Supporting Information

Microwave assisted synthesis of β-keto thioethers and furan derivatives by thiol directed multicomponent reactions

Asim Jana,[a] Prabhas Bhaumick[a] and Lokman H. Choudhury[a]*
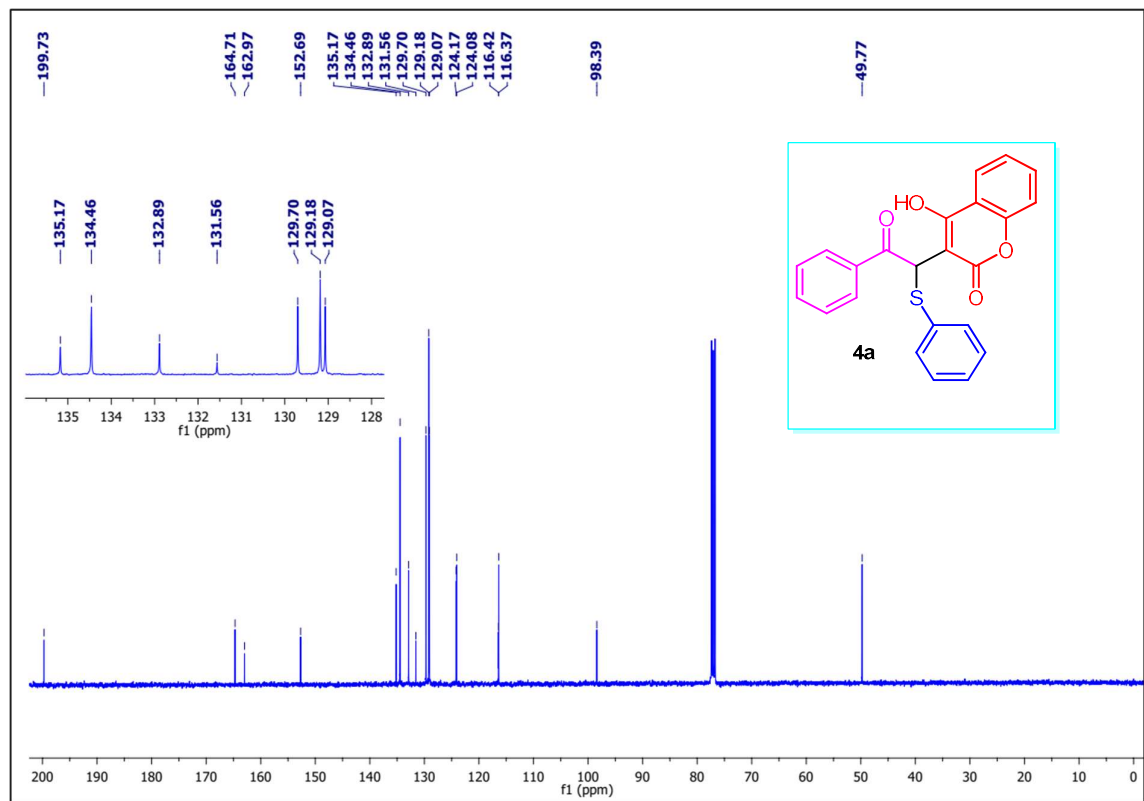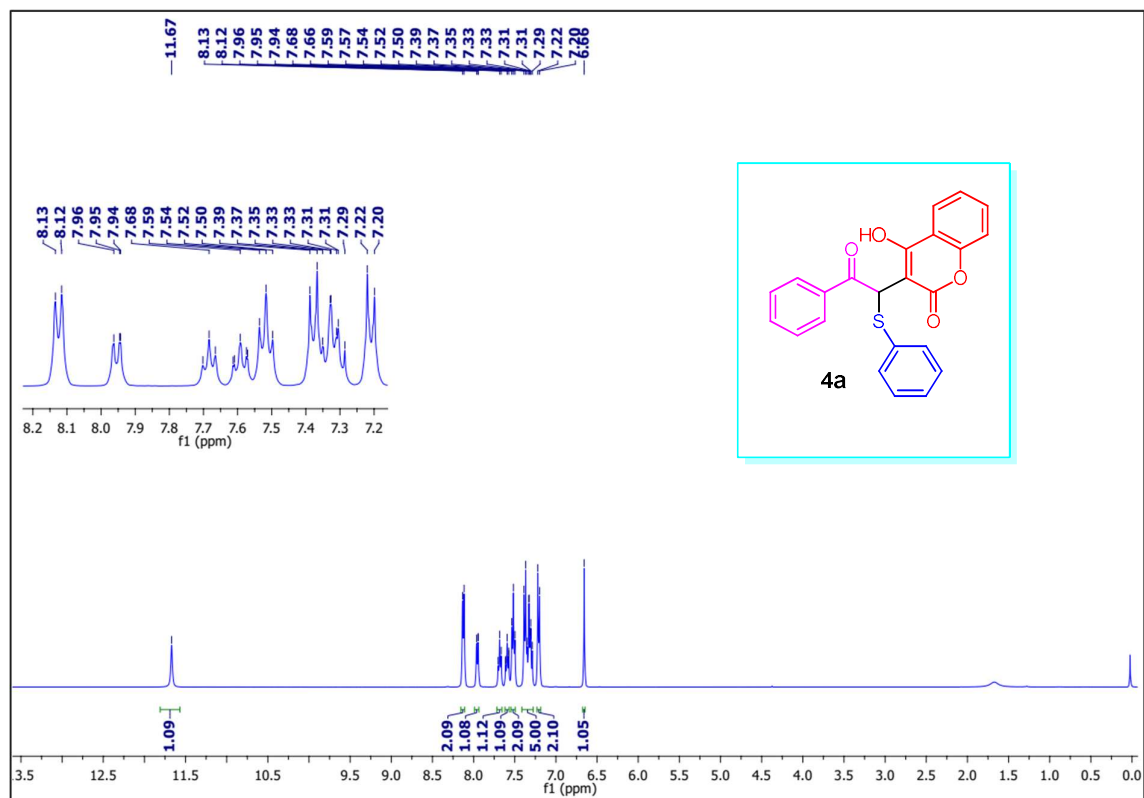
Department of Chemistry, Indian Institute of Technology Patna, Bihta, Patna-801106, India
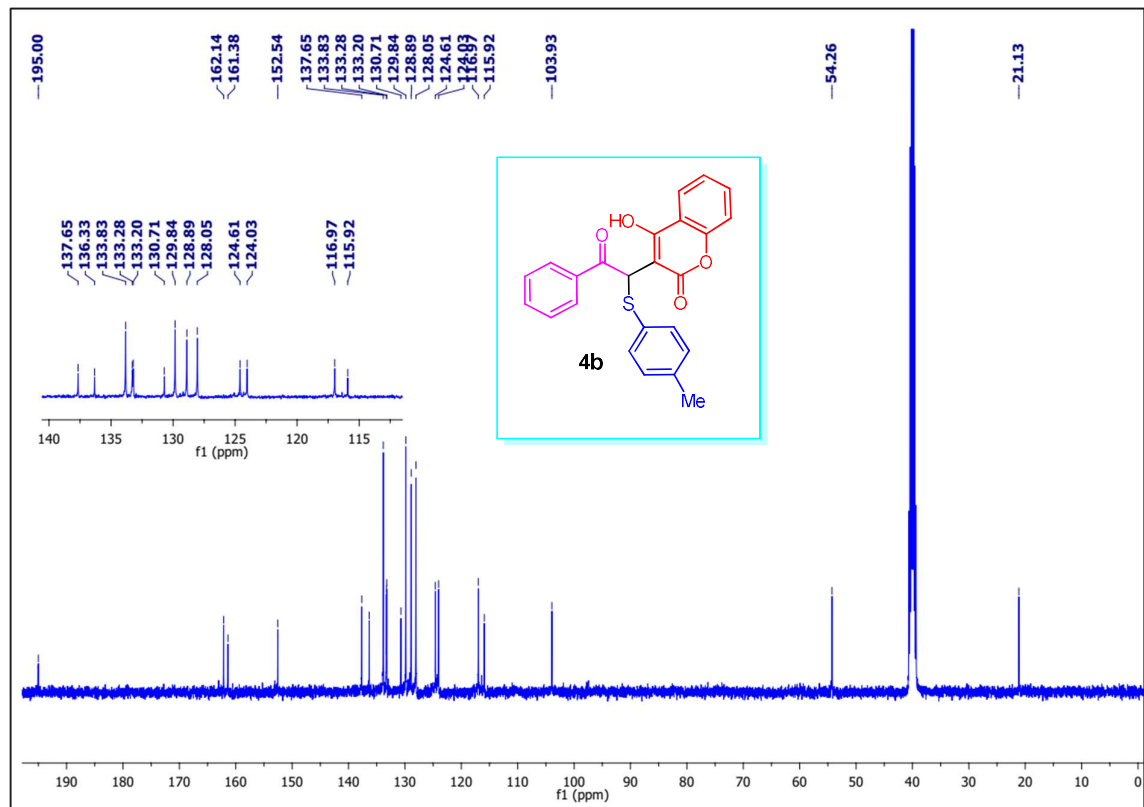
Table of contents:

