Supporting Information

Multicomponent synthesis of styryl linked benzo[*h*]pyrazolo[3,4-*b*]quinoline-5,6(10*H*)-diones by liquid assisted grinding

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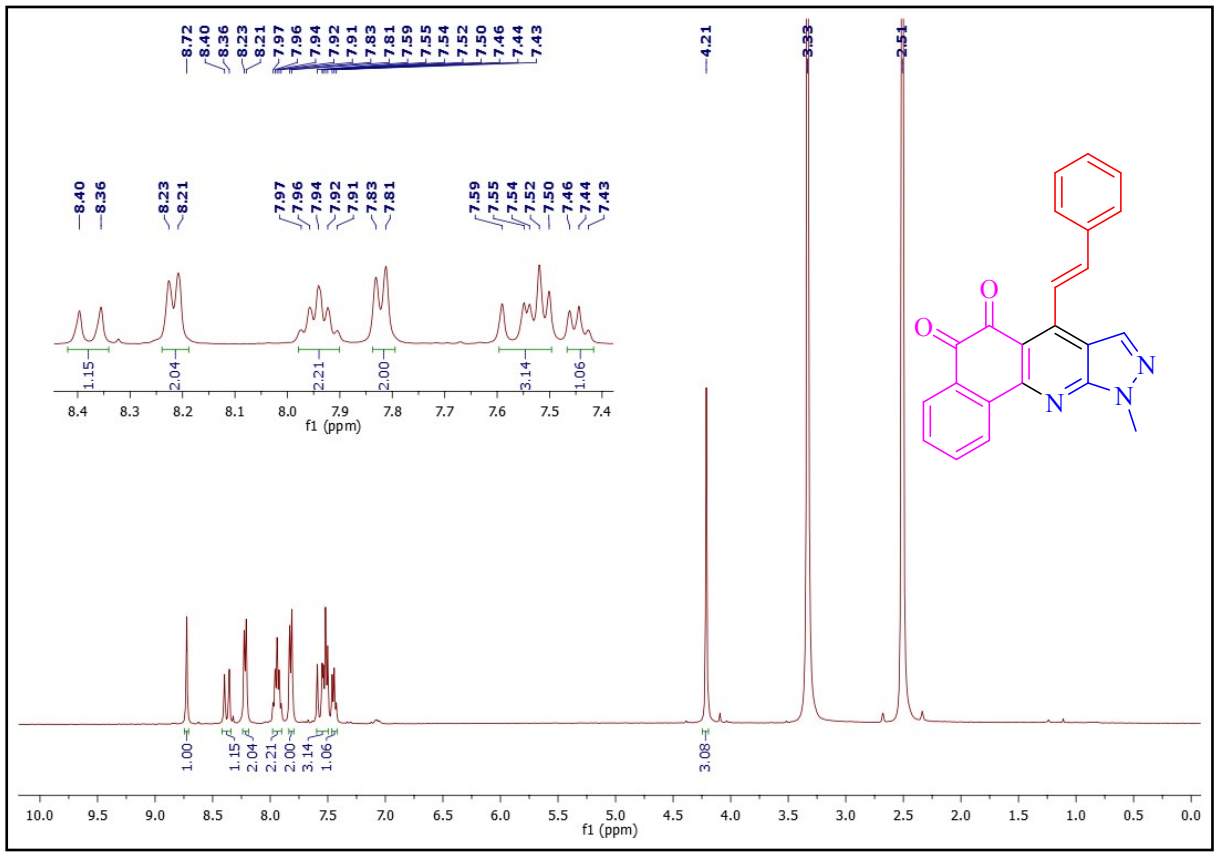
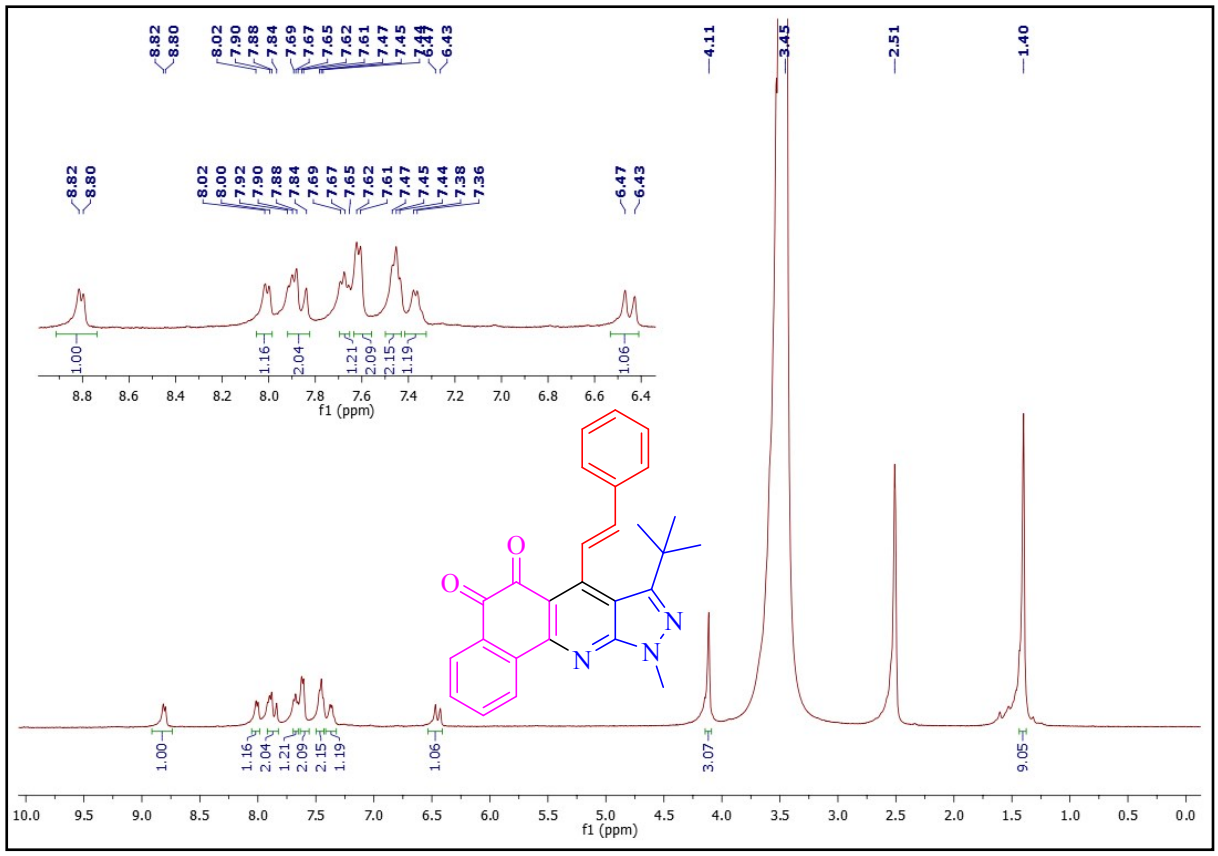
