Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Multicomponent synthesis of diphenyl 1,3-thiazole-barbituric acid hybrids and their fluorescence property studies

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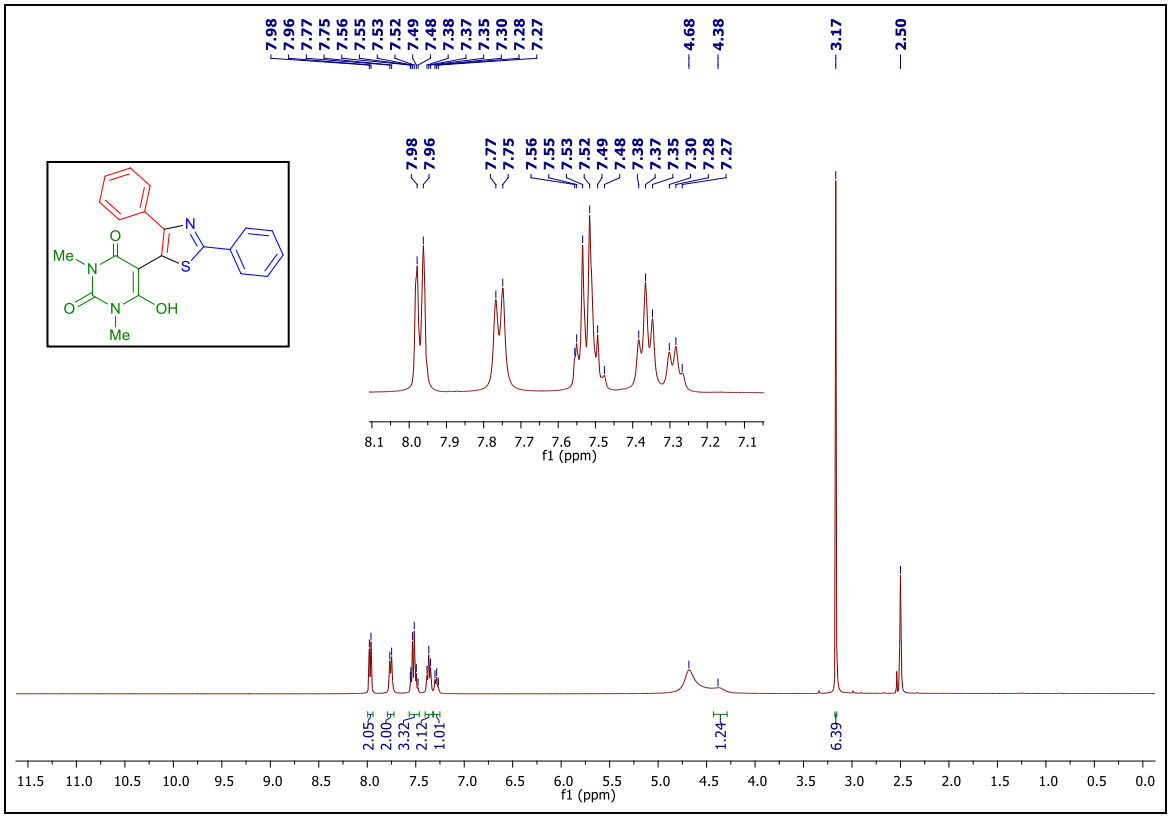
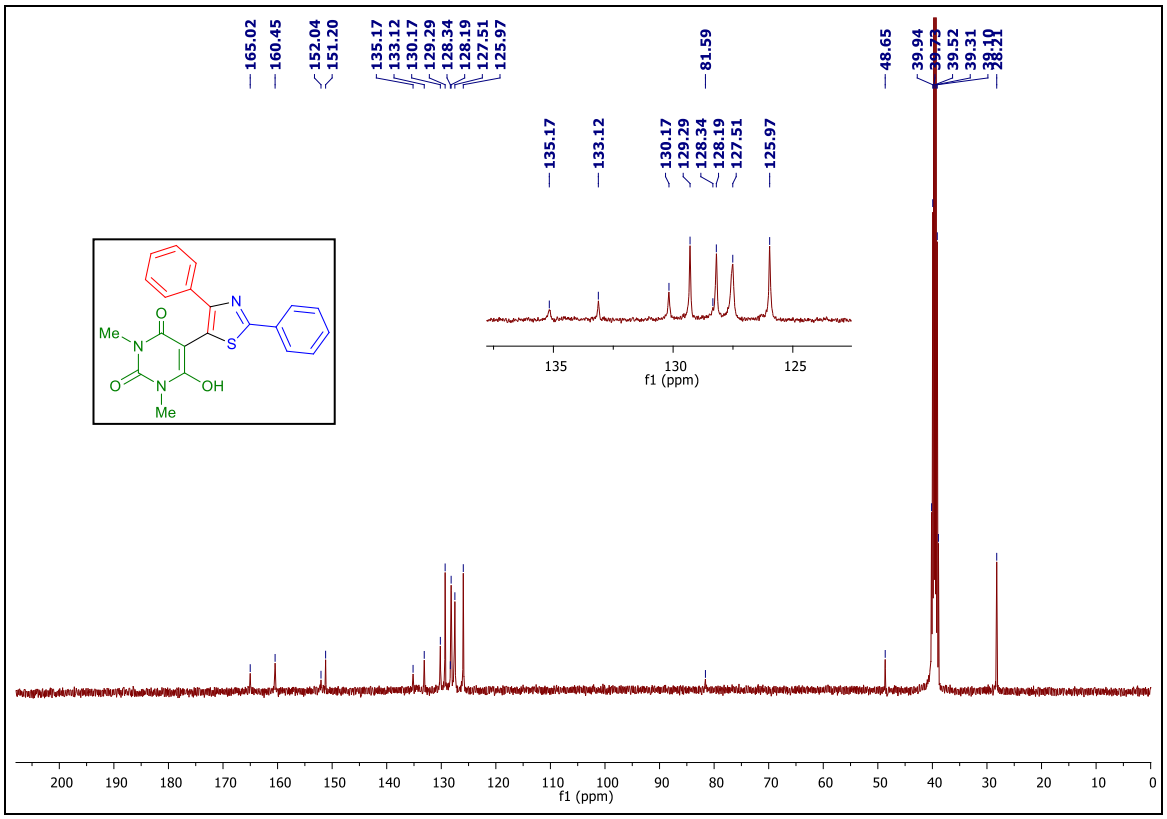
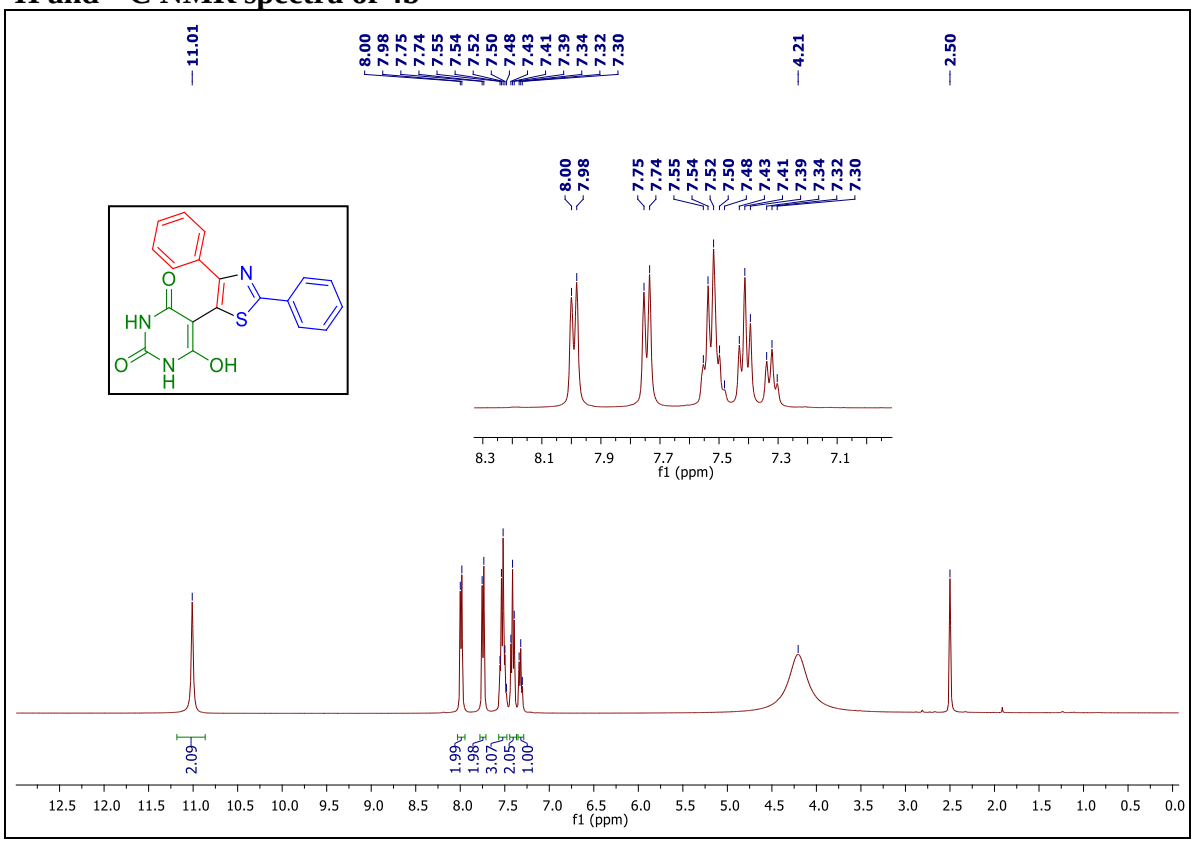
Copies of ^{1}H and ^{13}C NMR spectra of compounds