^{1}H &^{13}C Spectra of 4a

¹H &¹³C Spectra of 4b
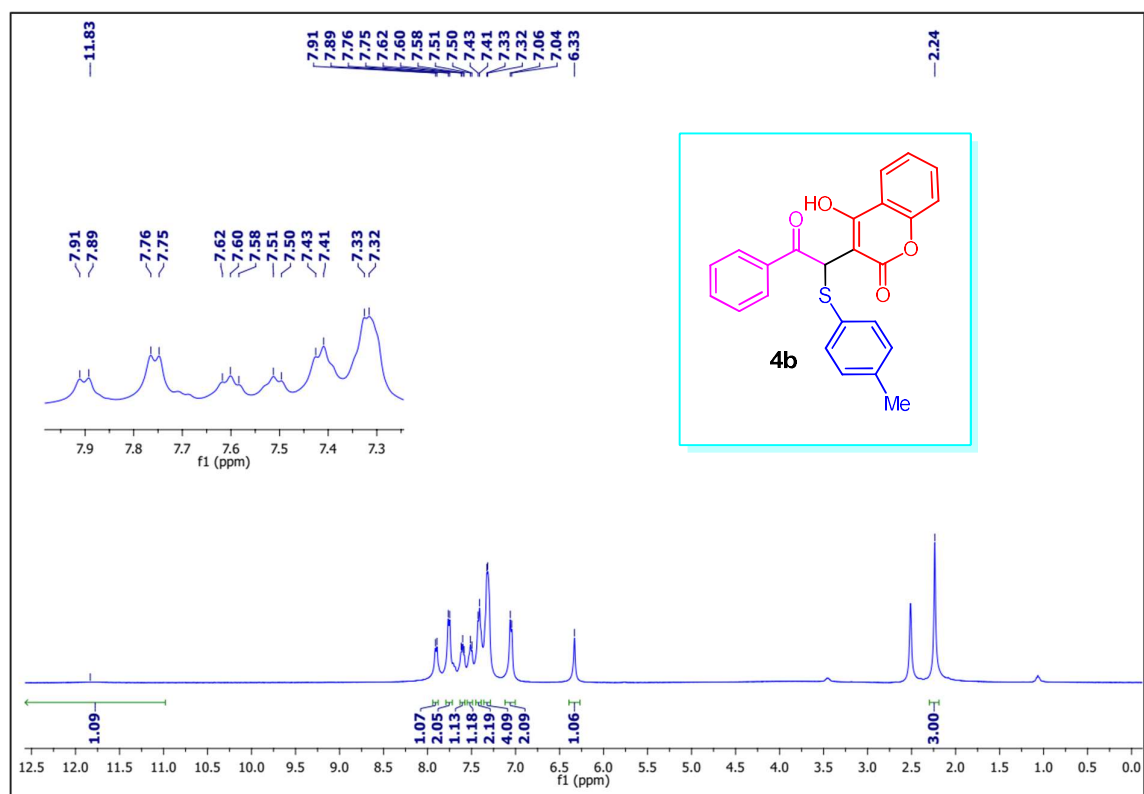
¹H &¹³C Spectra of 4c
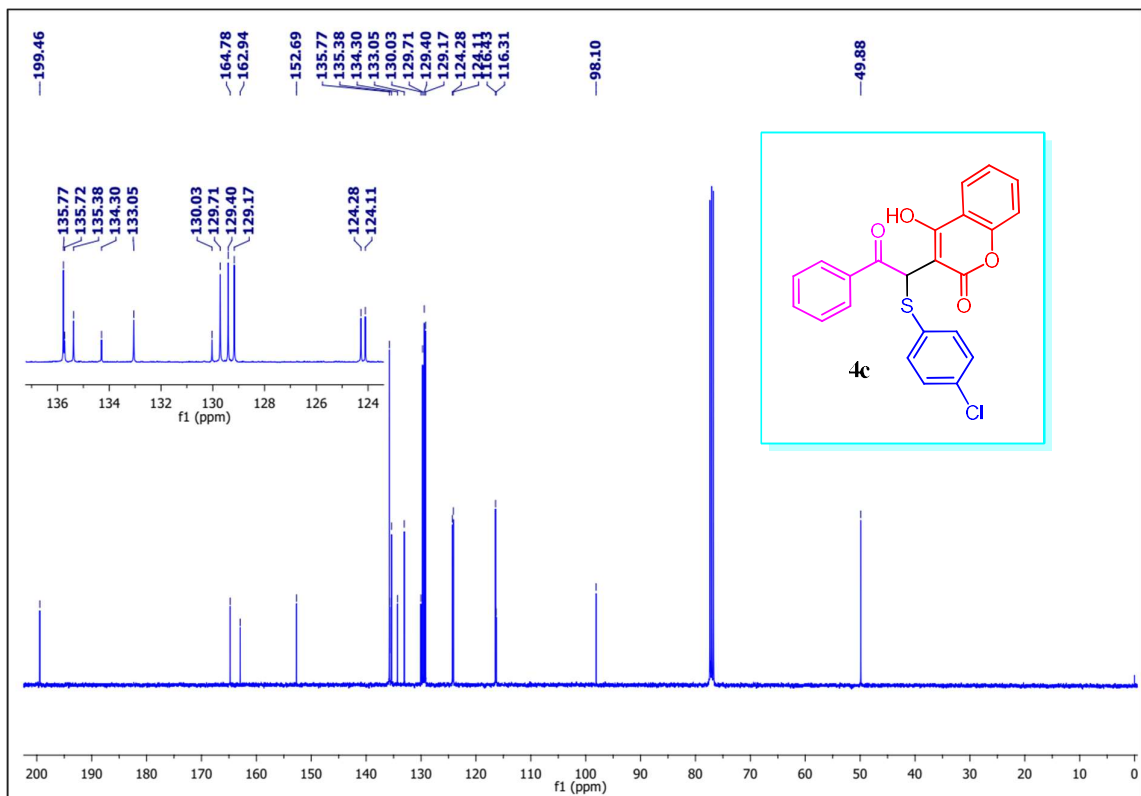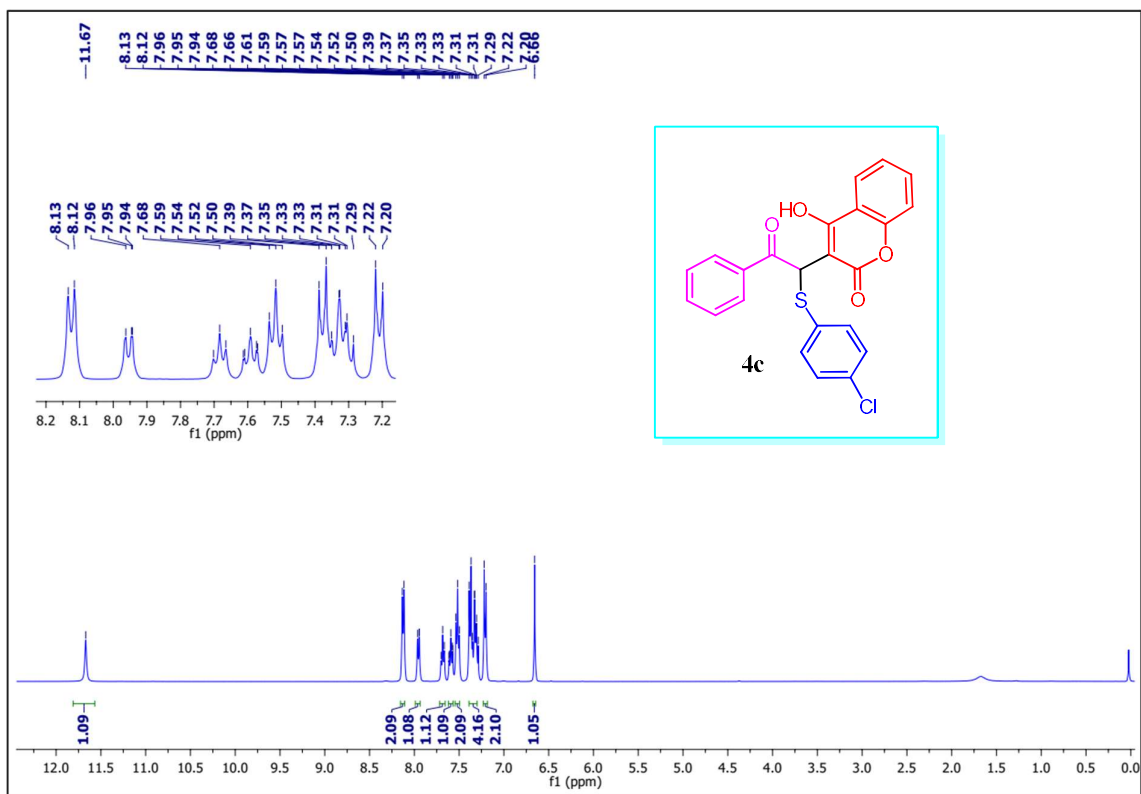
¹H &¹³C Spectra of 4d
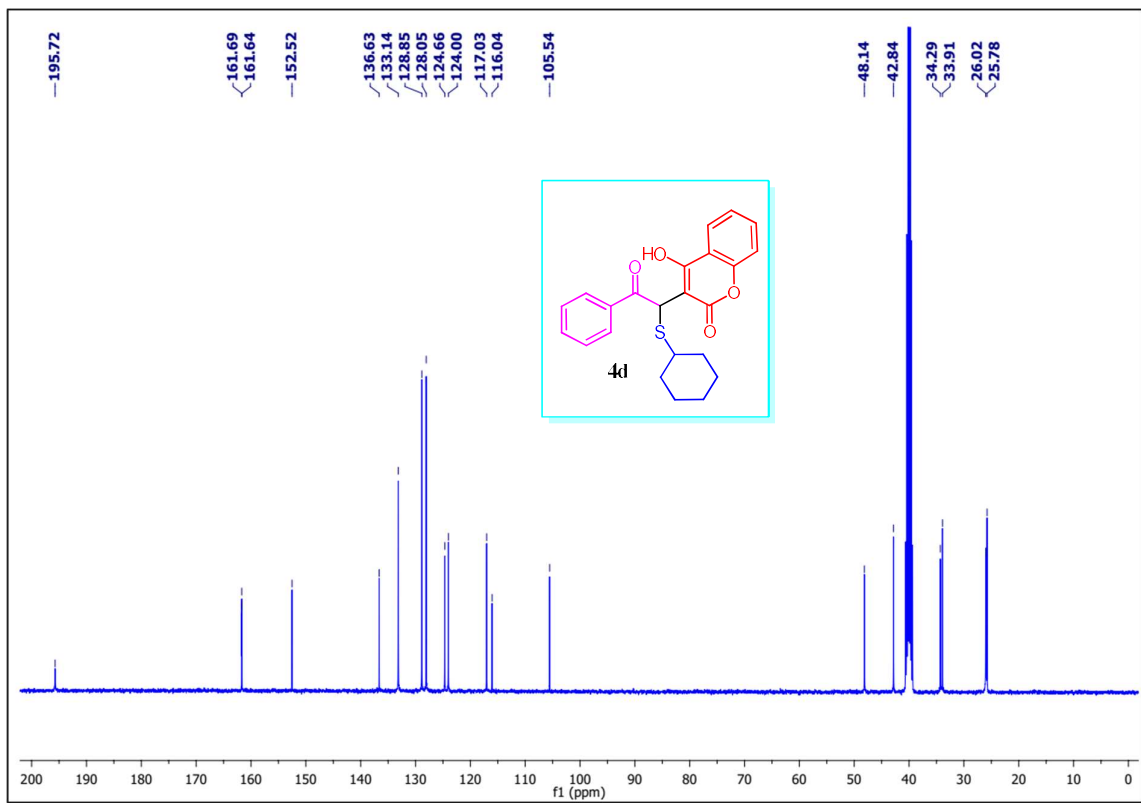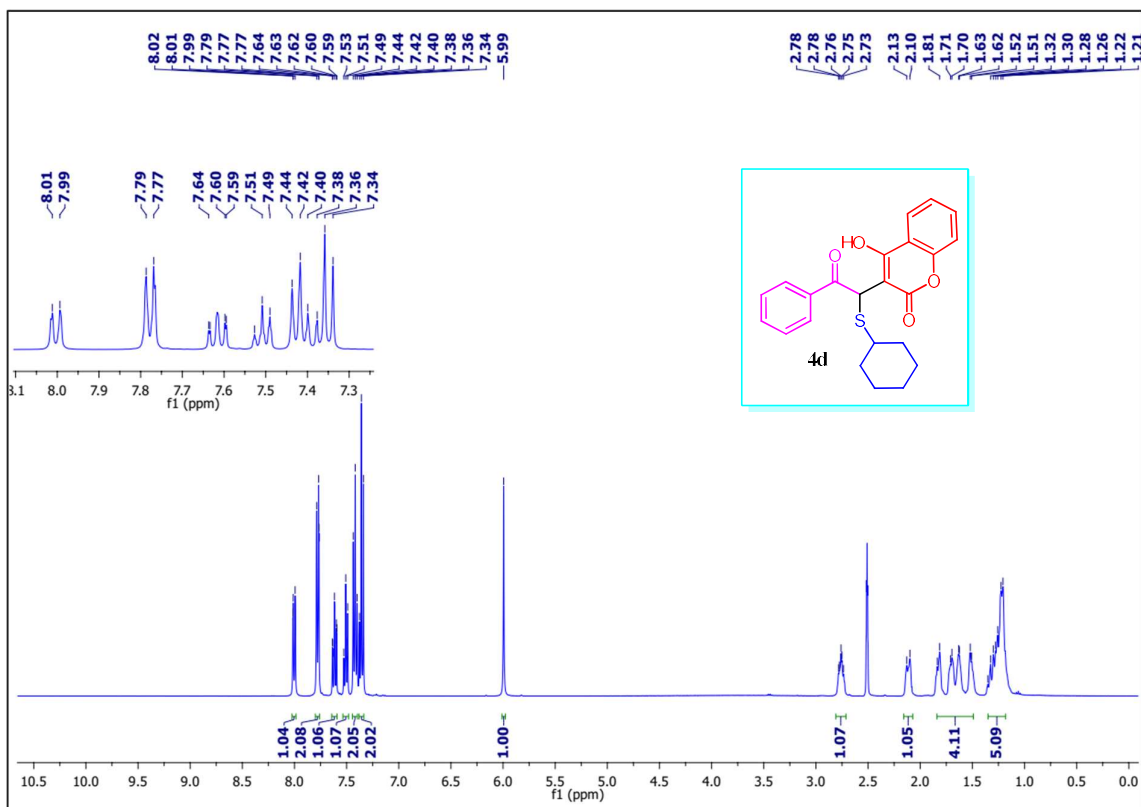
¹H &¹³C Spectra of 4e
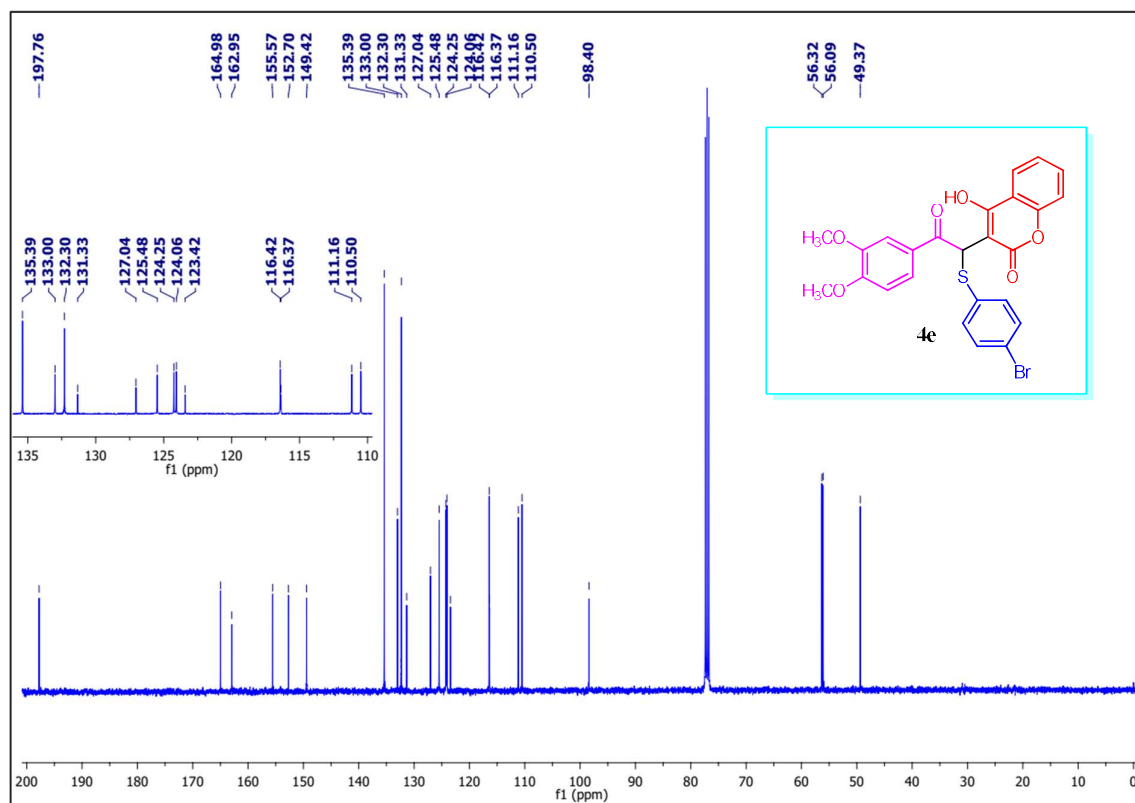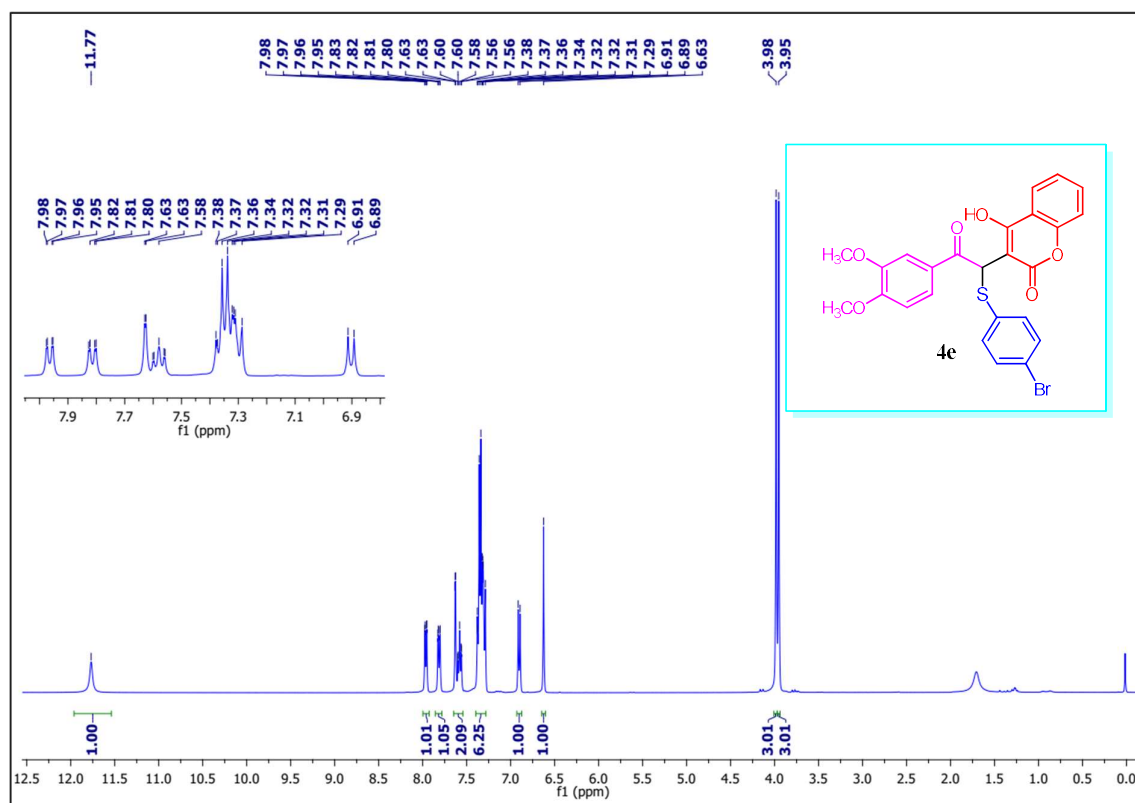
¹H &¹³C Spectra of 4f
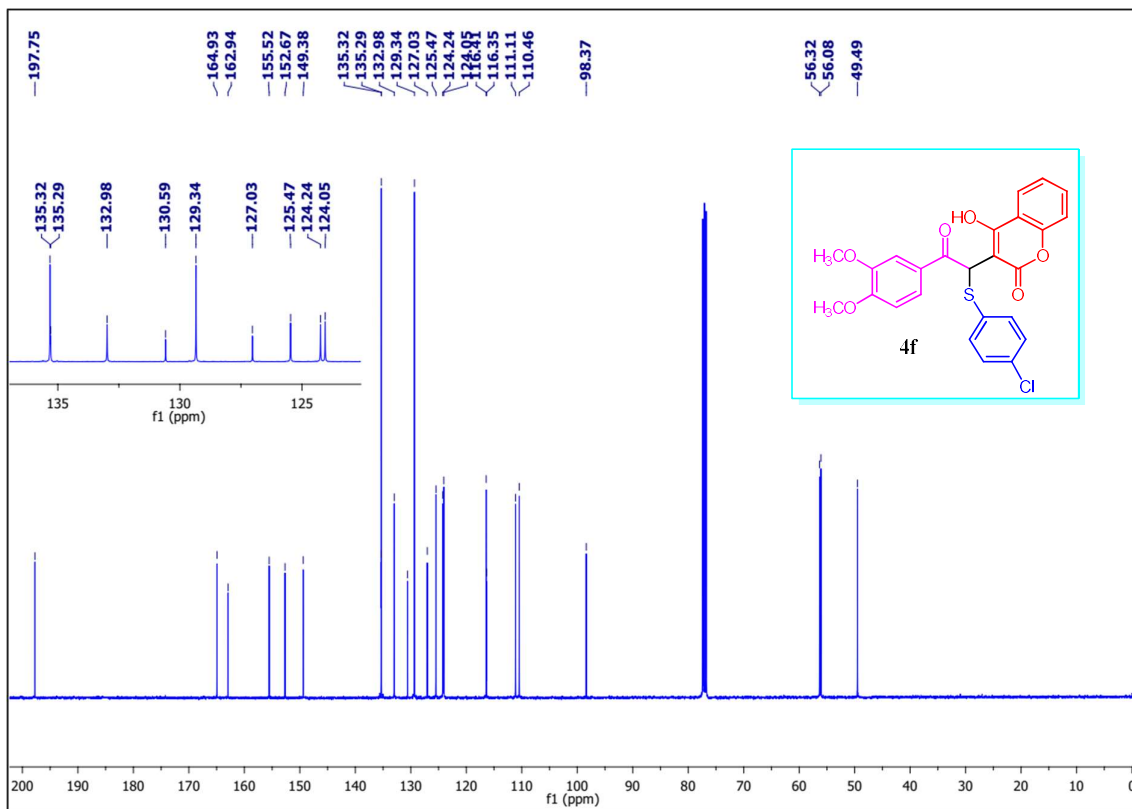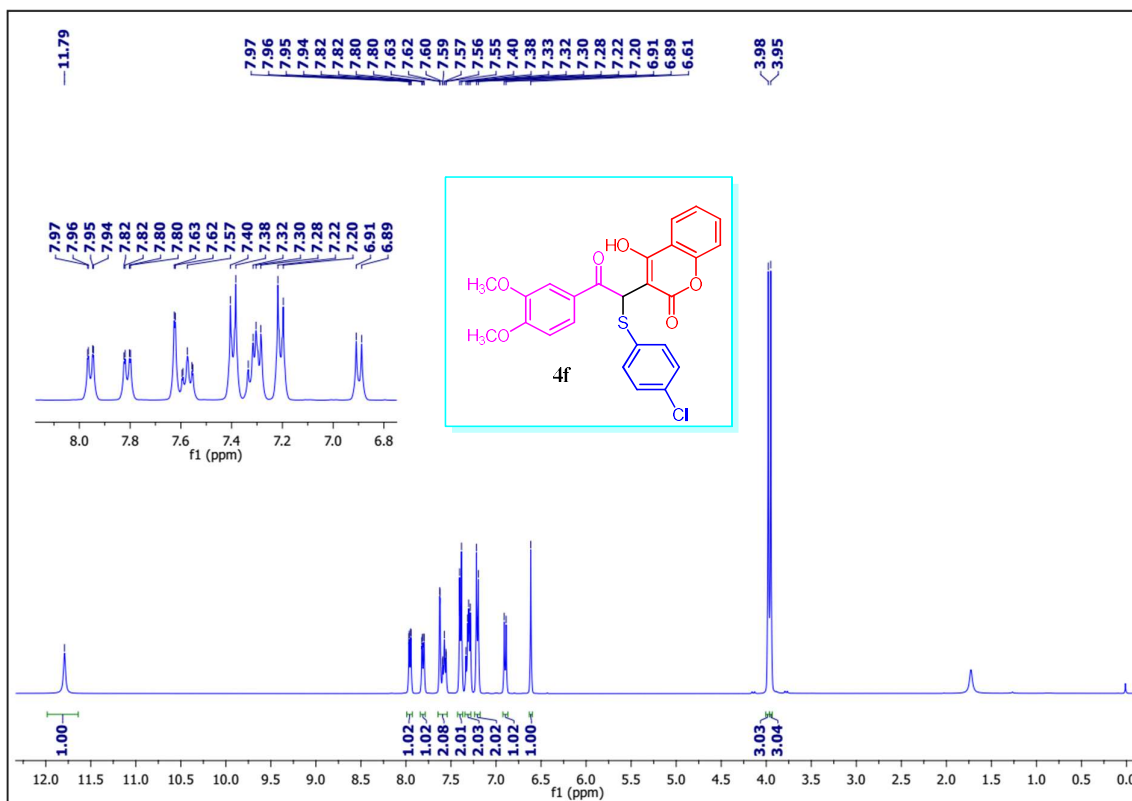
¹H &¹³C Spectra of 4g
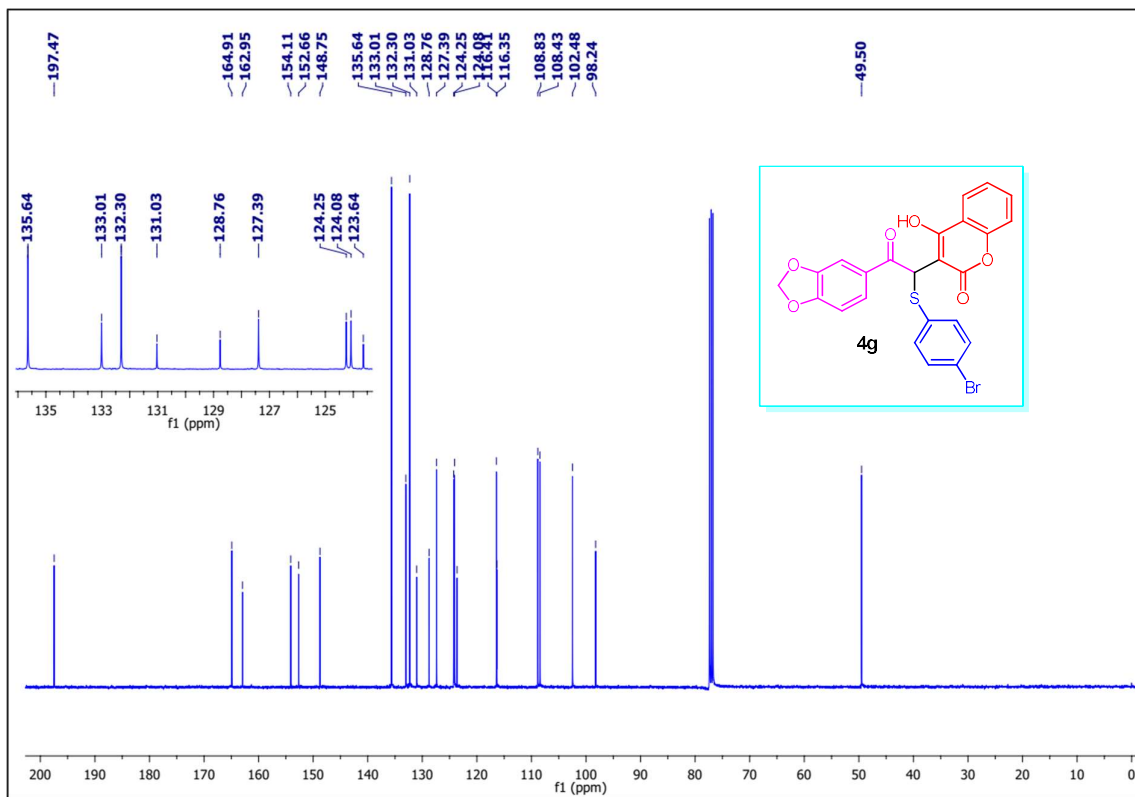
¹H &¹³C Spectra of 4h

