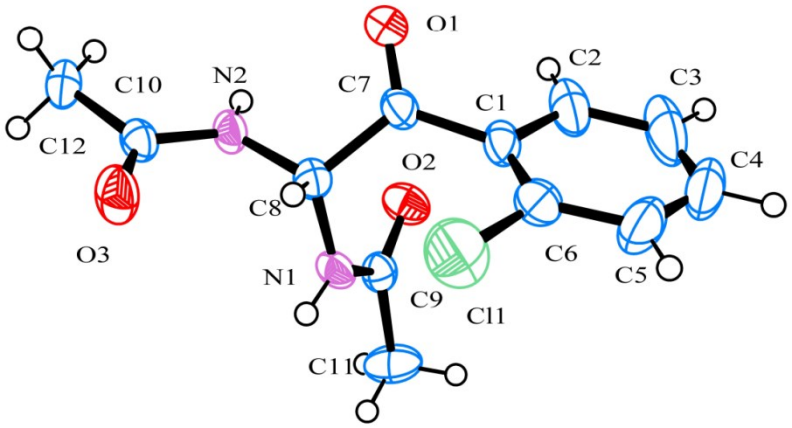

Figure S17. ORTEP representation of molecule **2l**, where the displacement ellipsoids were drawn at 50% probability level and hydrogen atoms is omitted for clarity.

MSR-03.cif

References

1. APEX3; Bruker AXS inc.: Madison, Wisconsin, USA.
2. X. Jiang, Y. Sun, J. Yao, Y. Cao, M. Kai, N. He, X. Zhang, Y. Wang, R. Wang, *Adv. Synth. Catal.* **2012**, *354*, 917-925.
3. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. Howard, H. Puschmann, *J.Appl. Crystallogr.* **2009**, *42*, 339-341.
4. L. Palatinus, G. Chapuis, *J. Appl. Crystallogr.* **2007**, *40*, 786-790.
5. G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, *64*, 112-122.