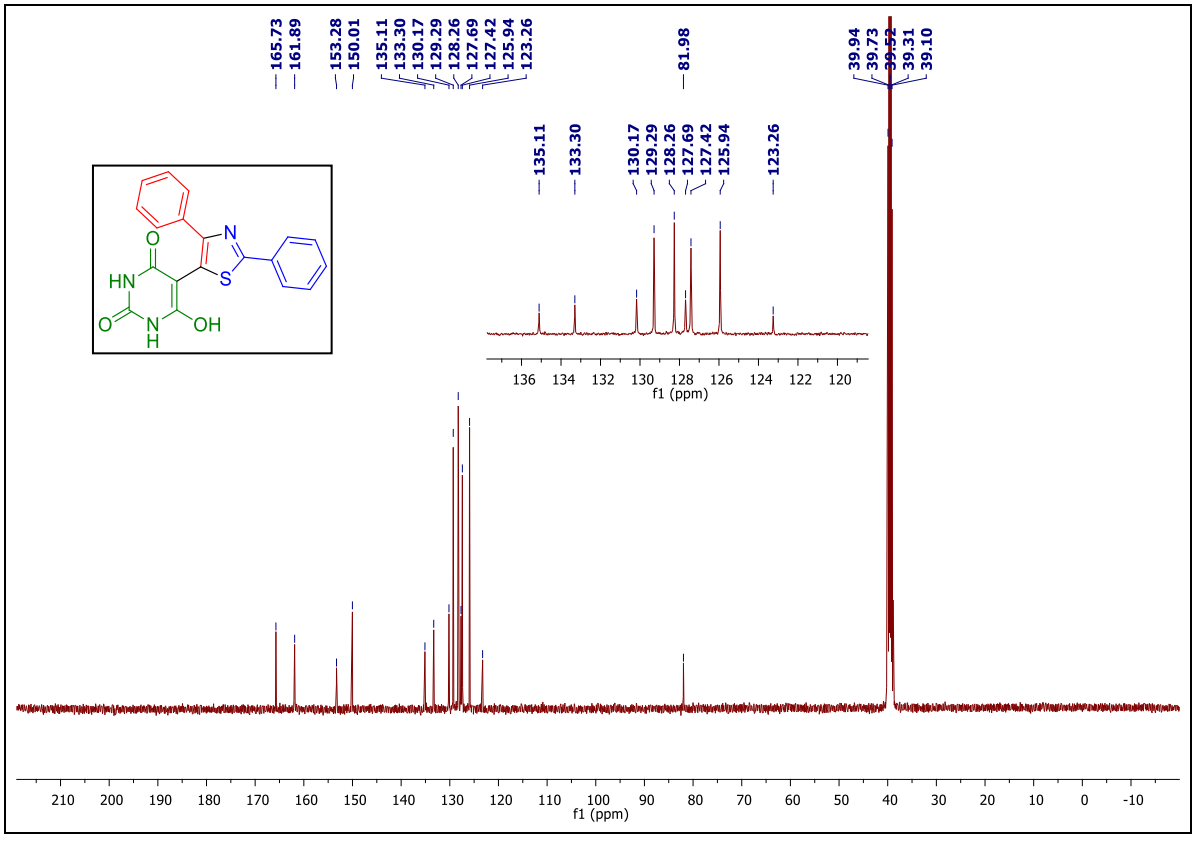
^{1}H and ^{13}C NMR spectra of 4a



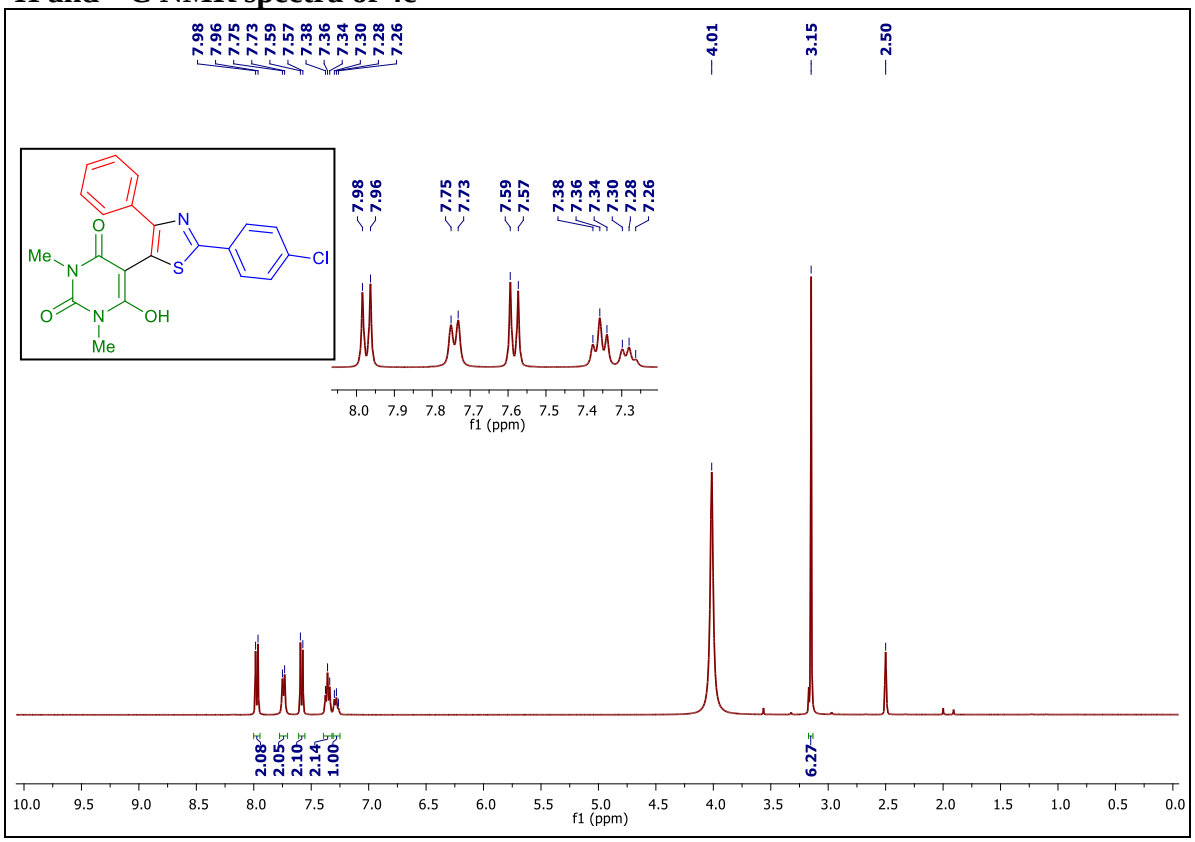


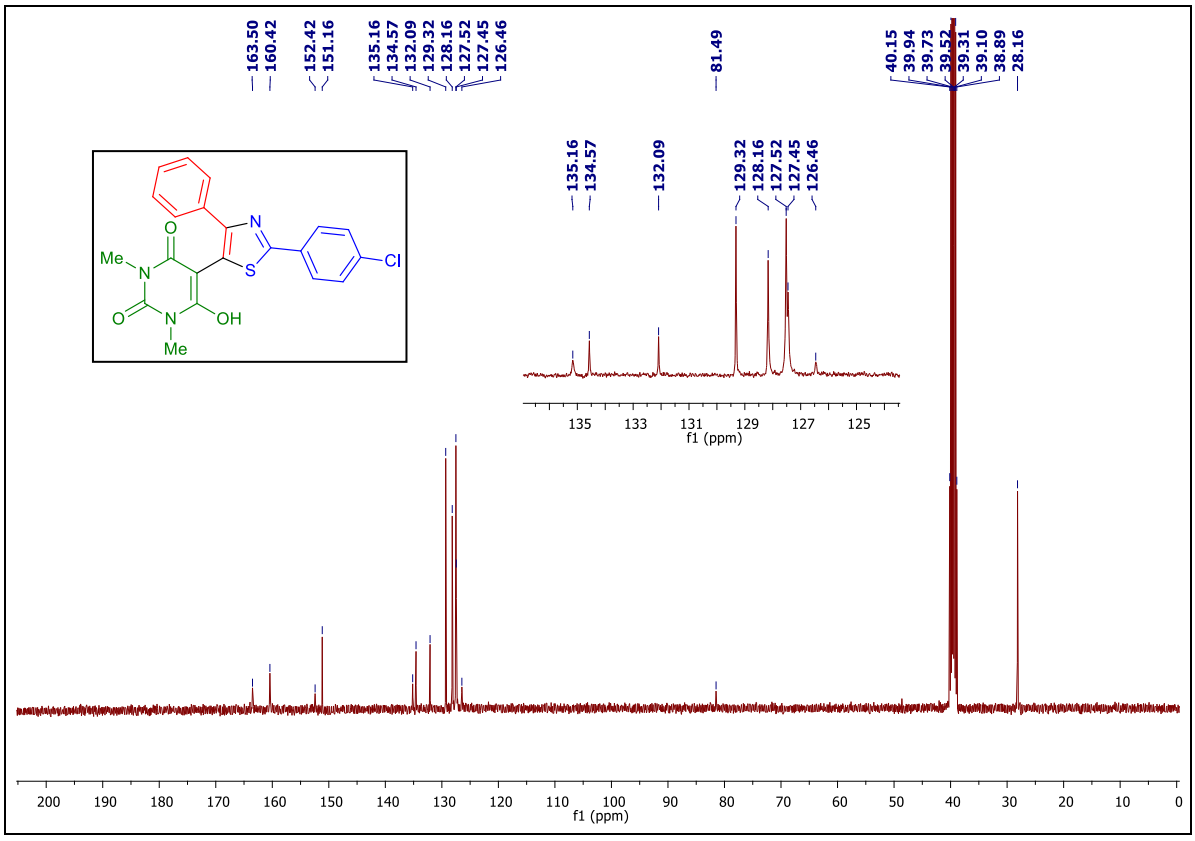
^{1}H and ^{13}C NMR spectra of 4b



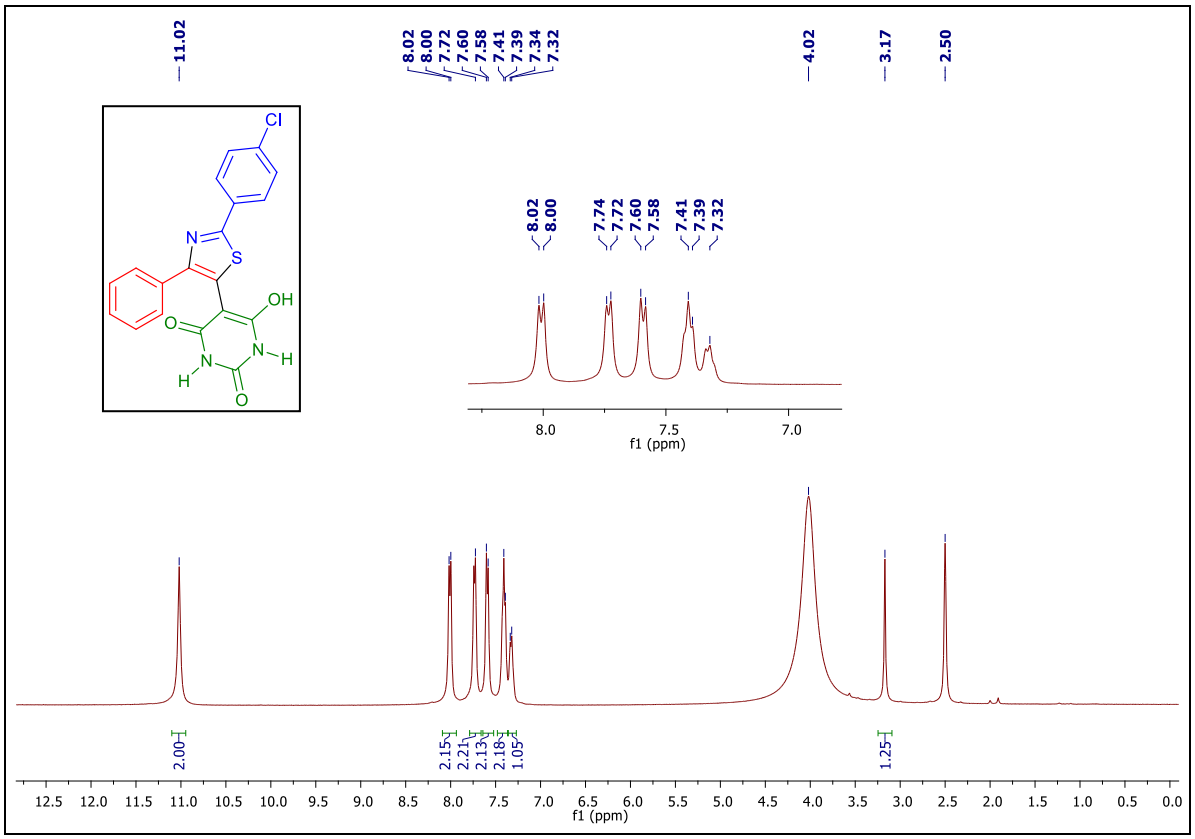


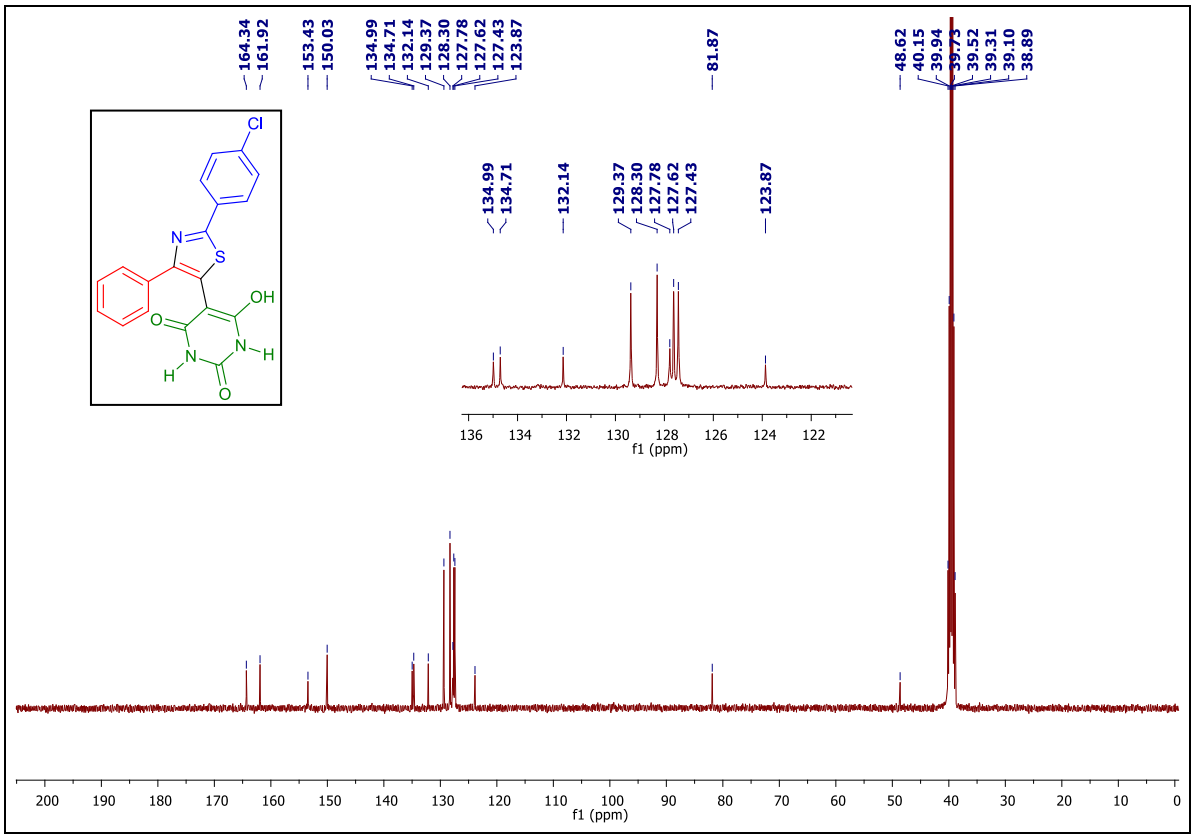
^{1}H and ^{13}C NMR spectra of 4c



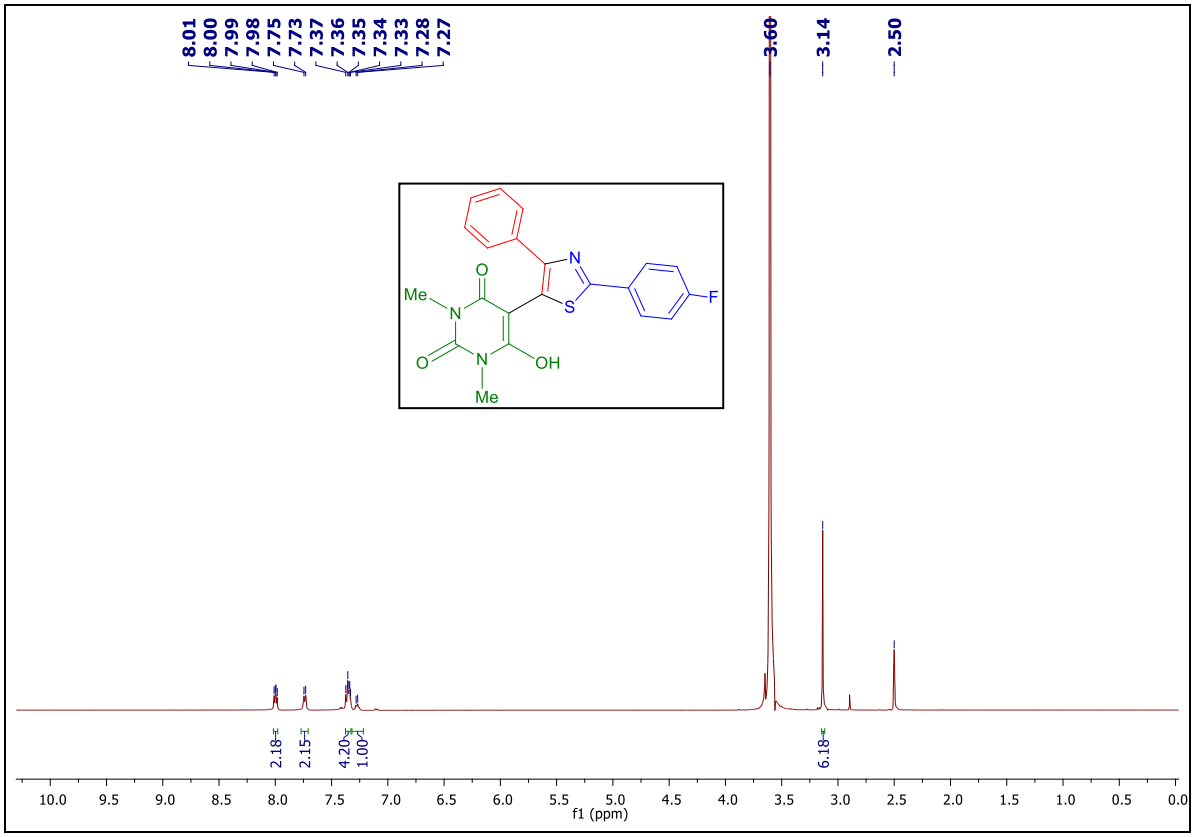


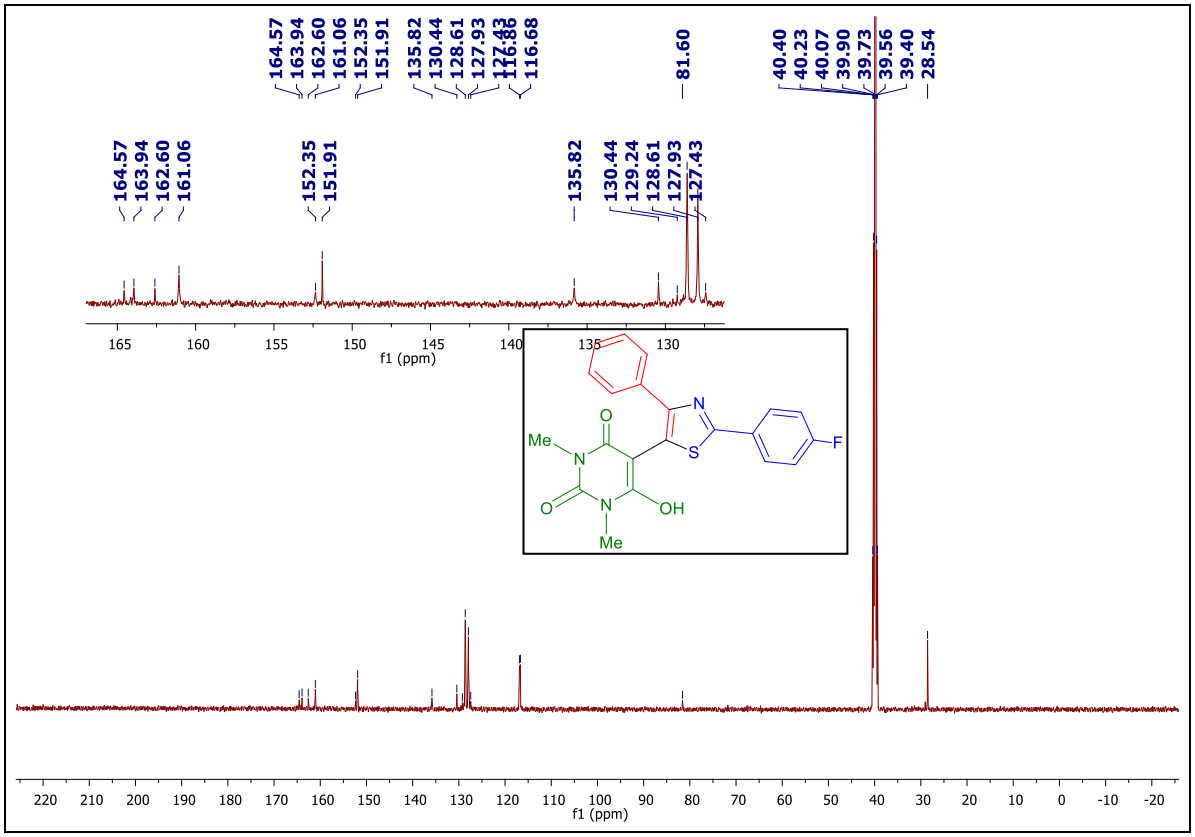
^{1}H and ^{13}C NMR spectra of 4d



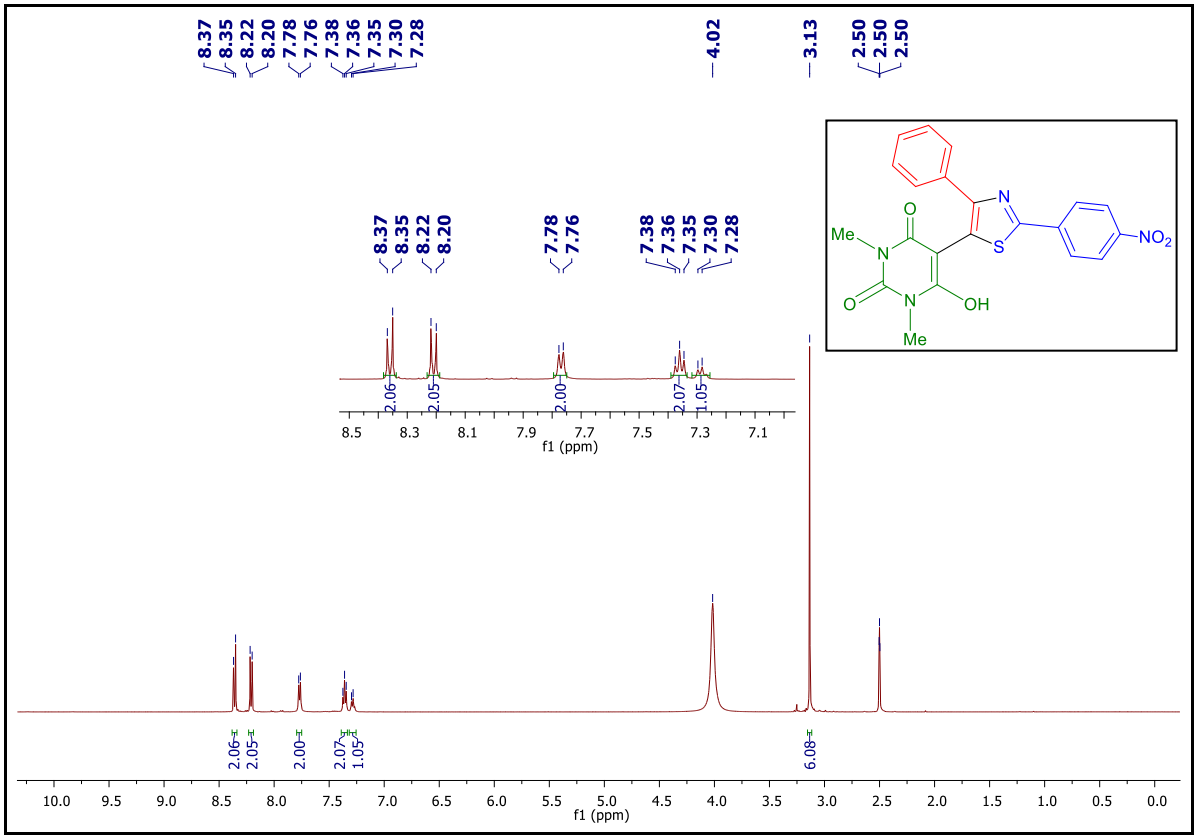


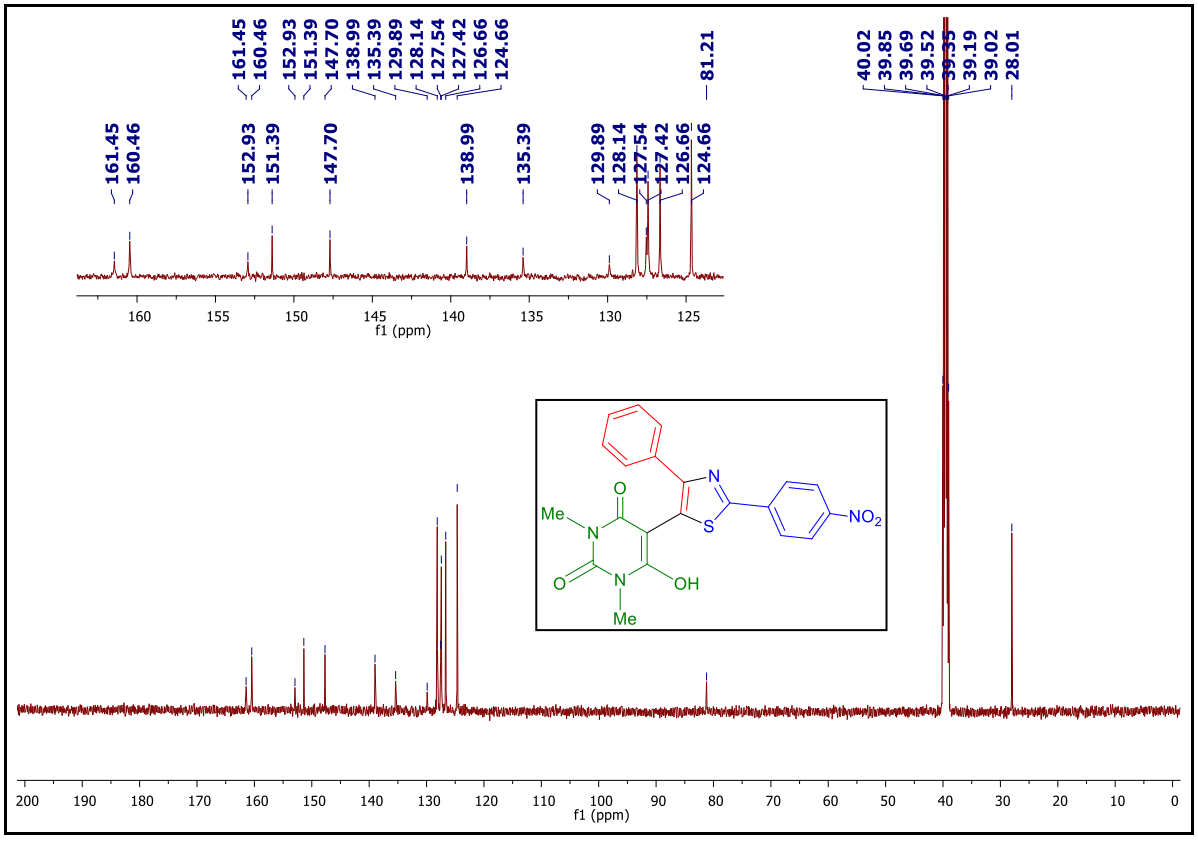
^{1}H and ^{13}C NMR spectra of 4e



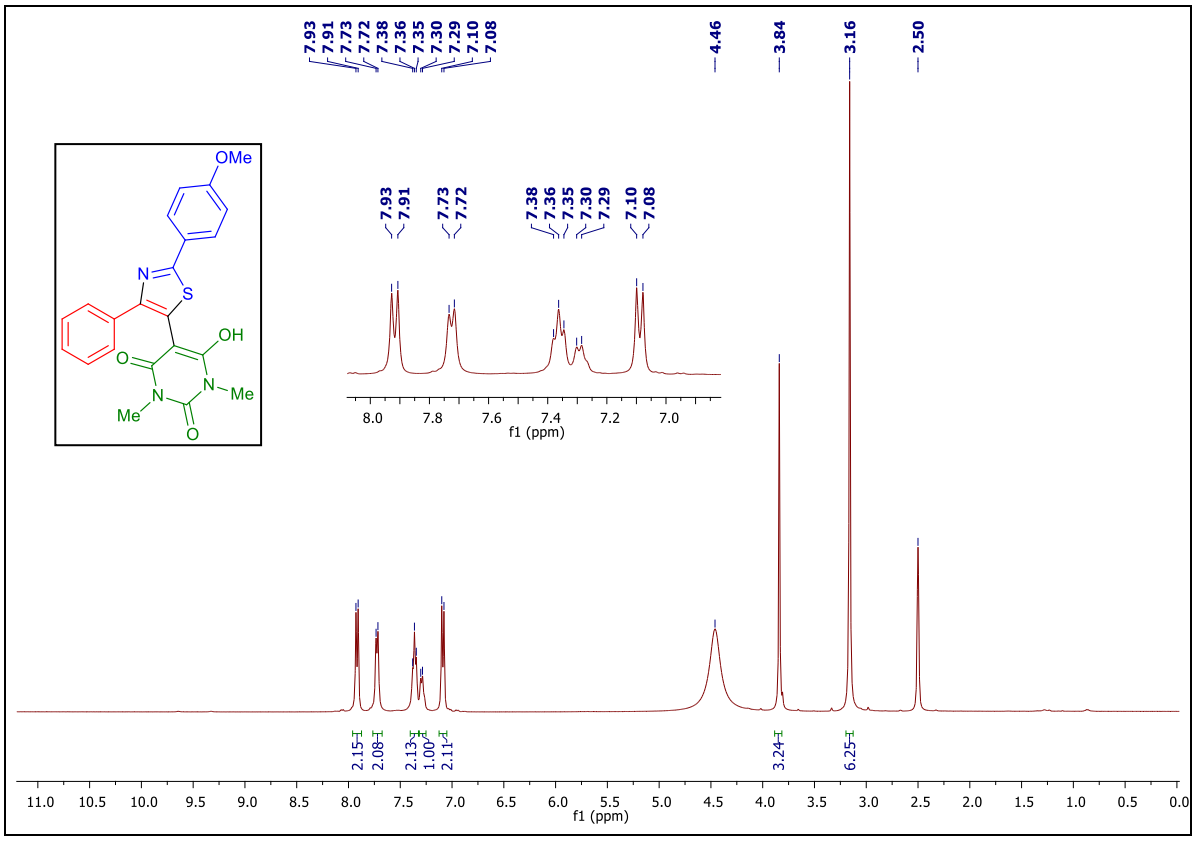


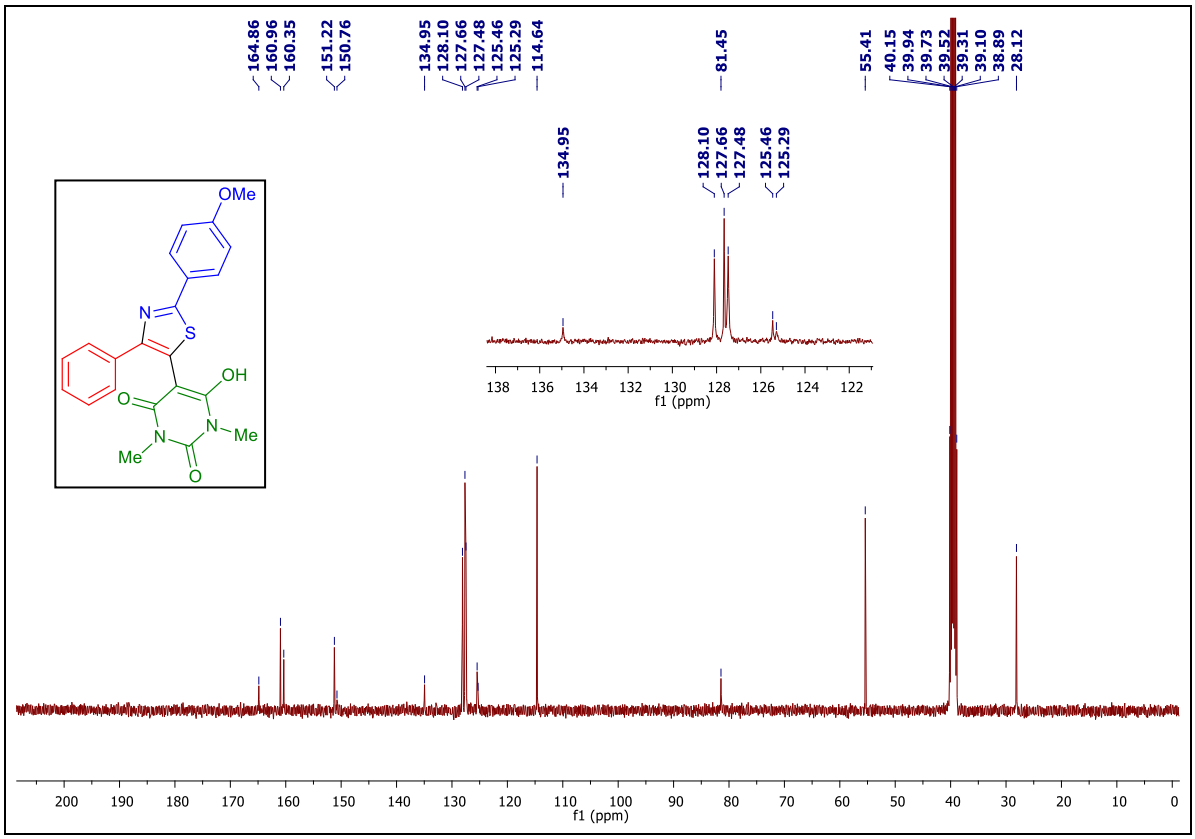
^{1}H and ^{13}C NMR spectra of 4f



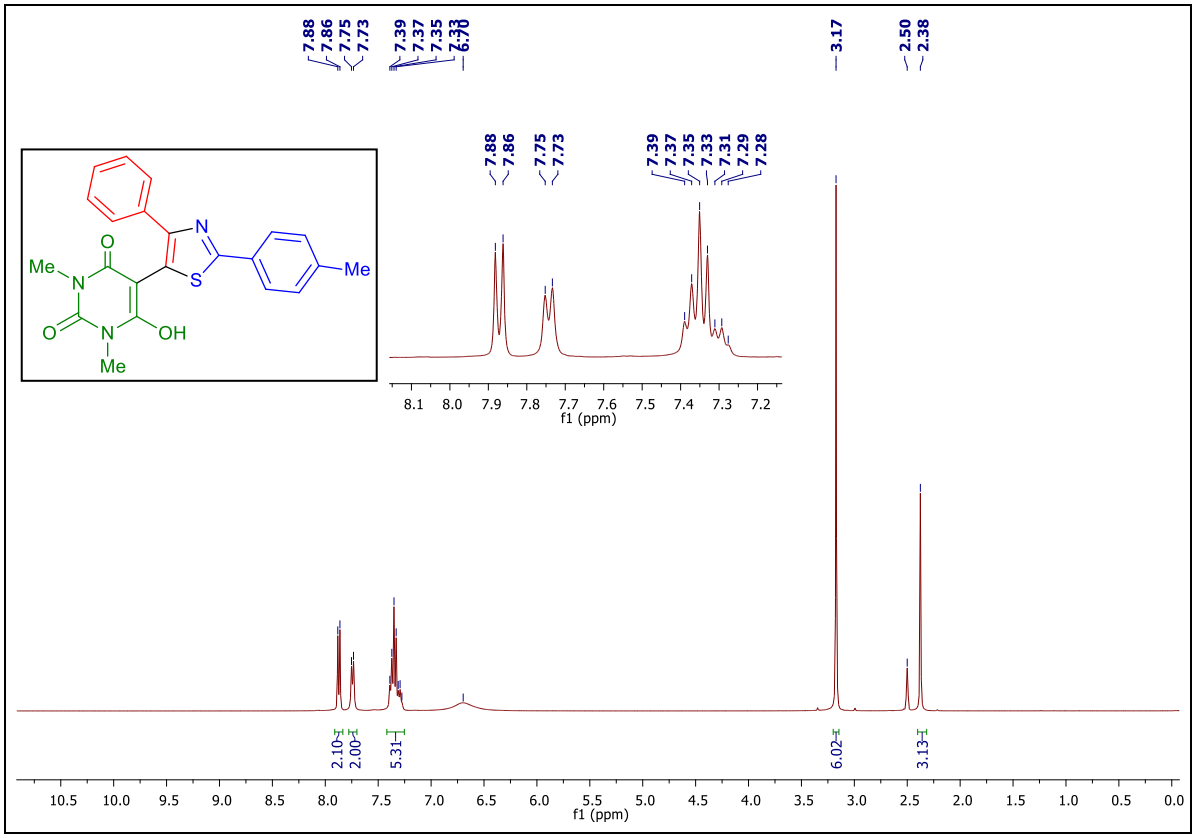


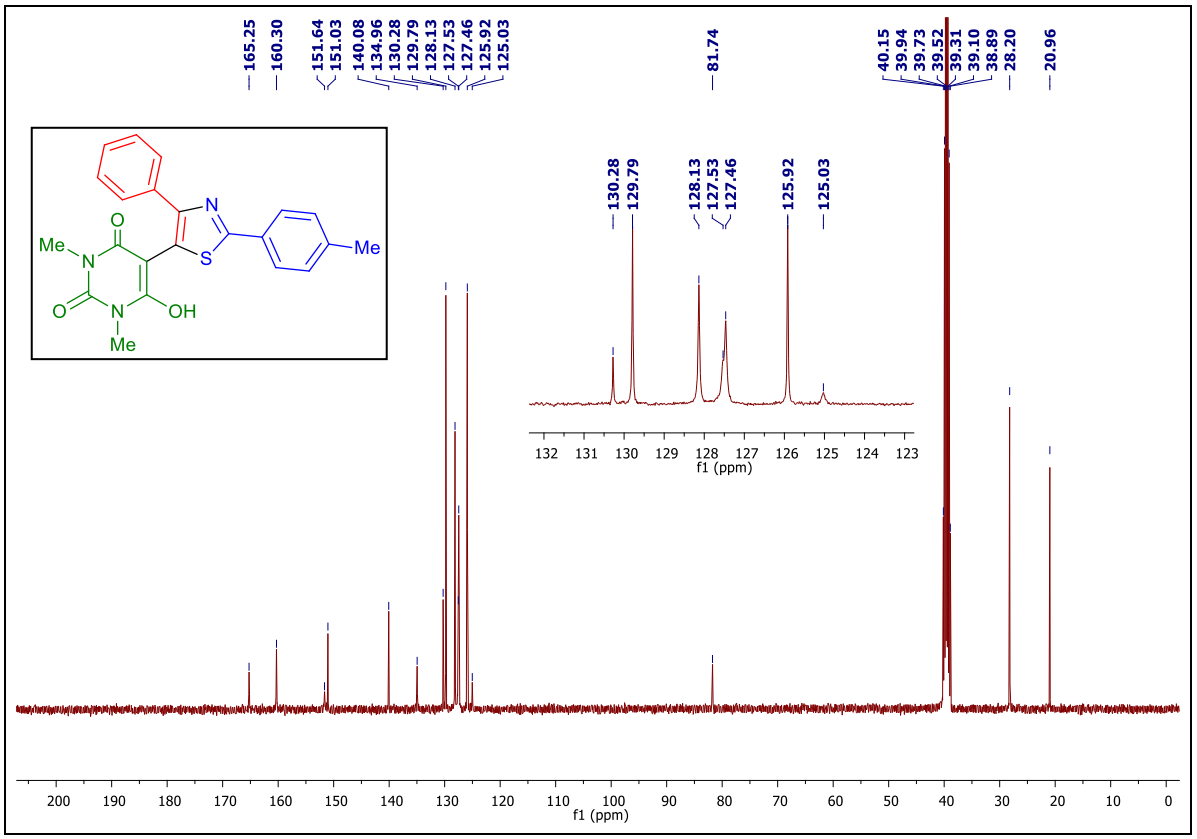
^{1}H and ^{13}C NMR spectra of 4g



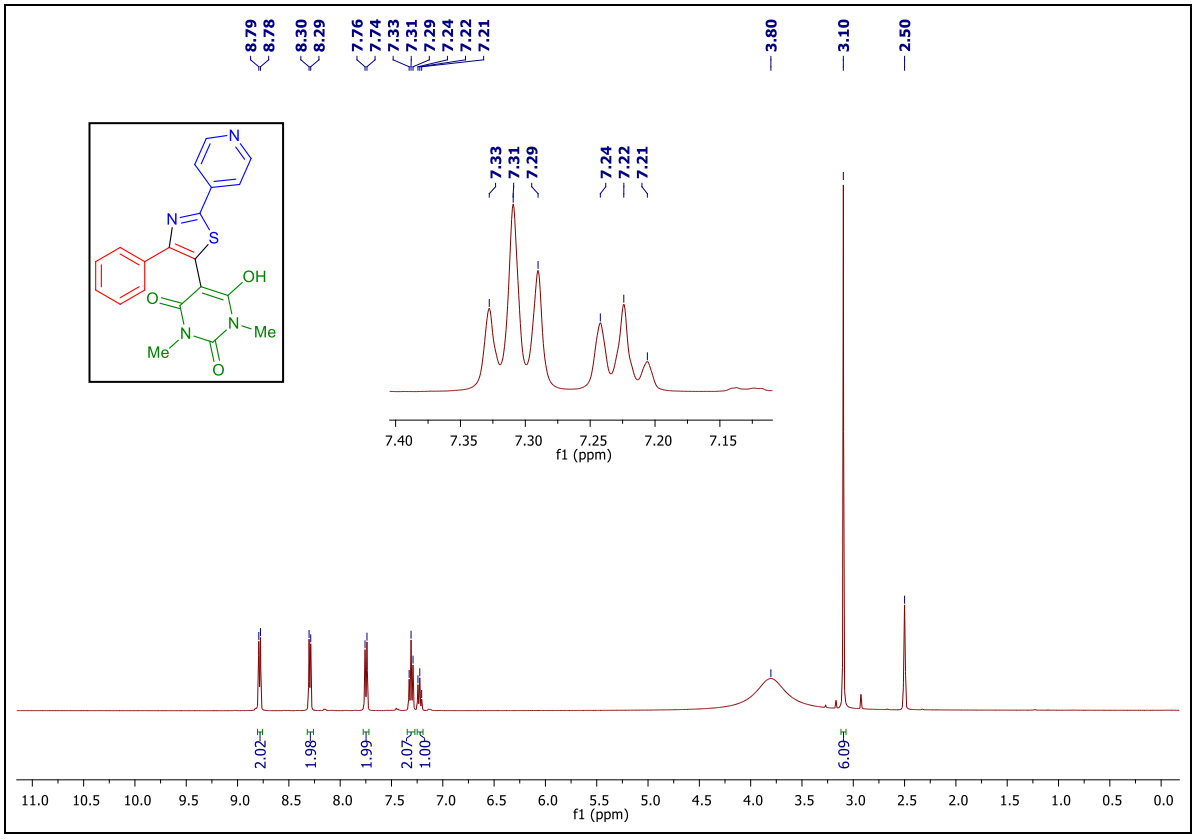