¹H &¹³C Spectra of 4i

¹H &¹³C Spectra of 4j

¹H &¹³C Spectra of 4k

¹H &¹³C Spectra of 4l

¹H & ¹³C Spectra of 4l

¹H &¹³C Spectra of 4m

^1H & ^{13}C Spectra of 4n

¹H &¹³C Spectra of 4o

^{1}H &^{13}C Spectra of 4p
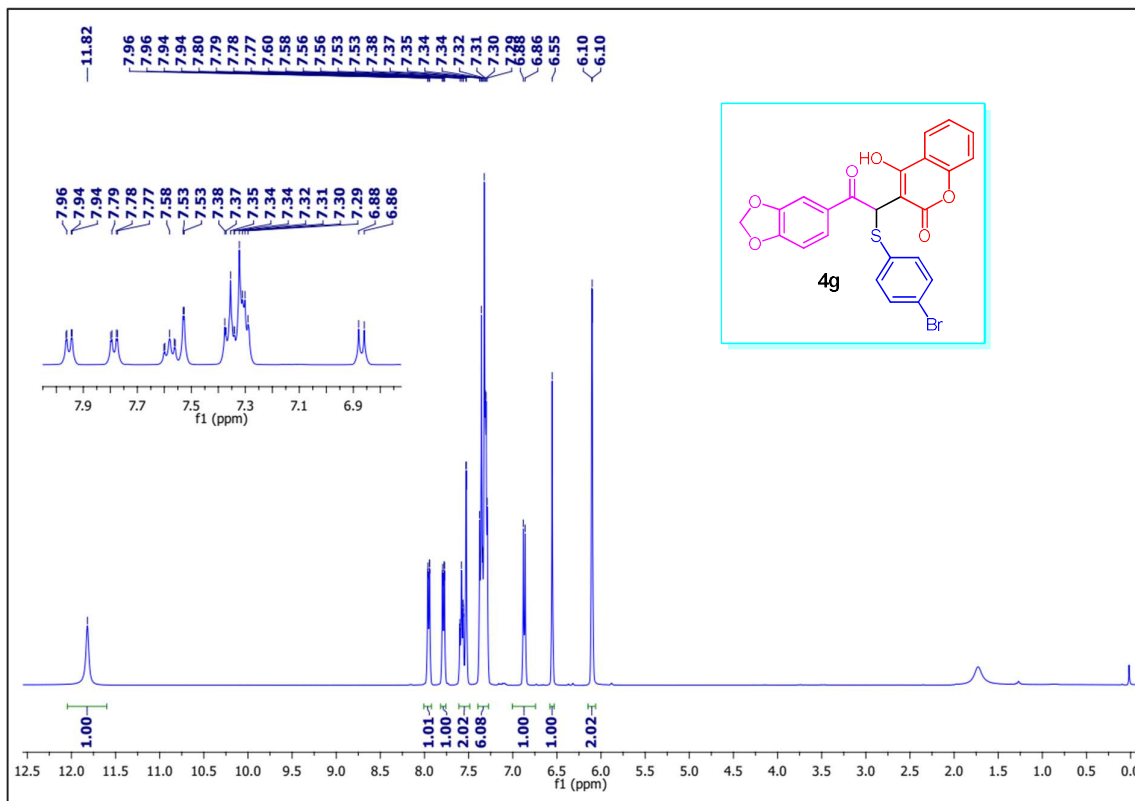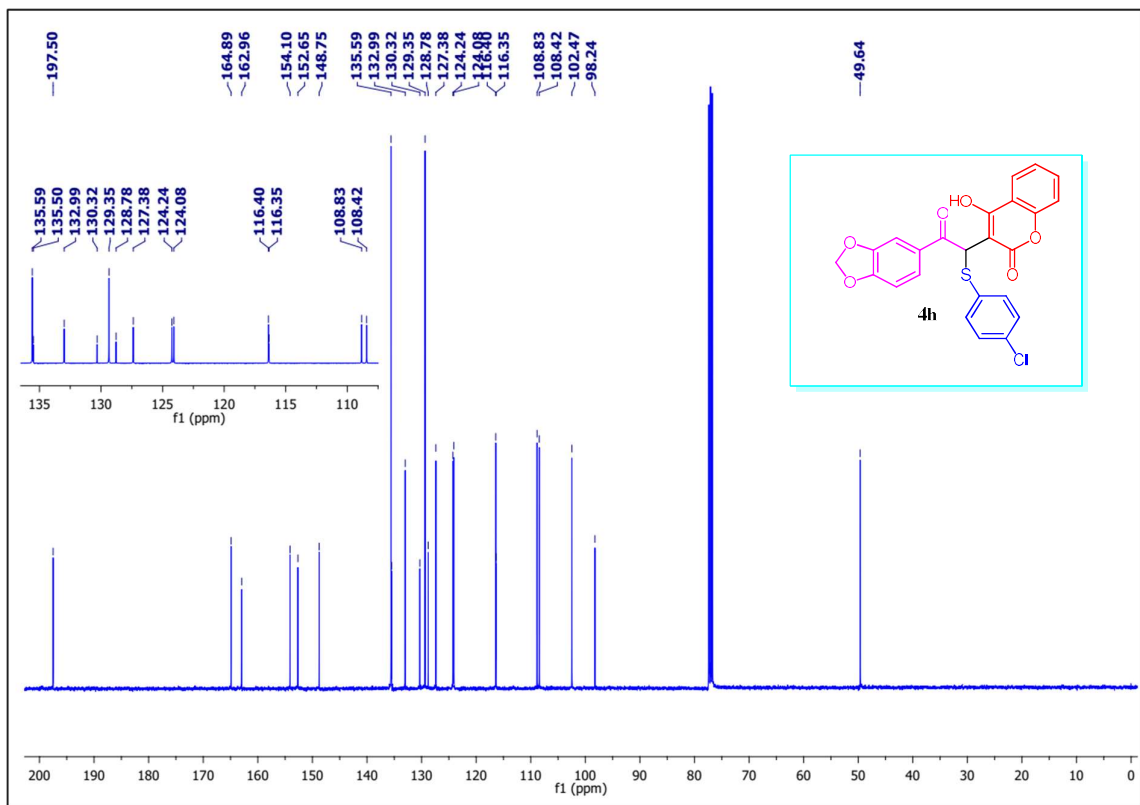
^{1}H &^{13}C Spectra of 4q
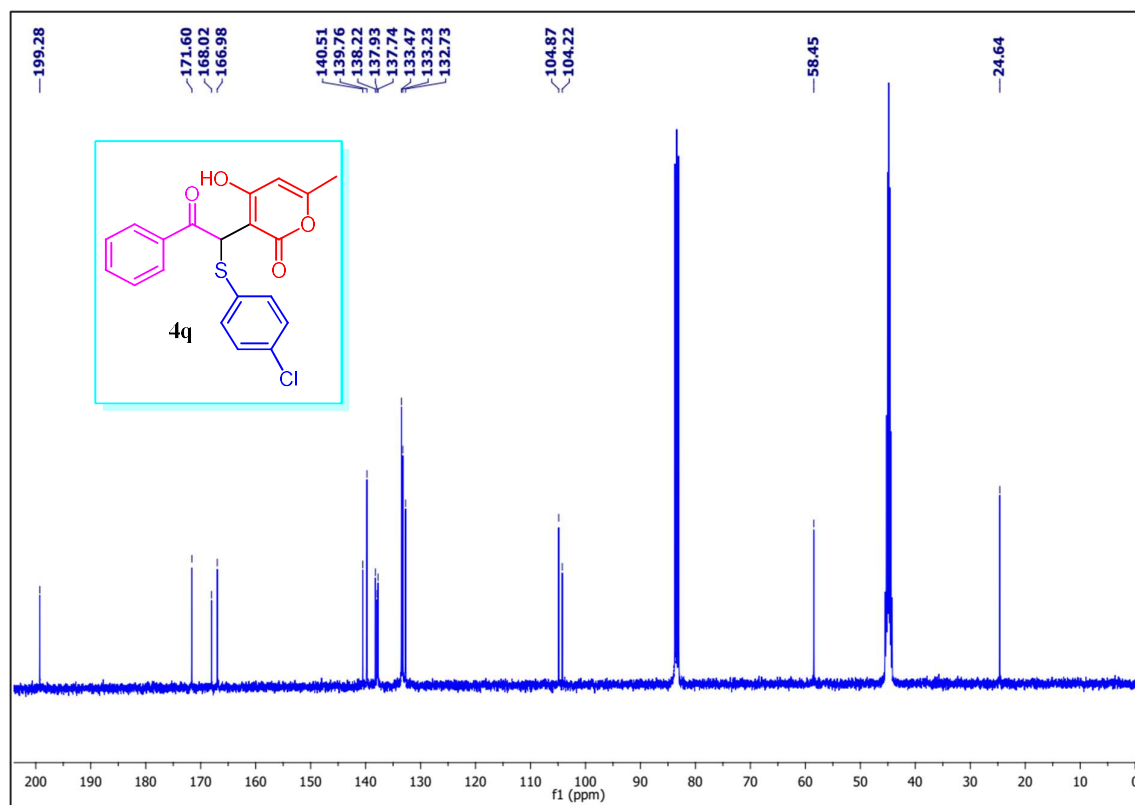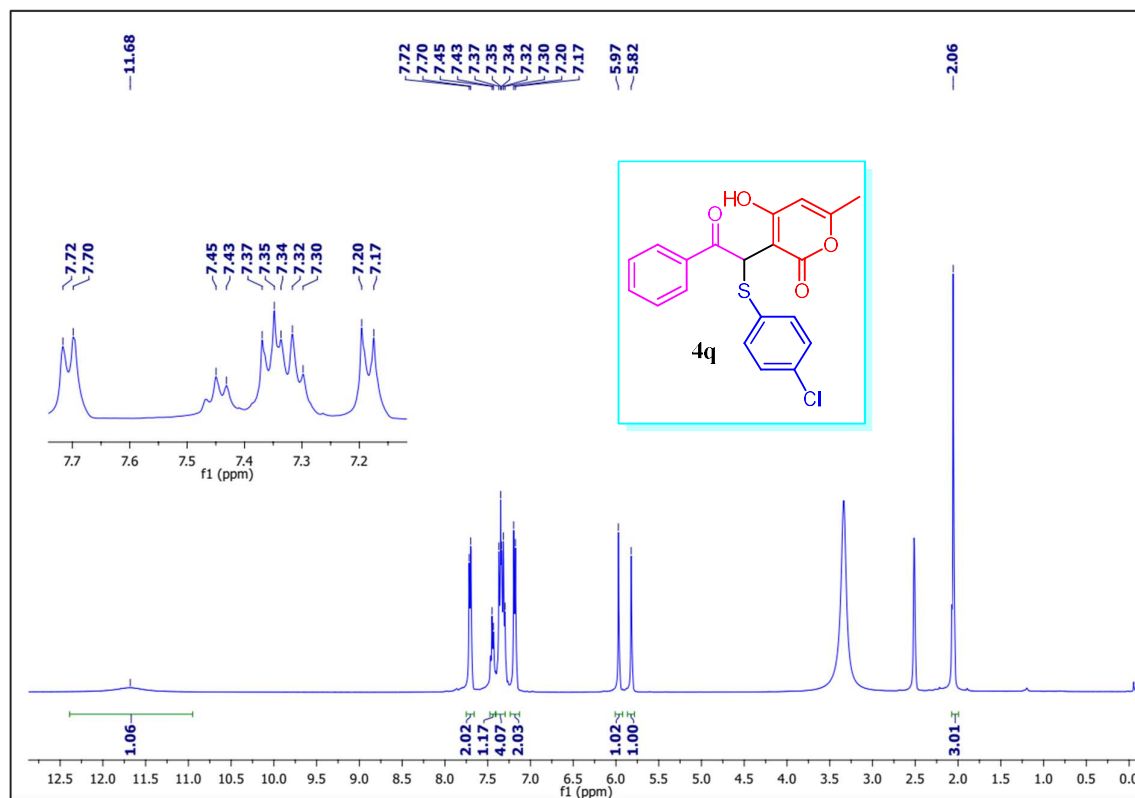
¹H &¹³C Spectra of 4r
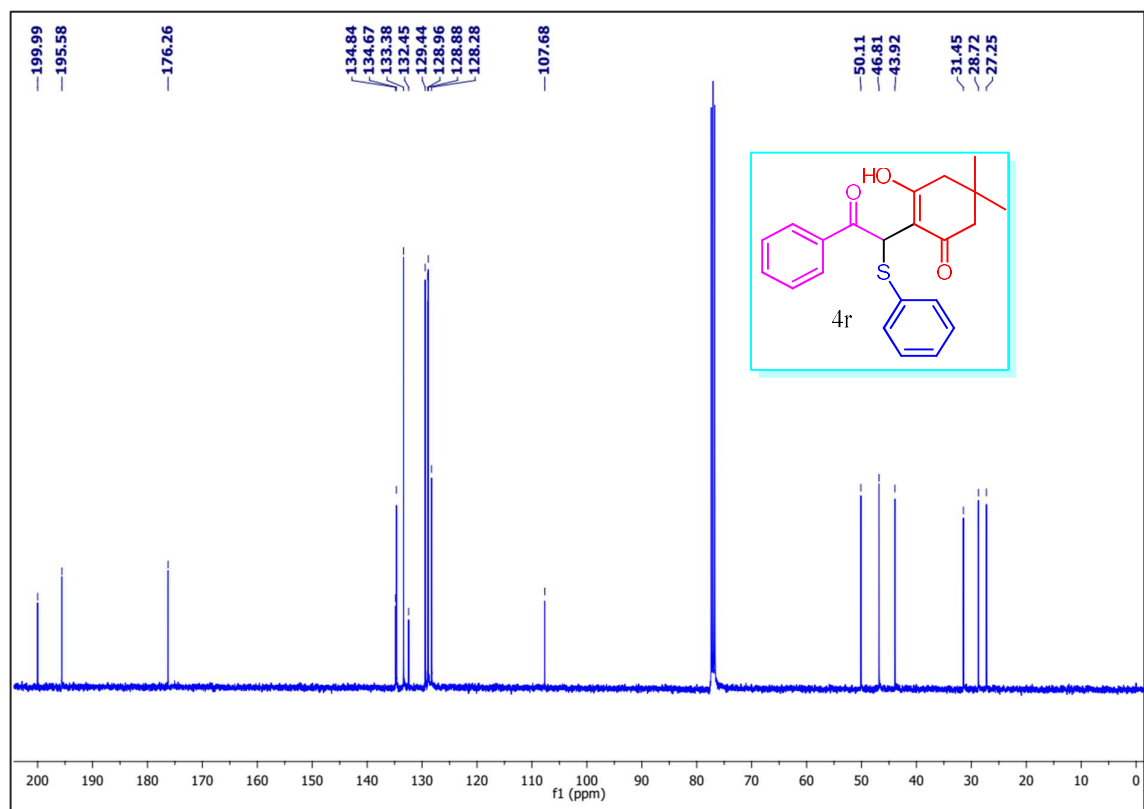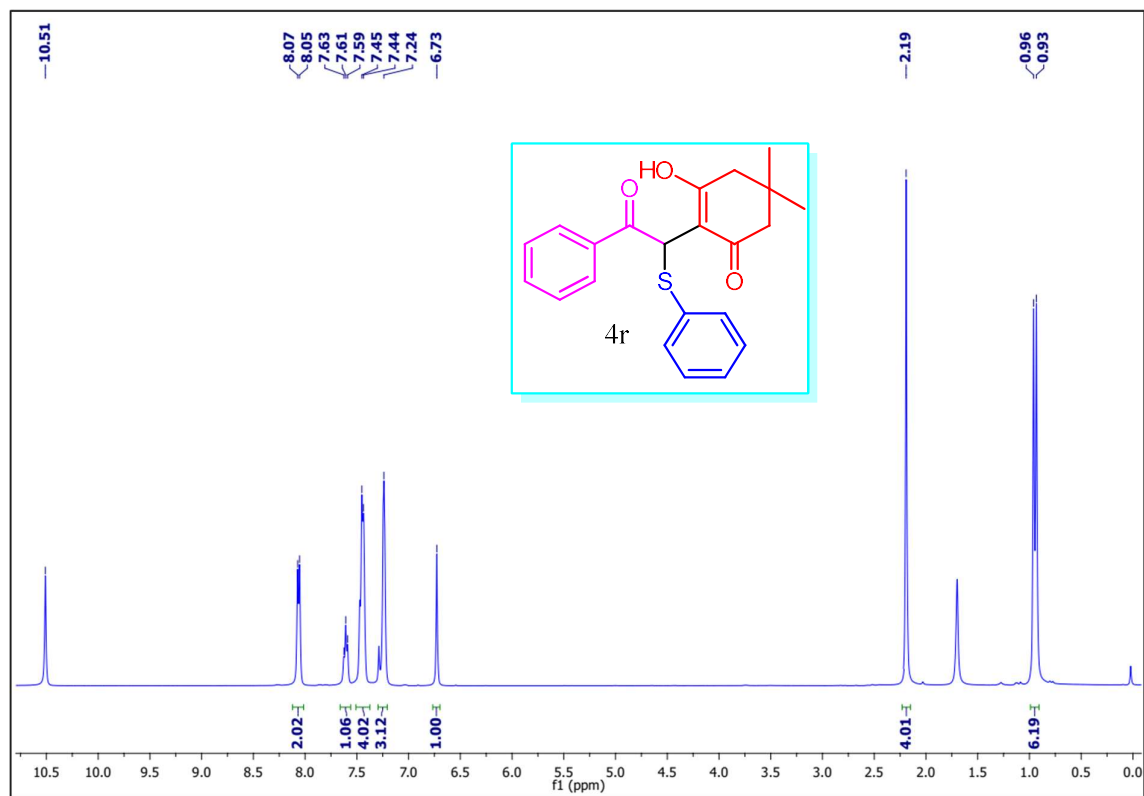
¹H &¹³C Spectra of 4s