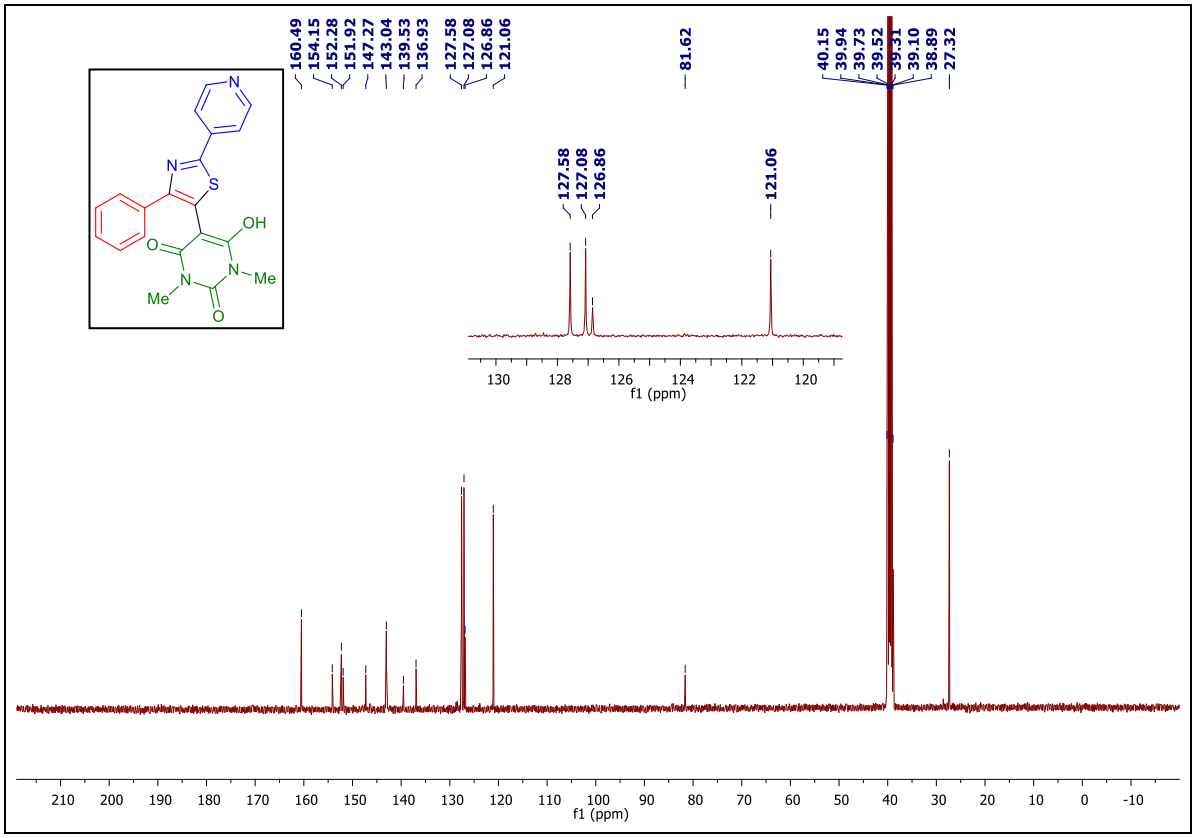
^{1}H and ^{13}C NMR spectra of 4h



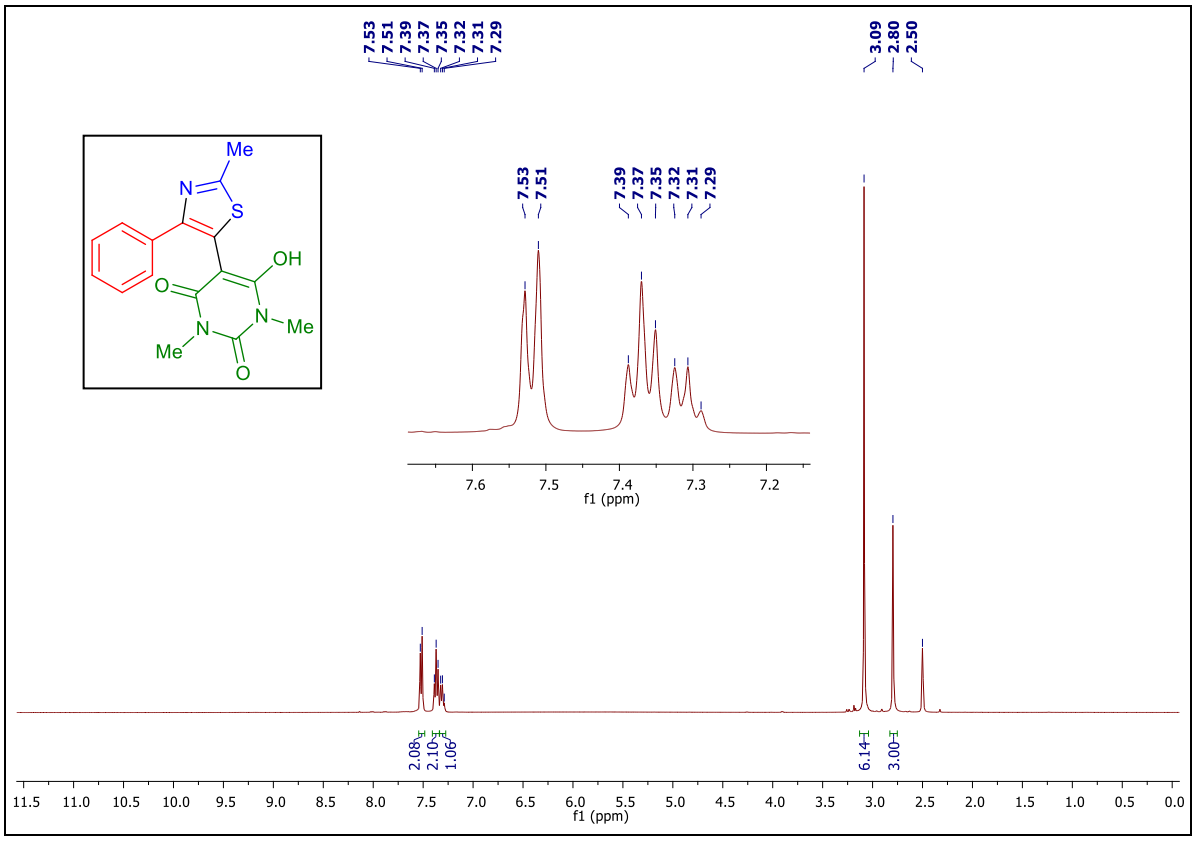


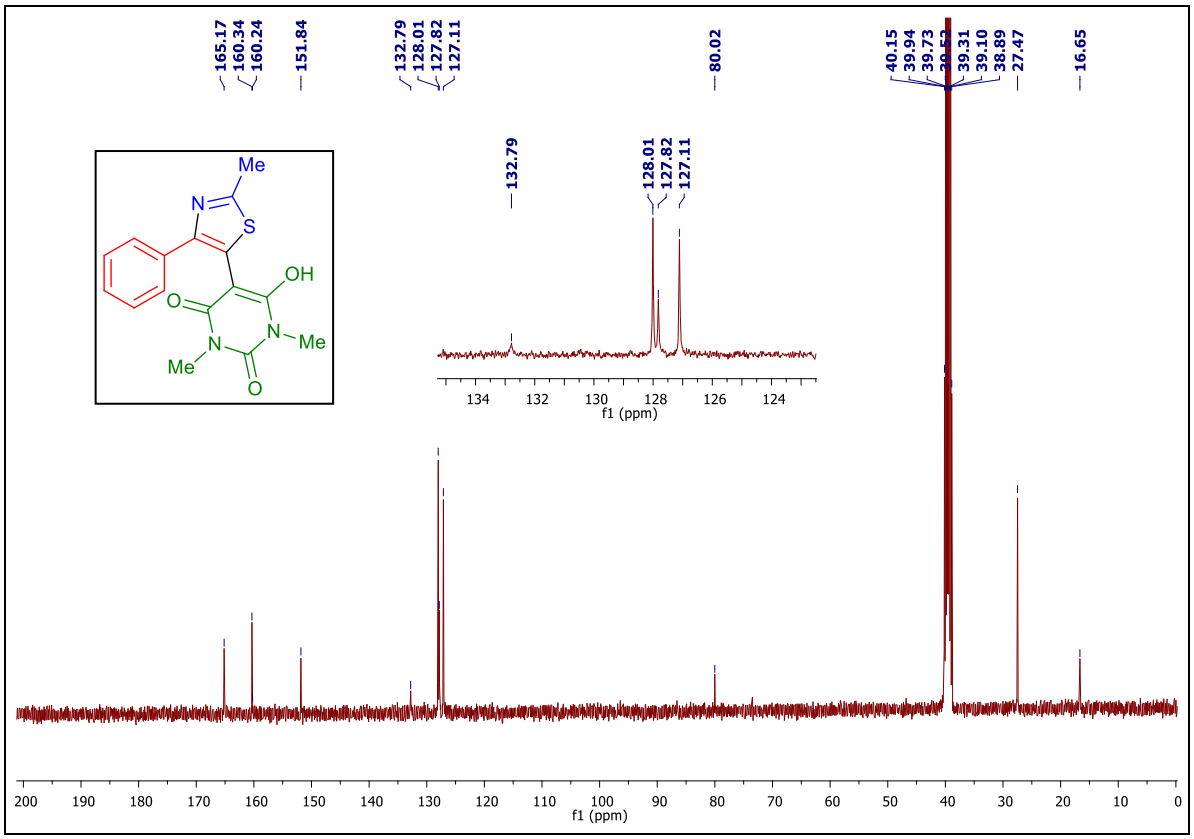
^{1}H and ^{13}C NMR spectra of 4i



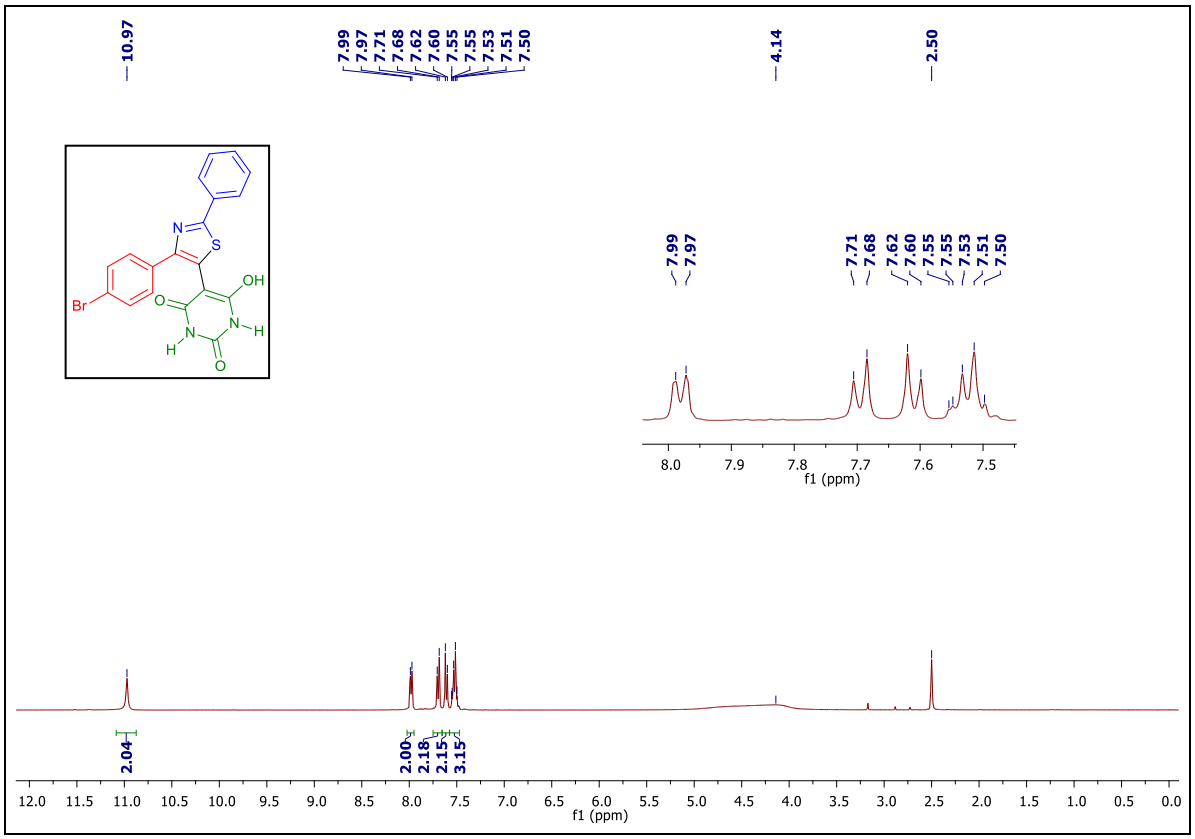


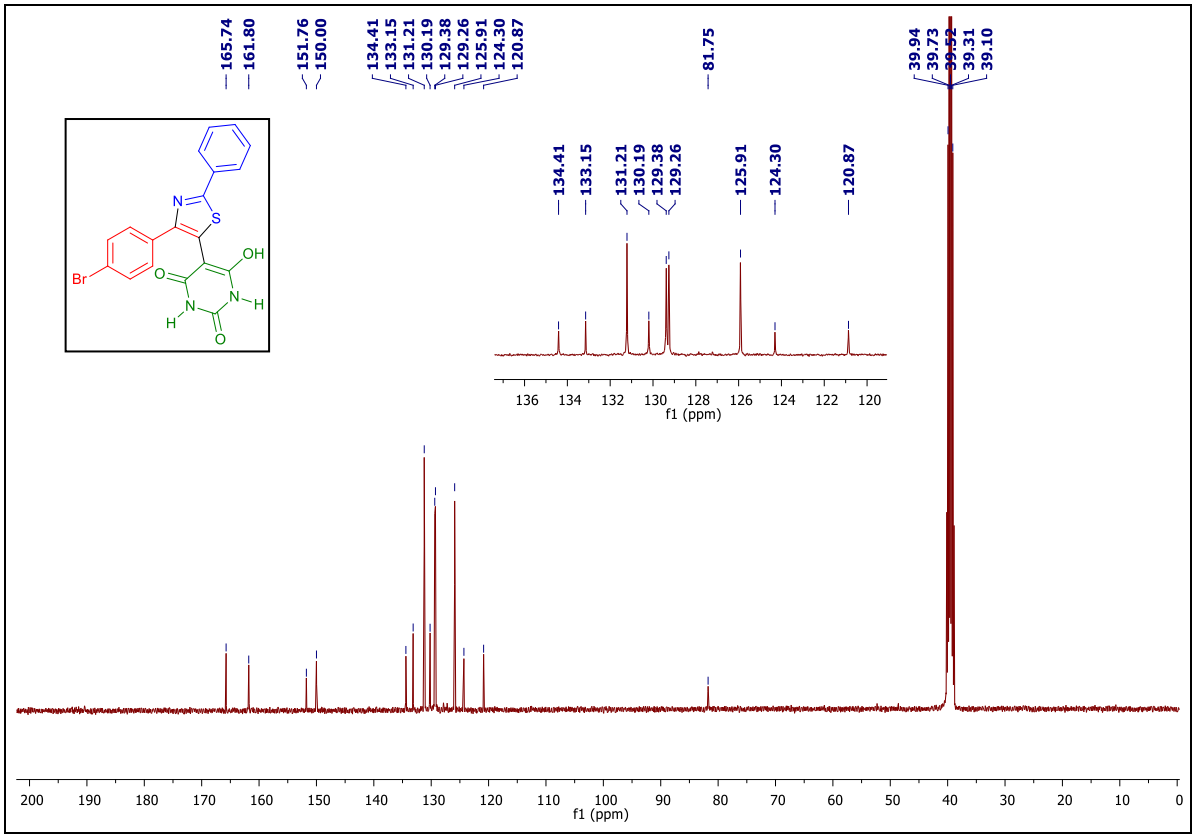
^{1}H and ^{13}C NMR spectra of 4j



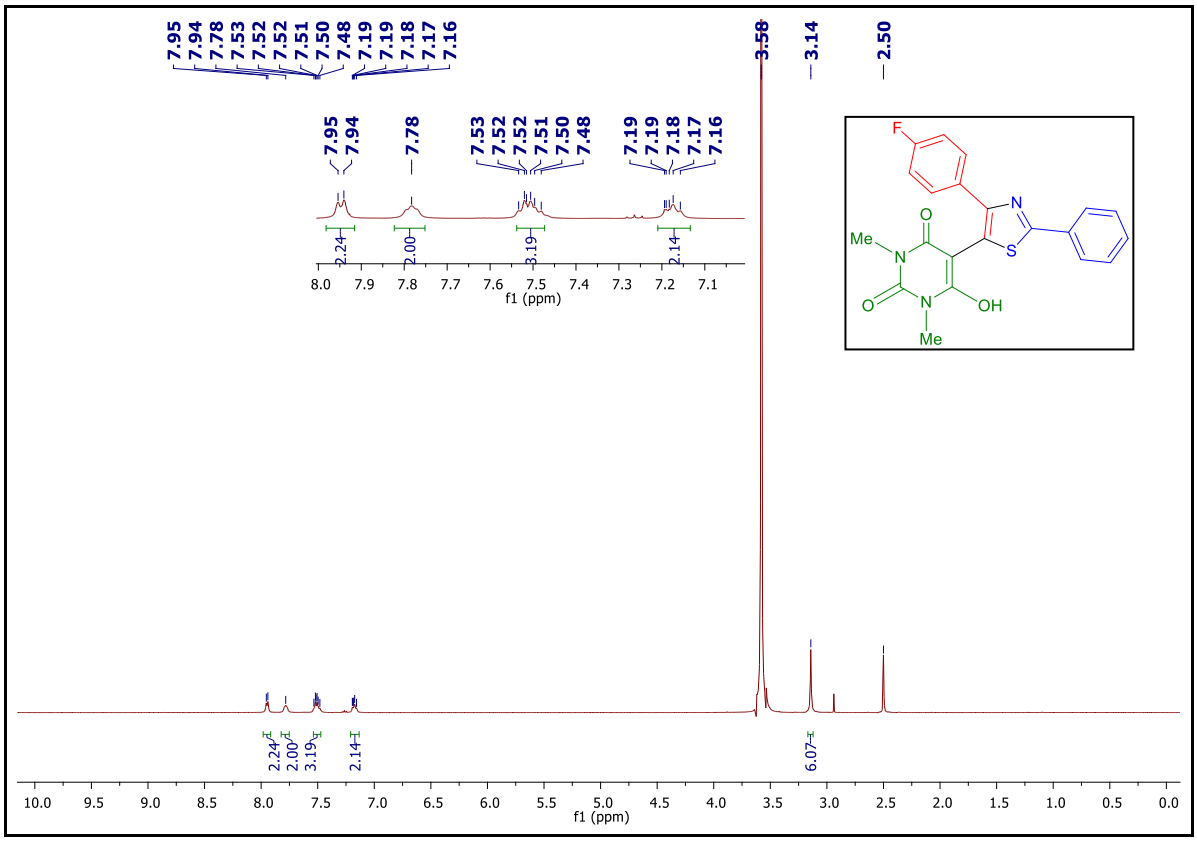


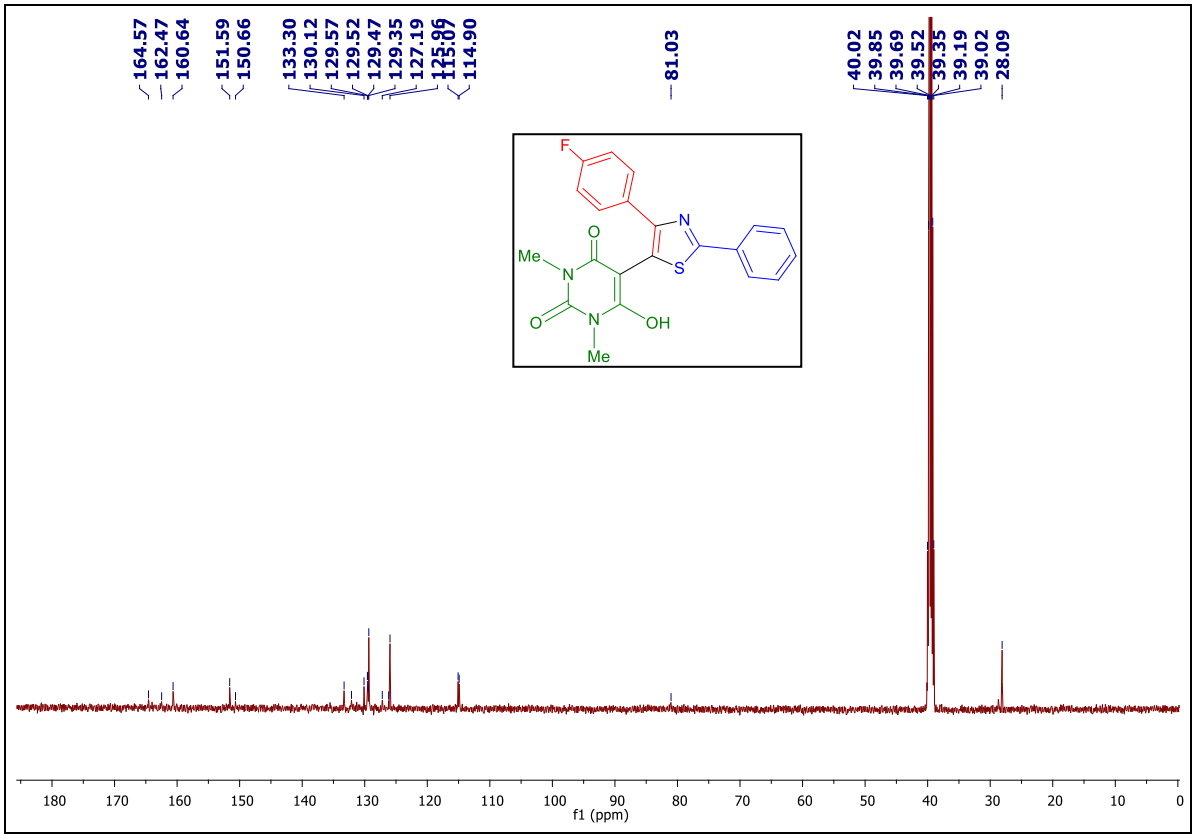
^{1}H and ^{13}C NMR spectra of 4k



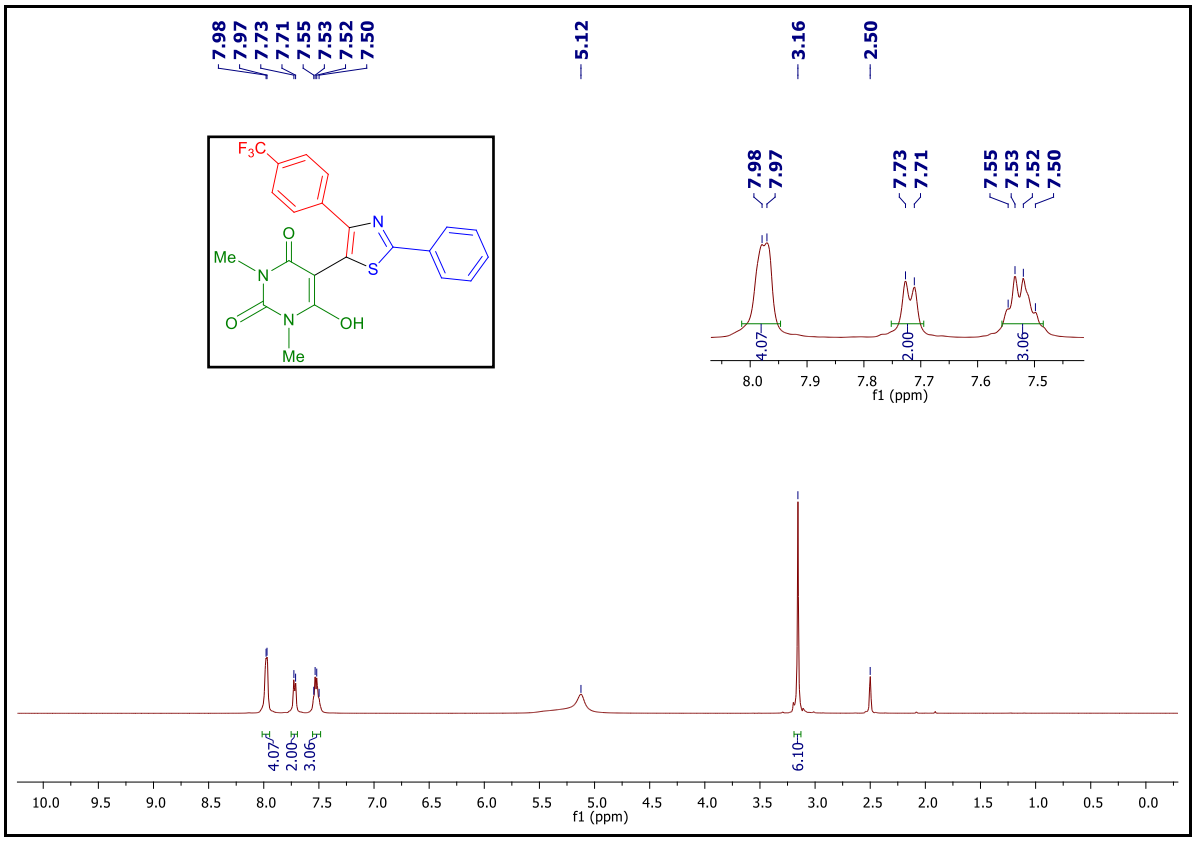


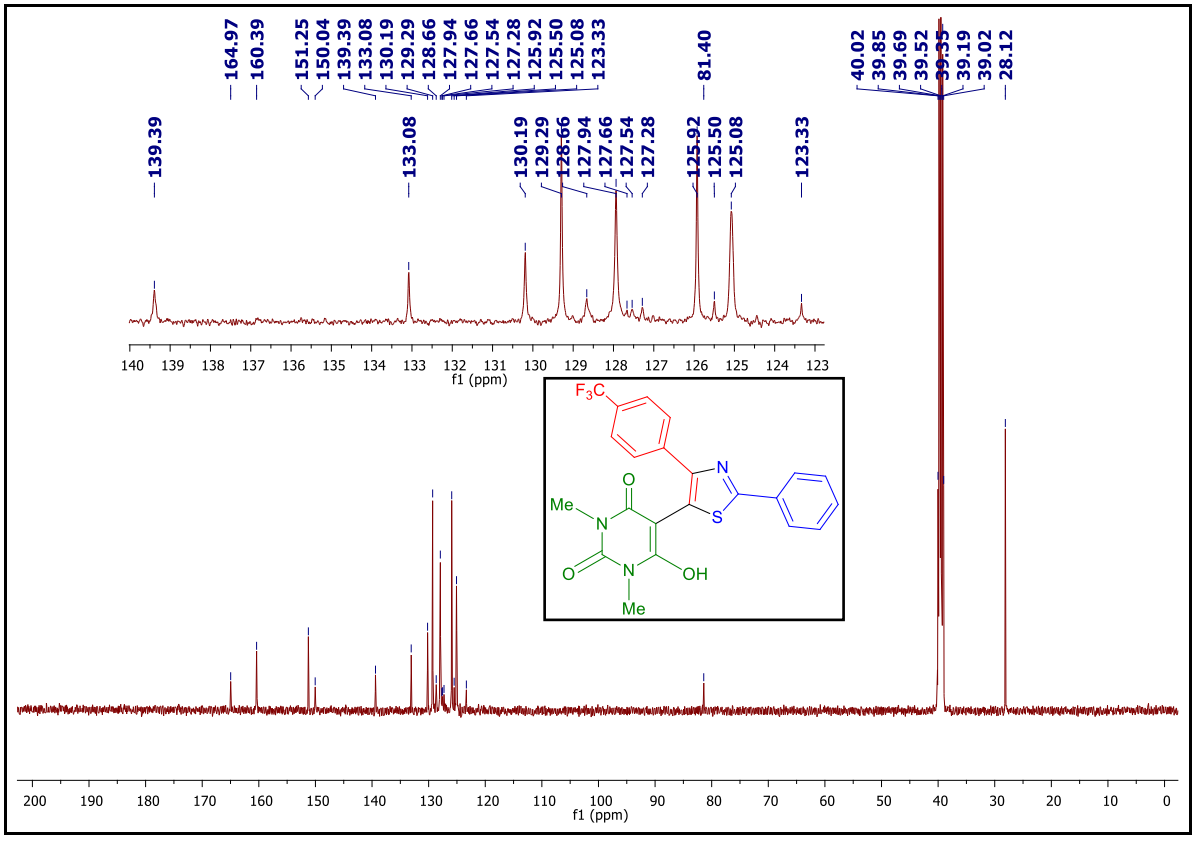
^{1}H and ^{13}C NMR spectra of 4l



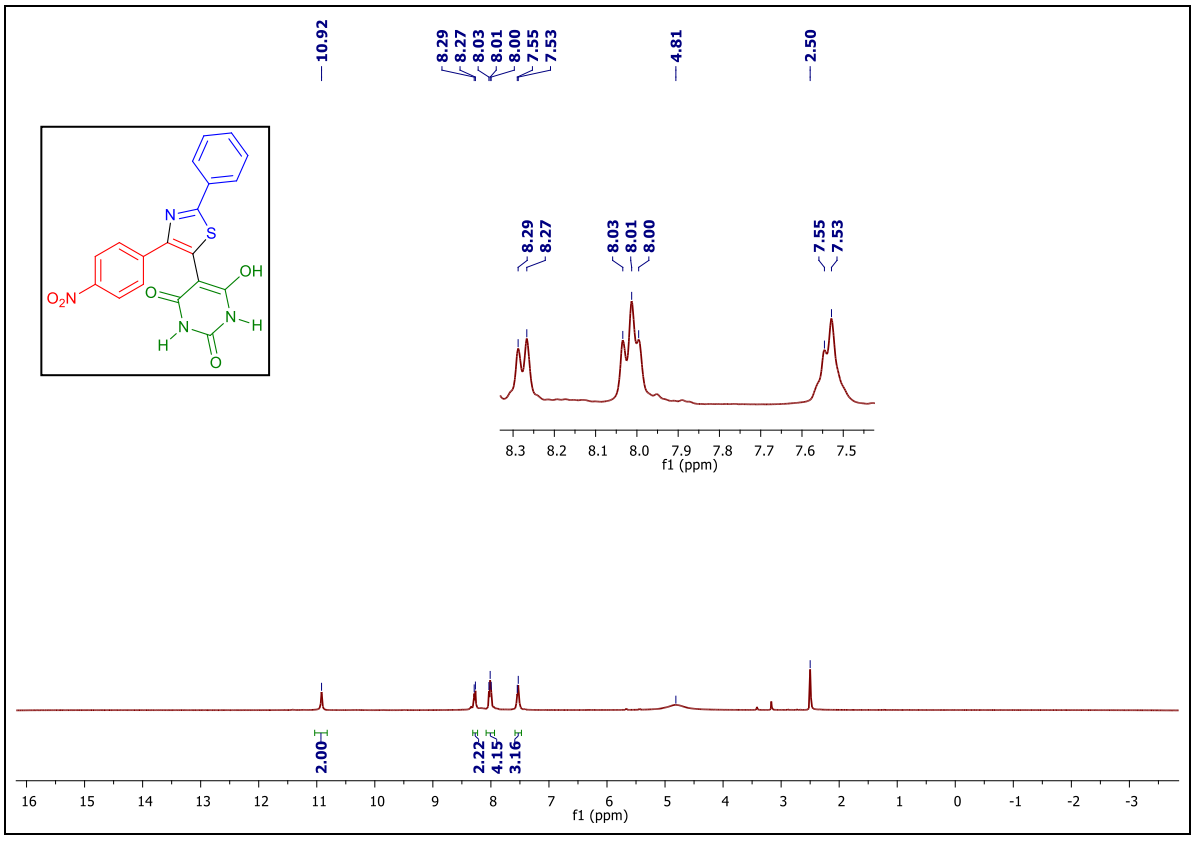


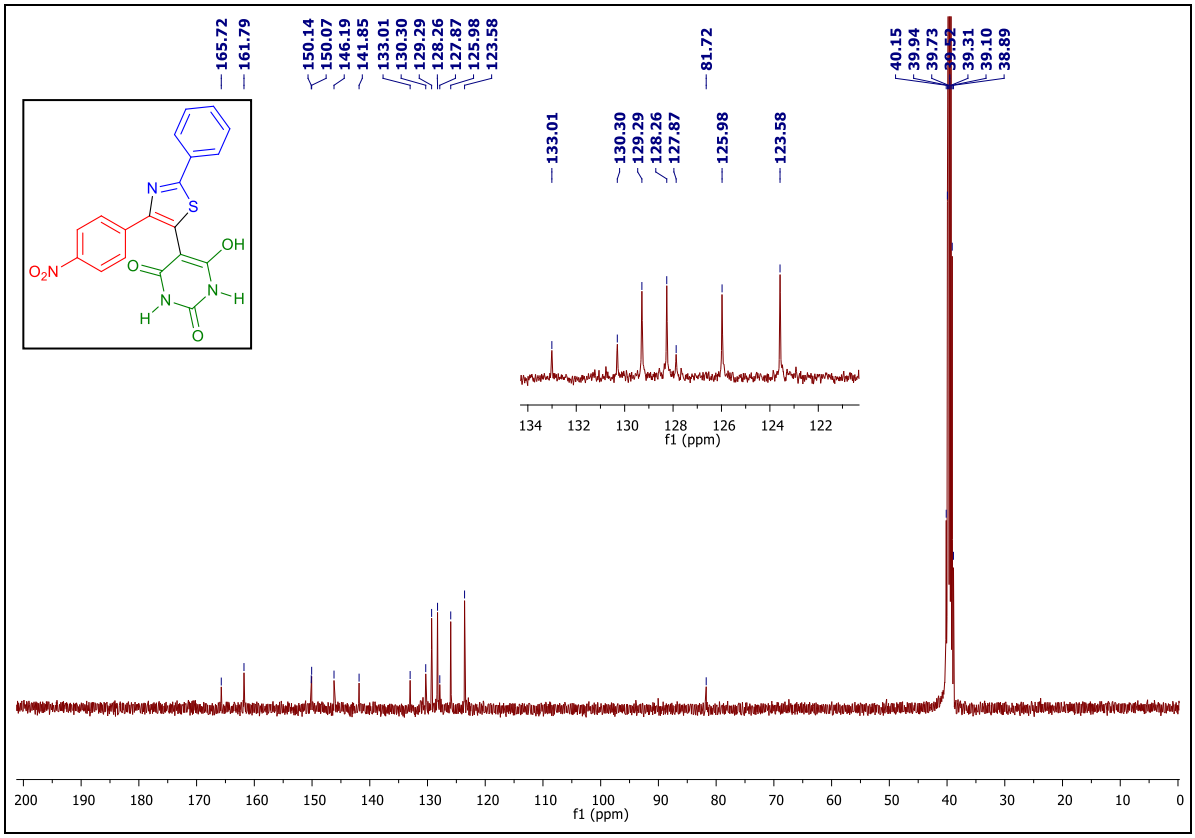
^{1}H and ^{13}C NMR spectra of 4m



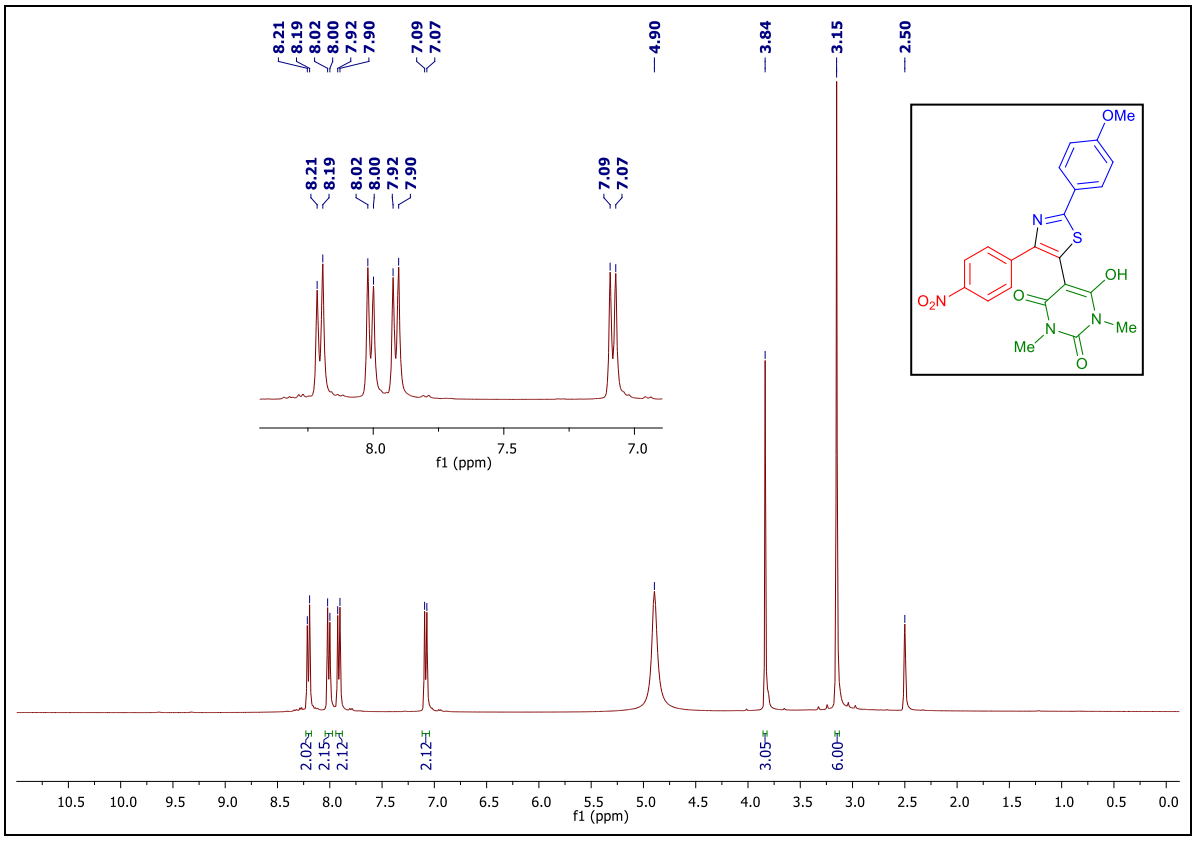


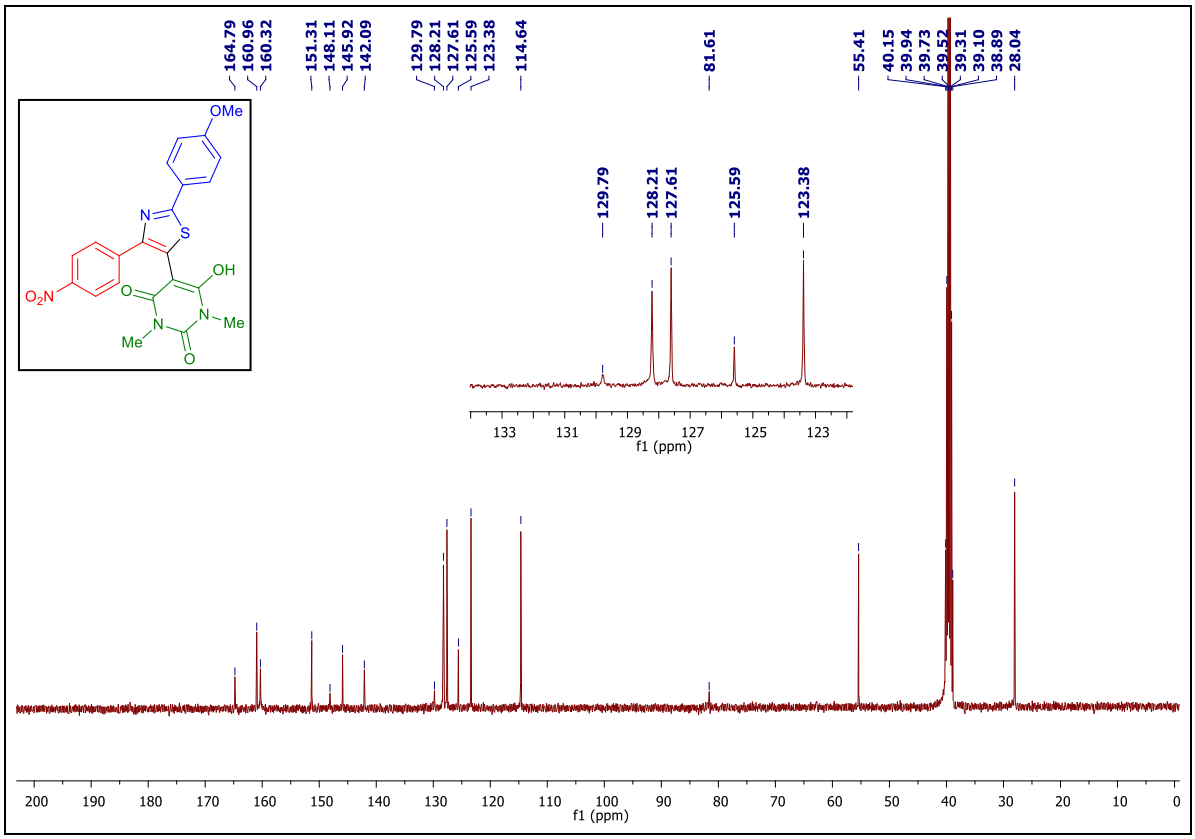
^{1}H and ^{13}C NMR spectra of 4n



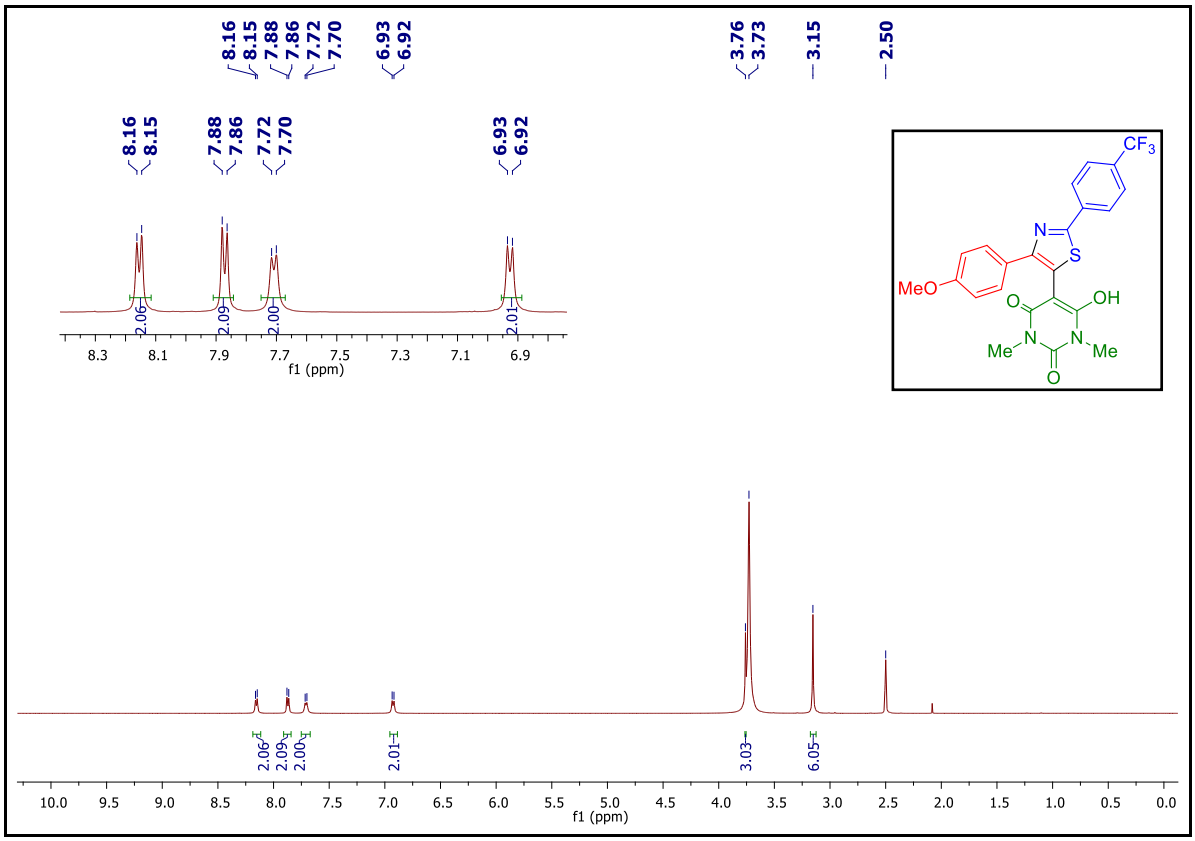


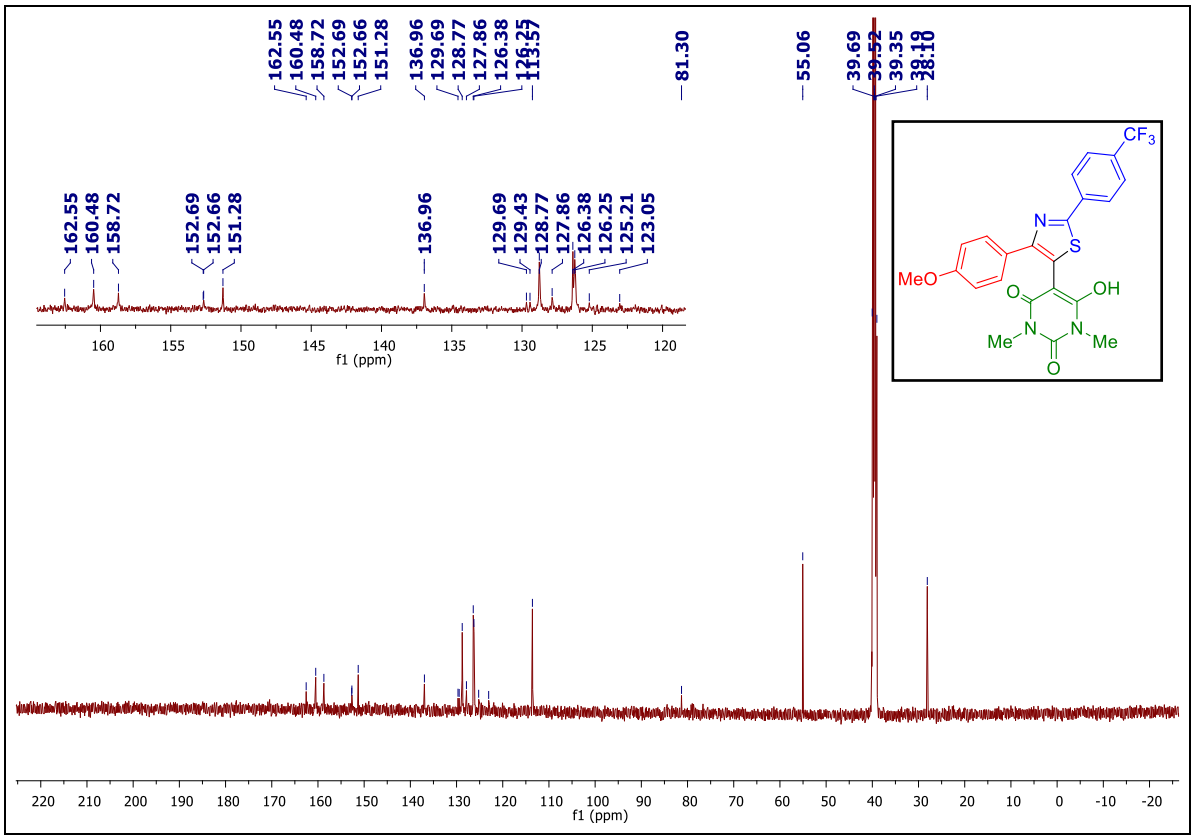
^{1}H and ^{13}C NMR spectra of 4o



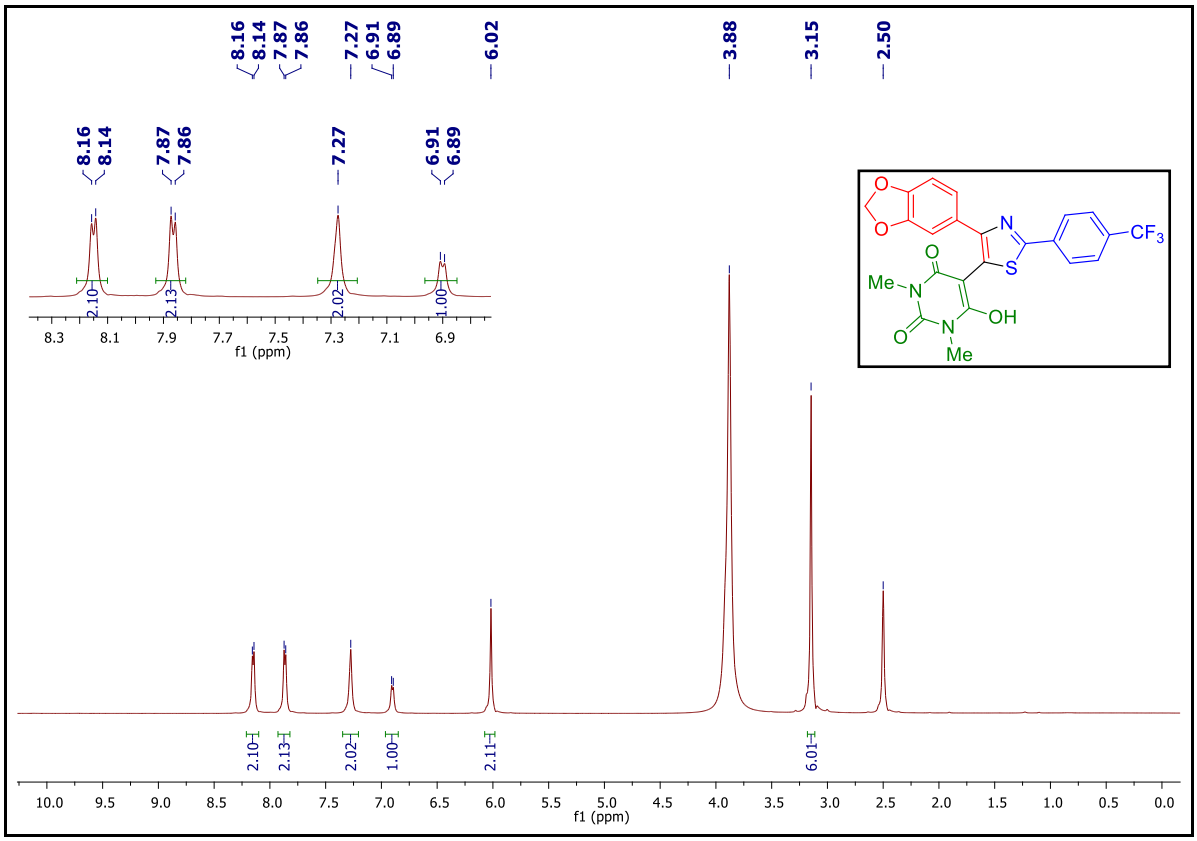


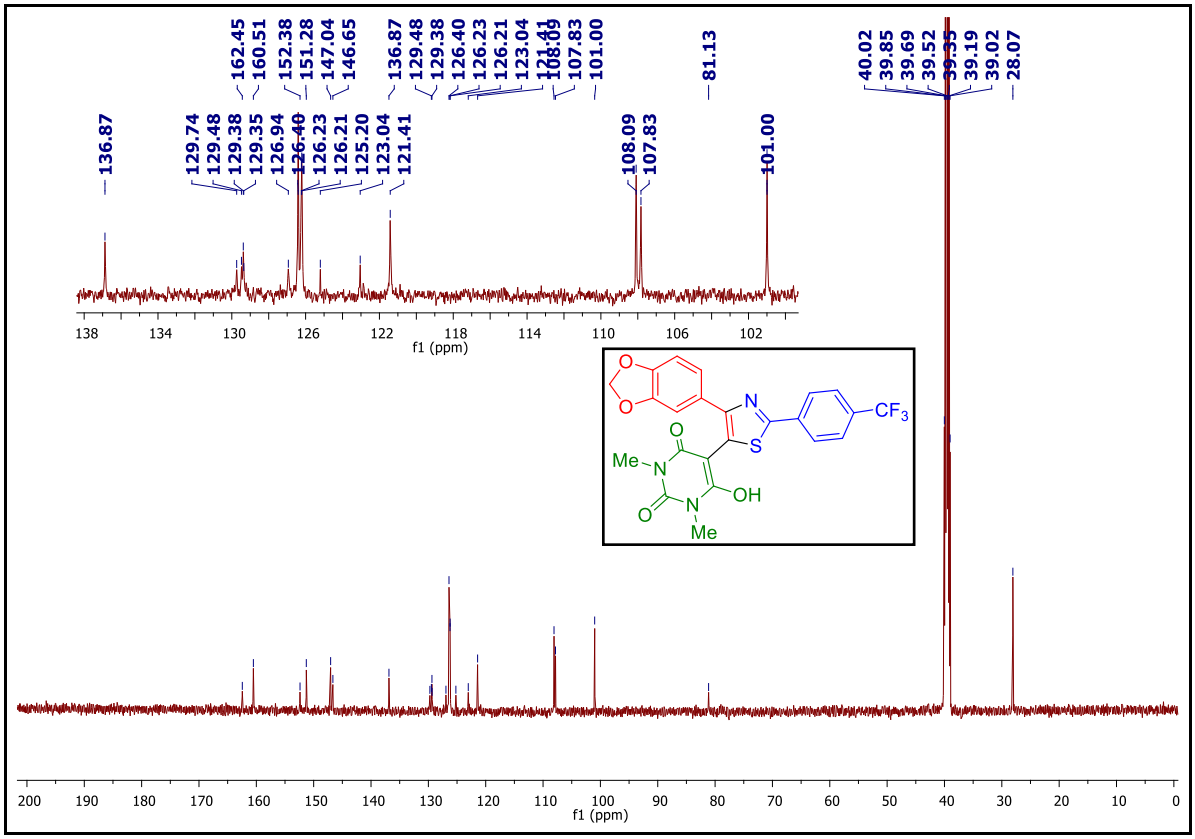
^{1}H and ^{13}C NMR spectra of 4p



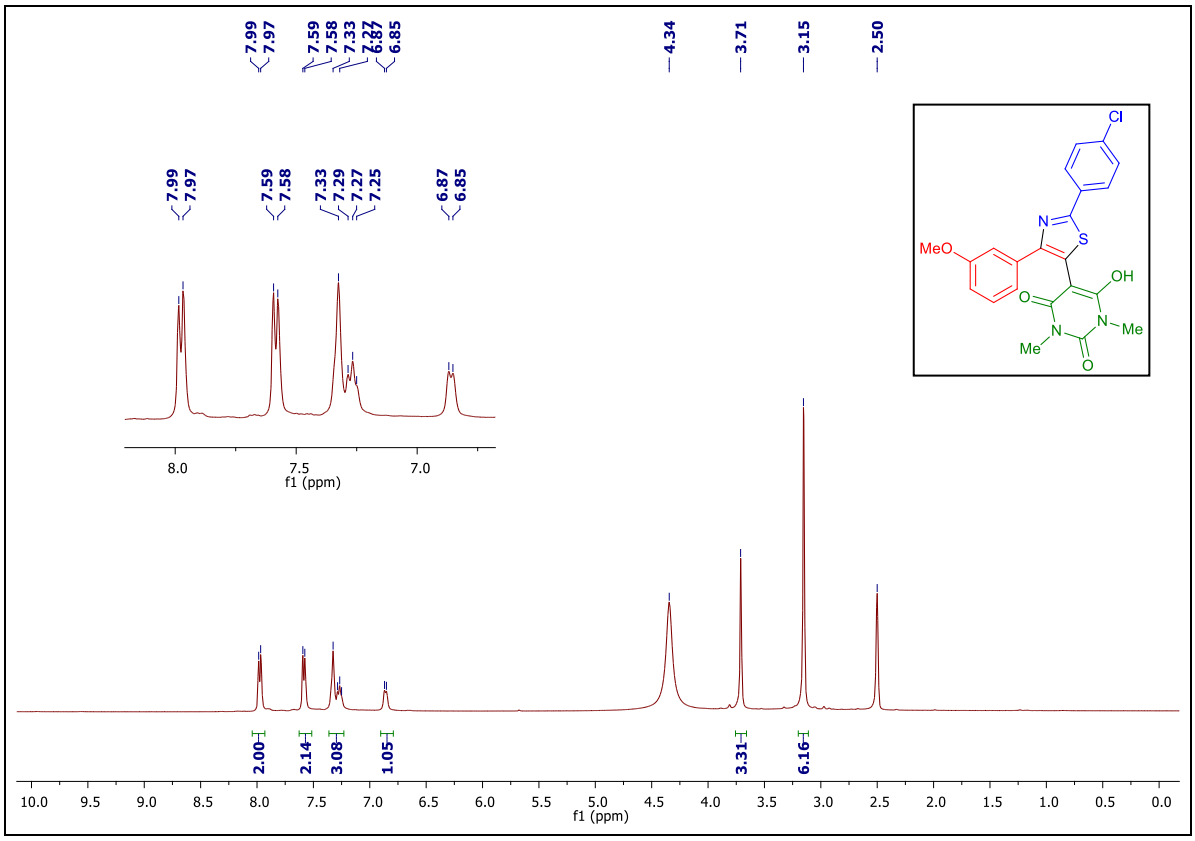


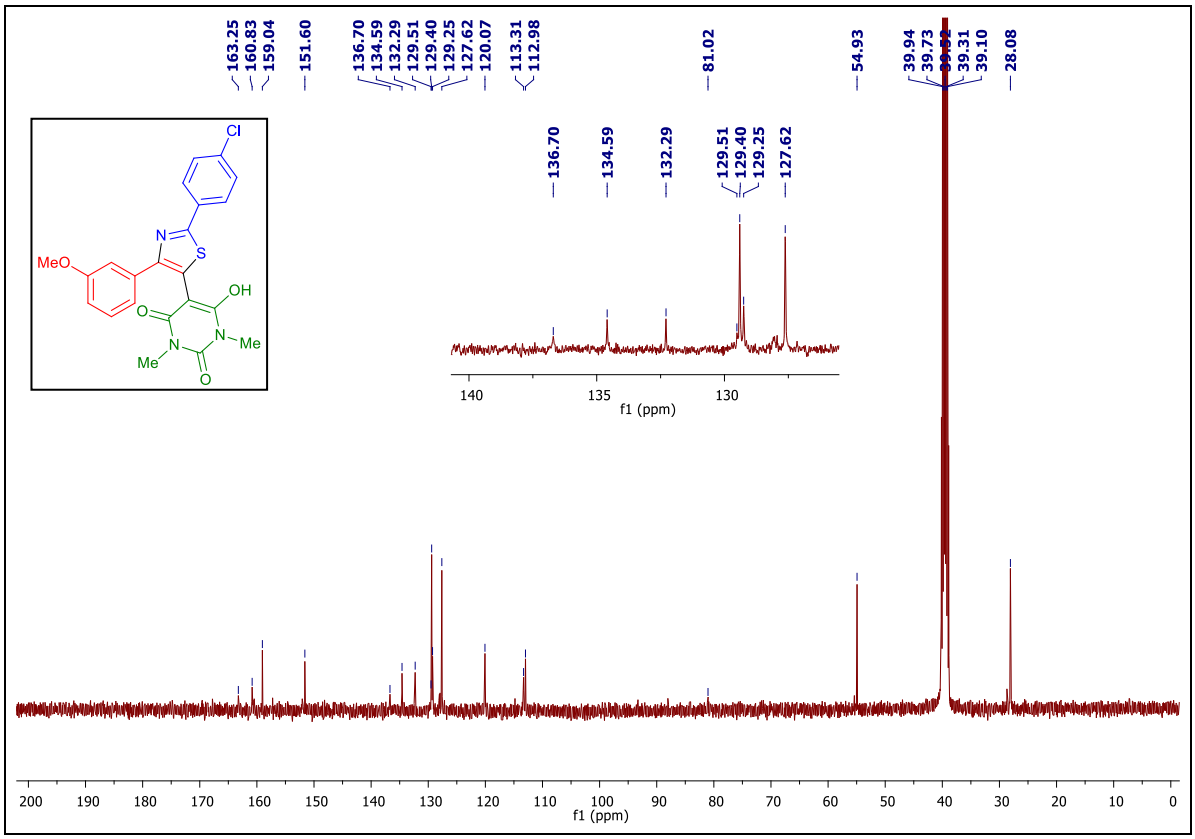
^{1}H and ^{13}C NMR spectra of 4q



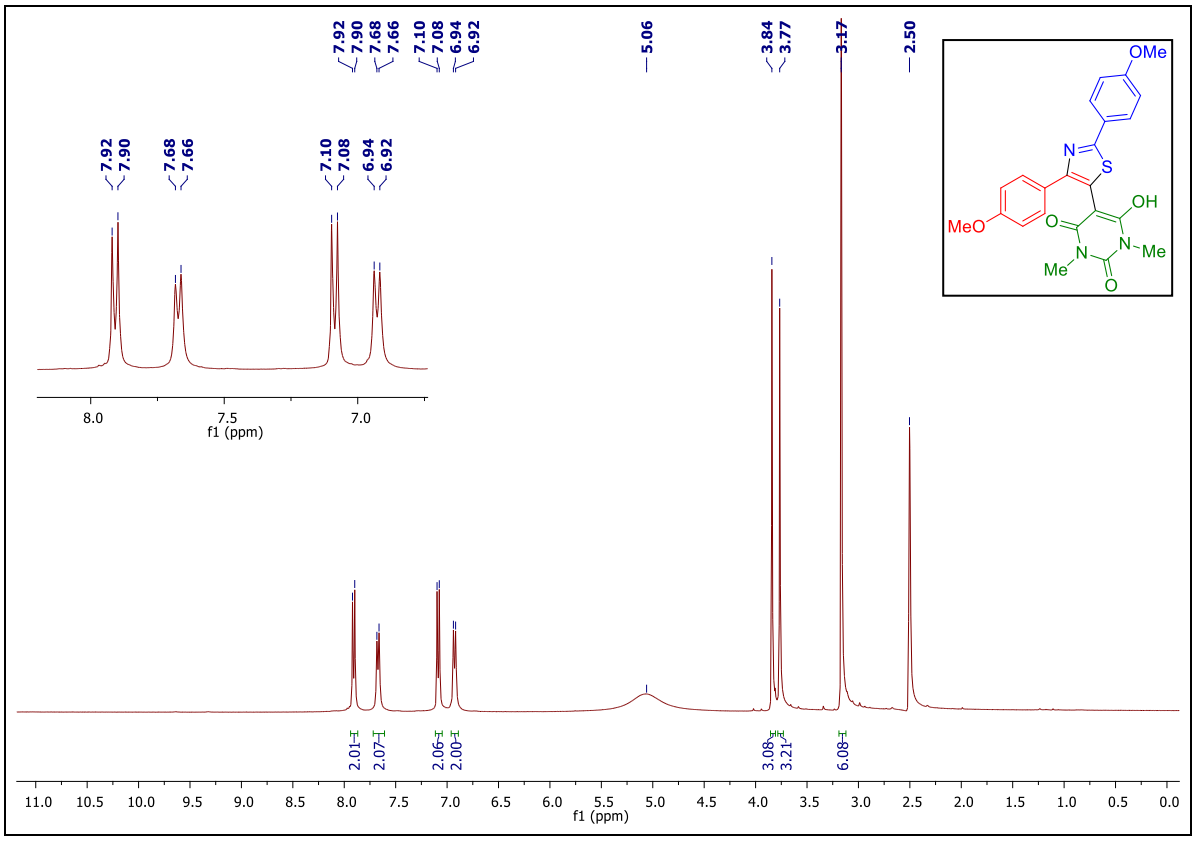


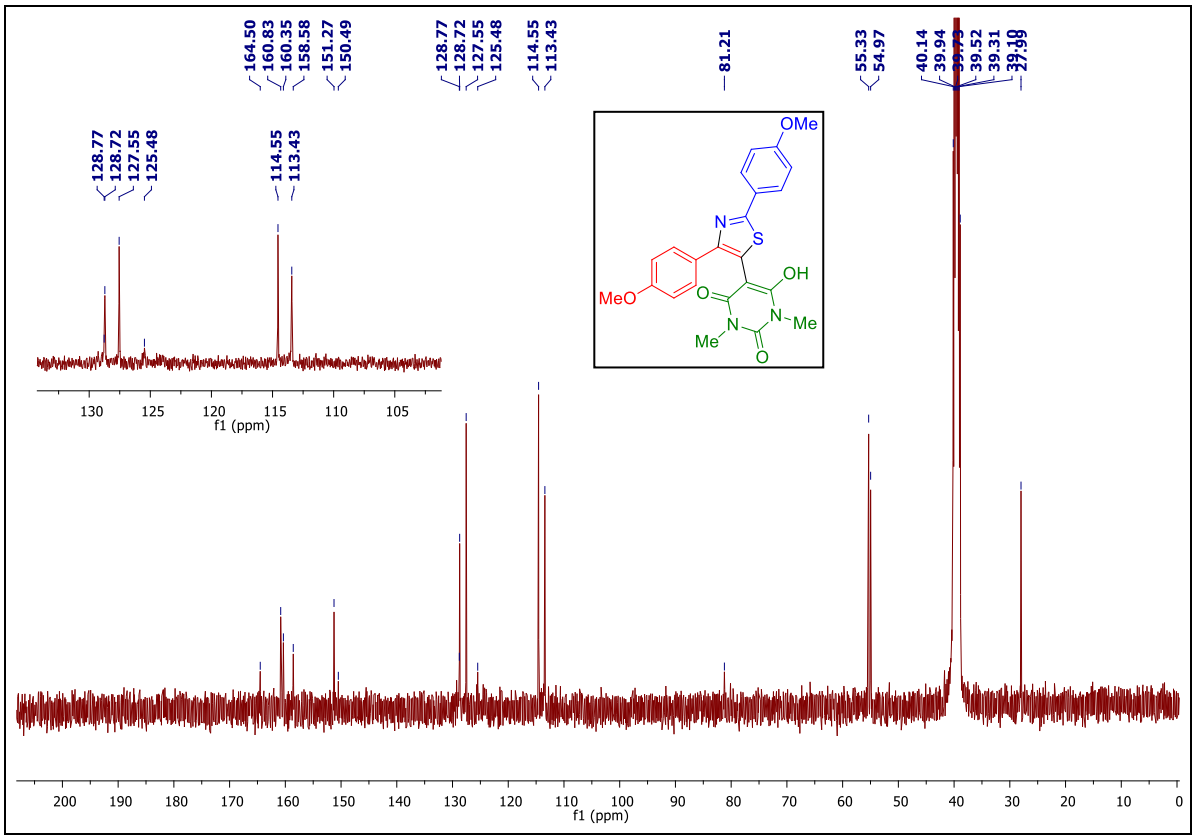
^{1}H and ^{13}C NMR spectra of 4r



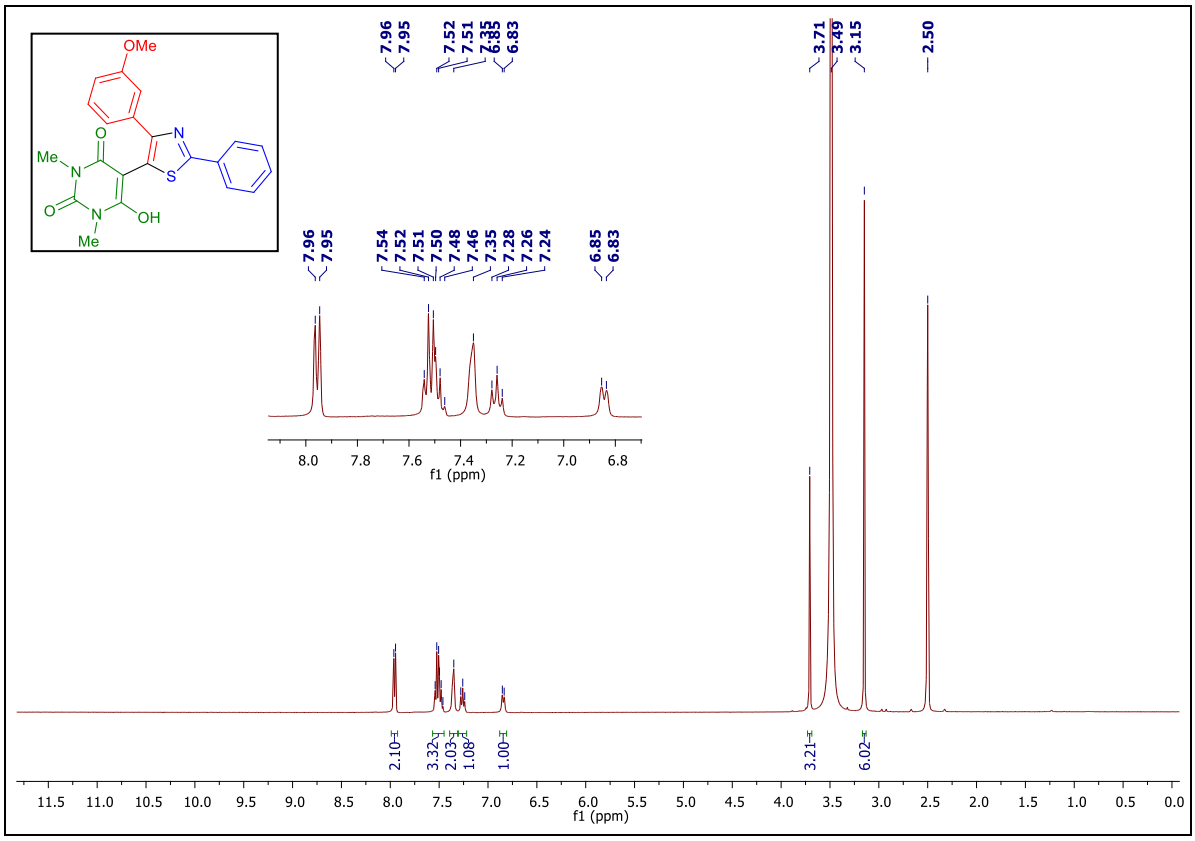


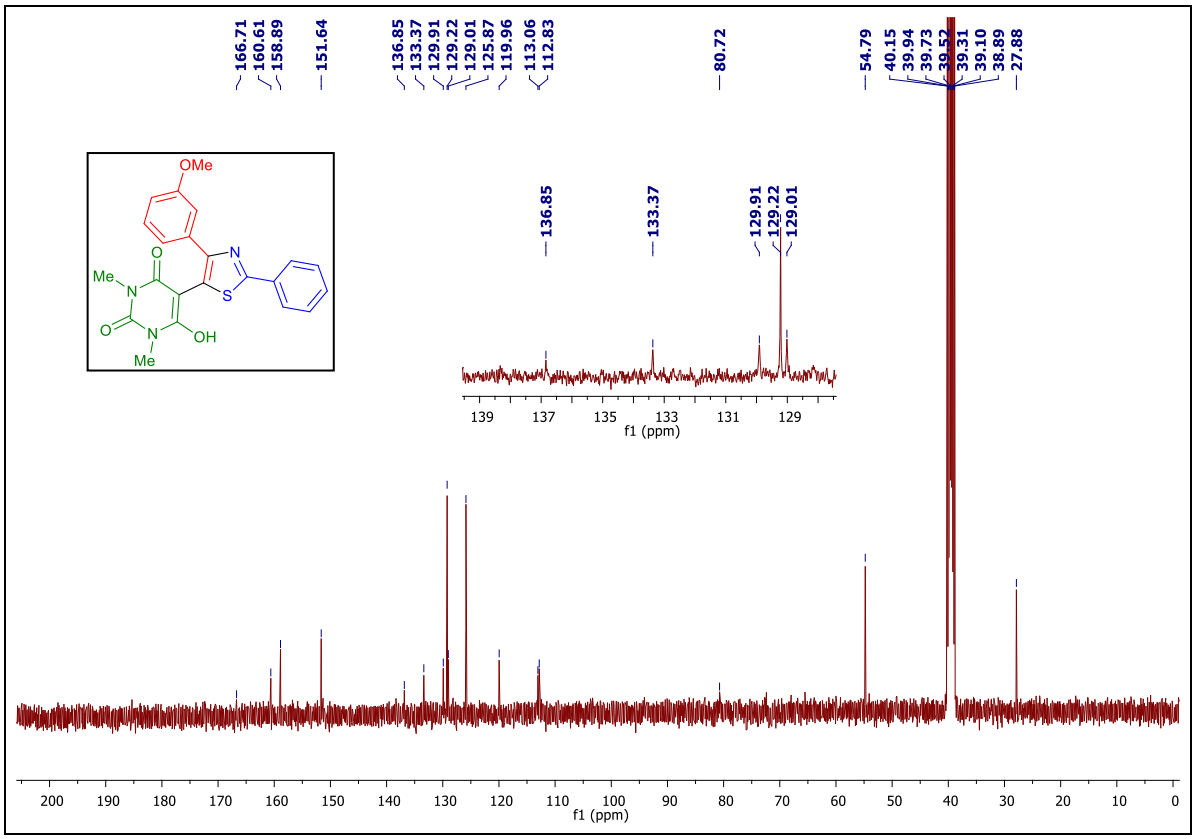
^{1}H and ^{13}C NMR spectra of 4s



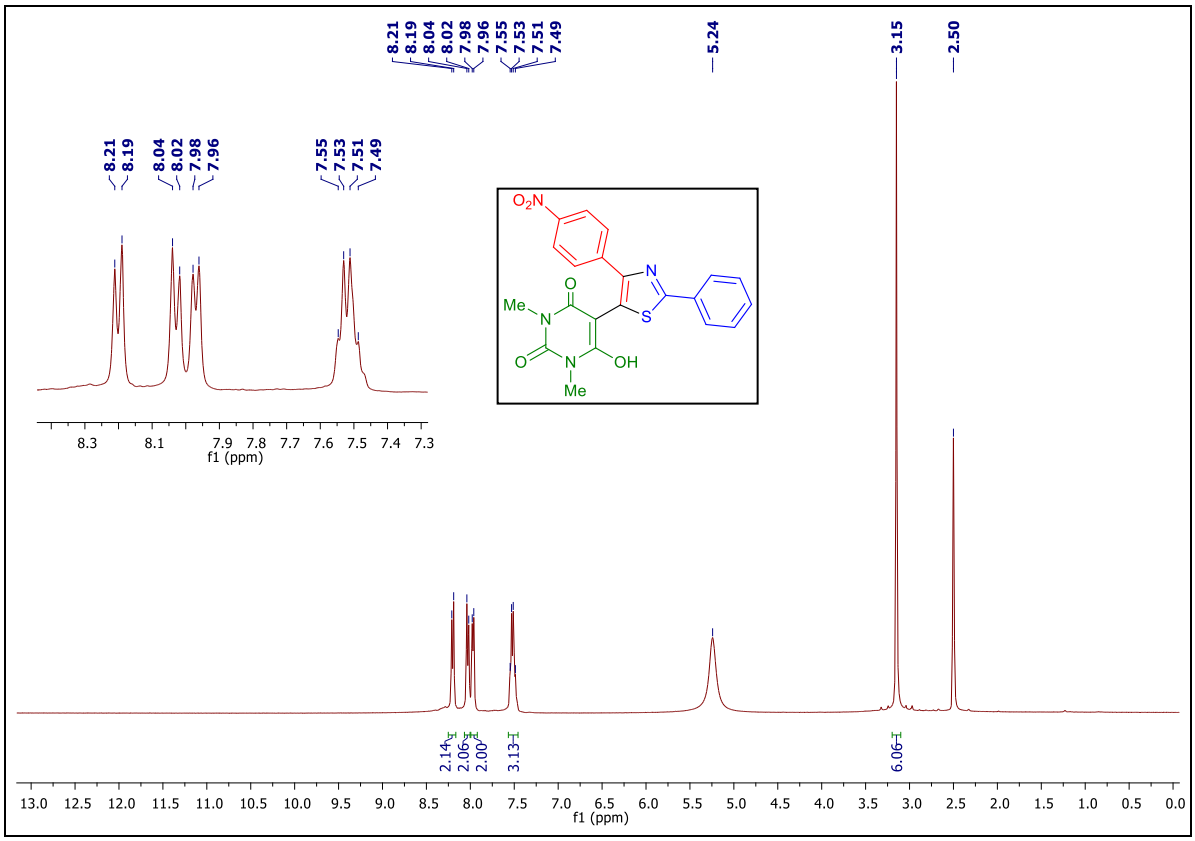


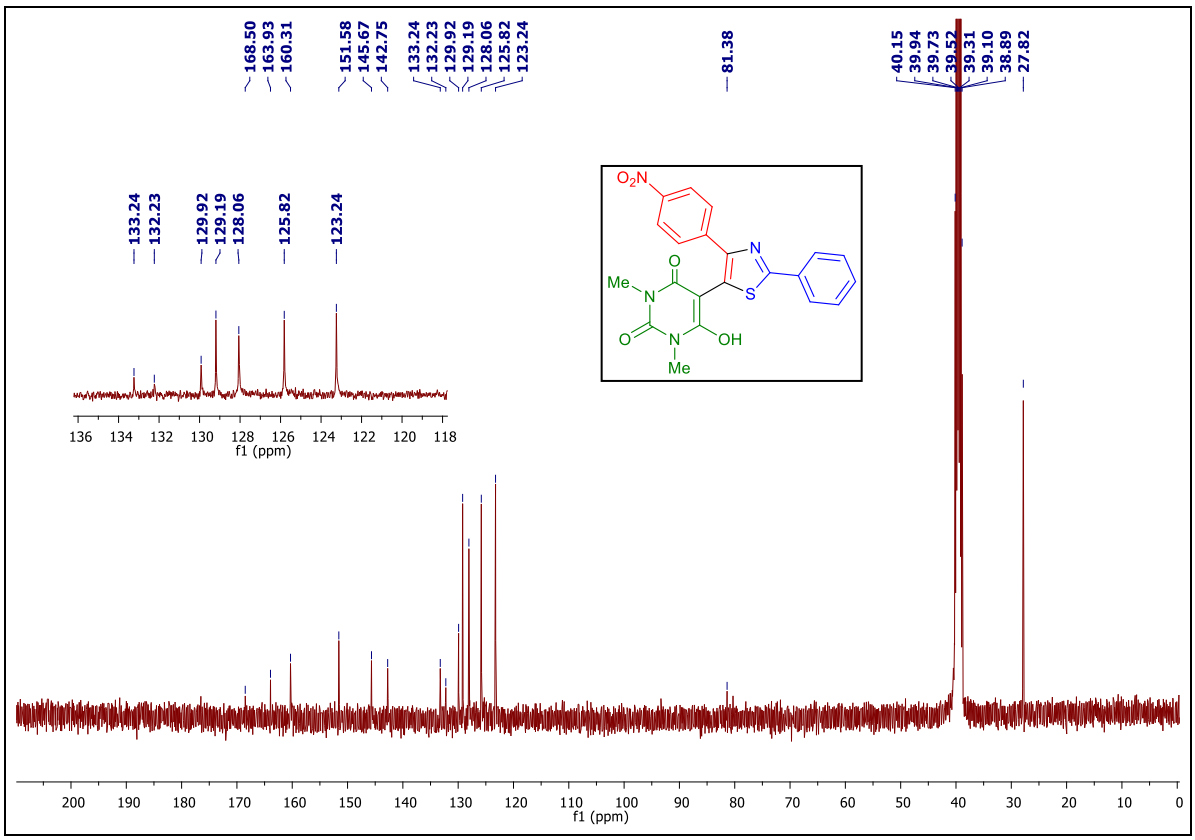
^{1}H and ^{13}C NMR spectra of 4t



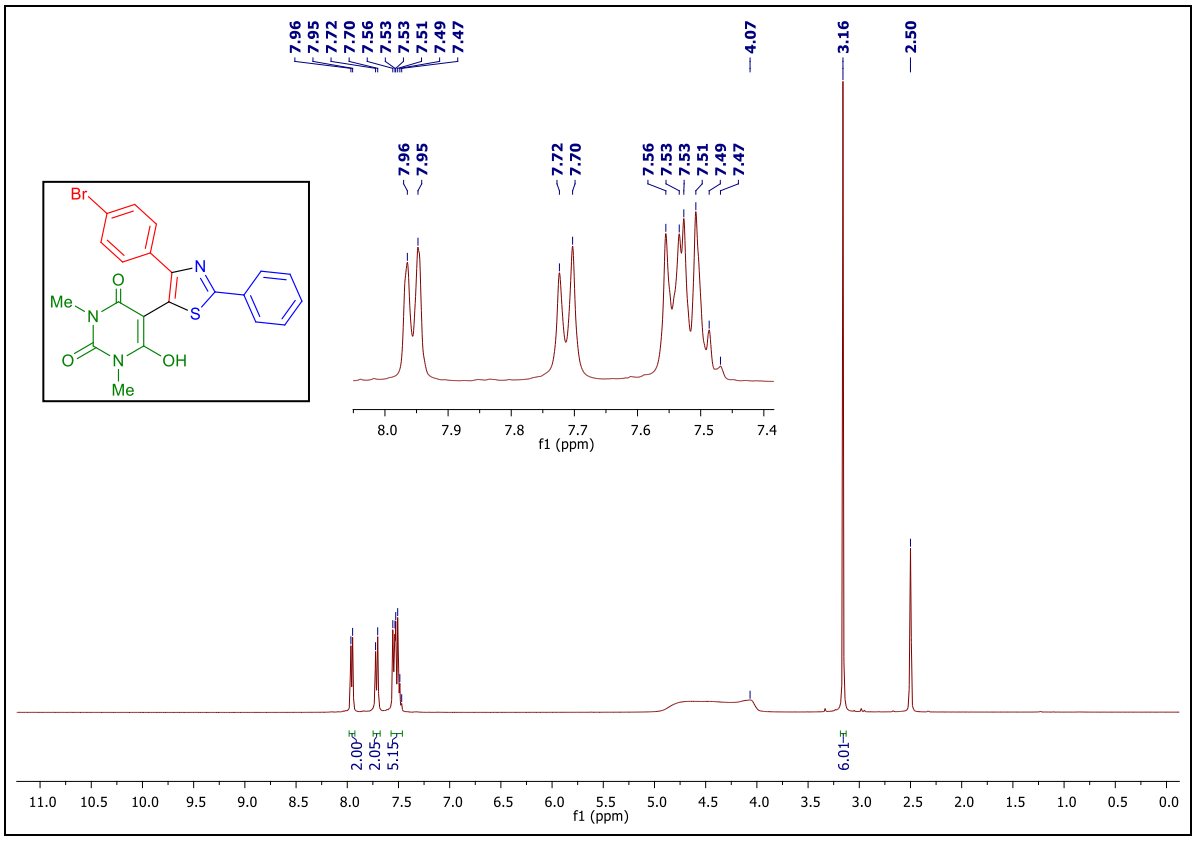


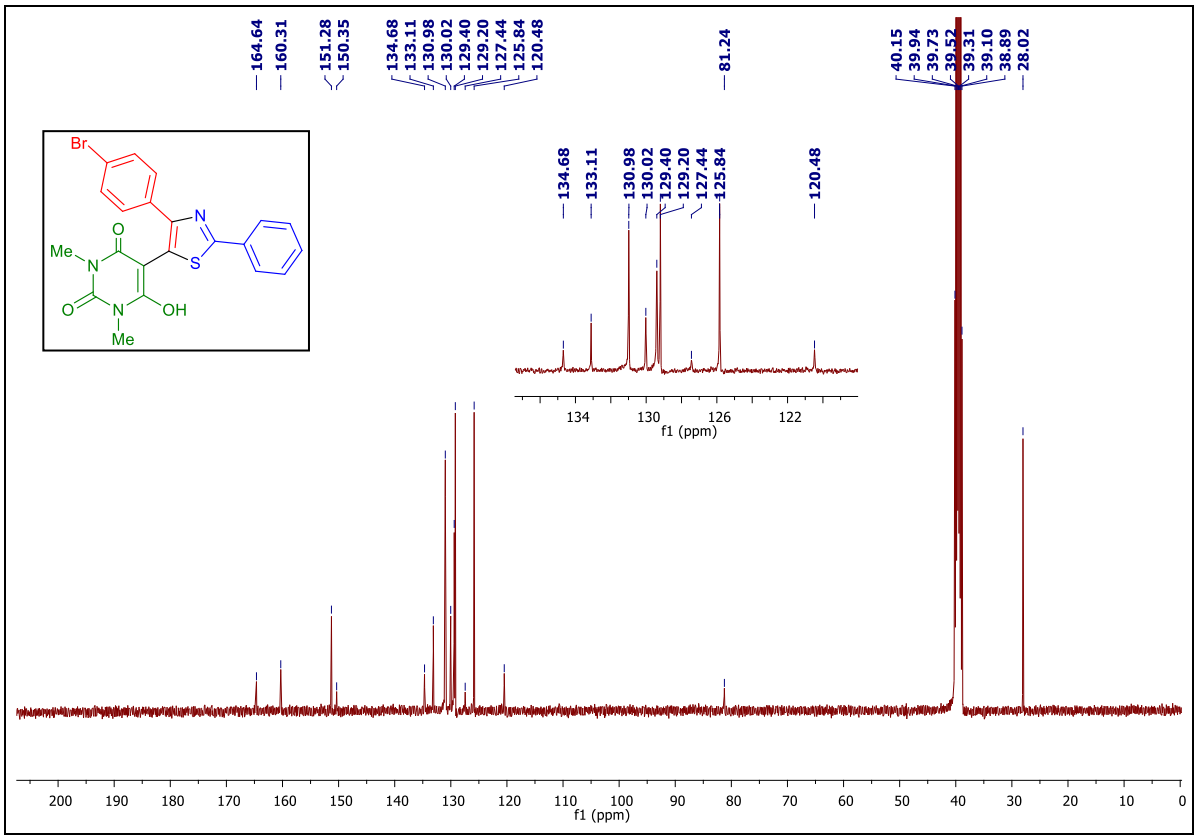
^{1}H and ^{13}C NMR spectra of 4u