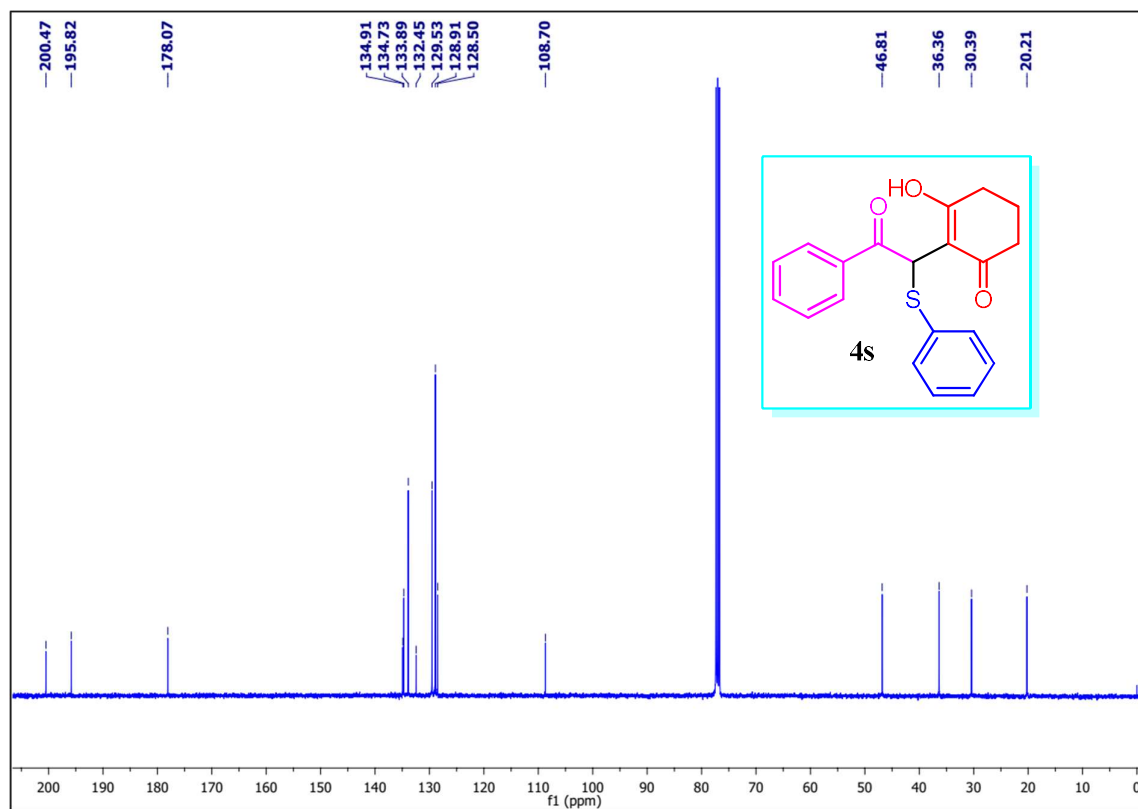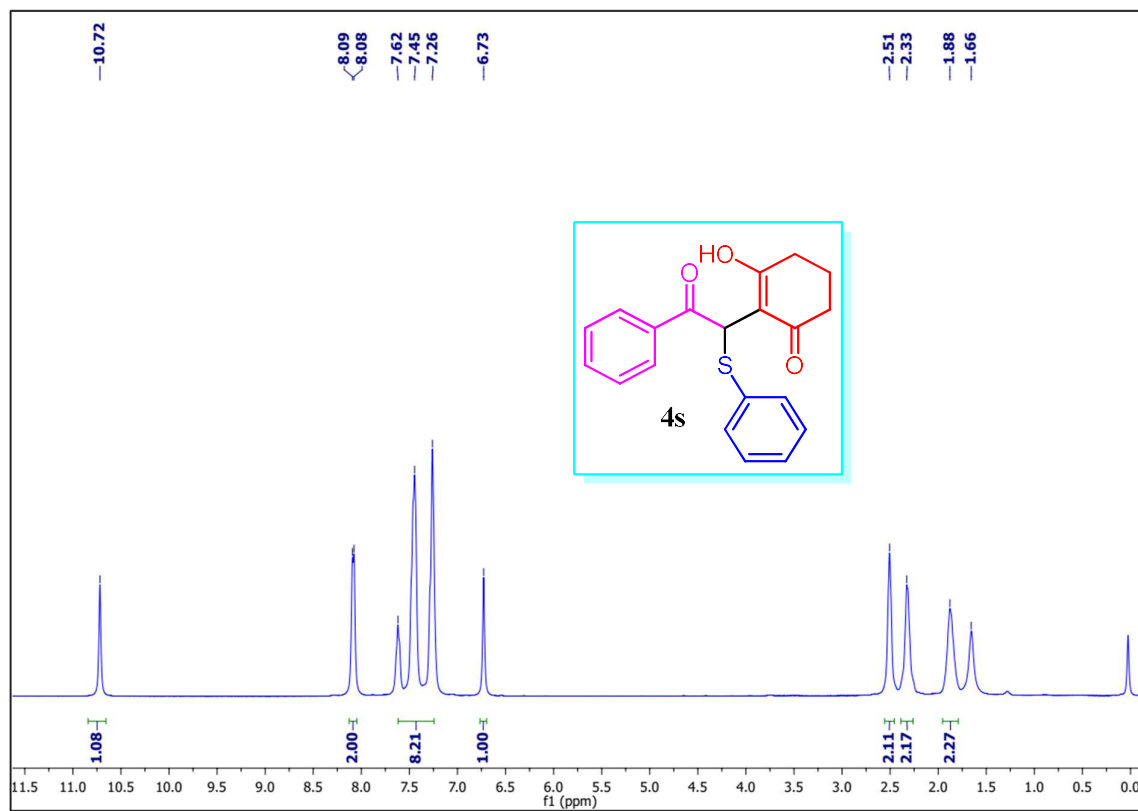
¹H &¹³C Spectra of 4t
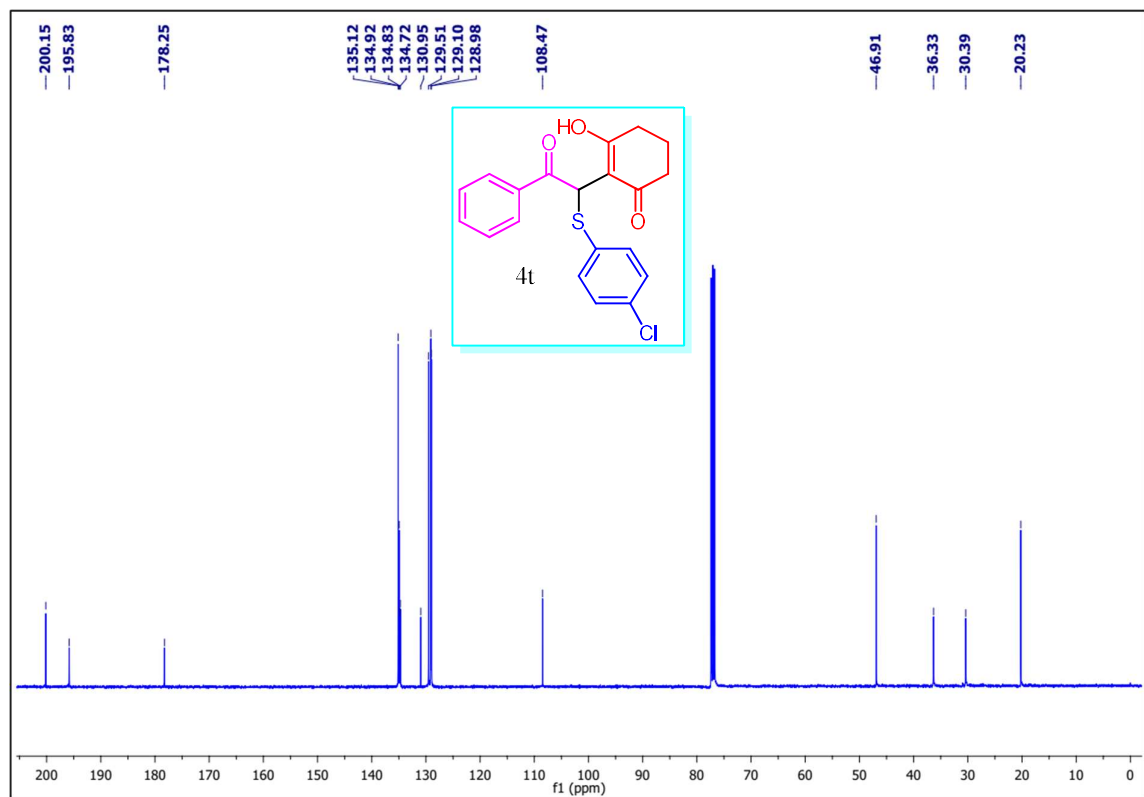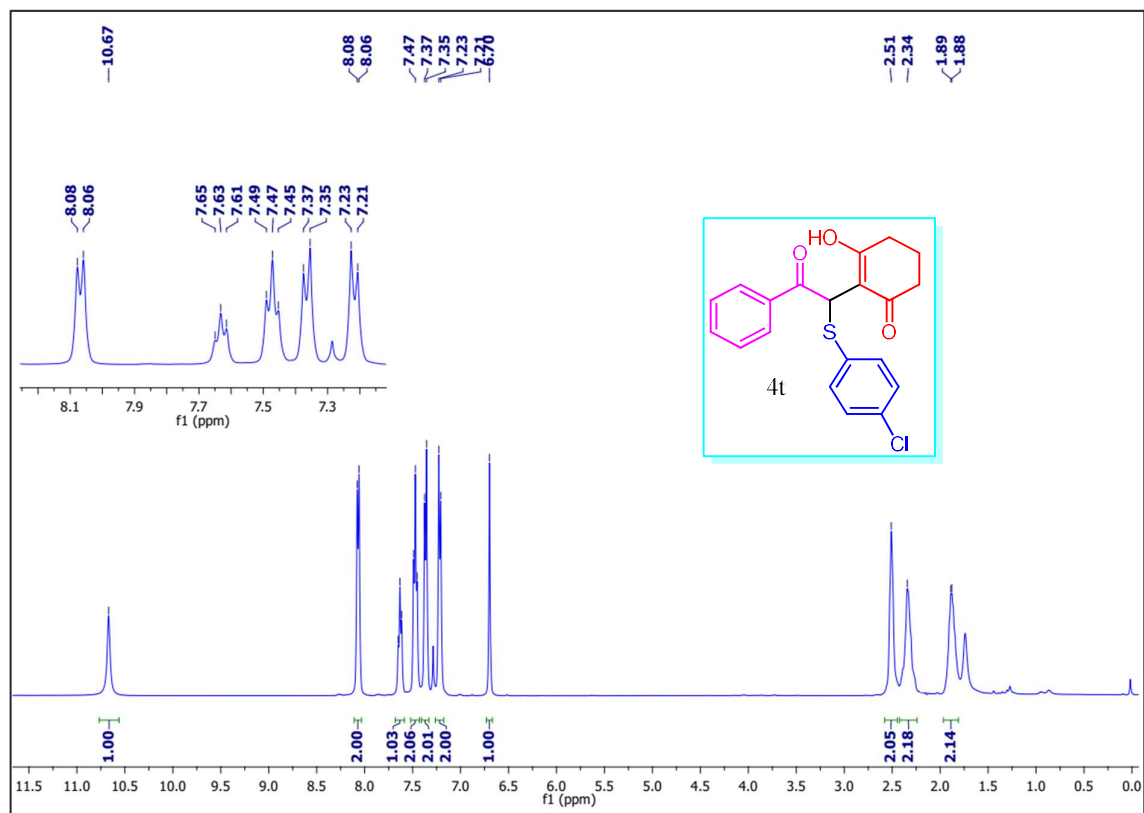
¹H &¹³C Spectra of 5
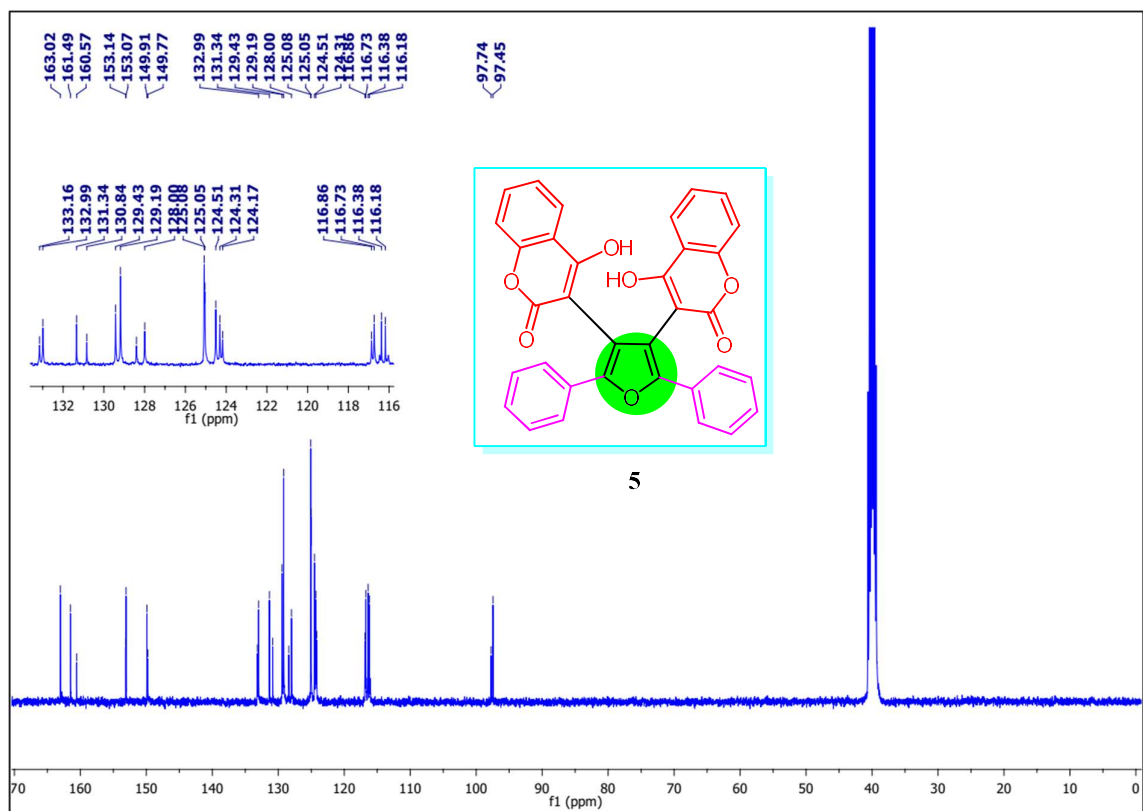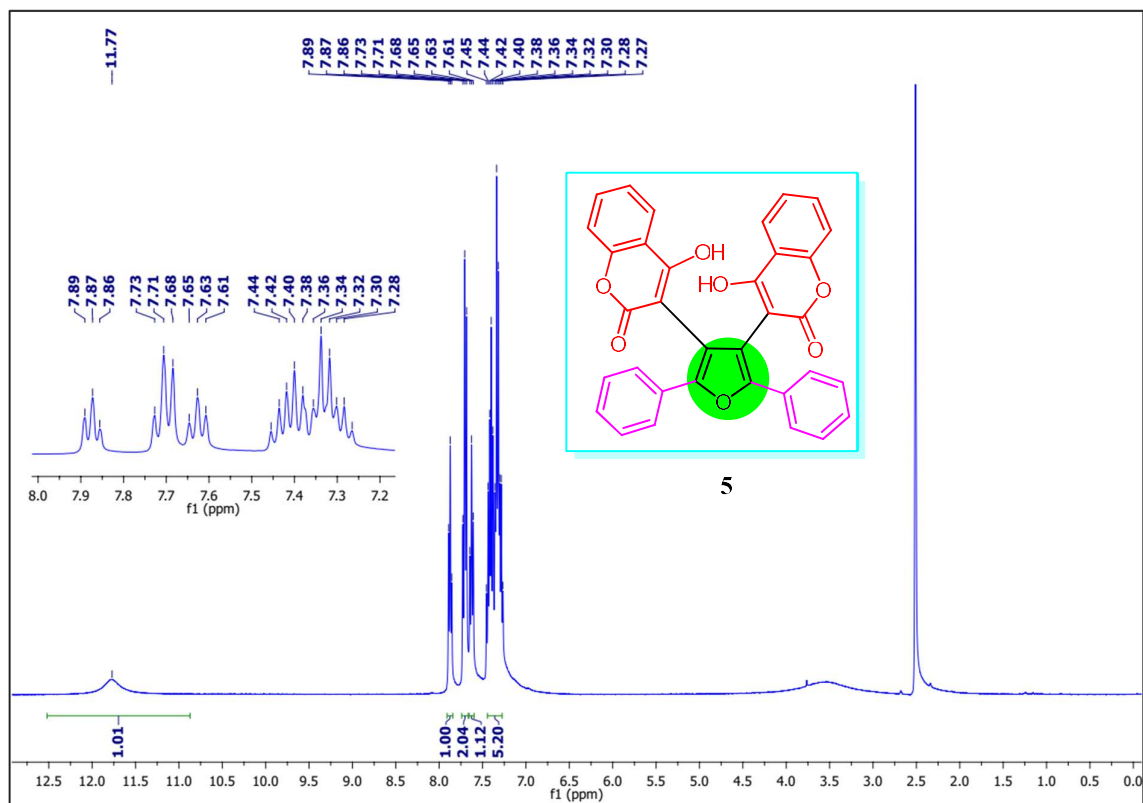
¹H &¹³C Spectra of 6a
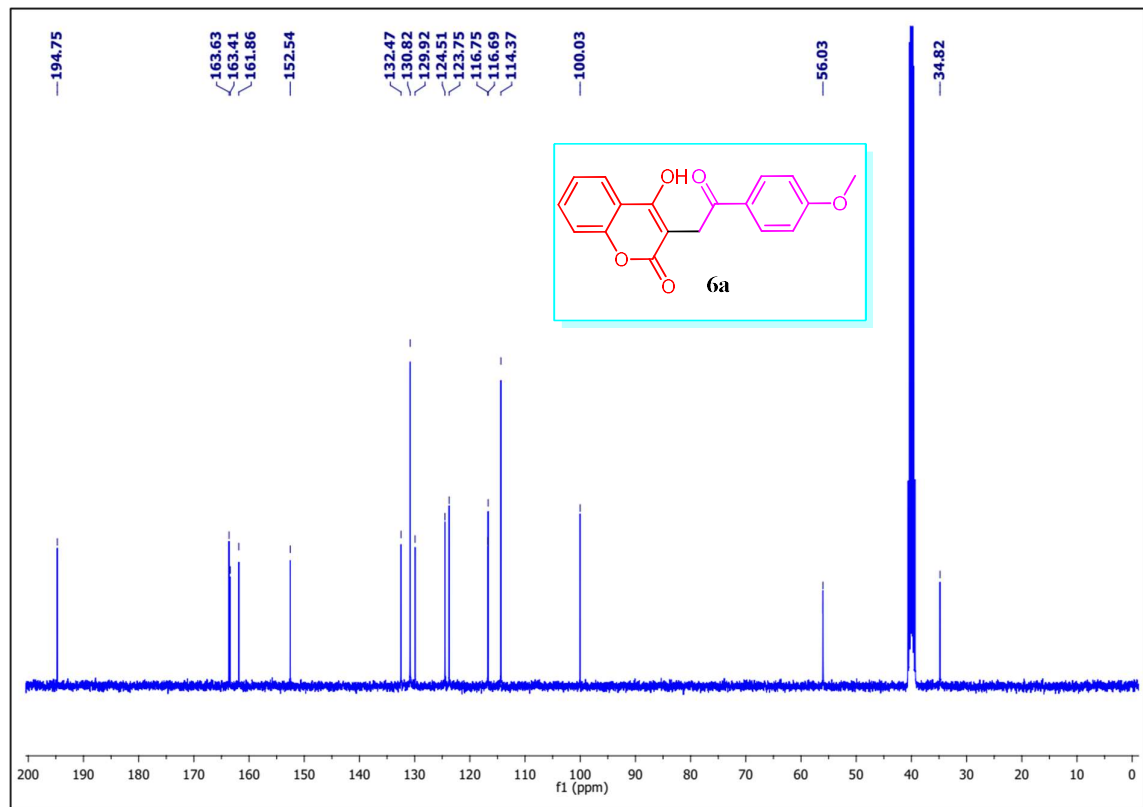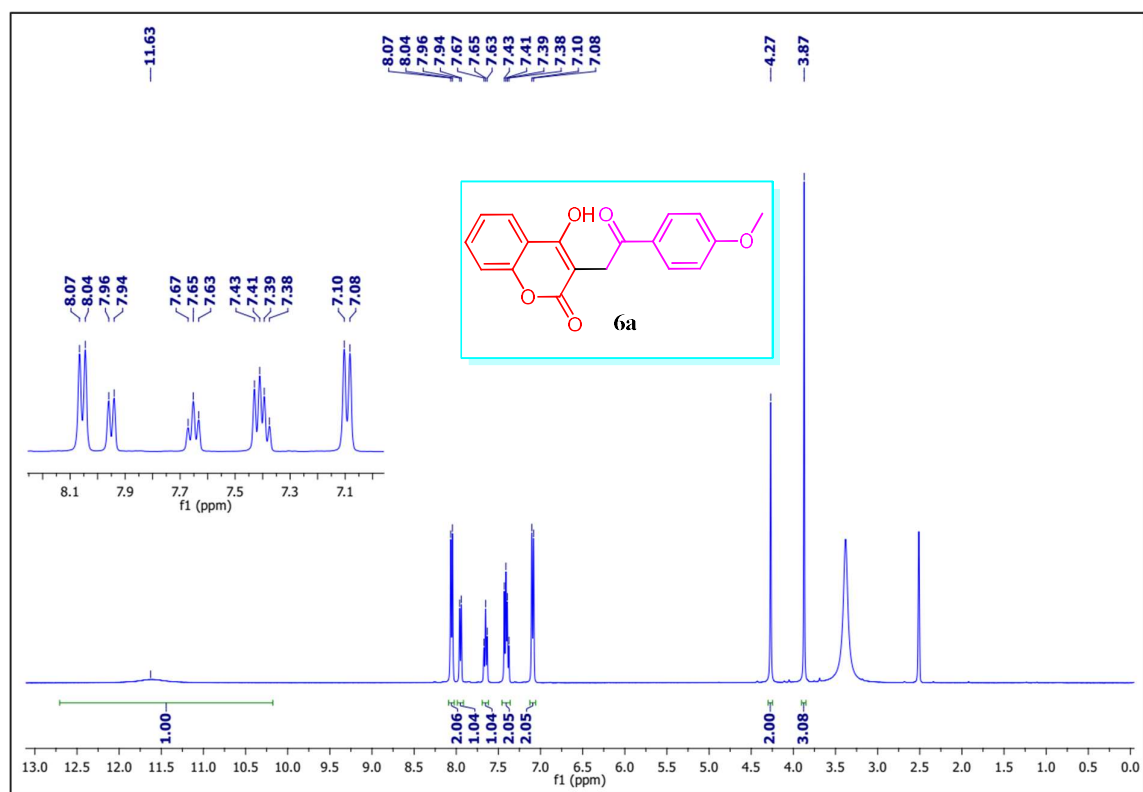
¹H &¹³C Spectra of 6b
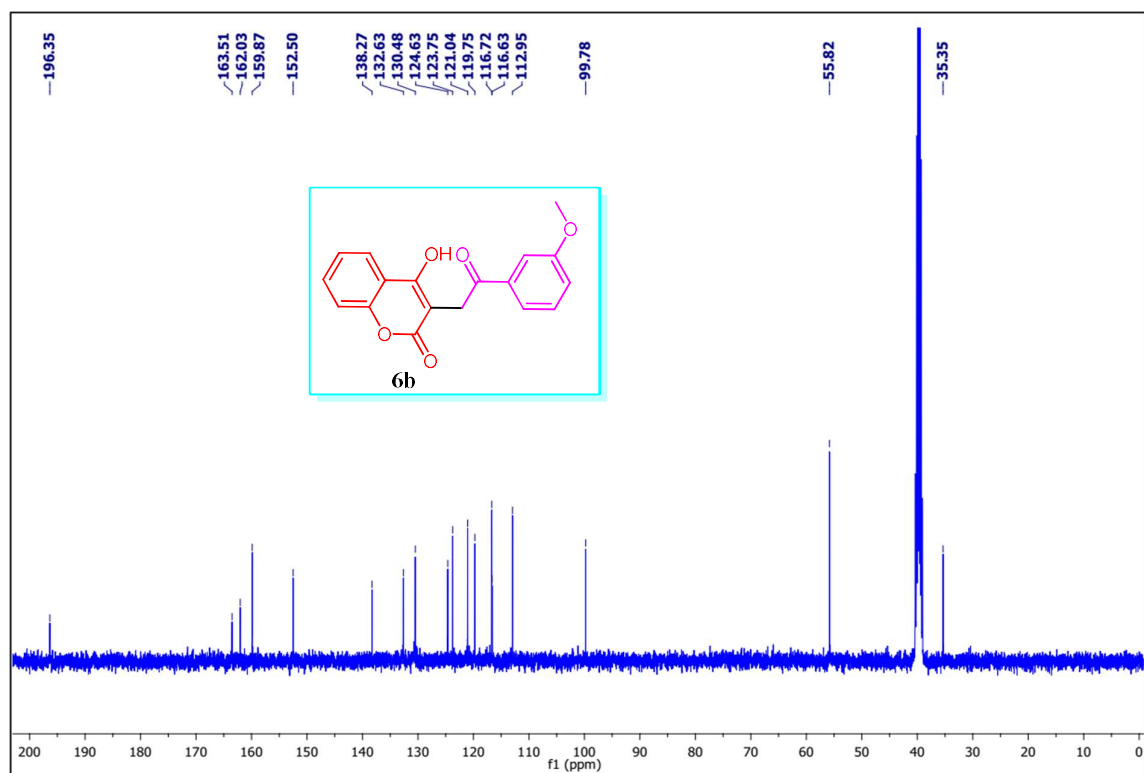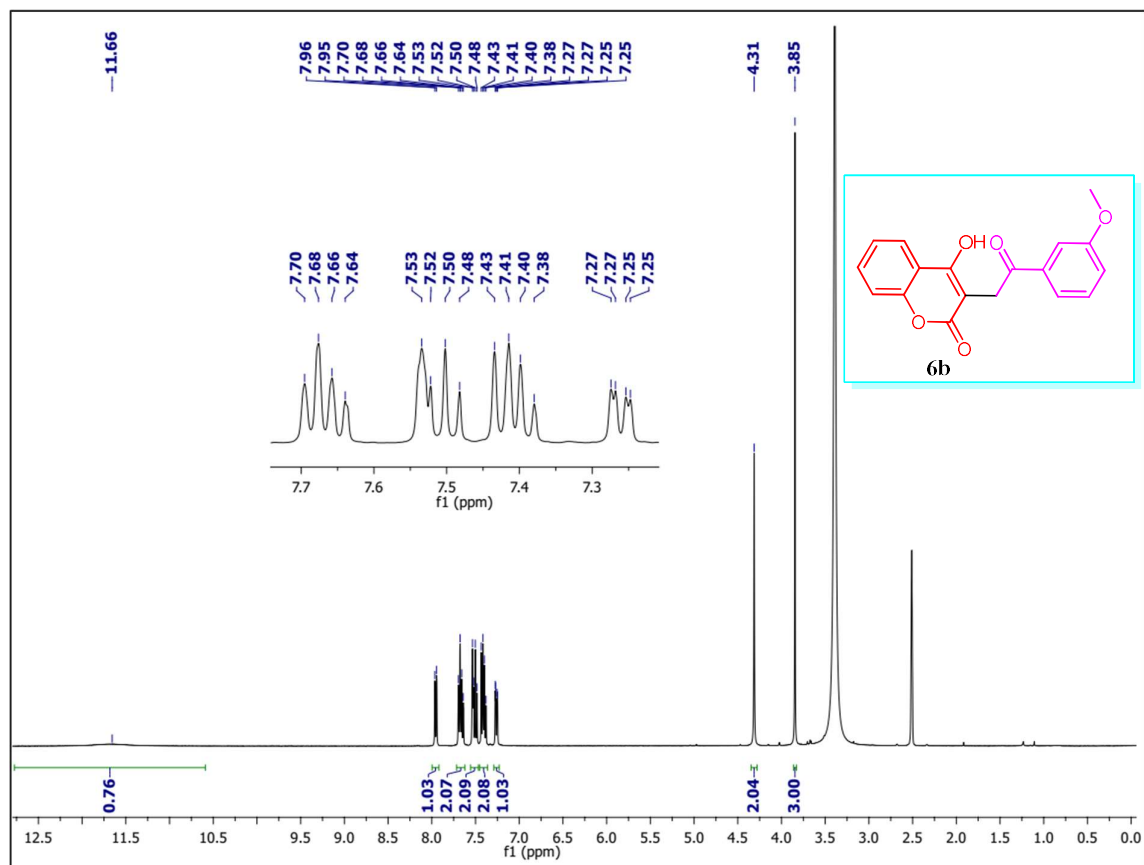
^{1}H &^{13}C Spectra of 6c
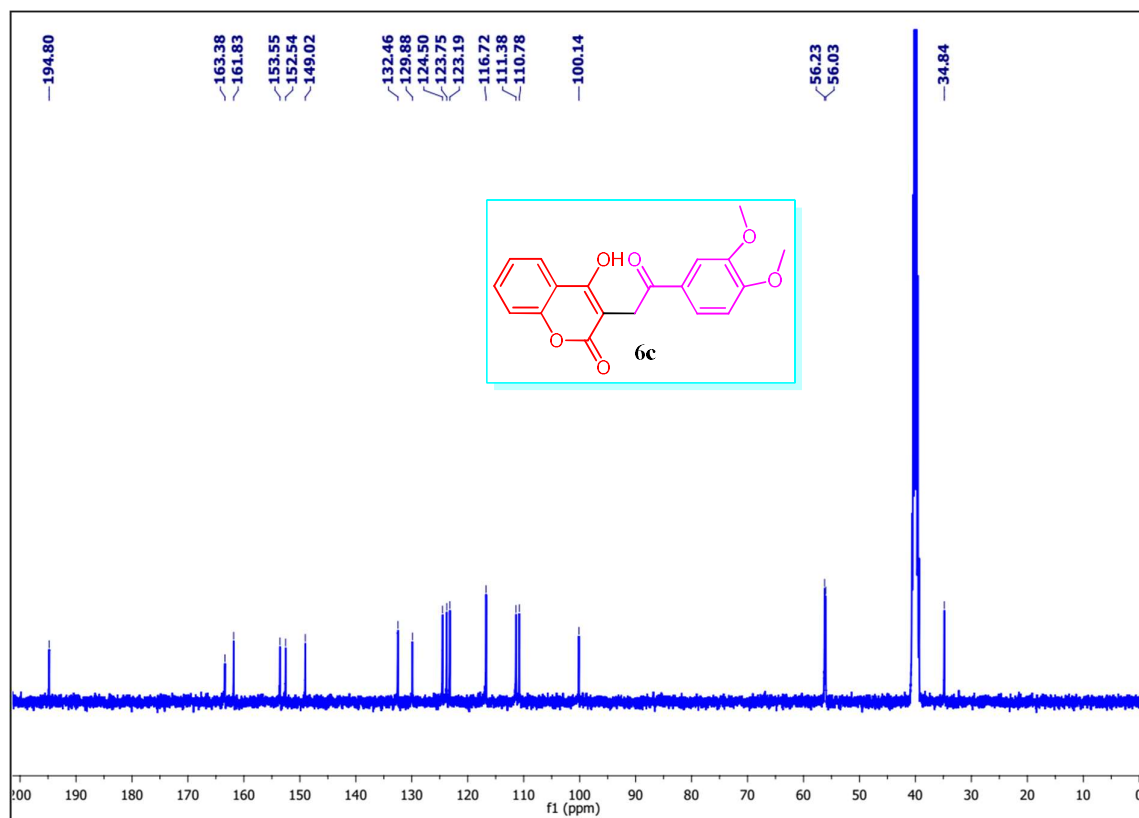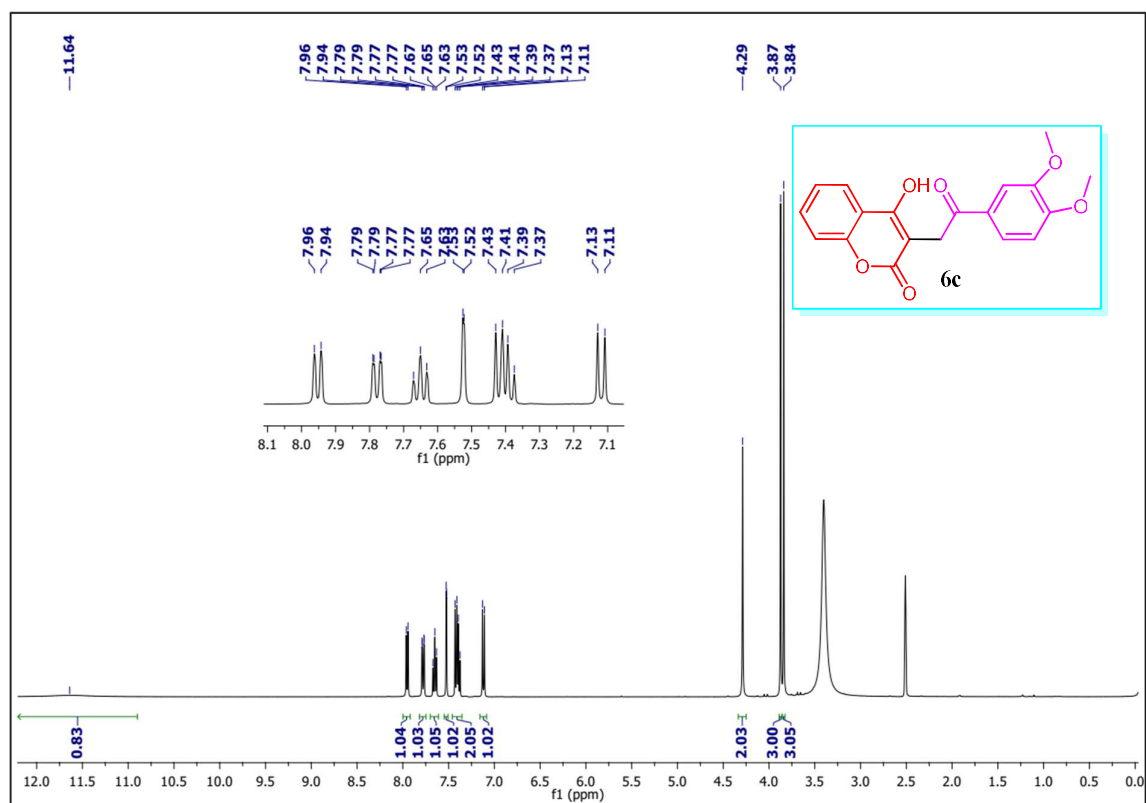
^{1}H &^{13}C Spectra of 6d
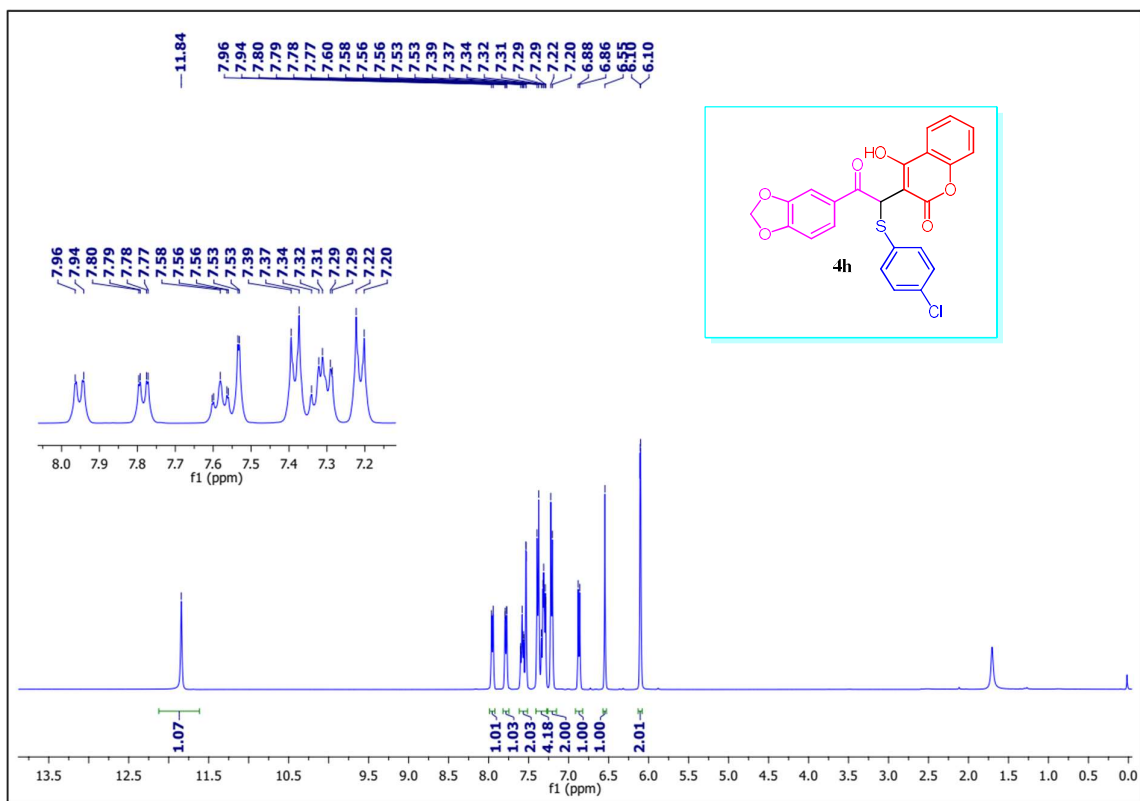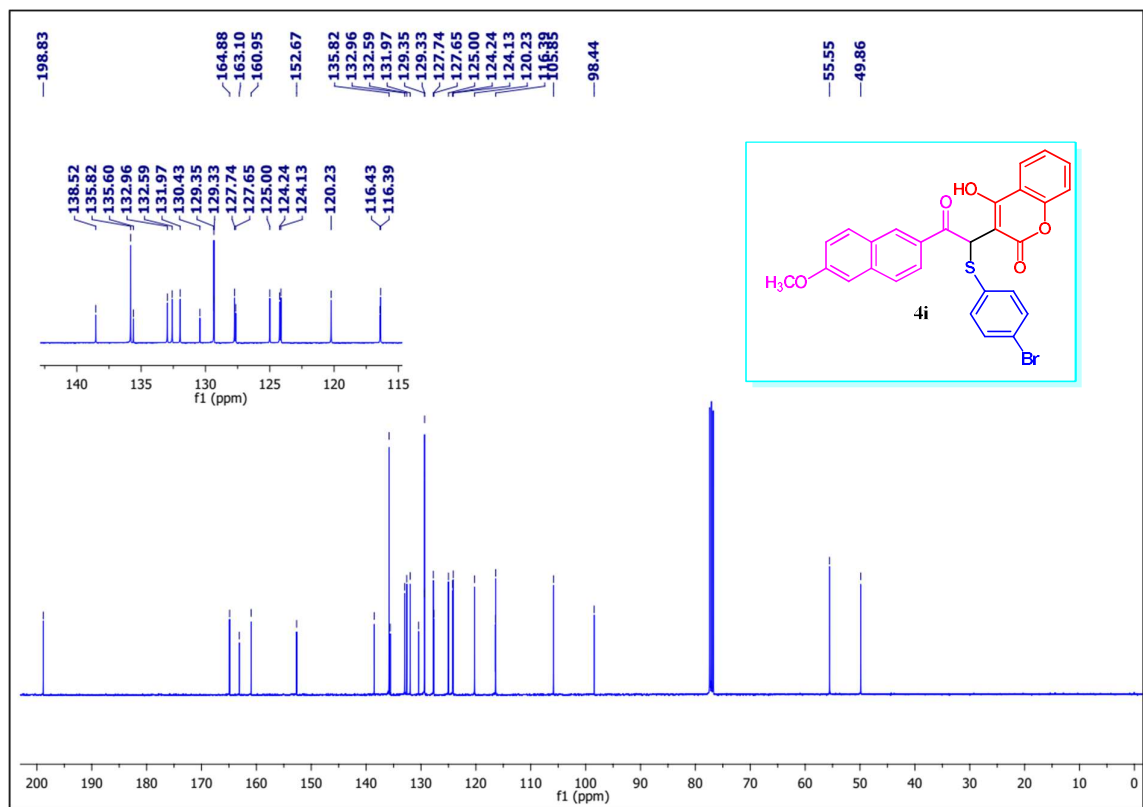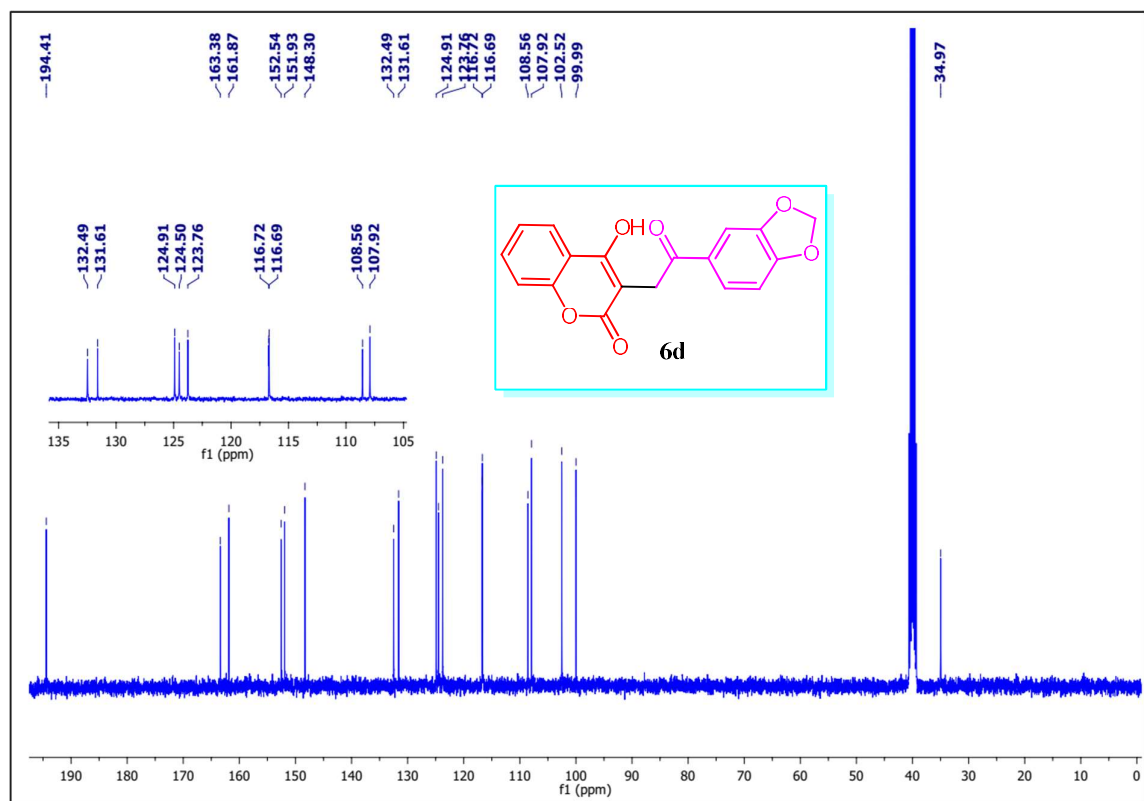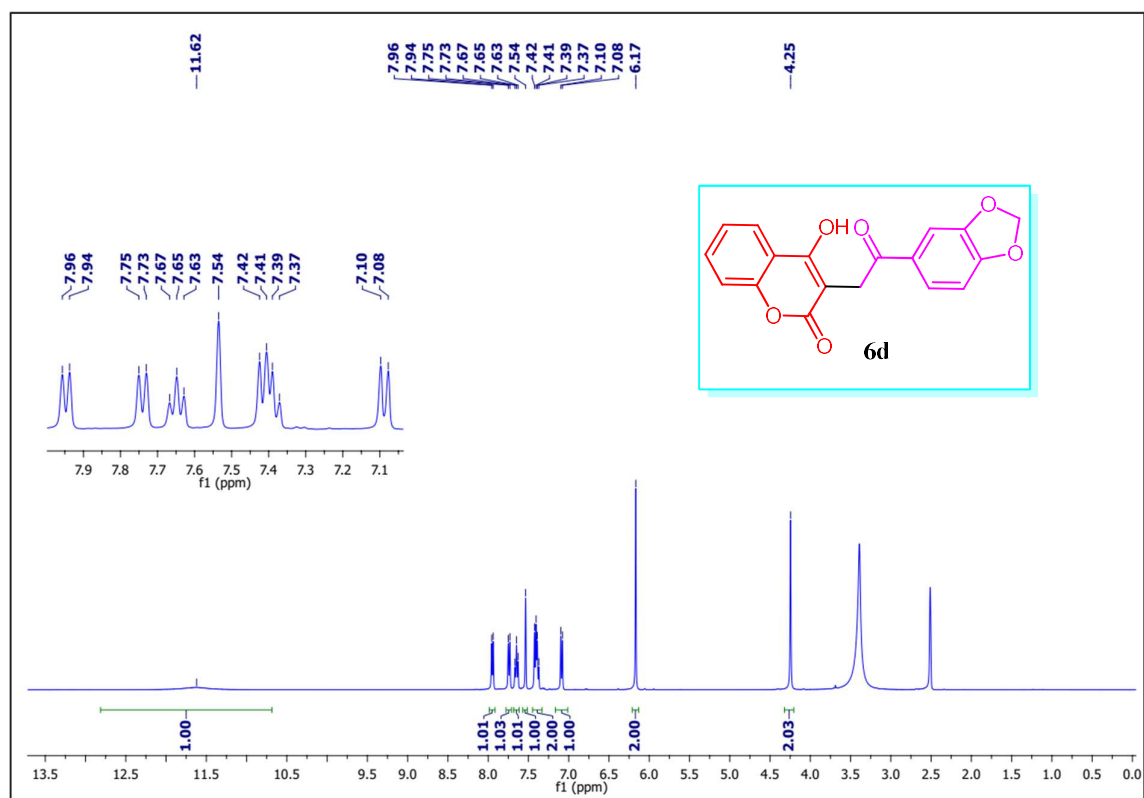
¹H &¹³C Spectra of 6e
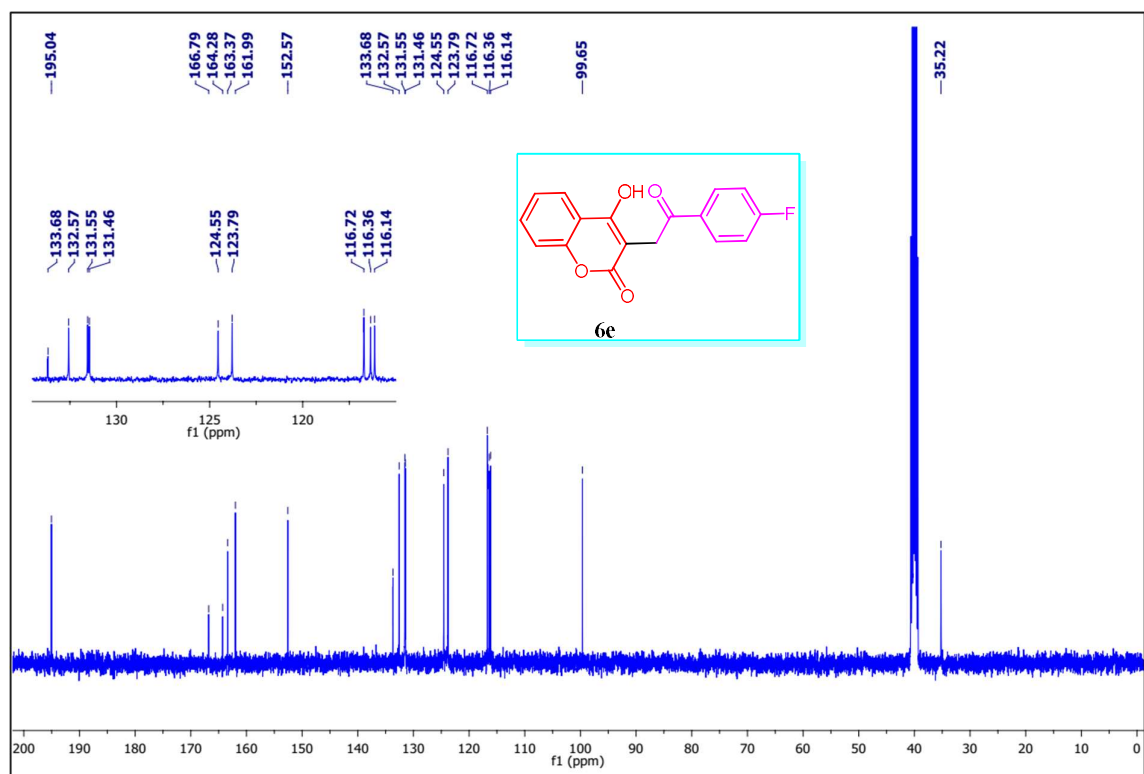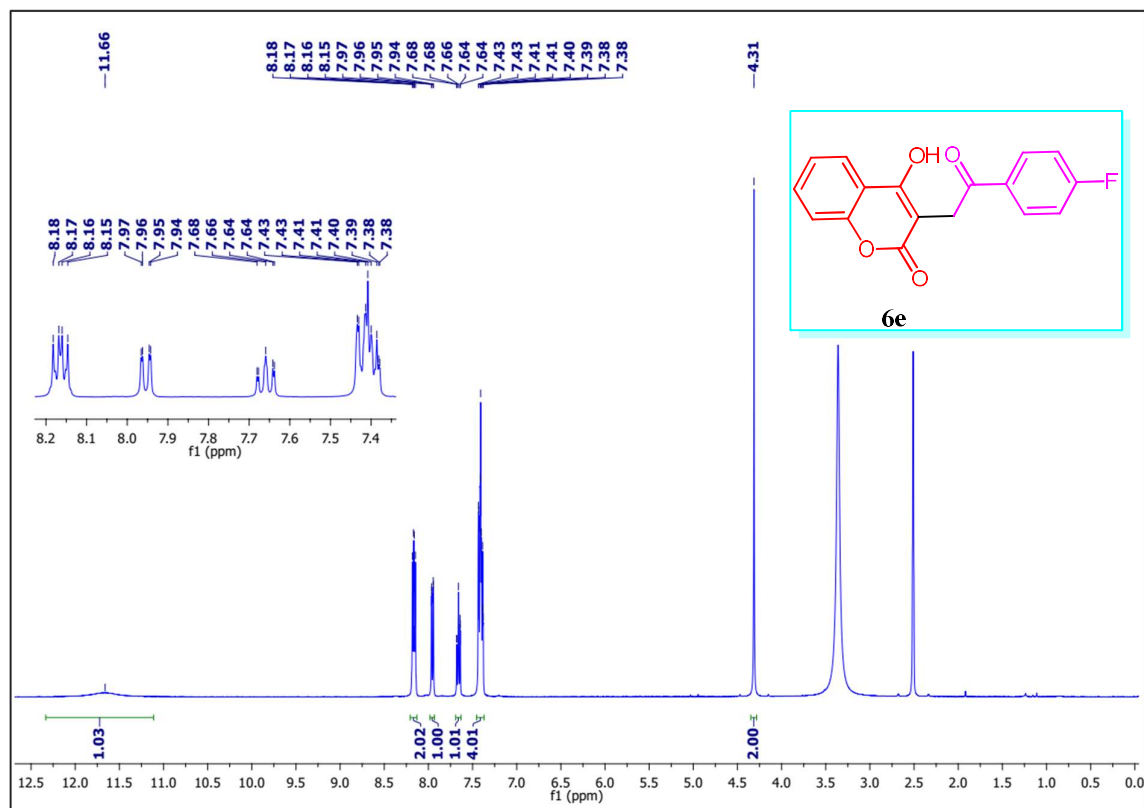
^{1}H &^{13}C Spectra of 7a
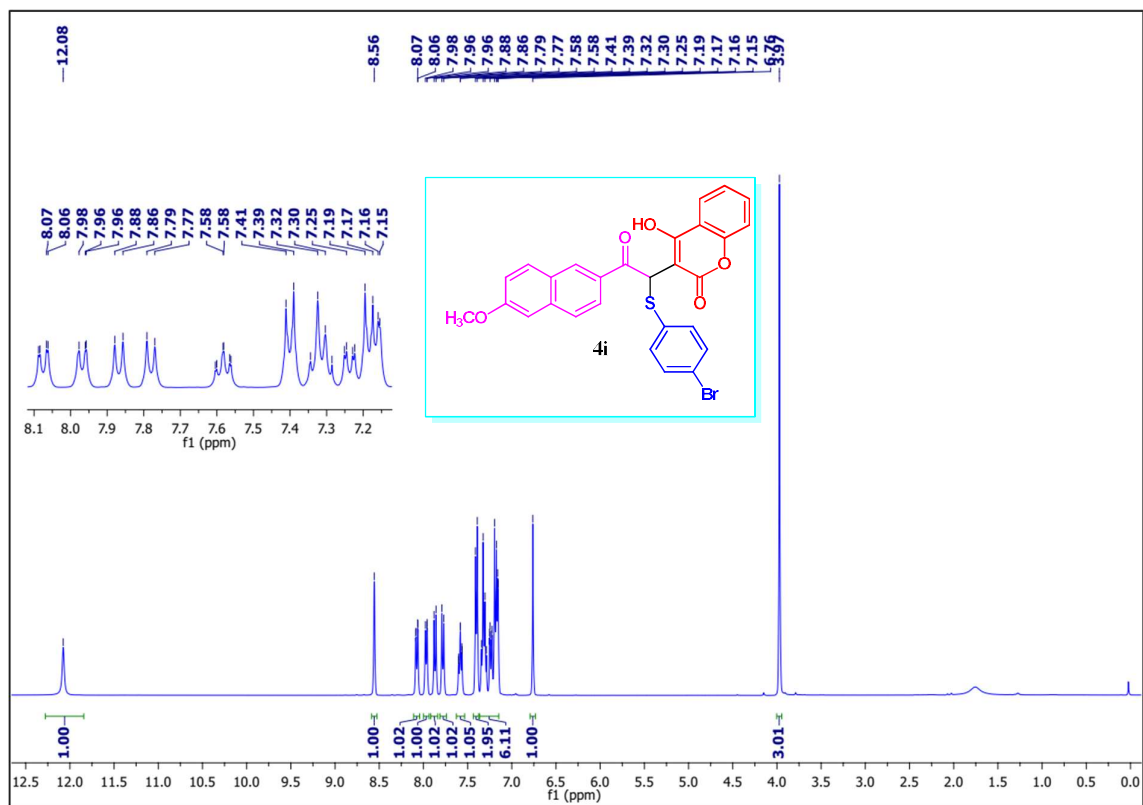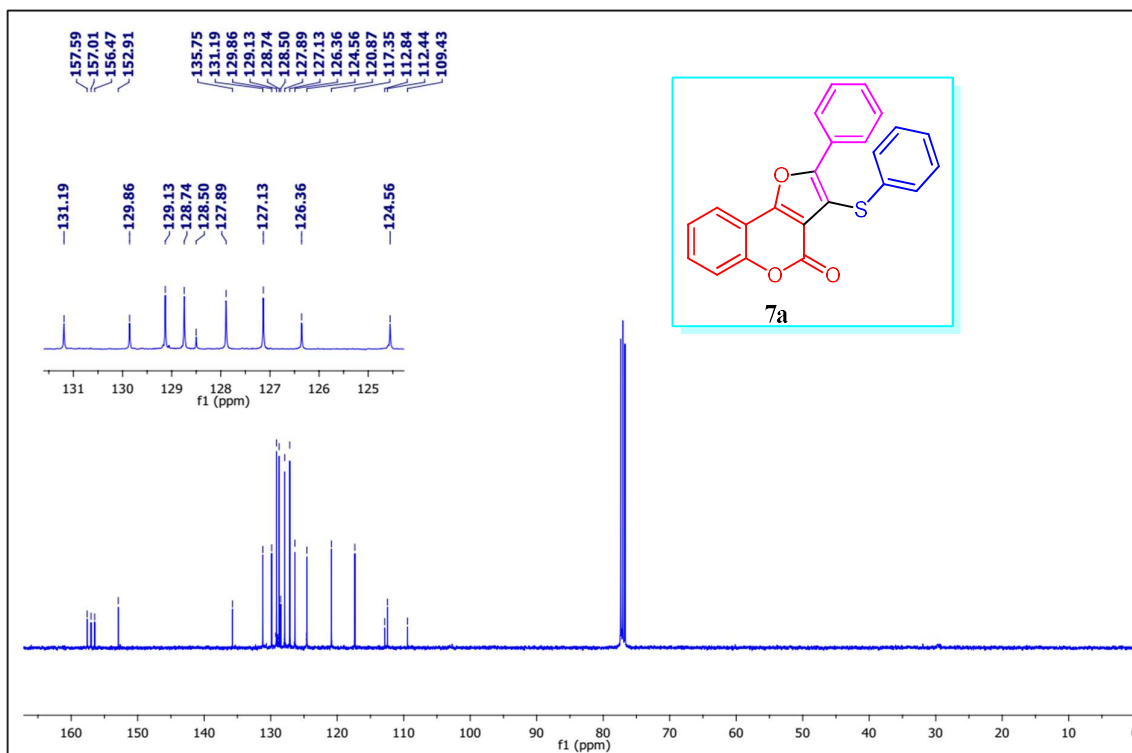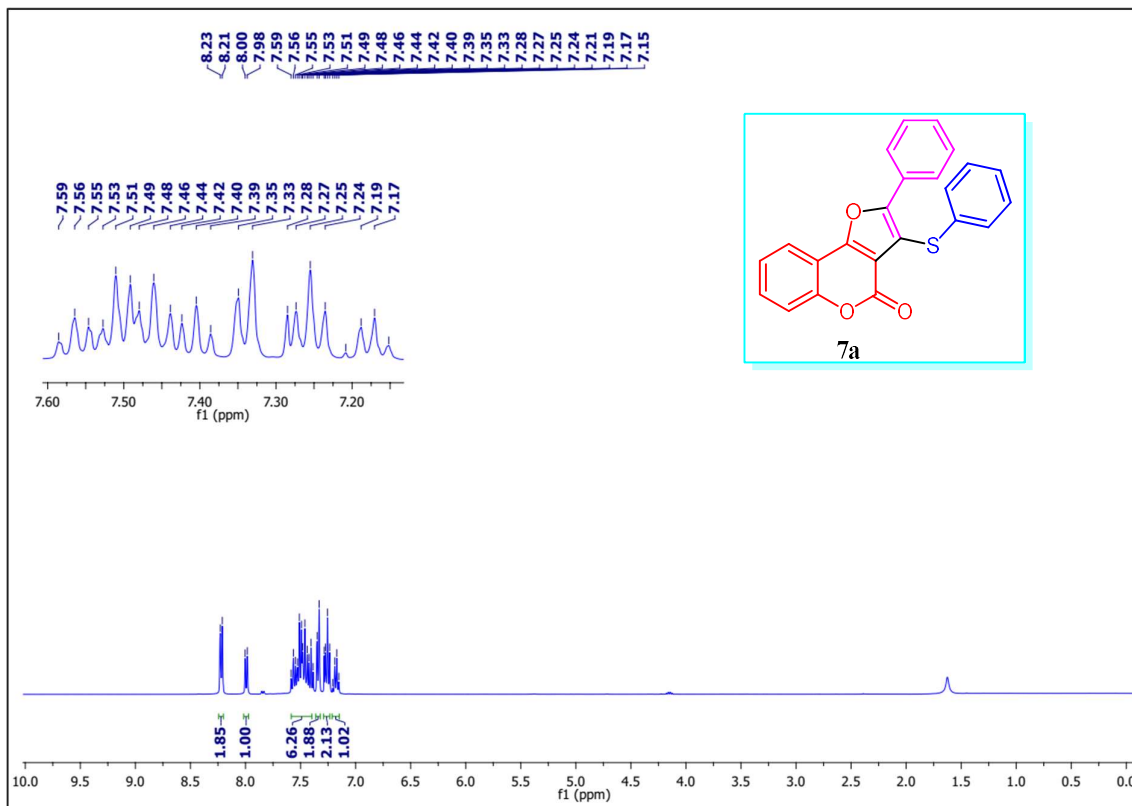
^{1}H &^{13}C Spectra of 7c