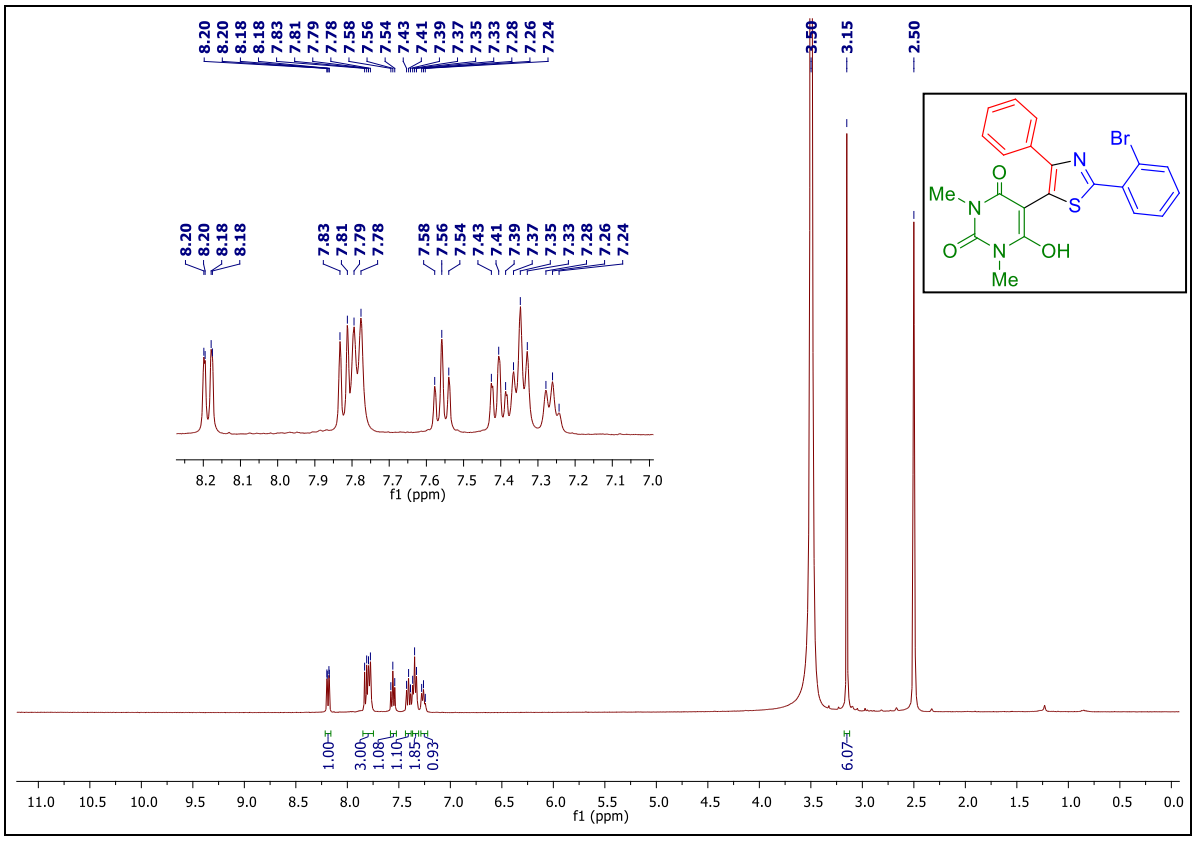


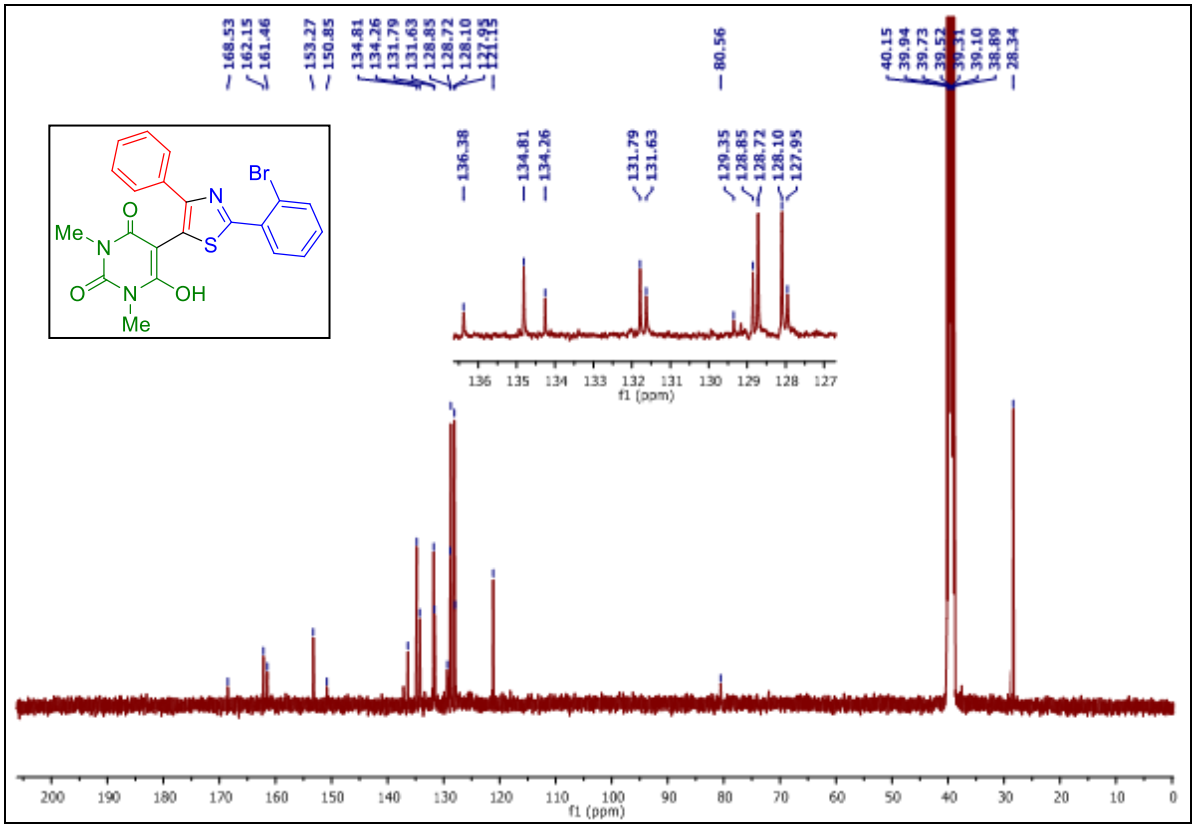
^{1}H and ^{13}C NMR spectra of 4v



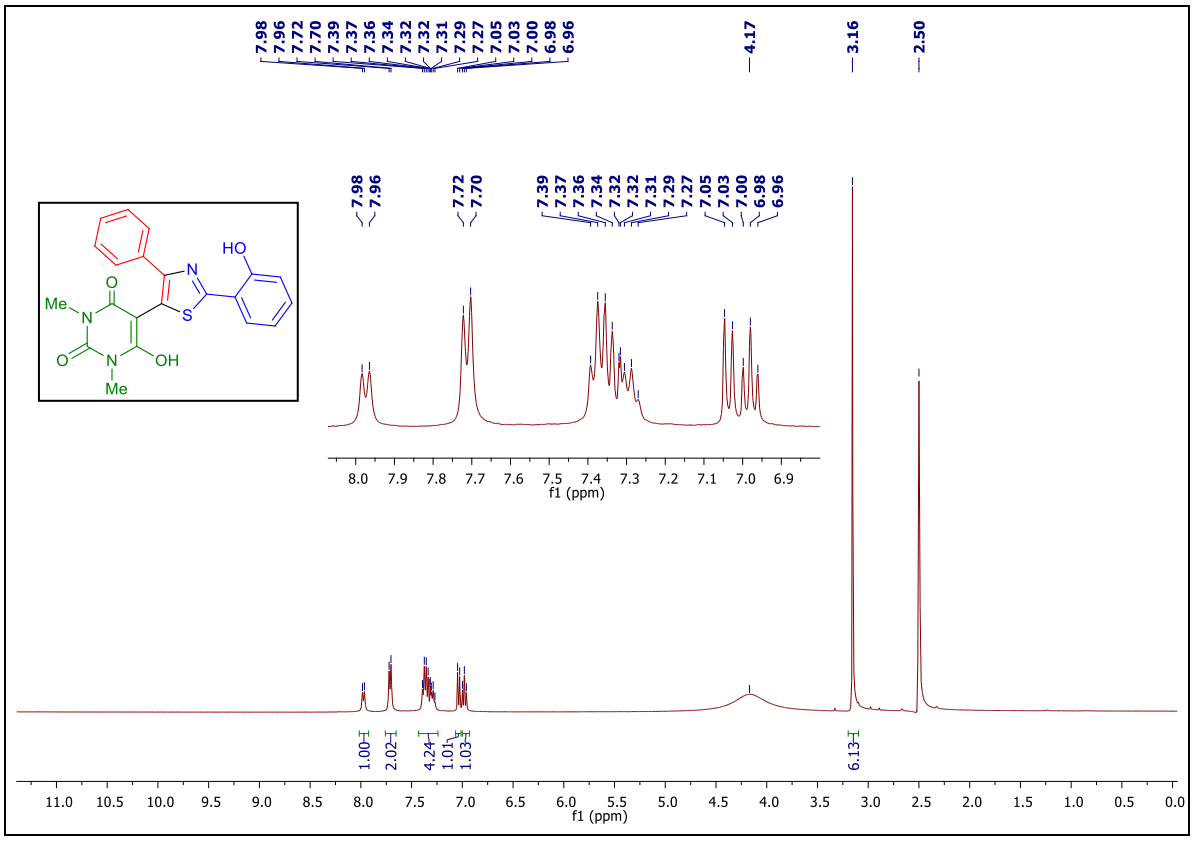


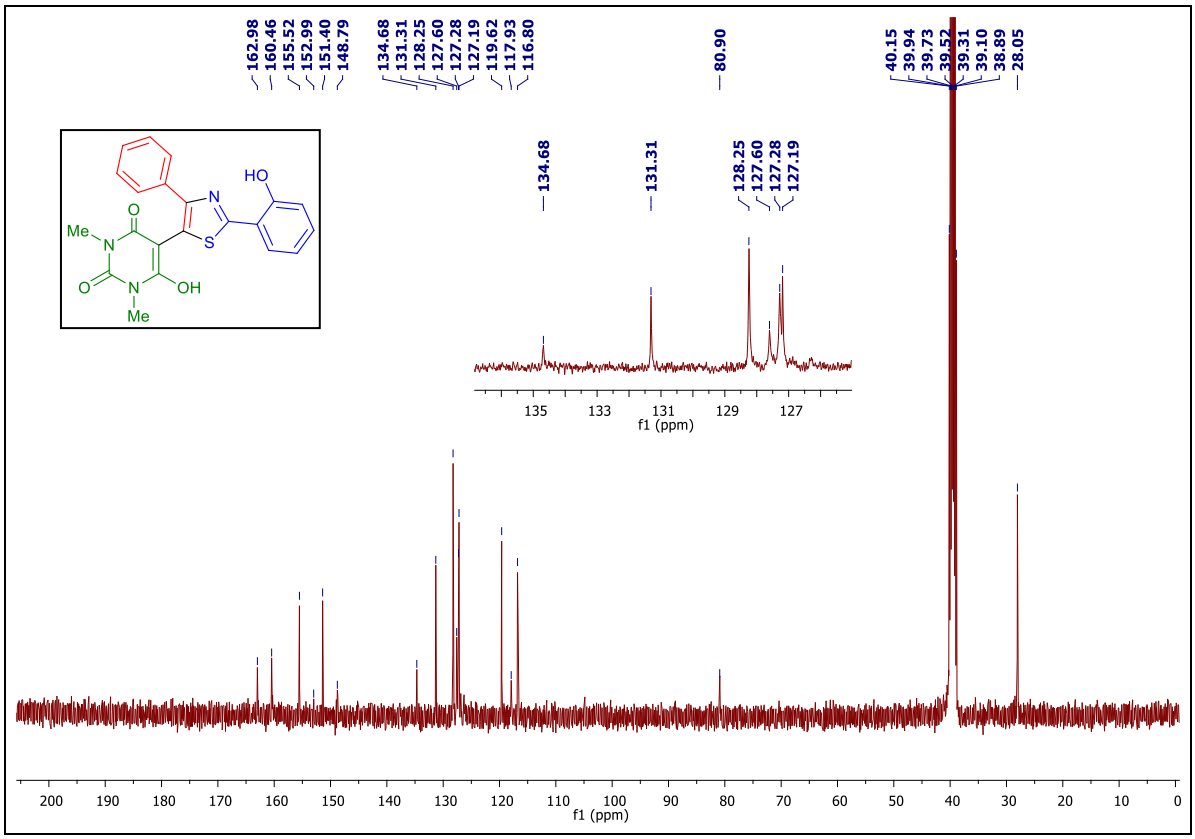
^{1}H and ^{13}C NMR spectra of 4w



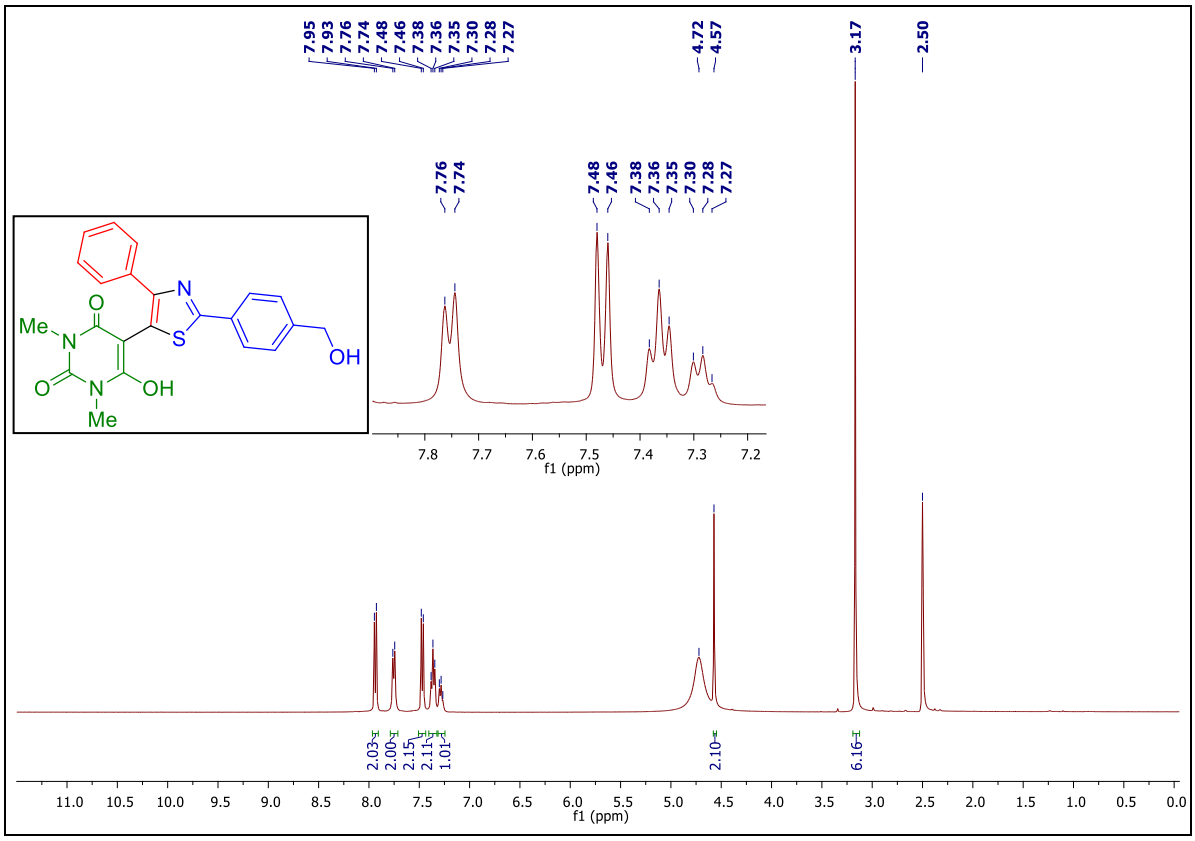


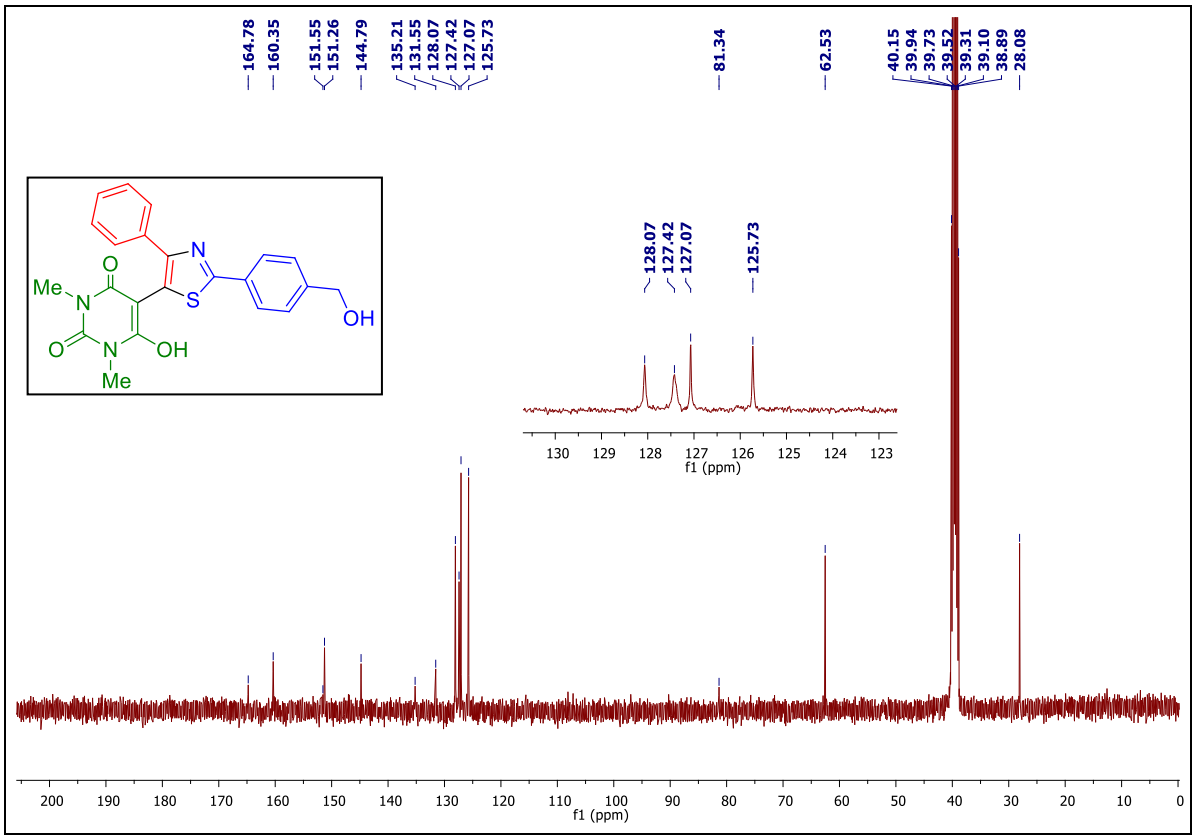
^{1}H and ^{13}C NMR spectra of 4x



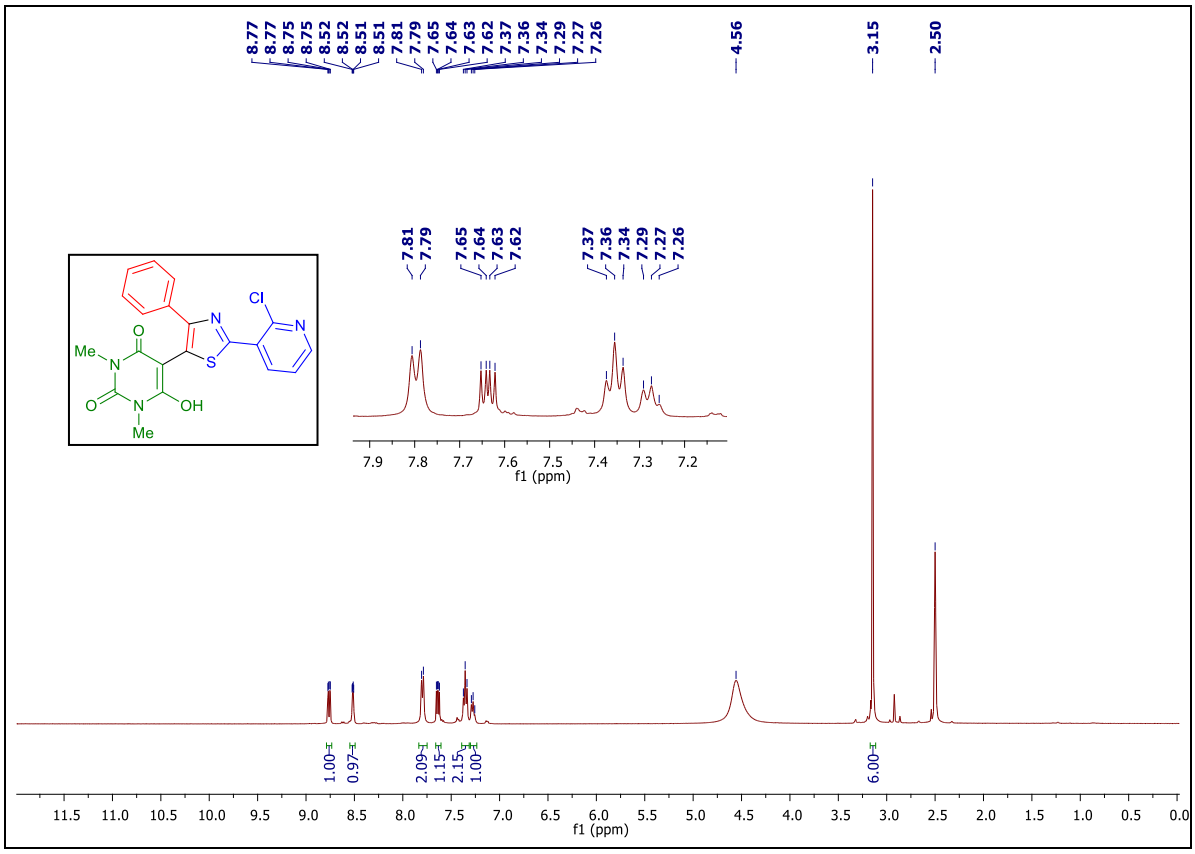


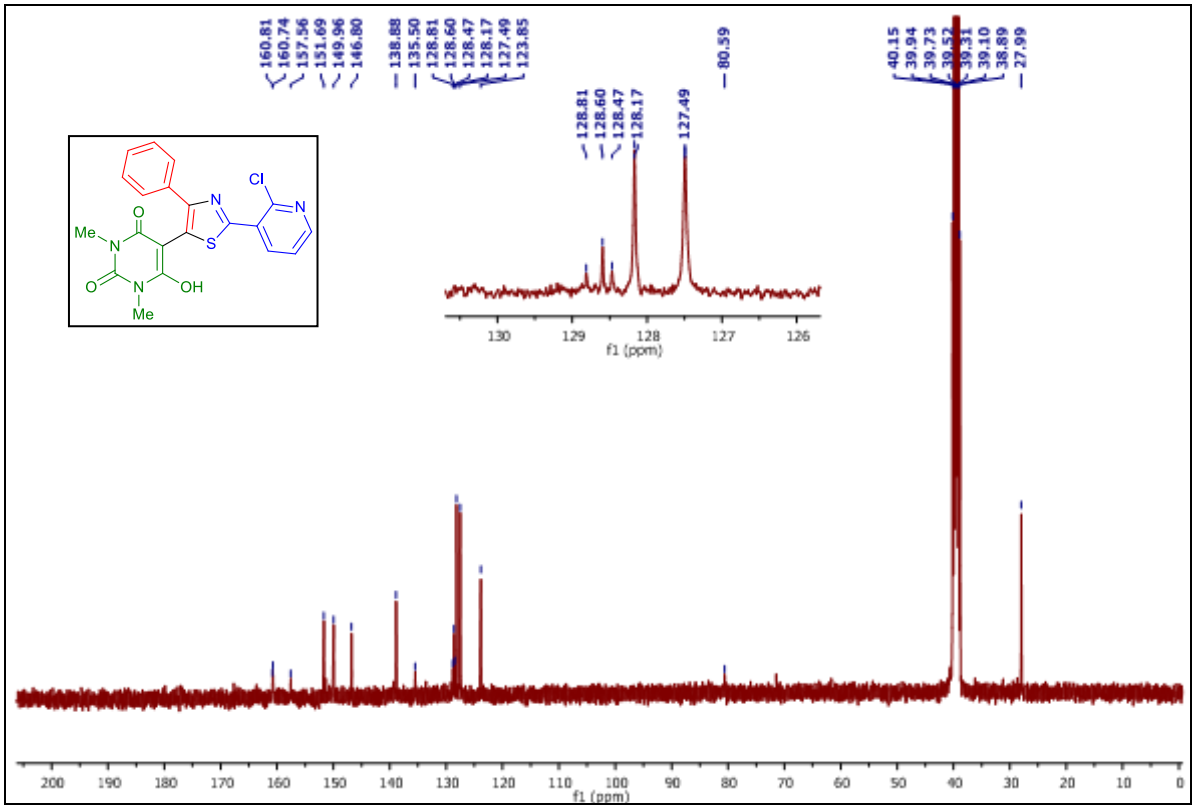
^{1}H and ^{13}C NMR spectra of 4y



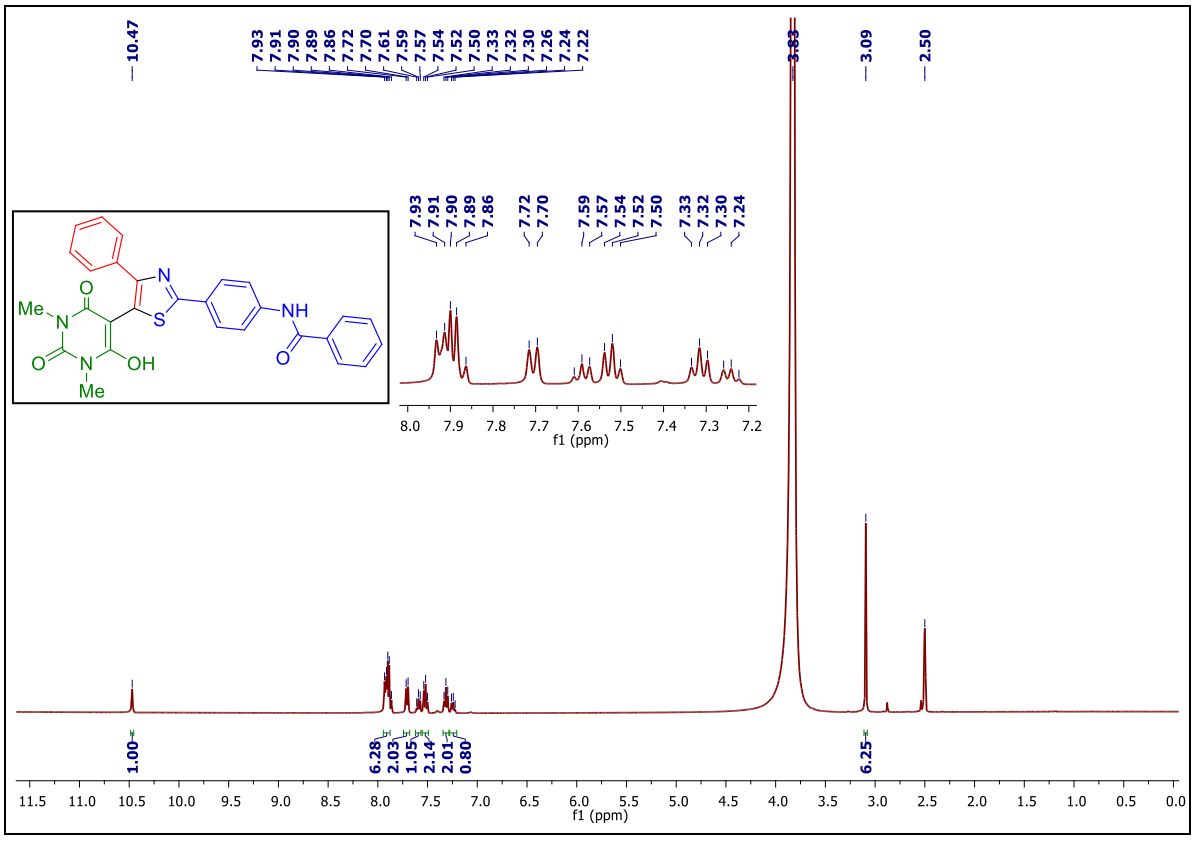


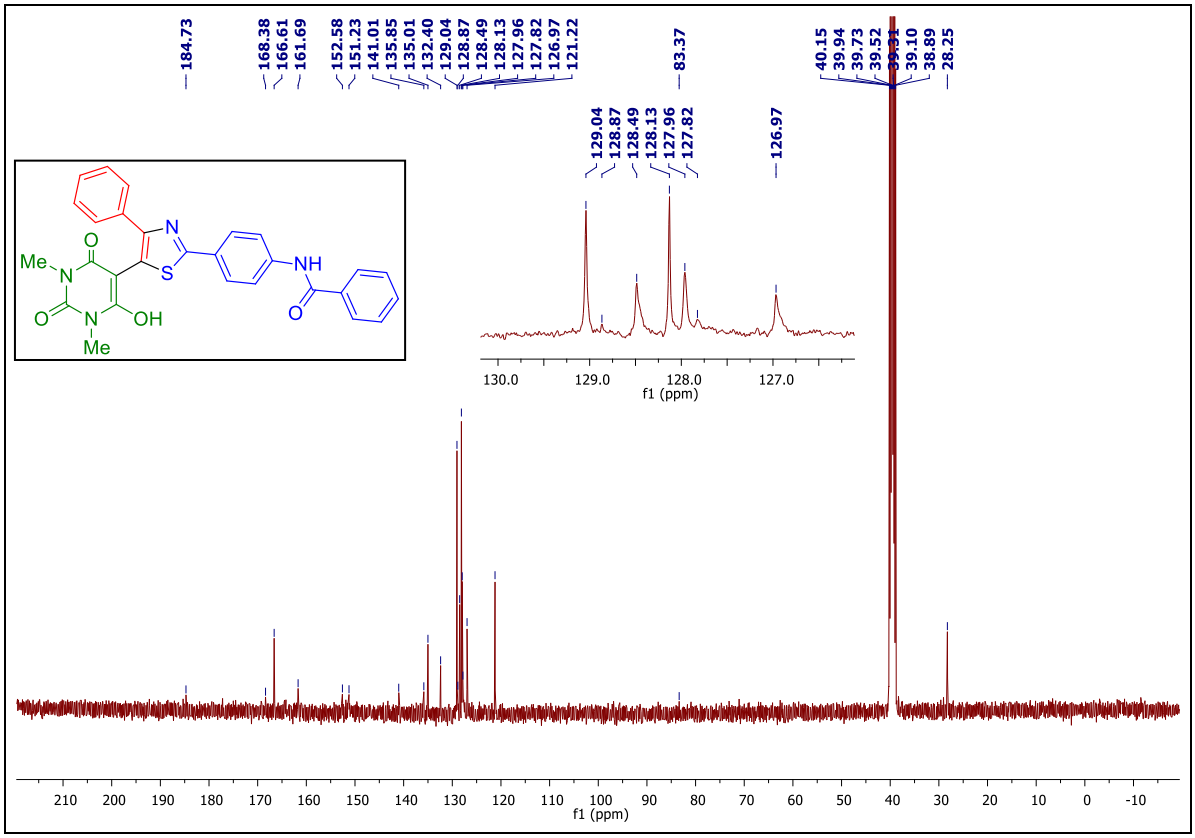
^{1}H and ^{13}C NMR spectra of 4z



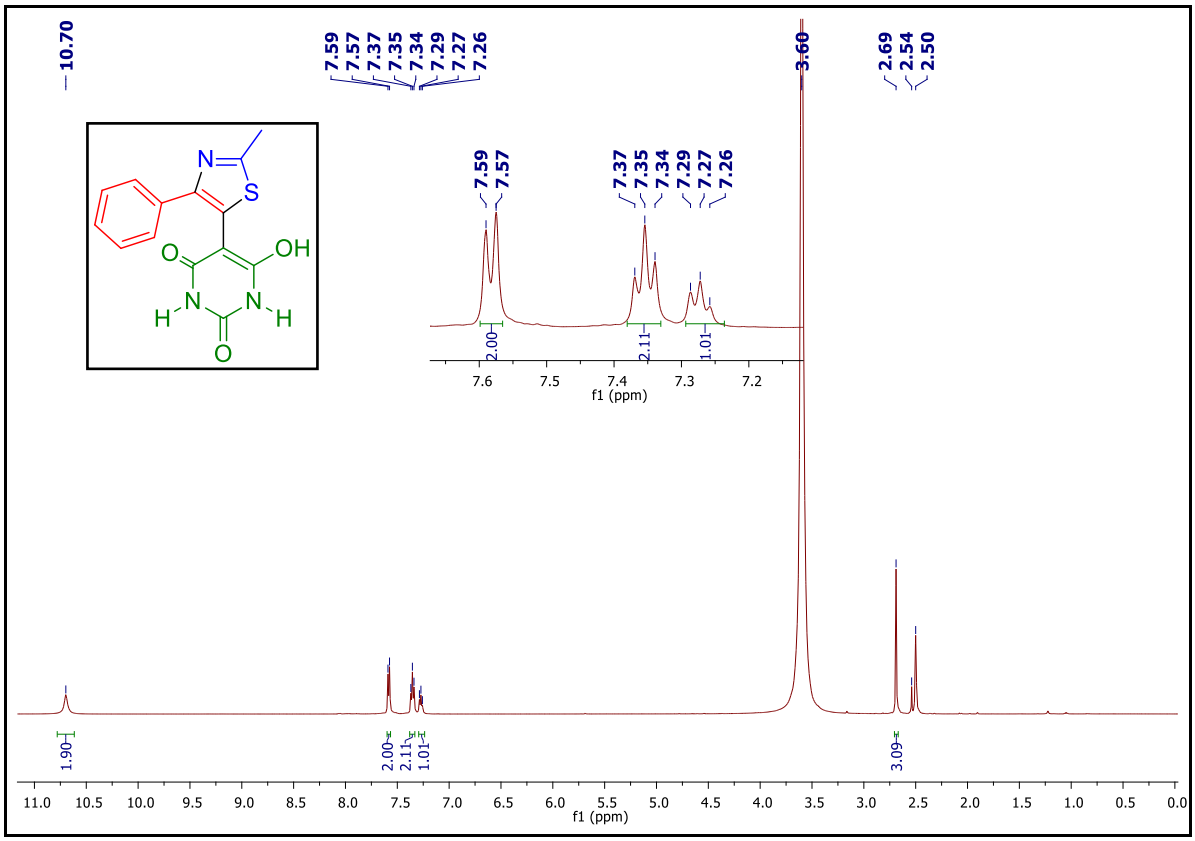


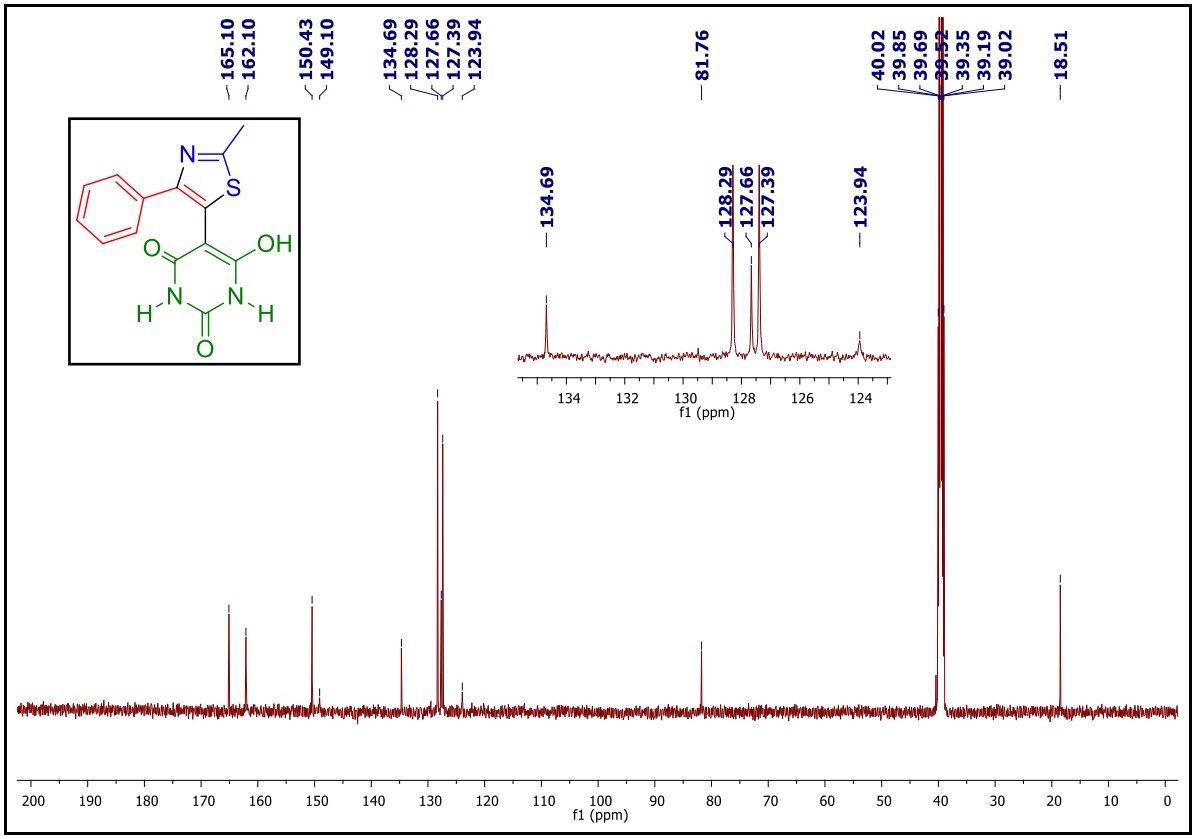
^{1}H and ^{13}C NMR spectra of 4aa



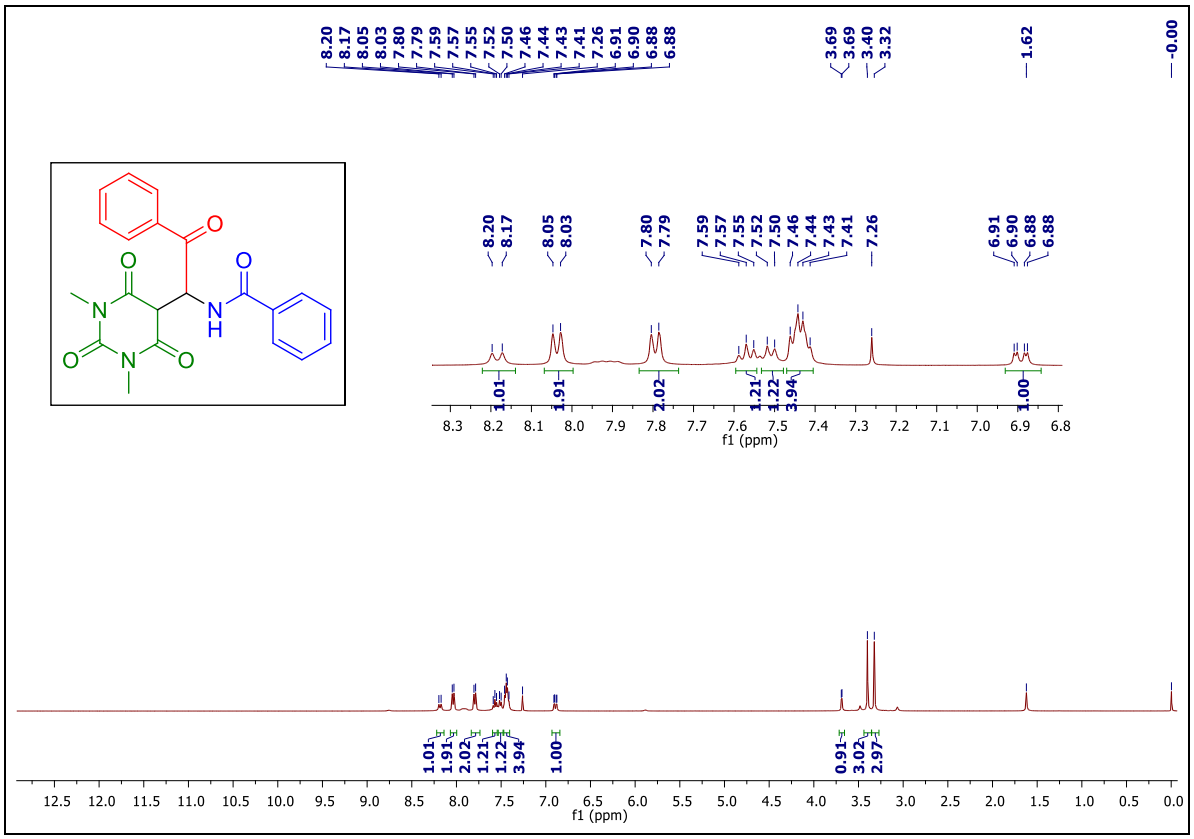


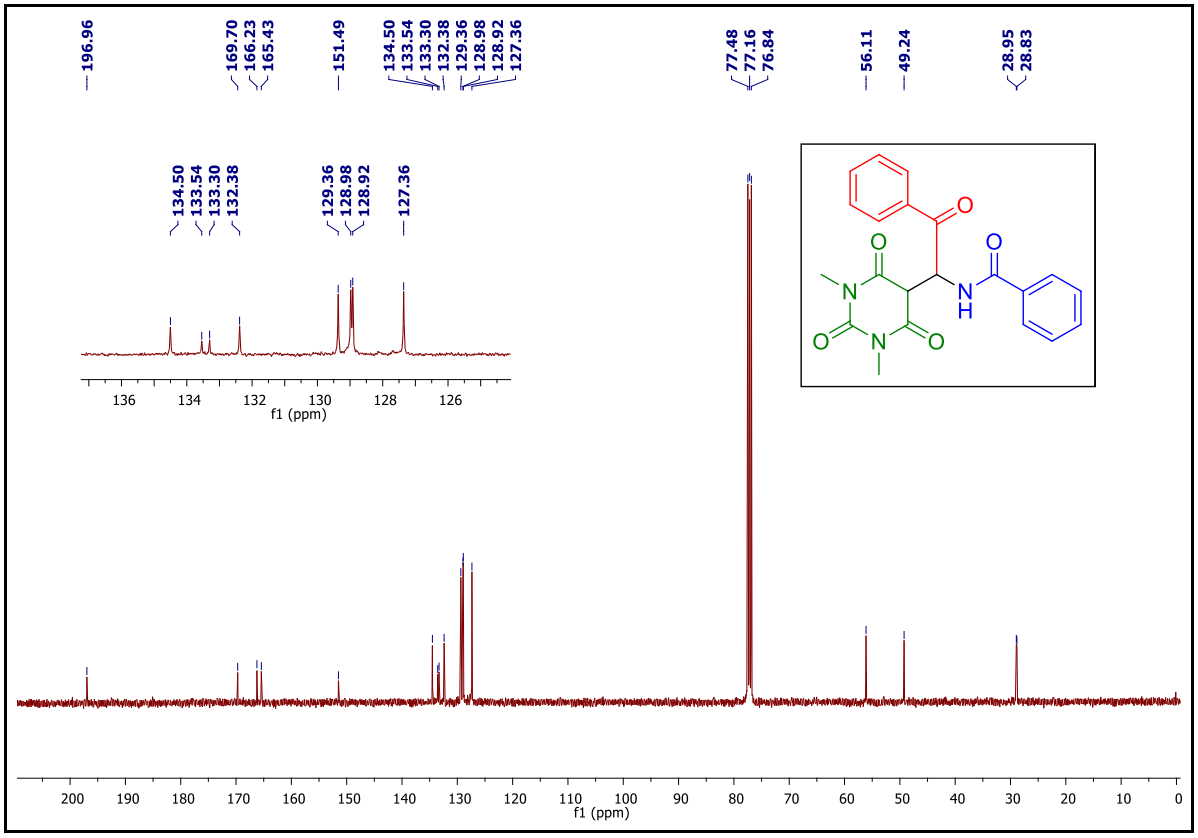