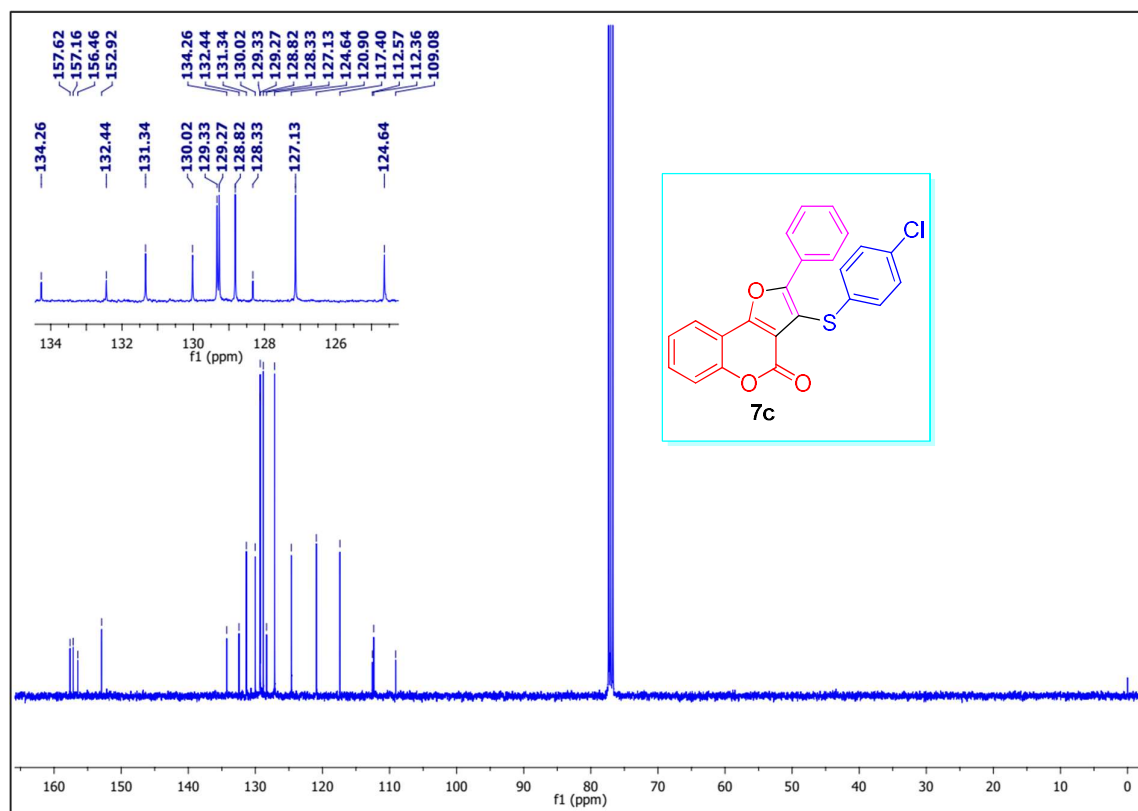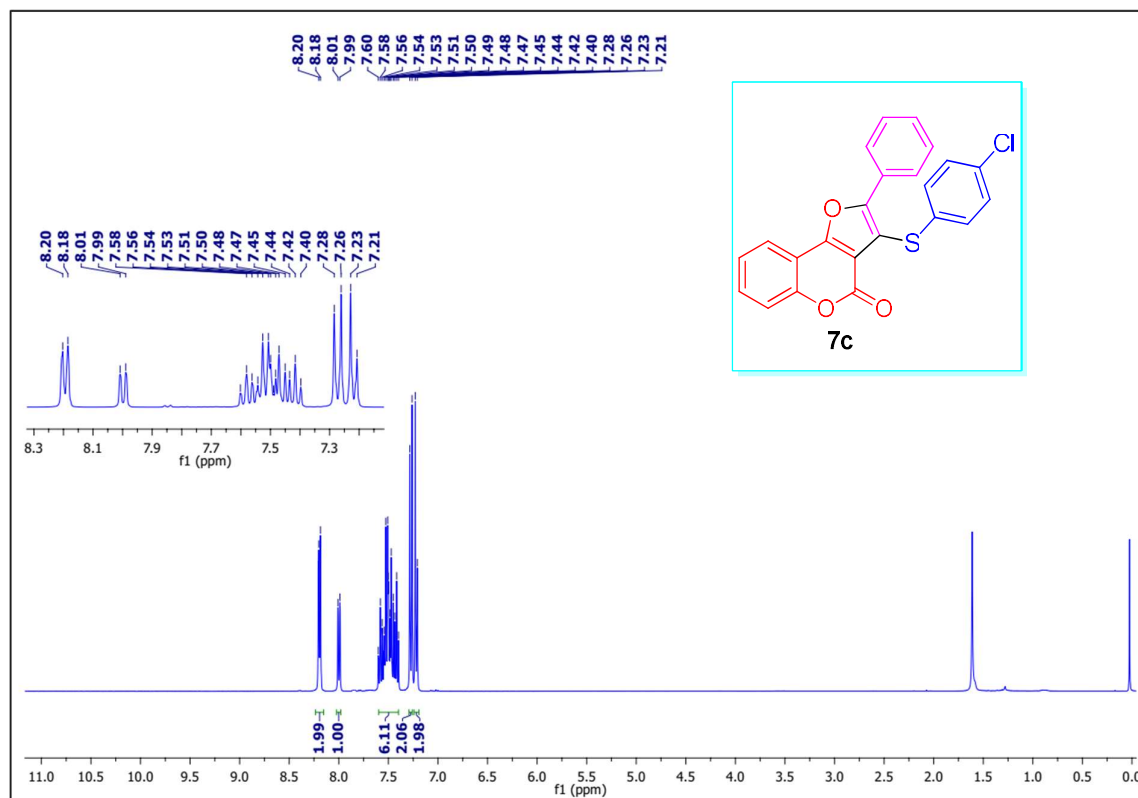
¹H &¹³C Spectra of 7j
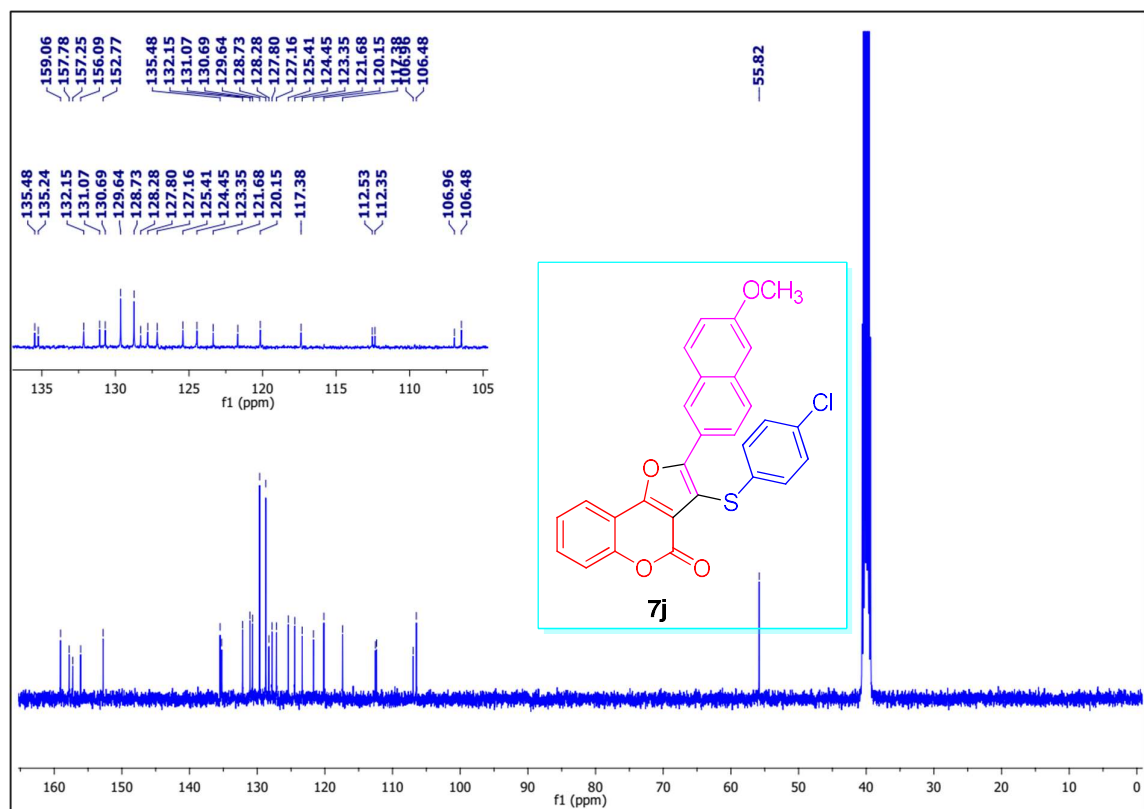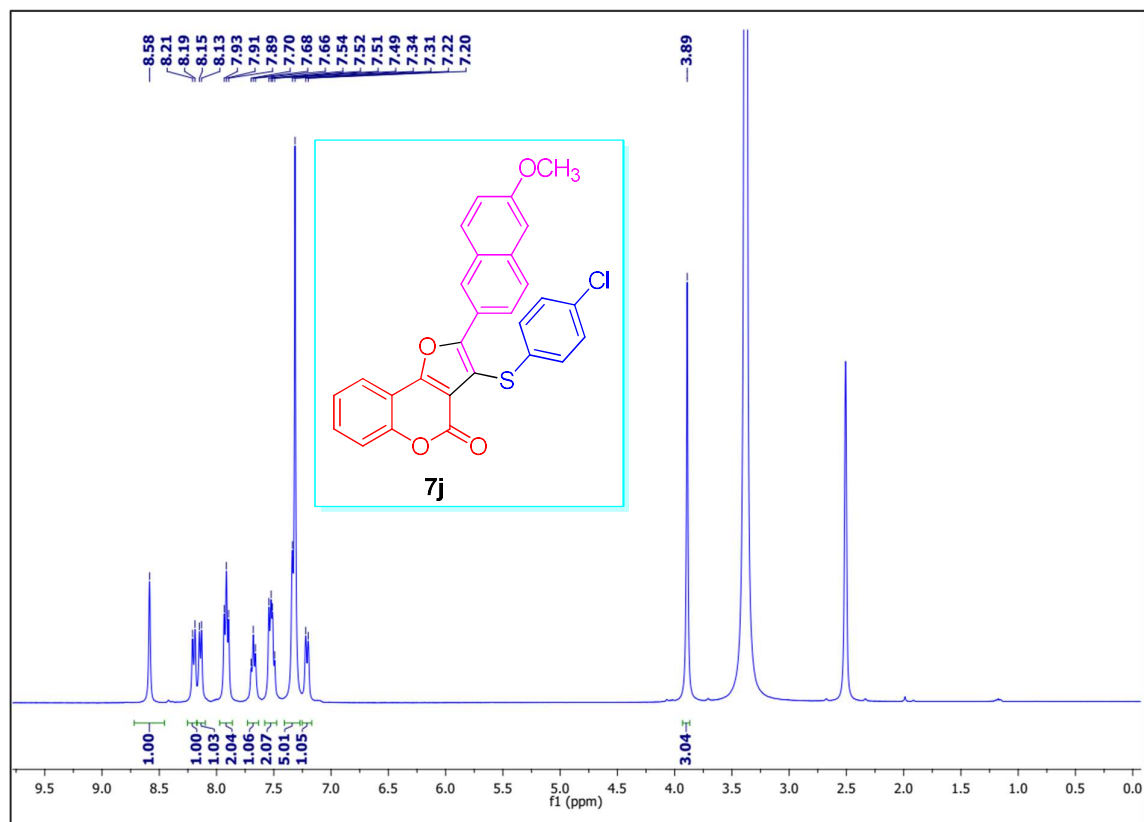
¹H &¹³C Spectra of 7r
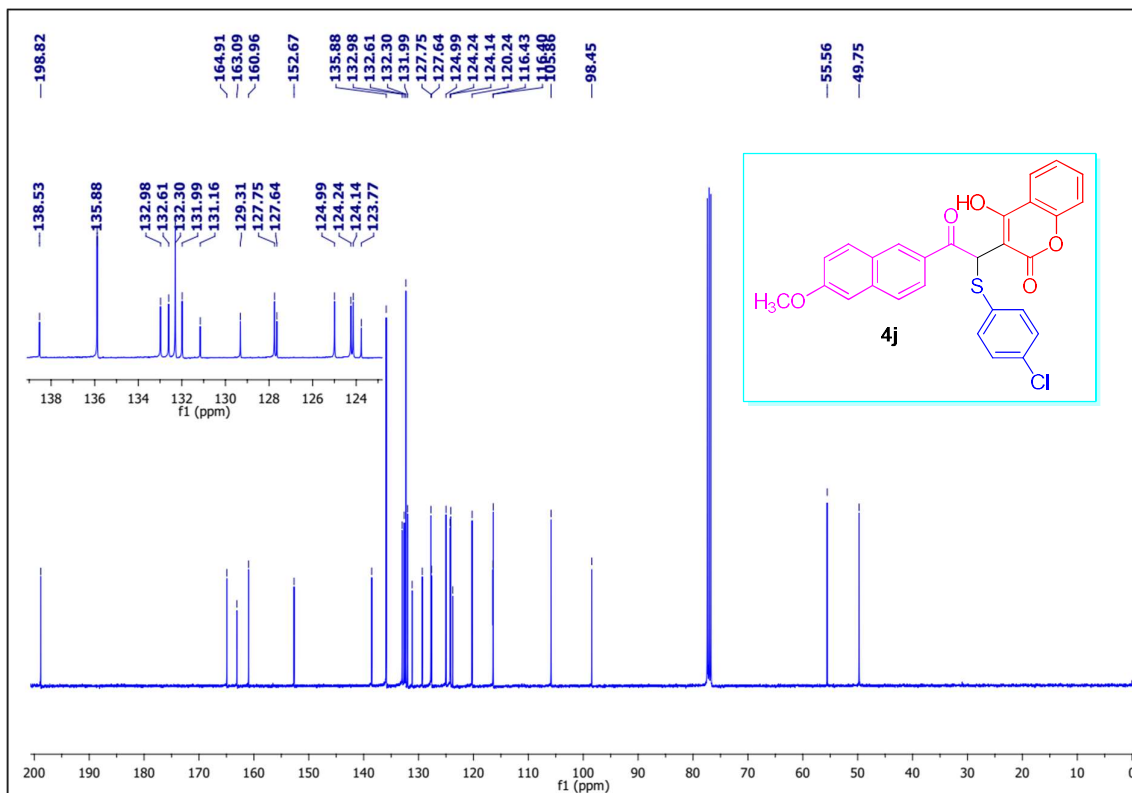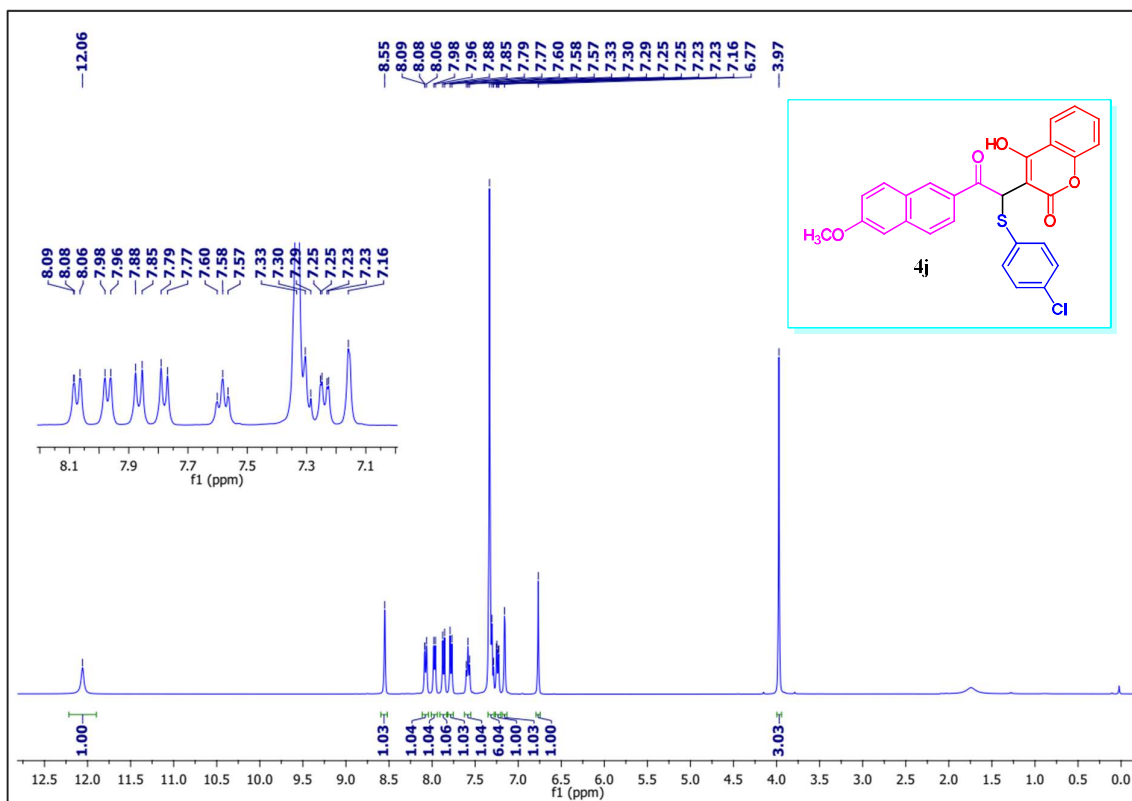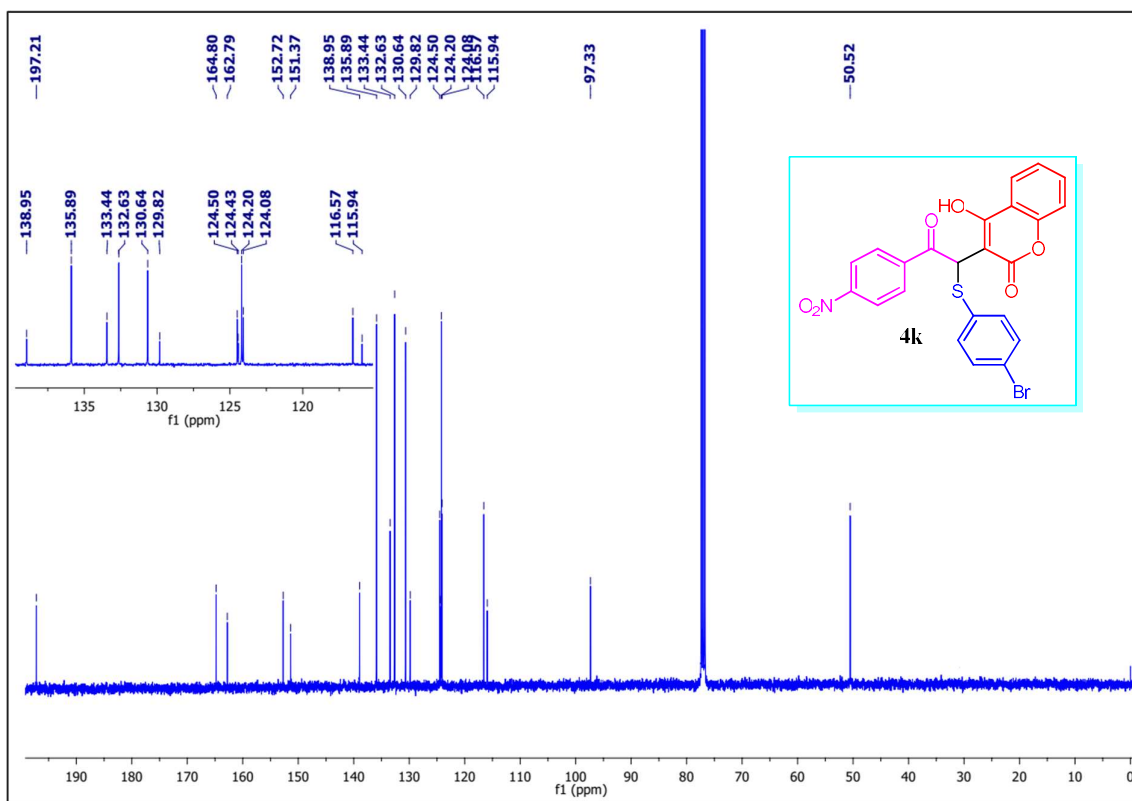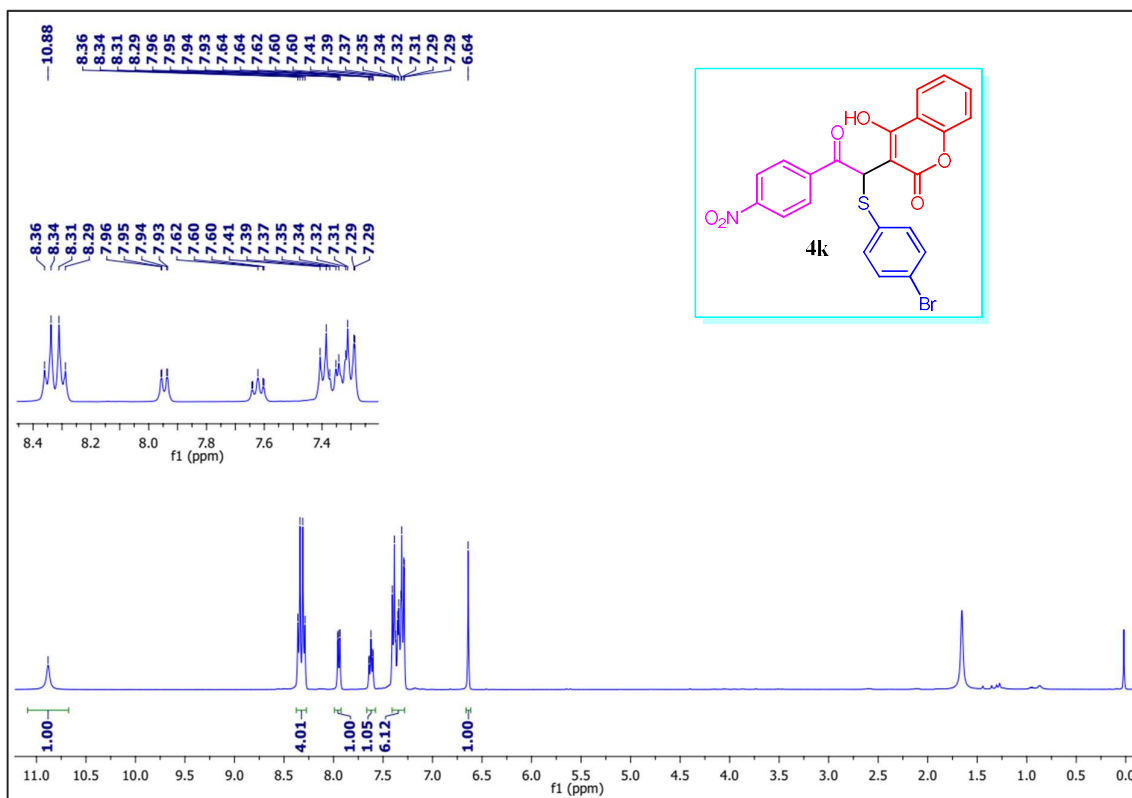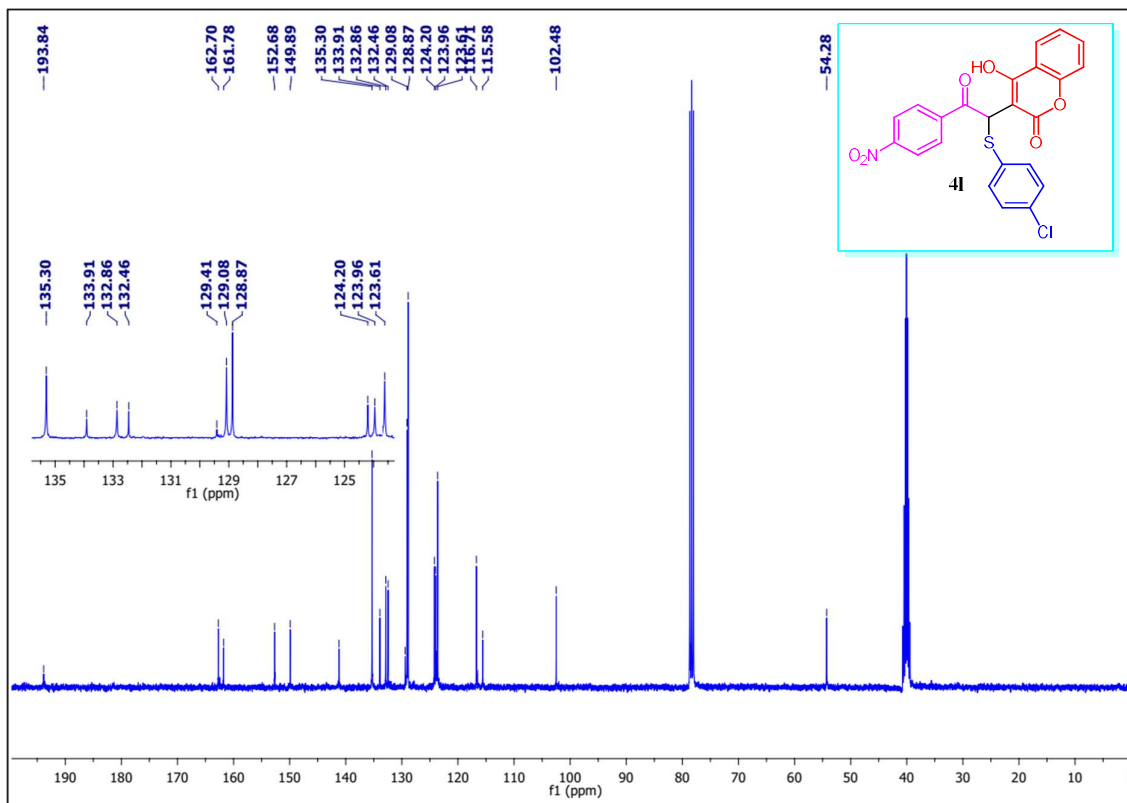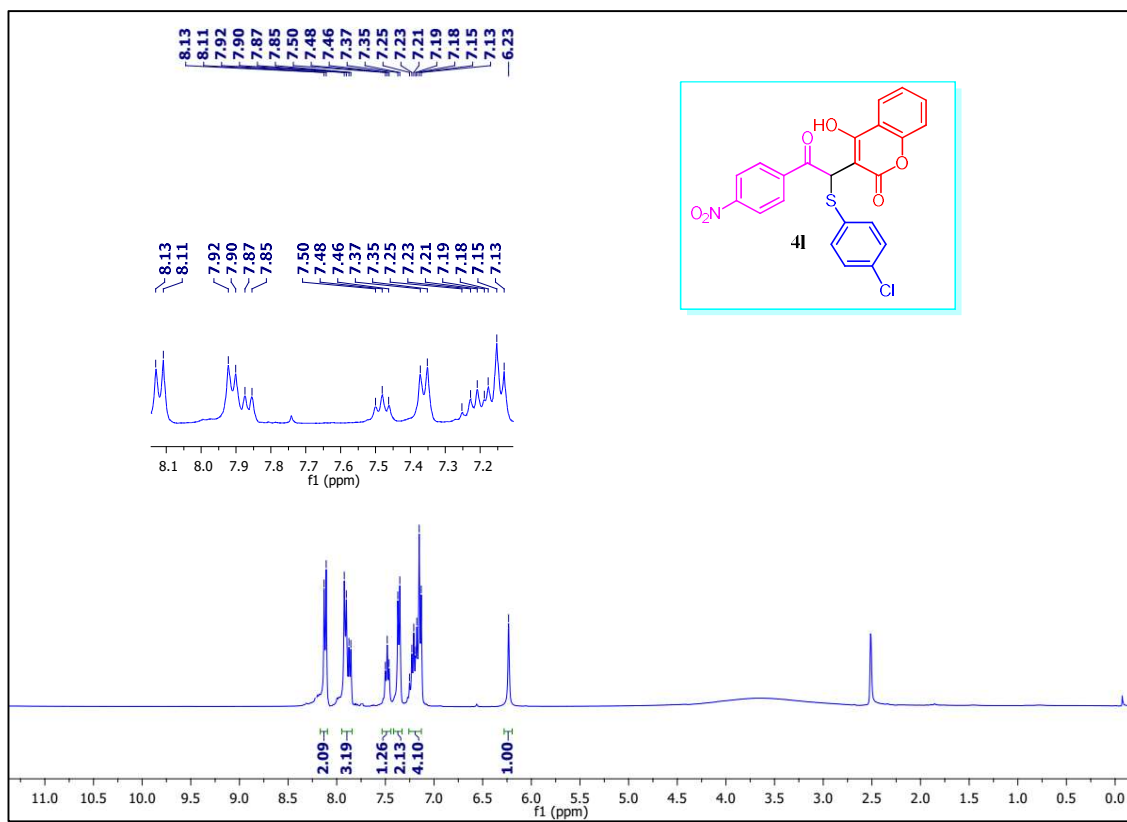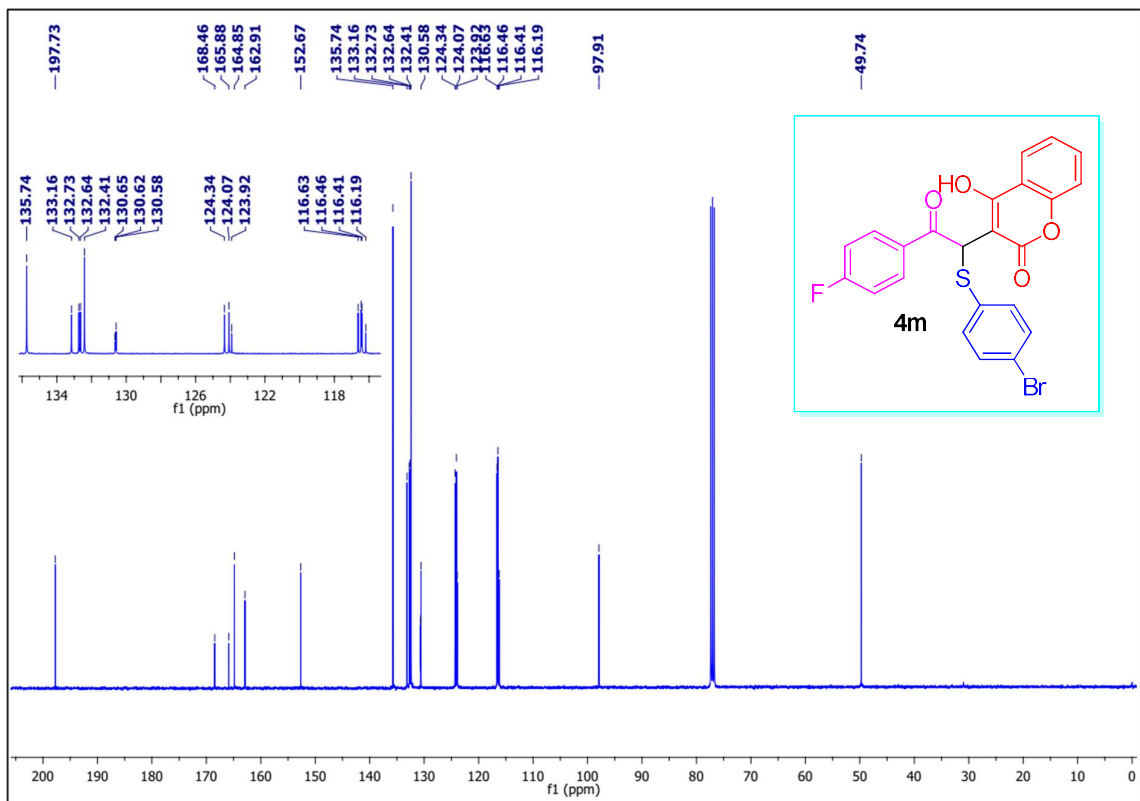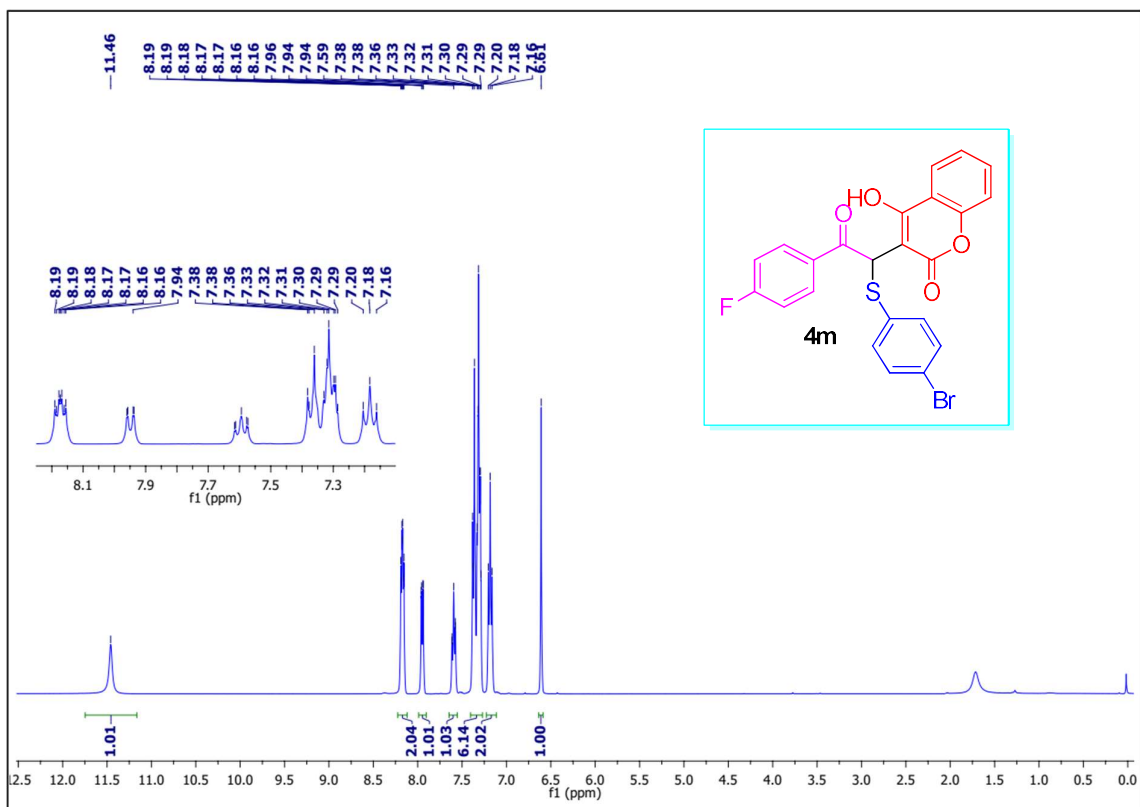