^{1}H and ^{13}C NMR spectra of 4bb



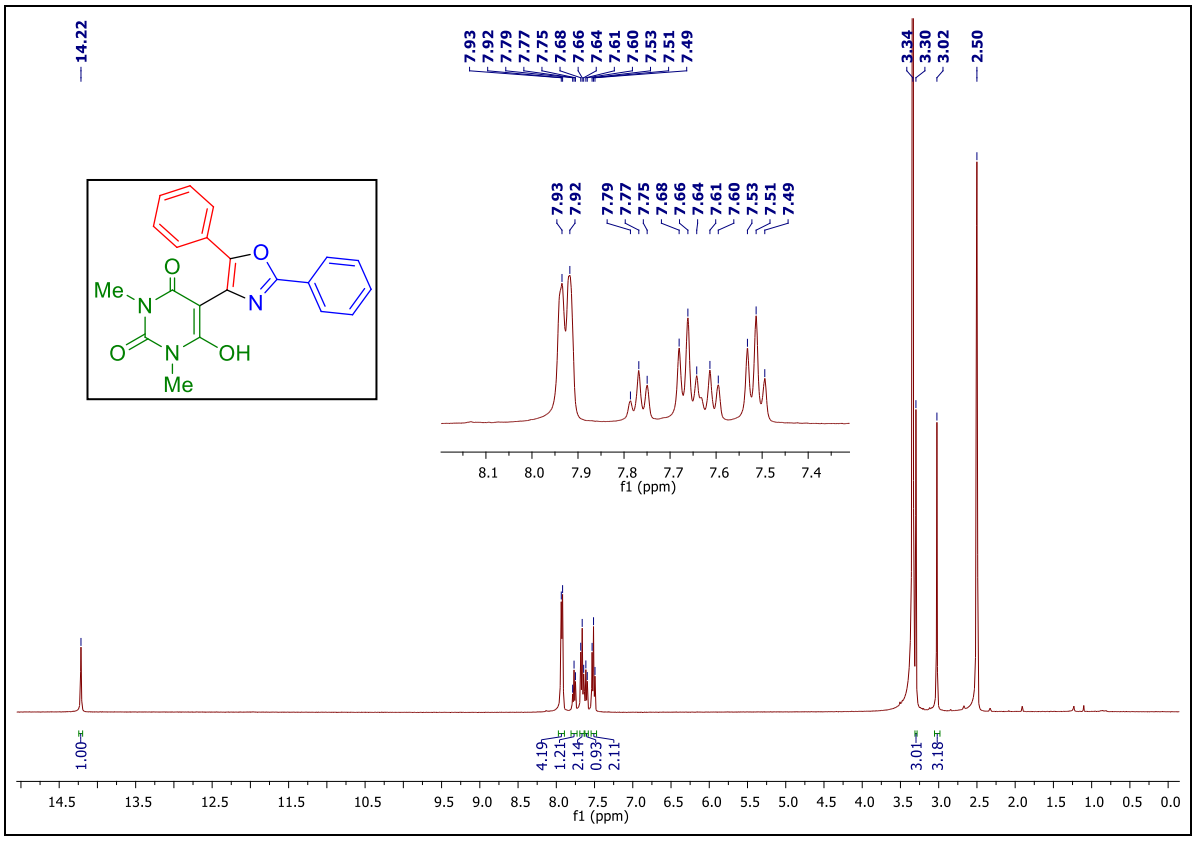


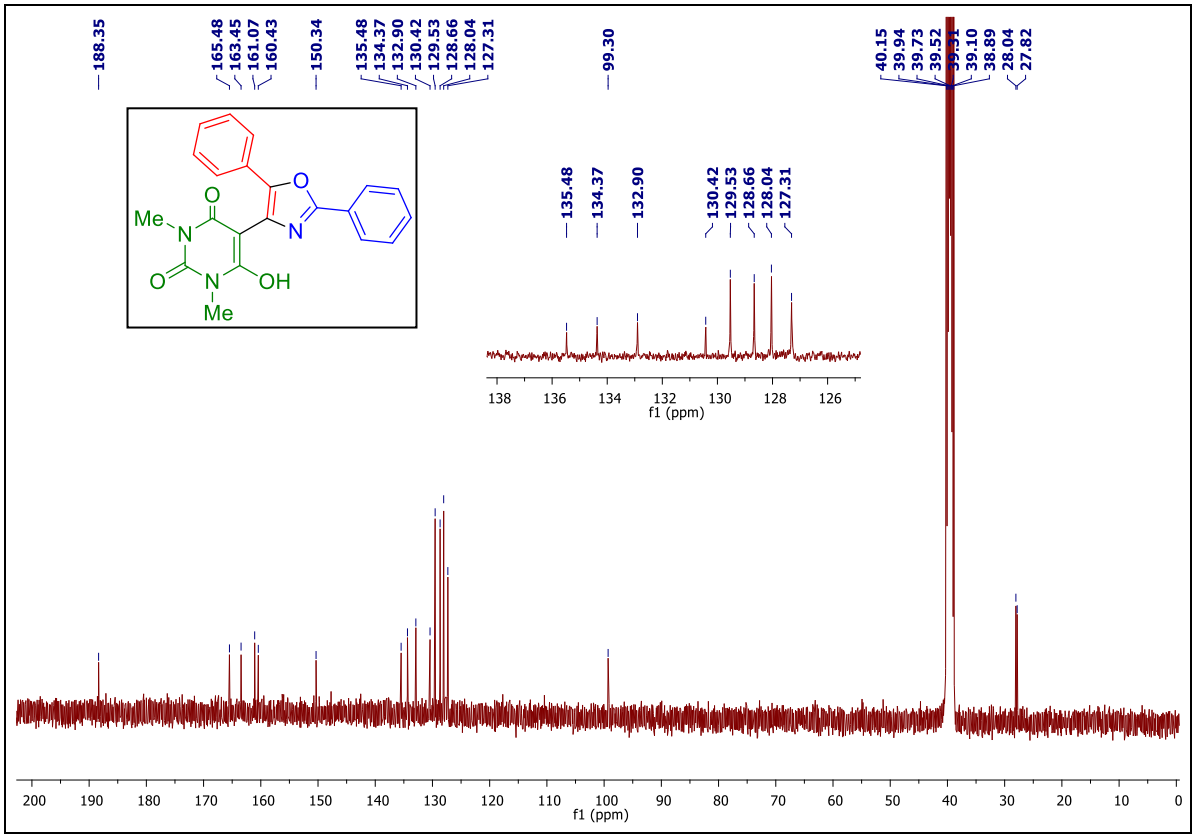
^{1}H and ^{13}C NMR spectra of 8a



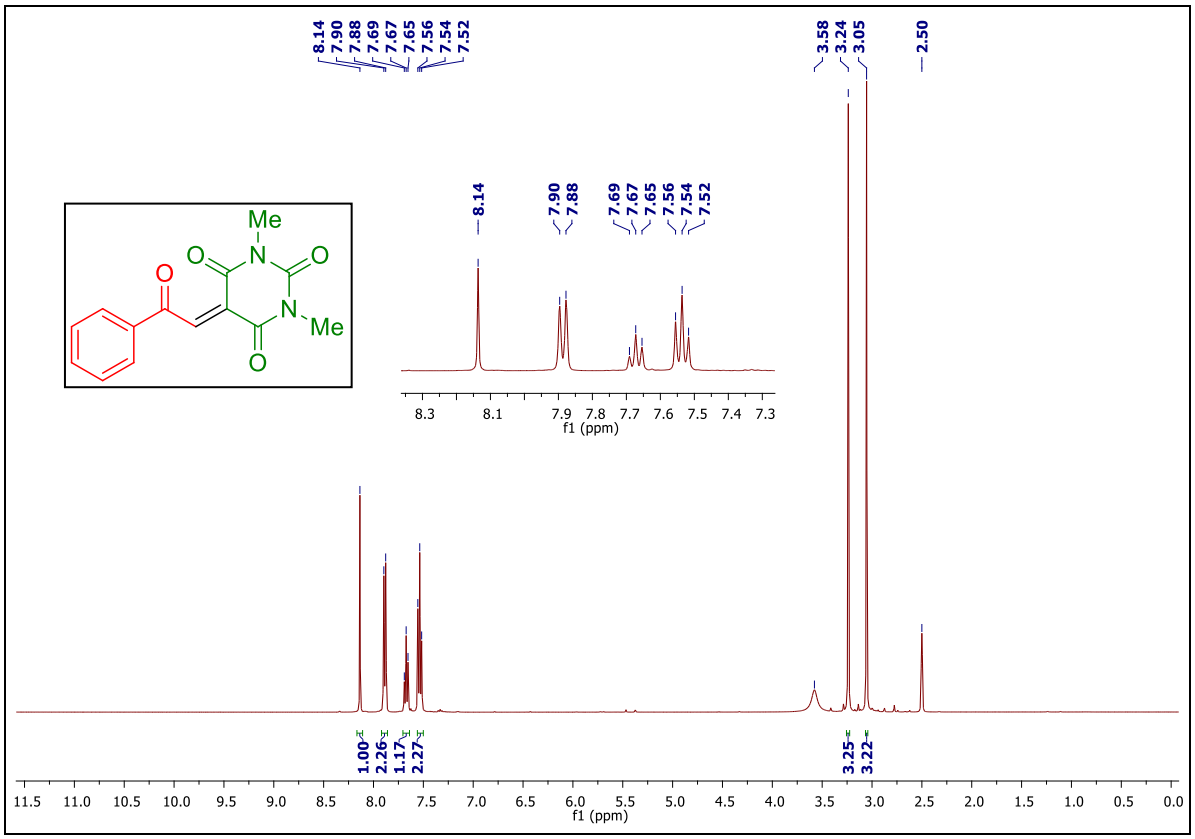


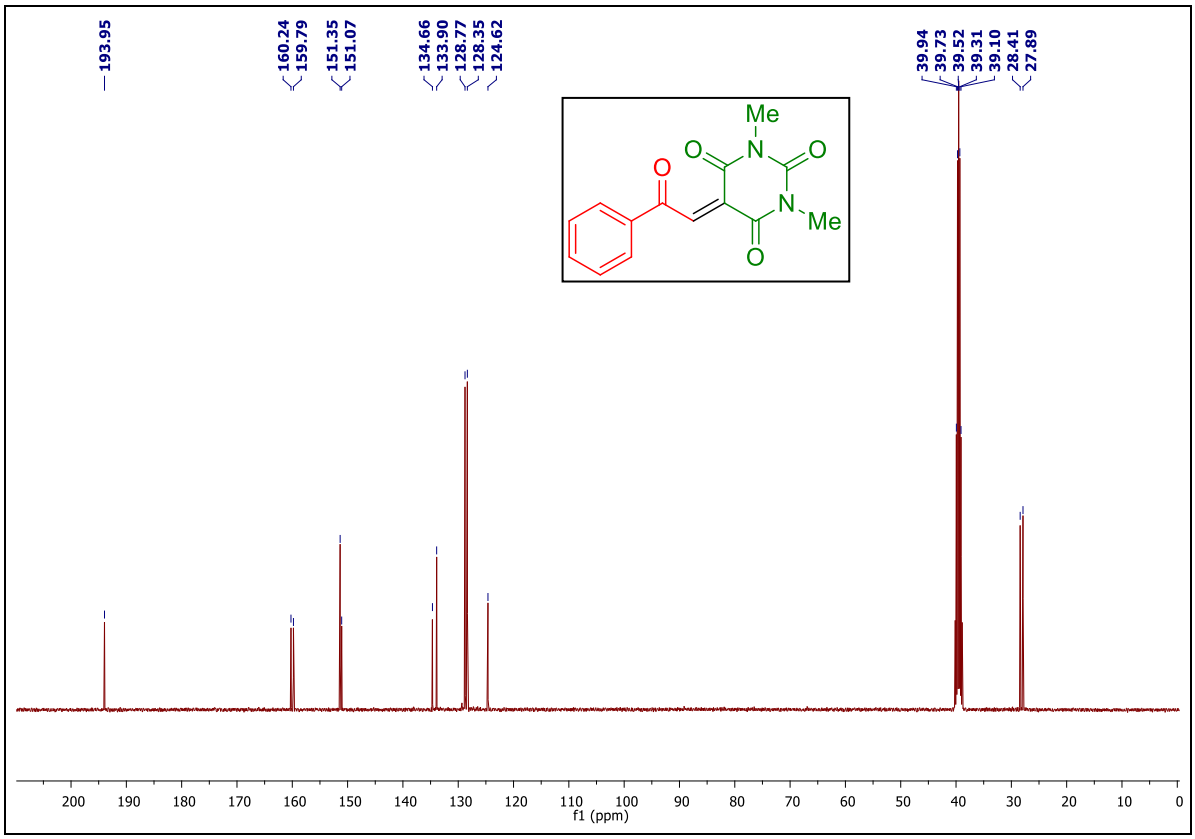
^{1}H and ^{13}C NMR spectra of 9a





^{1}H and ^{13}C NMR spectra of intermediate A





Crystal data of compound 4c:

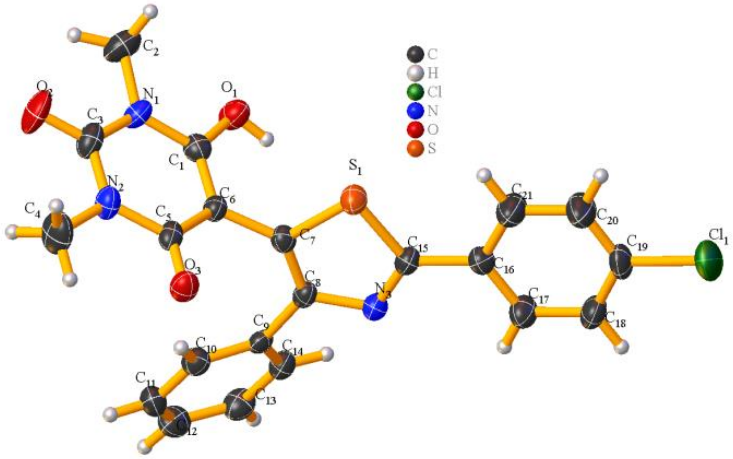


Figure S1. X-ray structure of **3c** with 50 % ellipsoidal probability (**CCDC 1979332**)

Table S1. Sample and crystal data for 4c

Identification code	MM_a	
Chemical formula	C_{21} H_{16} Cl N_3O_3S	
Formula weight	425.88 g/mol	
Temperature	298 K	
Wavelength	0.71073 Å	
Space group	P 21/n	
Unit cell dimensions	a = 10.525(1) Å	α = 90 °
	b = 8.9515(10) Å	β = 101.225(3) °
	c = 20.771(2) Å	γ = 90 °
Volume	1919.5(3) $Å^3$	
Z	4	
Density (calculated)	1.474 g/cm^3	
F(000)	880.0	

Crystal data of compound 8a:

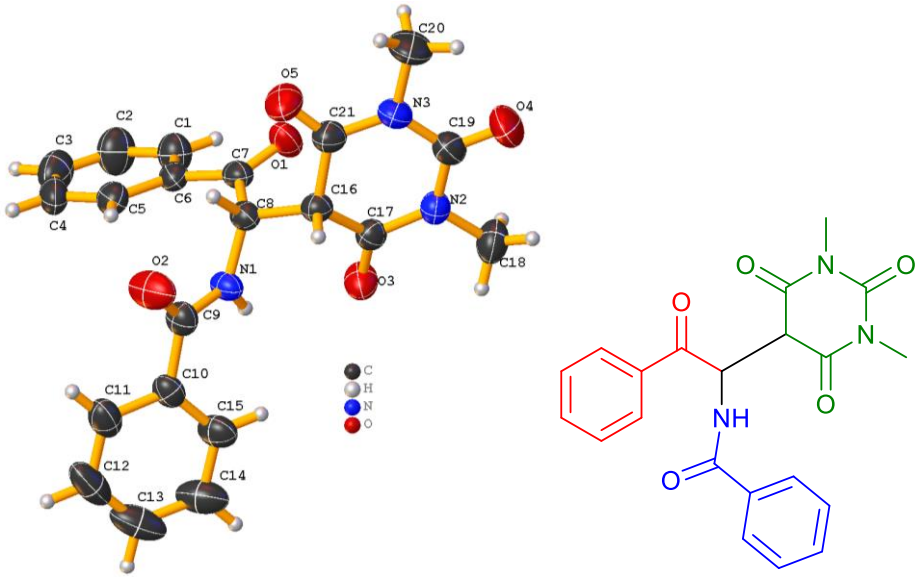


Figure S2: X-ray structure of **8a** with 50 % ellipsoidal probability (CCDC 1951758)

Table S2. Sample and crystal data for 8a

Identification code	oxazole_1	
Chemical formula	$C_{21}H_{19}N_3O_5$	
Formula weight	393.39 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal size	0.300 x 0.300 x 0.300 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.2908(7) Å	α = 64.421(2)°
	b = 11.5745(10) Å	β = 78.679(3)°
	c = 11.6052(11) Å	γ = 78.392(2)°
Volume	976.39(15) $Å^3$	
Z	2	
Density (calculated)	1.338 g/cm^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	412	

Quantum yield calcuataion:

Quantum yields were calculated with respect to quinine sulphate dihydrate in 0.1M H_2SO_4 as fluorescence standard.