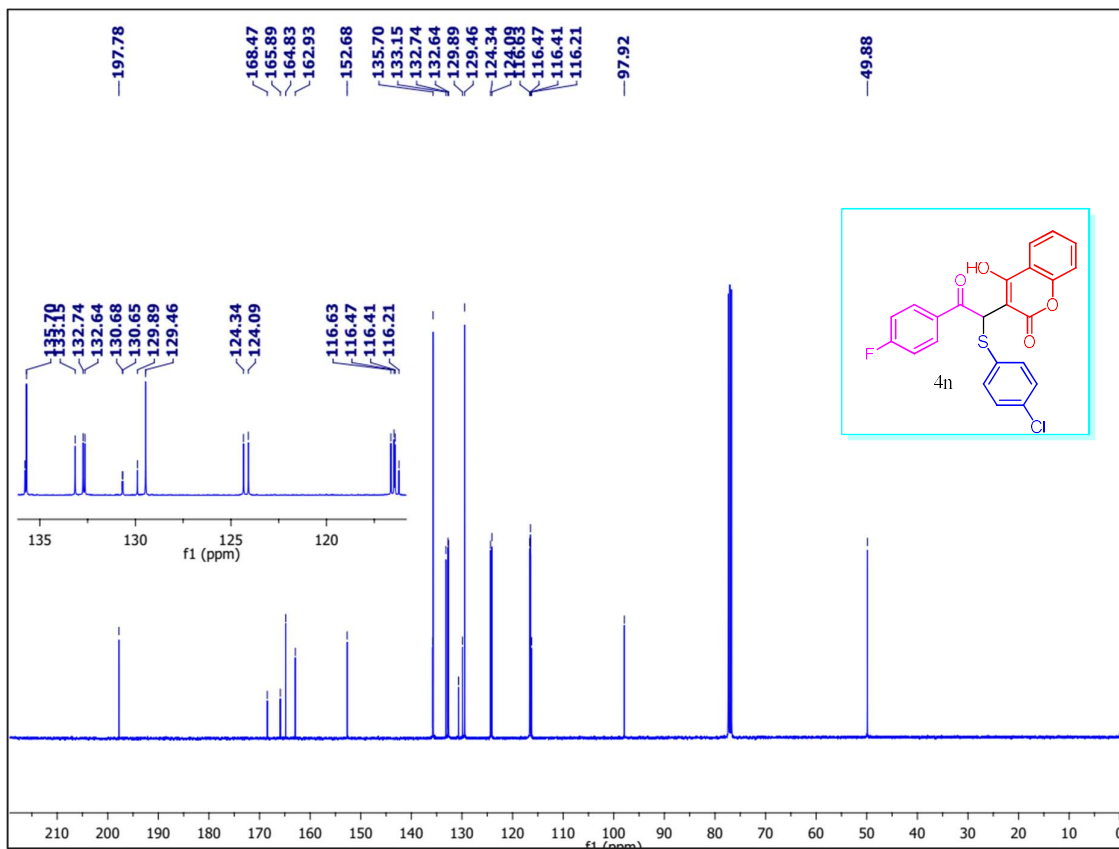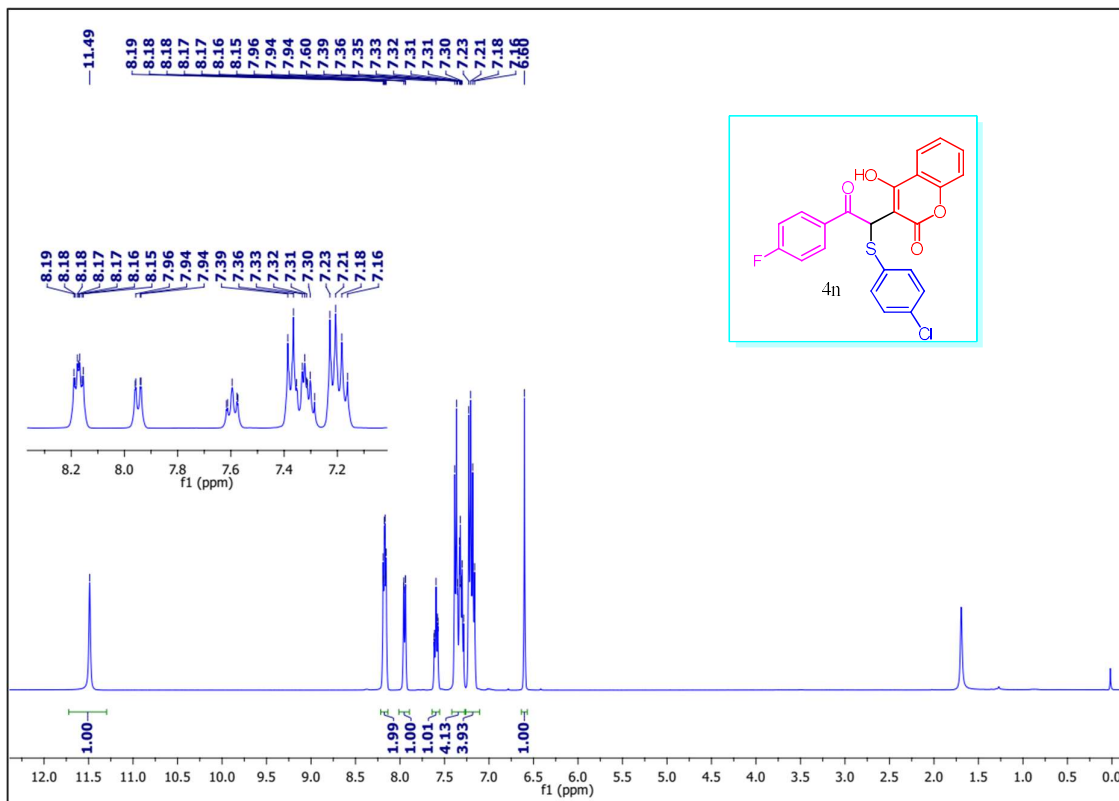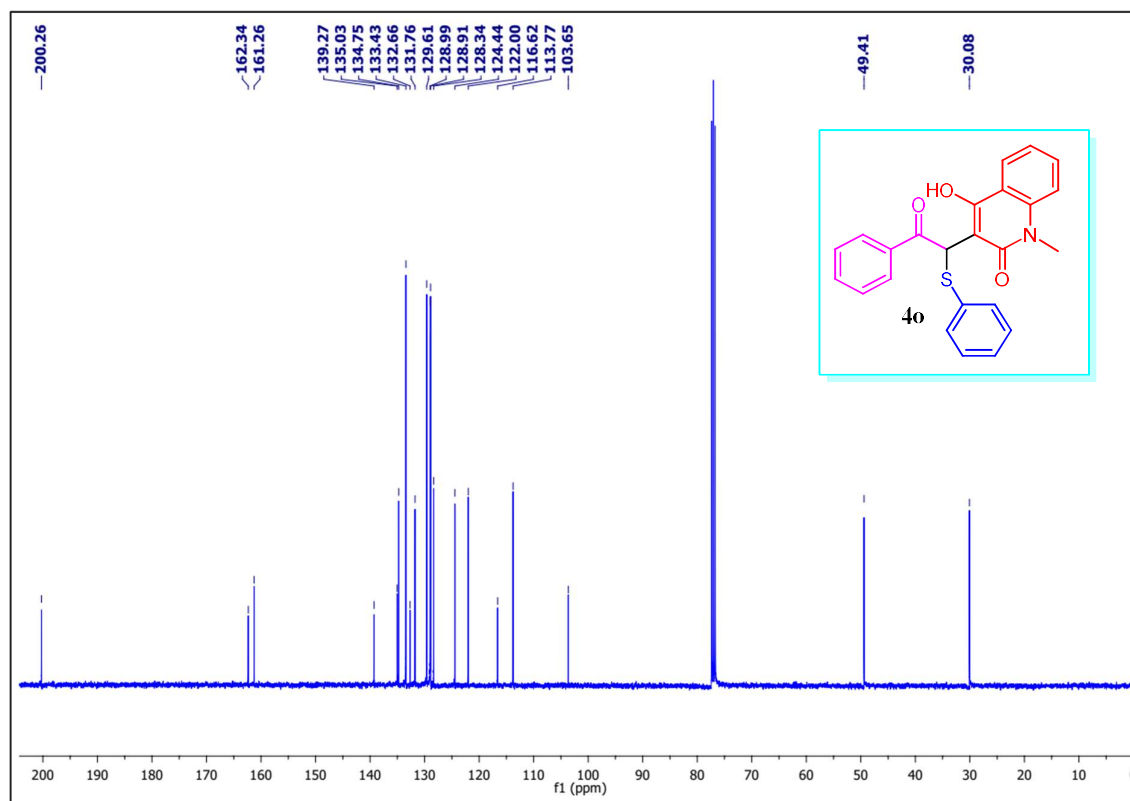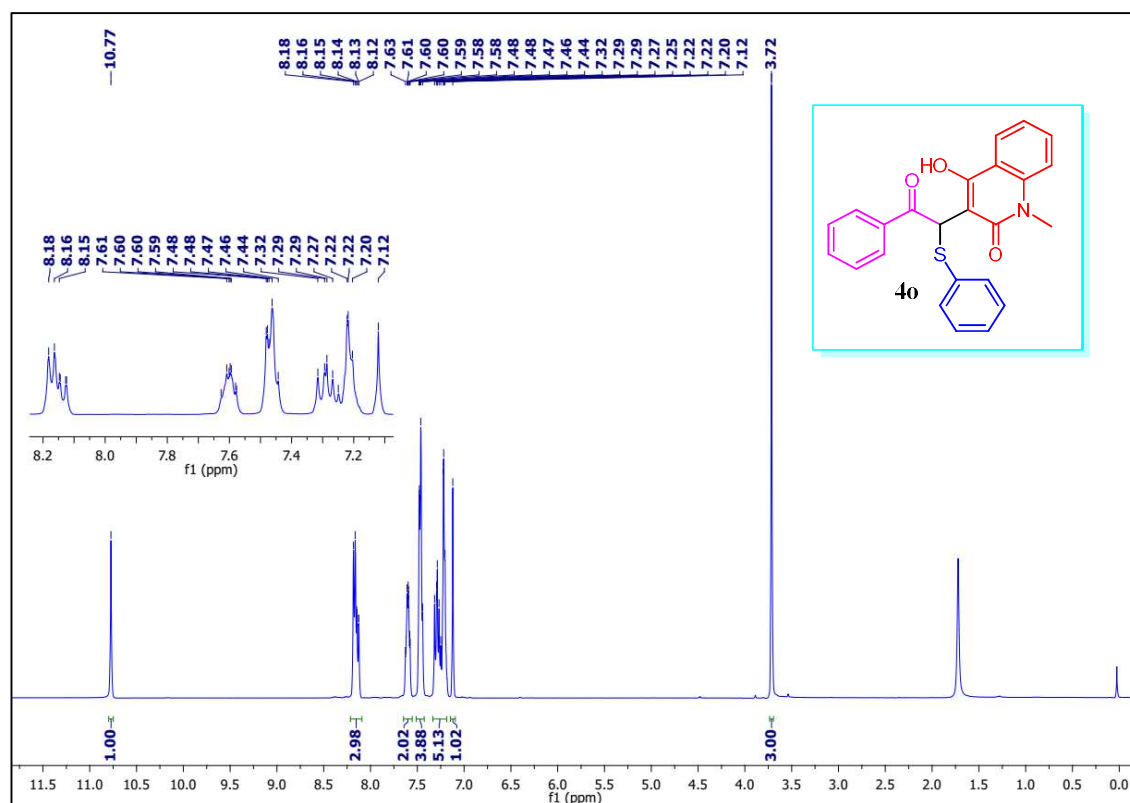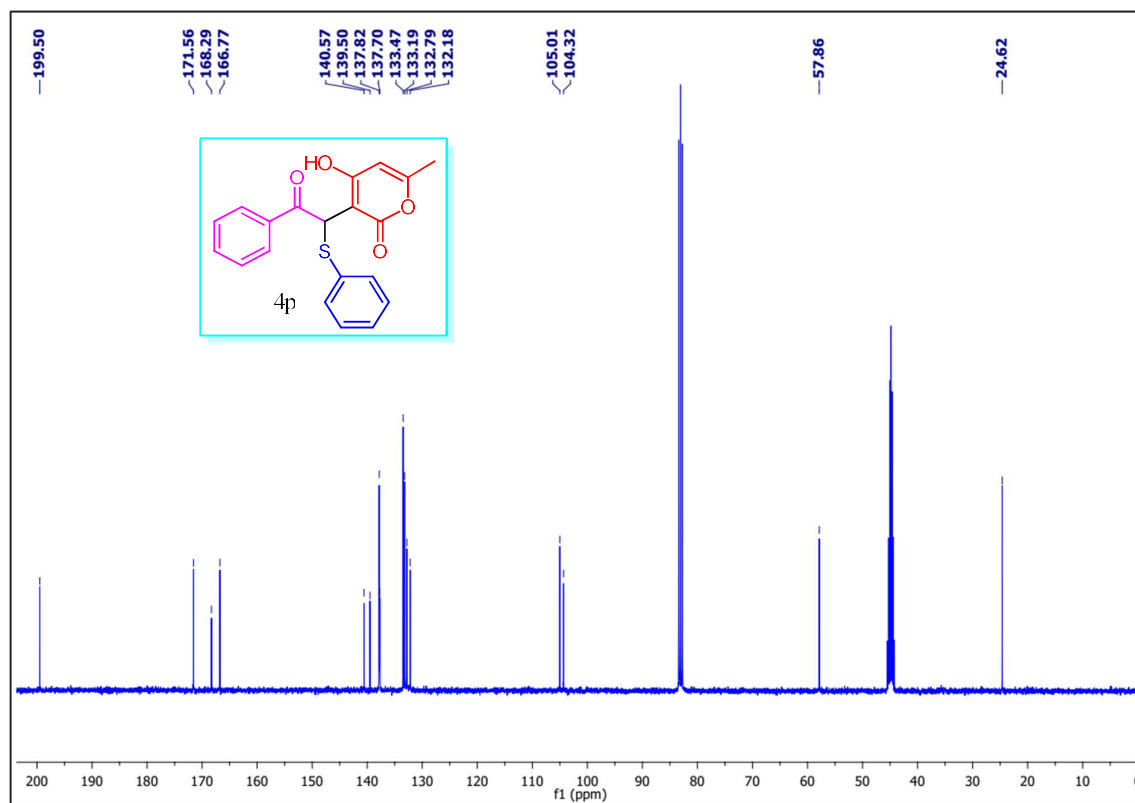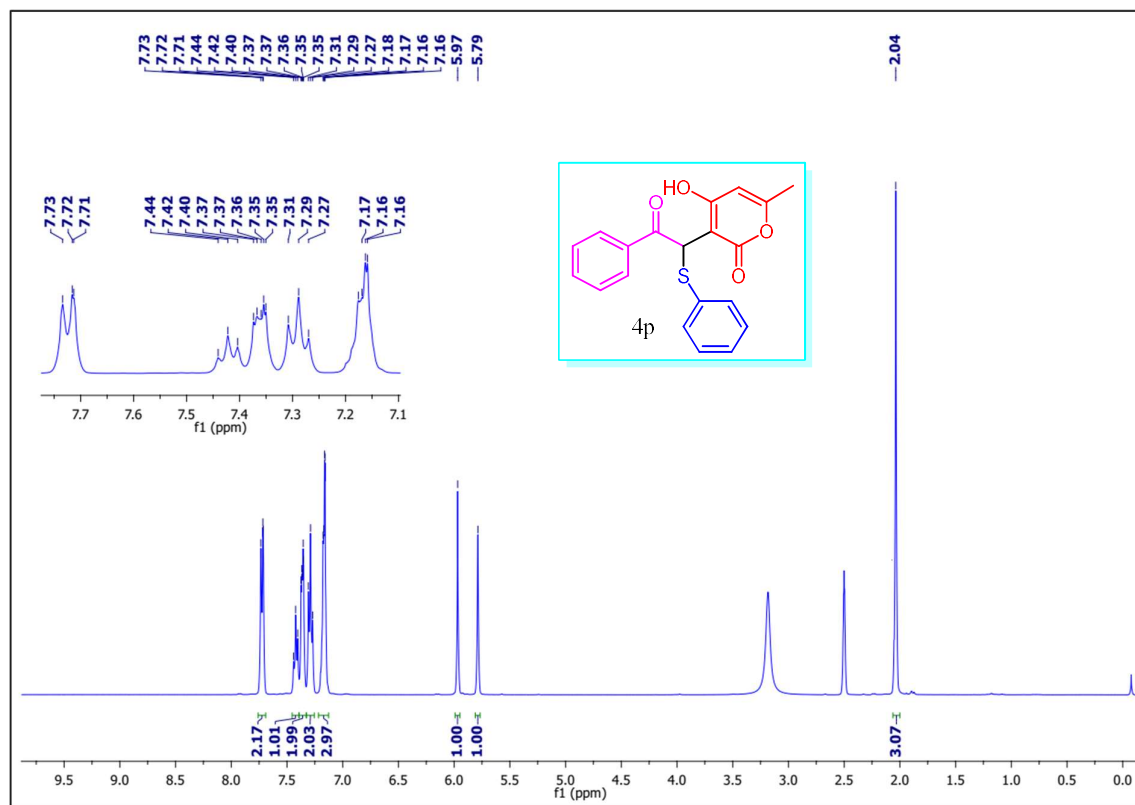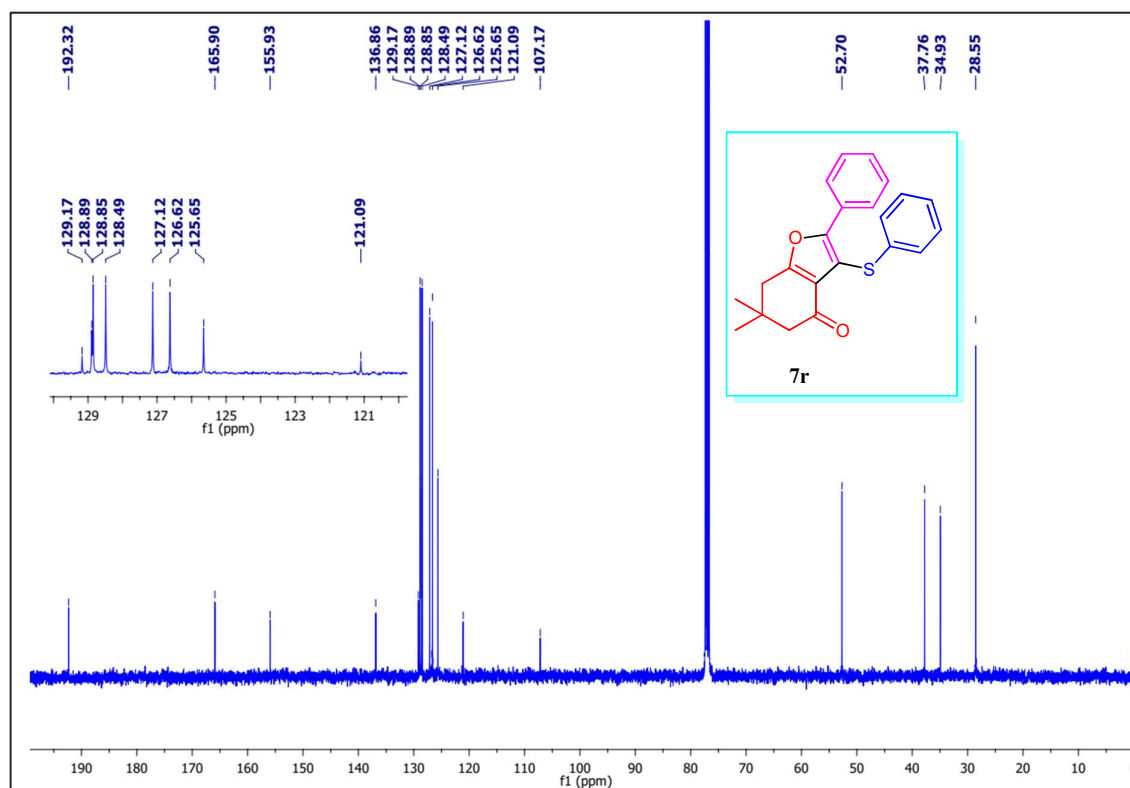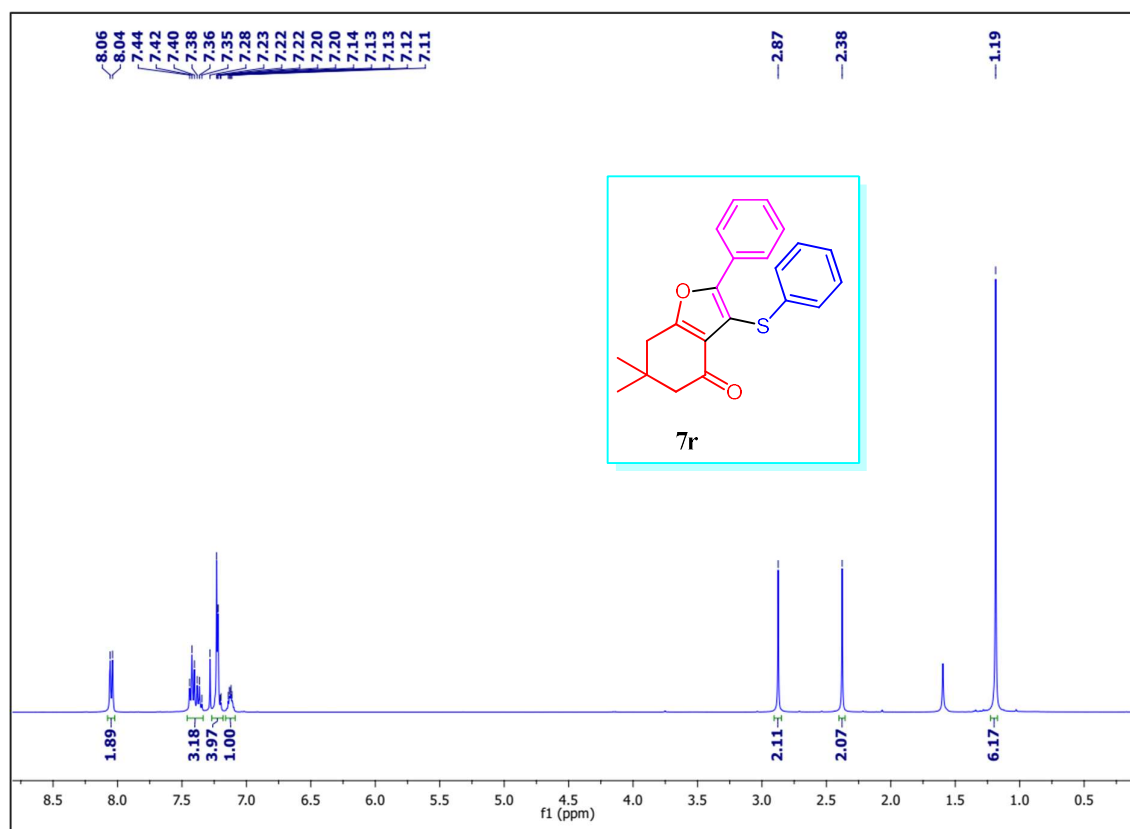
^{1}H &^{13}C Spectra of 7u
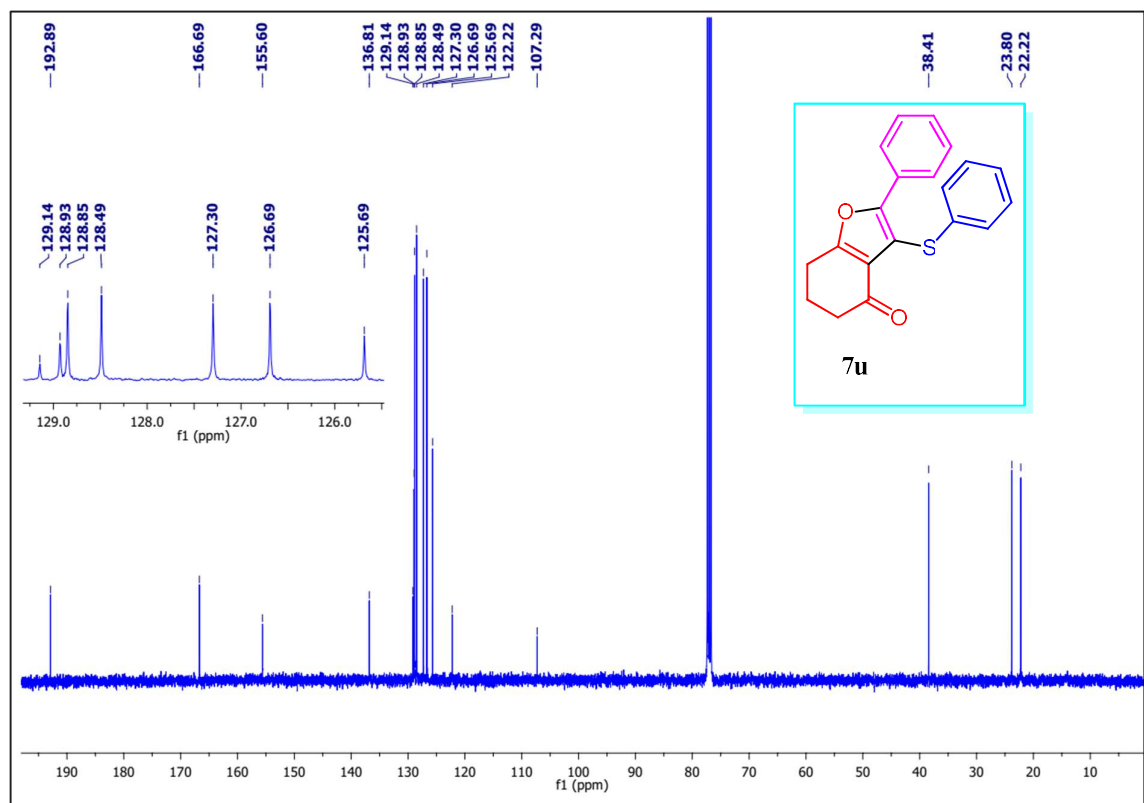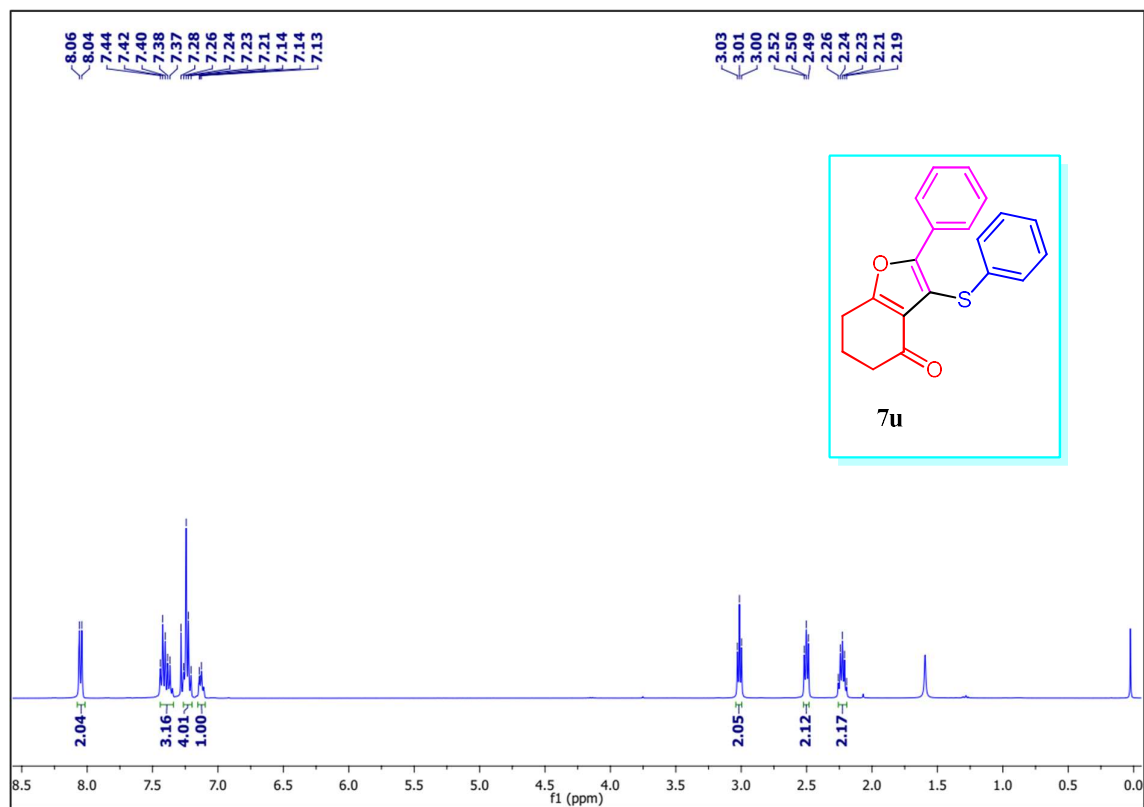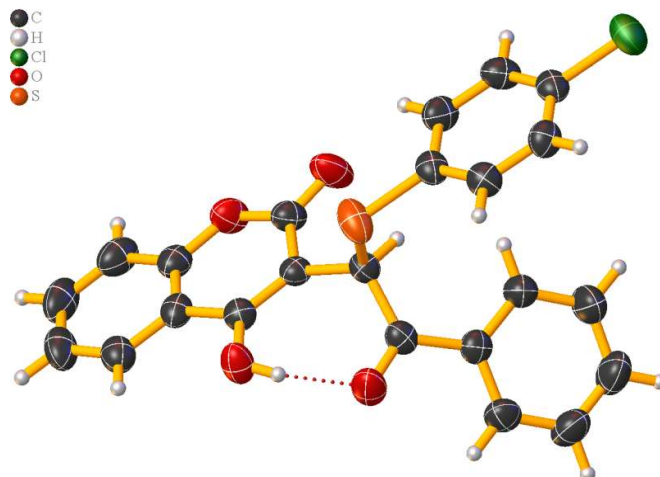
Figure S1. Ortep diagram of **4c** with 50% ellipsoidal probability (CCDC 1975421).