Ø = Quantum yield; λ abs max = Absorbance maxima

λ em max = Fluorescence emission maxima

Fluorescence quantum yields (Ø) were calculated according to the equation.[39]

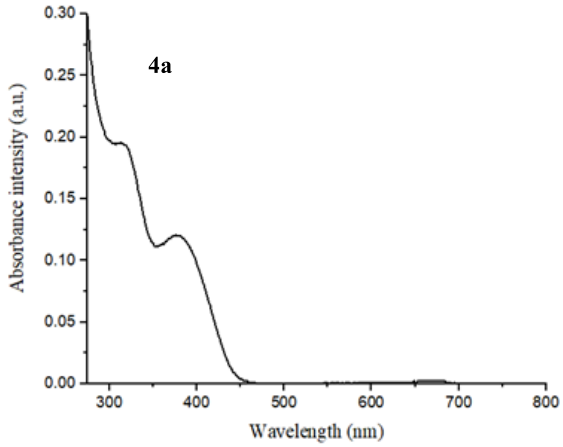
$$Ø = Ø_{std} \times [I_s / I_{std}] \times [A_{std} / A_s] \times [\eta_s / \eta_{std}]^2$$

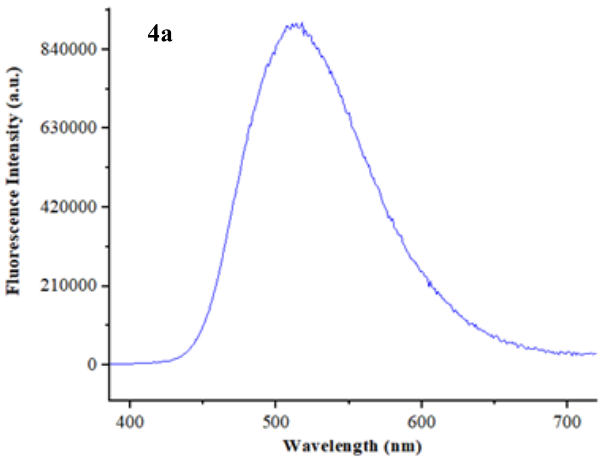
Where, Ø is the fluorescence quantum yield of the sample, $Ø_{std}$ is the quantum yield of the quinine sulphate dehydrate (Øf = 0.55, quinine sulphate dihydrate in 0.1 N H_2SO_4), I_s and I_{std} are the integrated emission intensities of the sample and the standard, respectively, A_s and A_{std} are the absorbance of the sample and the standard at the excitation wavelength, respectively, and η_s and η_{std} are the refractive index of the medium taken.

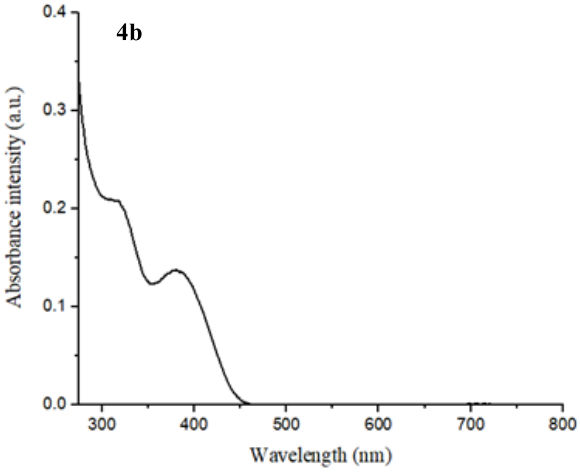
References:

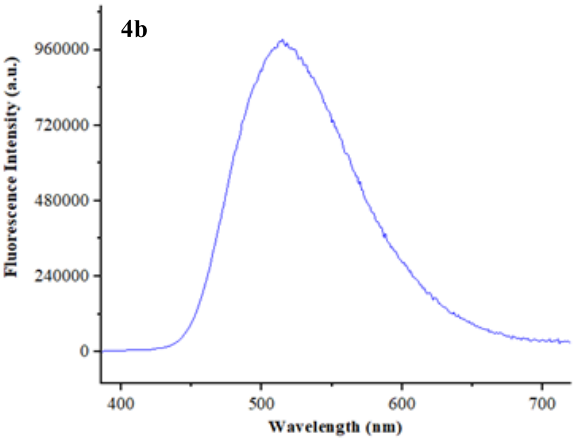
39. G. A. Crosby and J. N. Demas, *J. Phys. Chem*., 1971, **75**, 991.

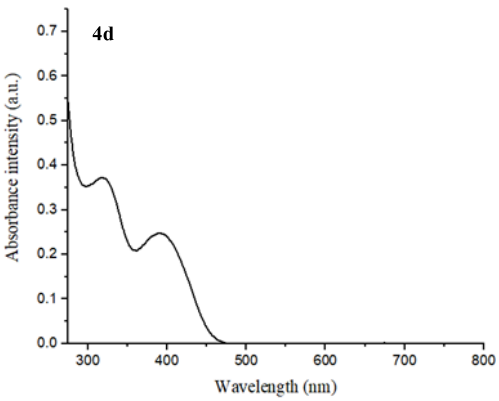
UV and fluorescence spectra of 4a-4s:

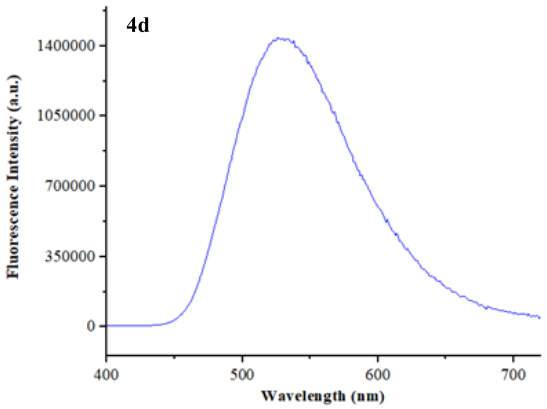


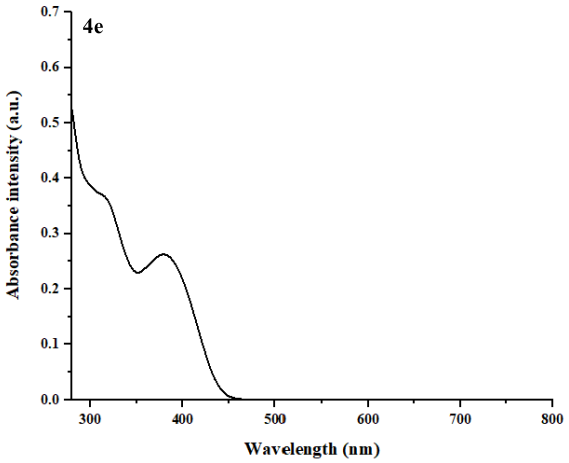








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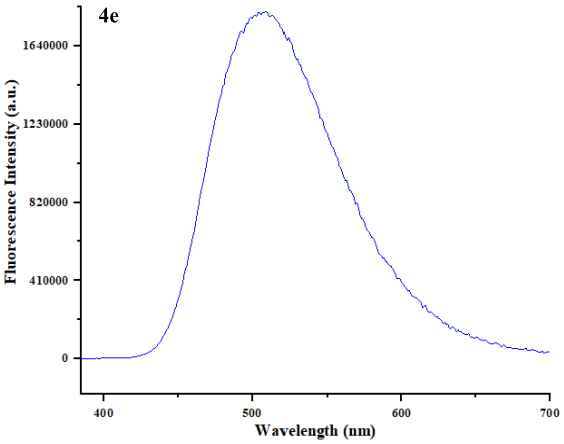
Absorbance intensity (a.u.)
Wavelength (nm)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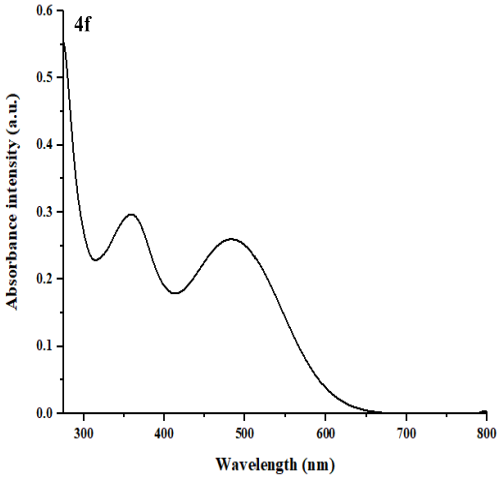
Fluorescence Intensity (a.u.)
Wavelength (nm)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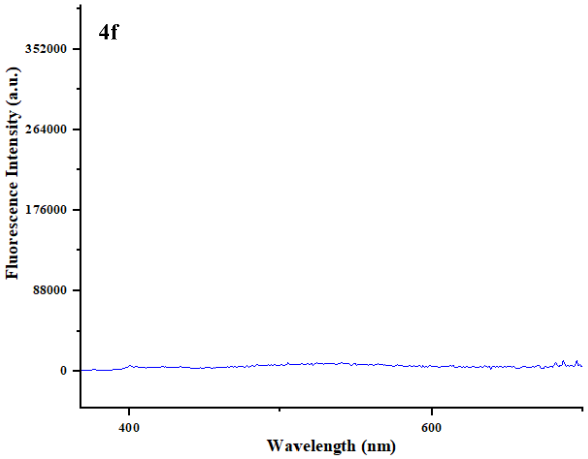
Absorbance intensity (a.u.)
Wavelength (nm)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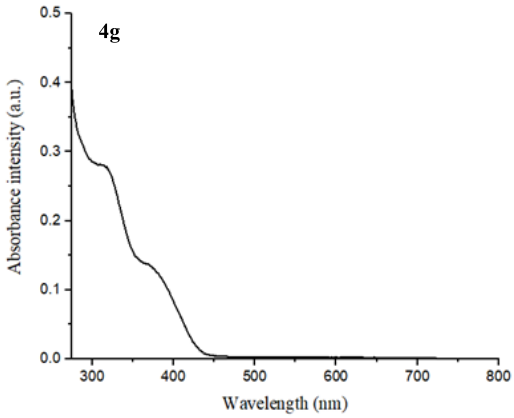
Wavelength (nm)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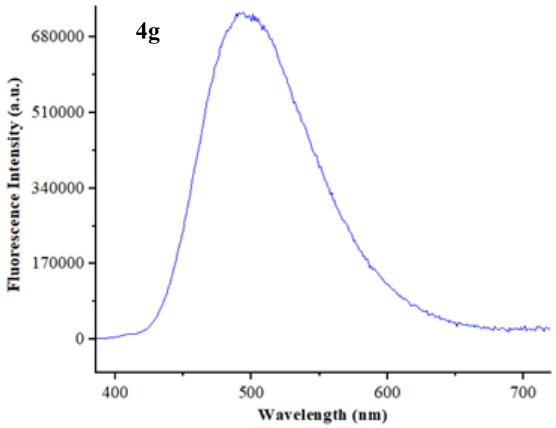
Absorbance intensity (a.u.)
Wavelength (nm)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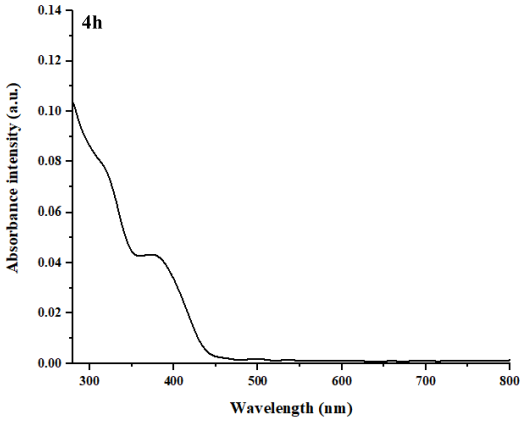
Fluorescence Intensity (a.u.)
Wavelength (nm)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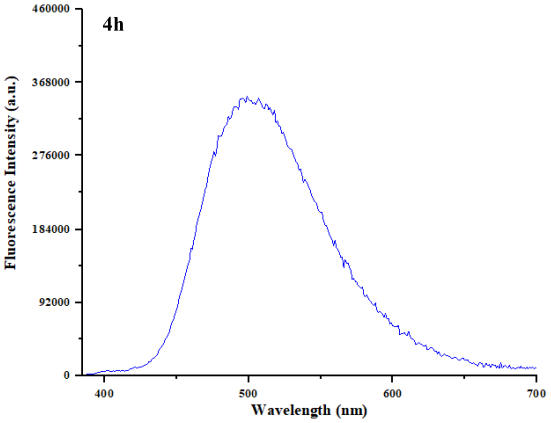
Wavelength (nm)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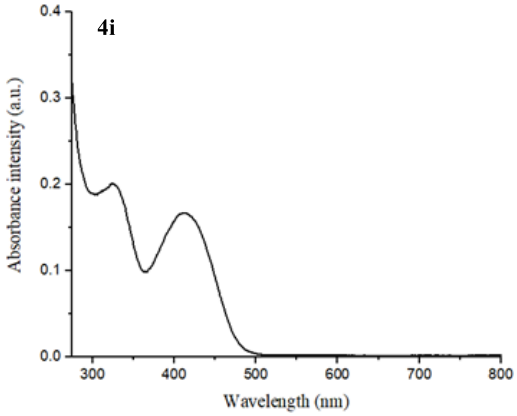
Wavelength (nm)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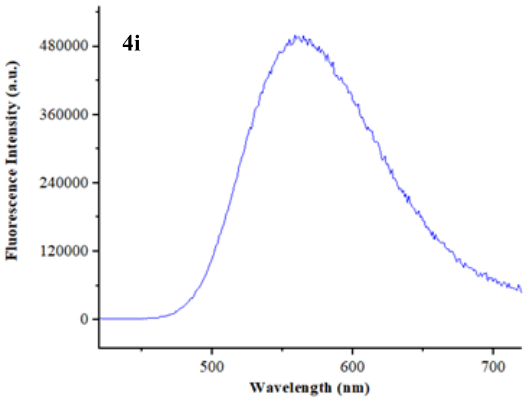
Wavelength (nm)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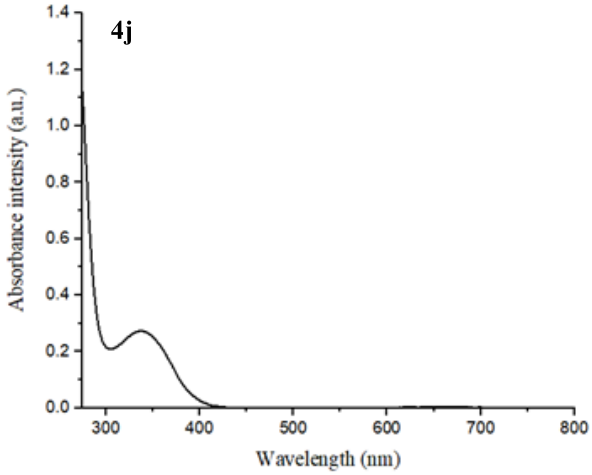
Wavelength (nm)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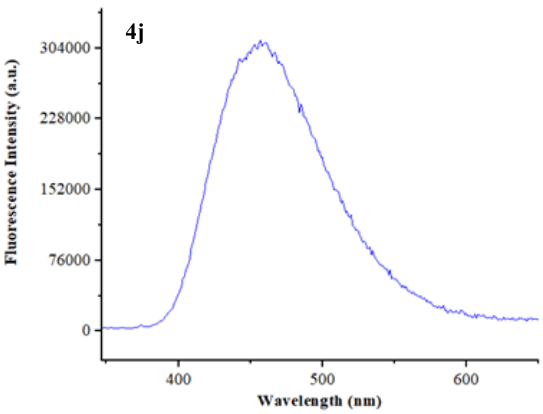
Wavelength (nm)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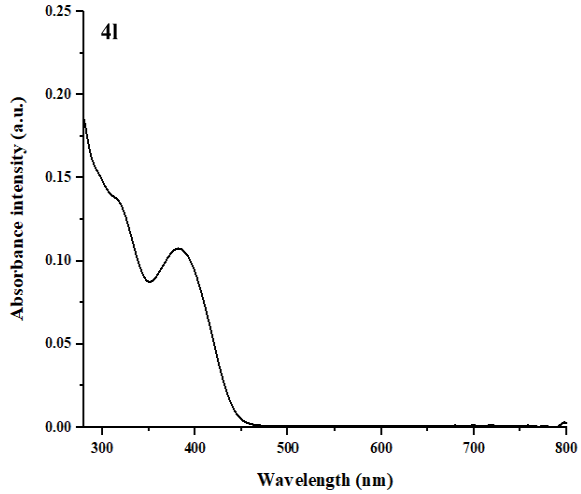
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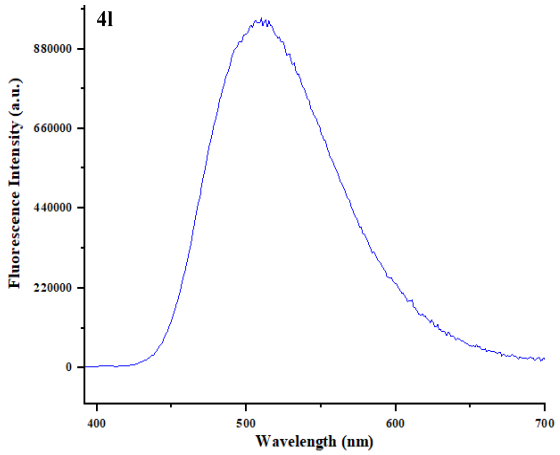
Wavelength (nm)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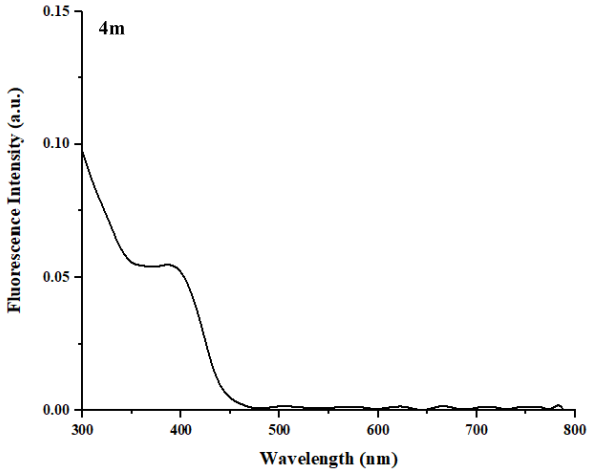
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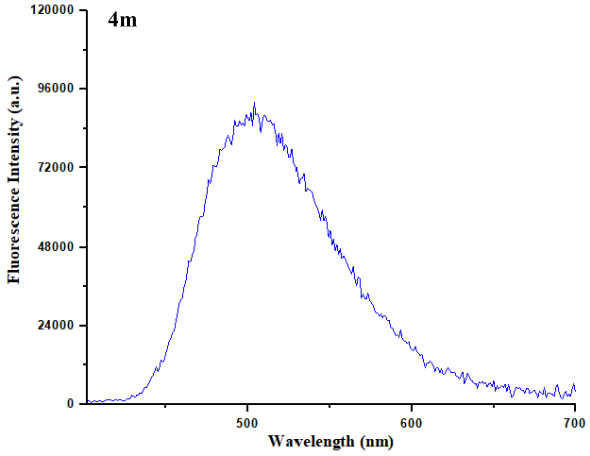
Wavelength (nm)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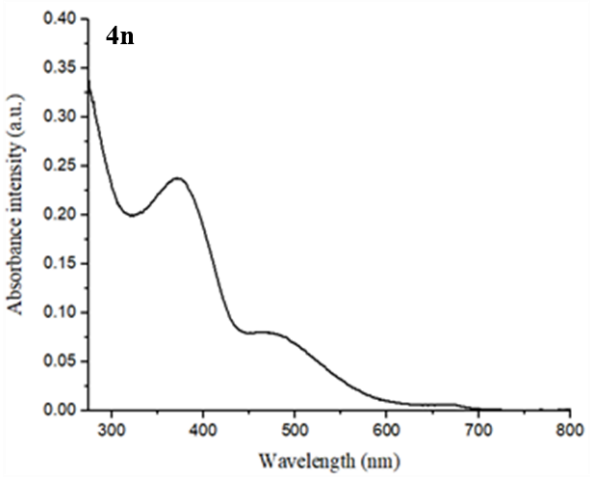
Wavelength (nm)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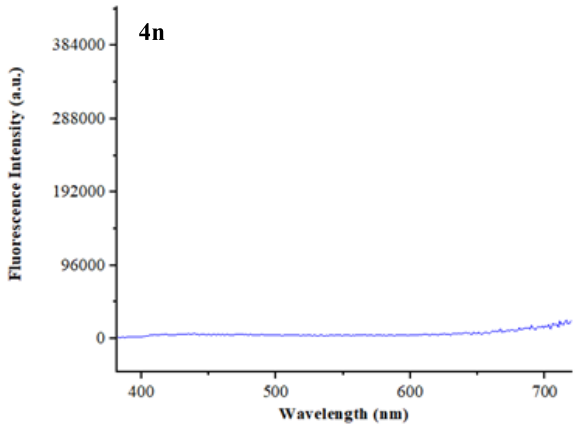
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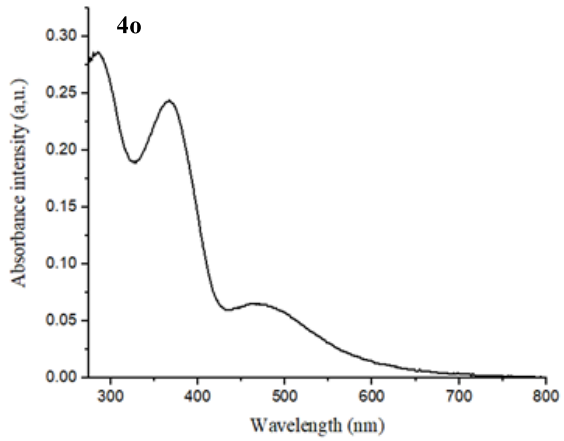
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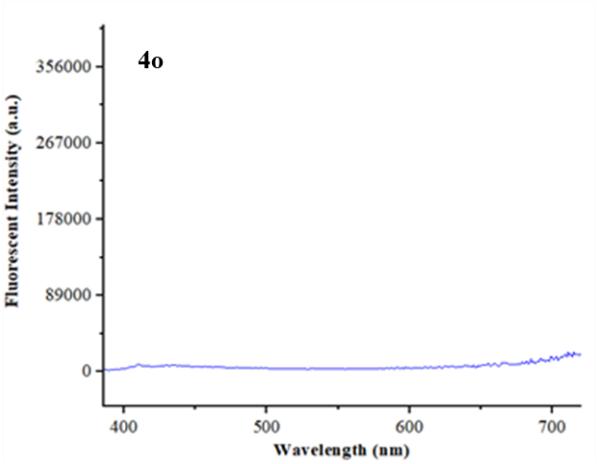
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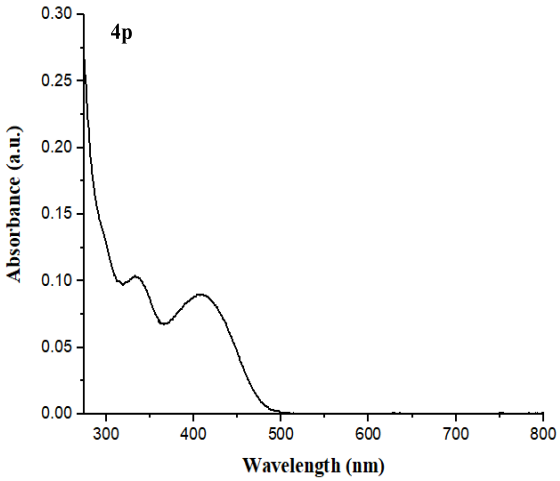
Wavelength (nm)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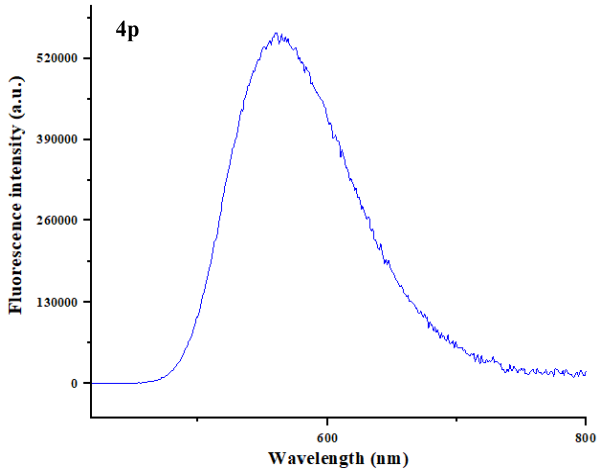
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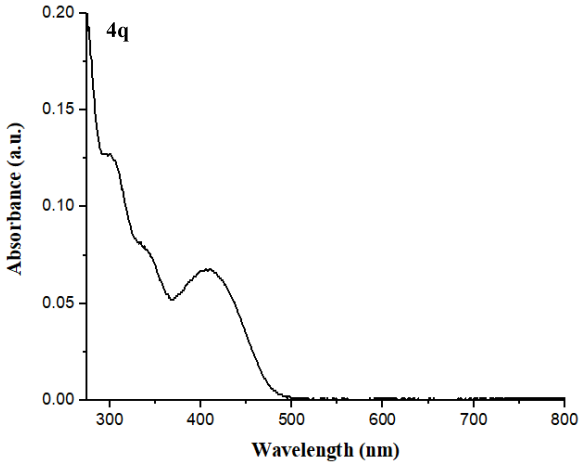
Wavelength (nm)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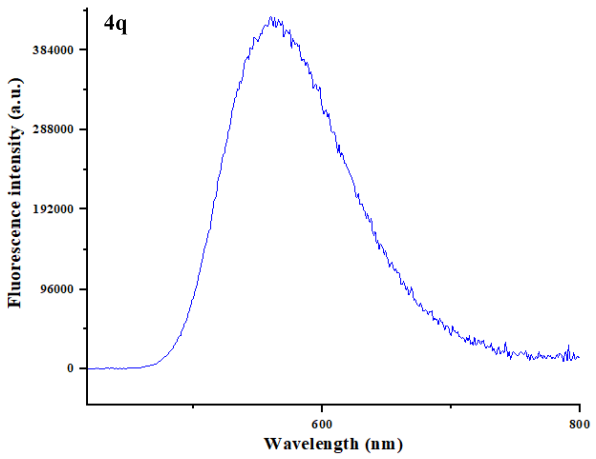
Wavelength (nm)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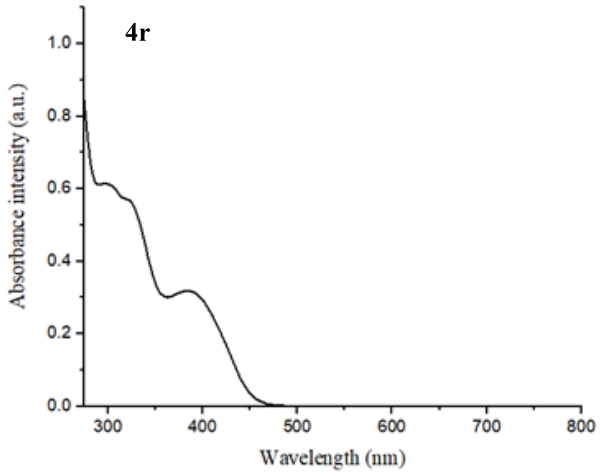
Wavelength (nm)


4r
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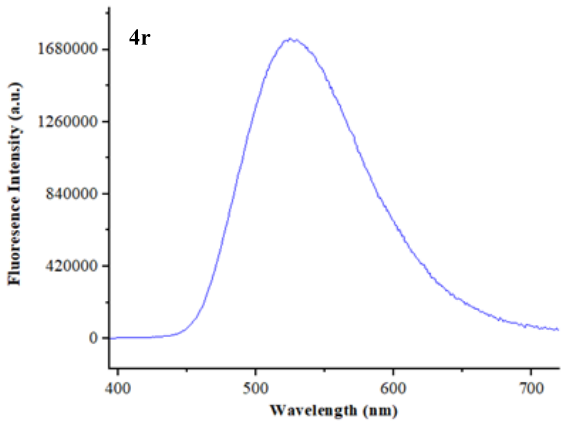
Wavelength (nm)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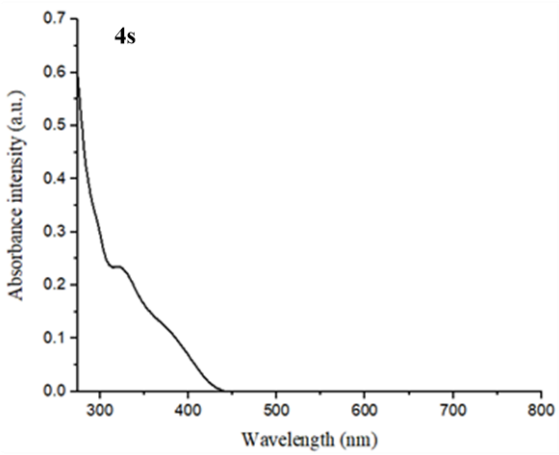
Fluoresence Intensity (a.u.)
Wavelength (nm)


4s
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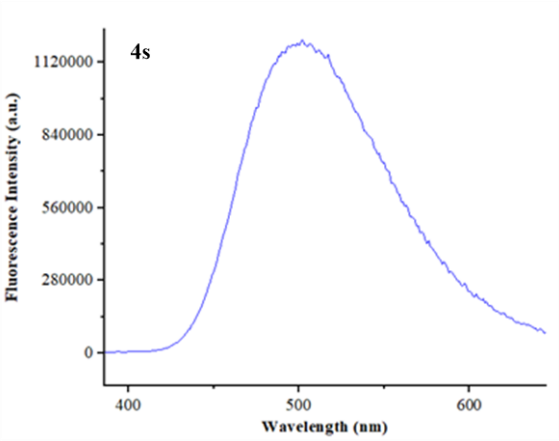
Wavelength (nm)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Fluorescence Intensity (a.u.)
Wavelength (nm)