Table S1. Crystal data for compound **4c**

Identification code	**4c**	
Chemical formula	C$_{23}$H$_{15}$ClO$_4$S	
Formula weight	422.86 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	
	a = 8.7831(8) Å	α = 99.835(2)°
Unit cell dimensions	b = 8.9008(7) Å	β = 100.128(2)°
	c = 13.3834(12) Å	γ = 106.436(2)°

Volume	960.54(14) Å^3
Z	2
Density (calculated)	1.462 g/cm^3
Absorption coefficient	0.336 mm^{-1}
F(000)	436
Theta range for data collection	2.49 to 25.50°
Index ranges	-10≤ h≤ 10, -10≤ k≤ 10, -16≤ l≤ 16
Reflections collected	26141
Independent reflections	3571 [R(int) = 0.0258]
Max. and min. transmission	0.9040 and 0.9040
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick 2014)
Function minimized	$\Sigma \, w(F_o{}^2 - F_c{}^2)^2$
Data / restraints / parameters	3571 / 0 / 264
Goodness-of-fit on F^2	1.039
Final R indices	2945 data; I>2σ(I) R1 = 0.0391, wR2 = 0.0938
	all data R1 = 0.0505, wR2 = 0.1010
Weighting scheme	w=1/[σ^2(F$_o{}^2$)+(0.0400P)^2+0.5229P], where P=(F$_o{}^2$+2F$_c{}^2$)/3
Extinction coefficient	0.0094(15)
Largest diff. peak and hole	0.403 and -0.267 eÅ^{-3}
R.M.S. deviation from mean	0.039 eÅ^{-3}
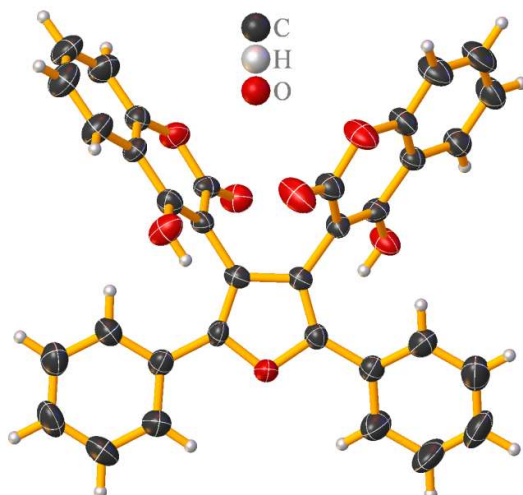
Figure S2. Ortep diagram of **5** with 50% ellipsoidal probability; one molecule of **5** and two disordered DMSO molecules have been removed for clearty (CCDC 1975422).

Table S2. Crystal data for compound **5.**

Identification code	**5**	
Chemical formula	$C_{72}H_{52}O_{16}S_2$	
Formula weight	1237.26 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal size	0.050 x 0.100 x 0.300 mm	
Crystal system	triclinic	
Space group	P -1	
	a = 13.7724(13) Å	α = 80.591(2)°
Unit cell dimensions	b = 15.3172(15) Å	β = 65.912(2)°
	c = 15.8809(15) Å	γ = 82.455(2)°
Volume	3009.5(5) Å^3	
Z	2	

Density (calculated)	1.365 g/cm^3
Absorption coefficient	0.162 mm^{-1}
F(000)	1288
Theta range for data collection	2.54 to 18.87°
Index ranges	-12≤h≤12, -13≤k≤13, -14≤l≤14
Reflections collected	25696
Independent reflections	4753 [R(int) = 0.0534]
Max. and min. transmission	0.9920 and 0.9810
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick 2014)
Function minimized	Σ w(F$_o^2$ - F$_c^2$)^2
Data / restraints / parameters	4753 / 106 / 865
Goodness-of-fit on F^2	1.023
Final R indices	3647 data; I>2σ(I) R1 = 0.0397, wR2 = 0.0907
	all data R1 = 0.0599, wR2 = 0.1022
Weighting scheme	w=1/[σ^2(F$_o^2$)+(0.0454P)^2+2.3442P], where P=(F$_o^2$+2F$_c^2$)/3
Extinction coefficient	0.0035(4)
Largest diff. peak and hole	0.233 and -0.168 eÅ^{-3}
R.M.S. deviation from mean	0.033 eÅ^{-3}