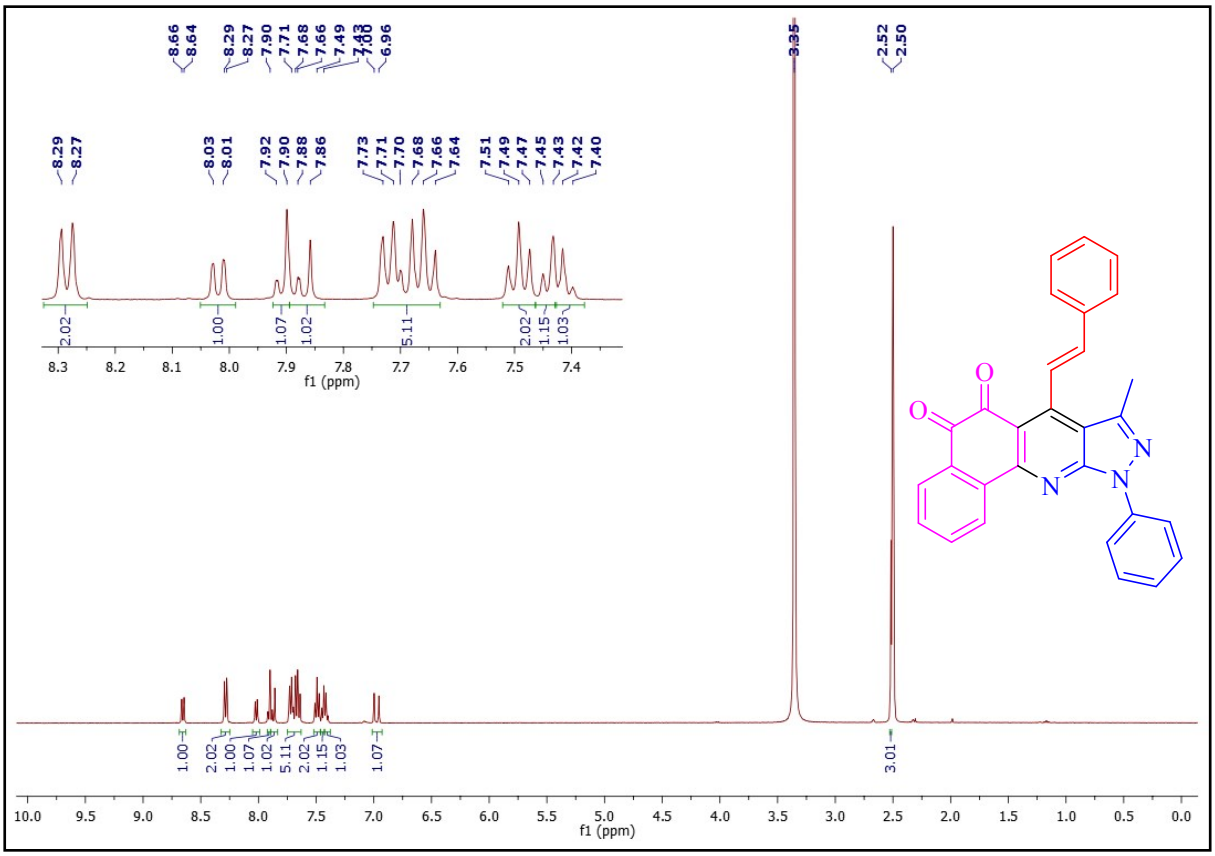
^{1}H NMR Spectra of Compound 4a



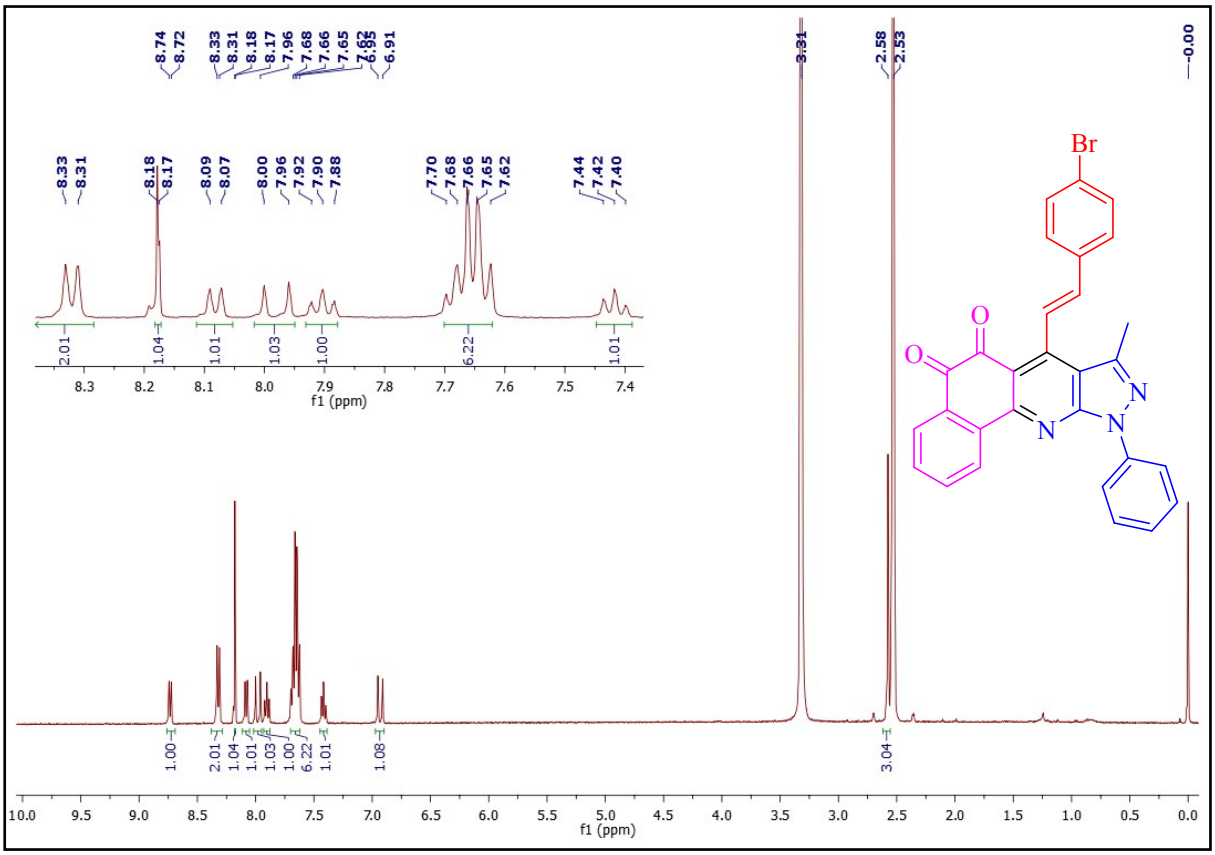
^{1}H NMR Spectra of Compound 4b



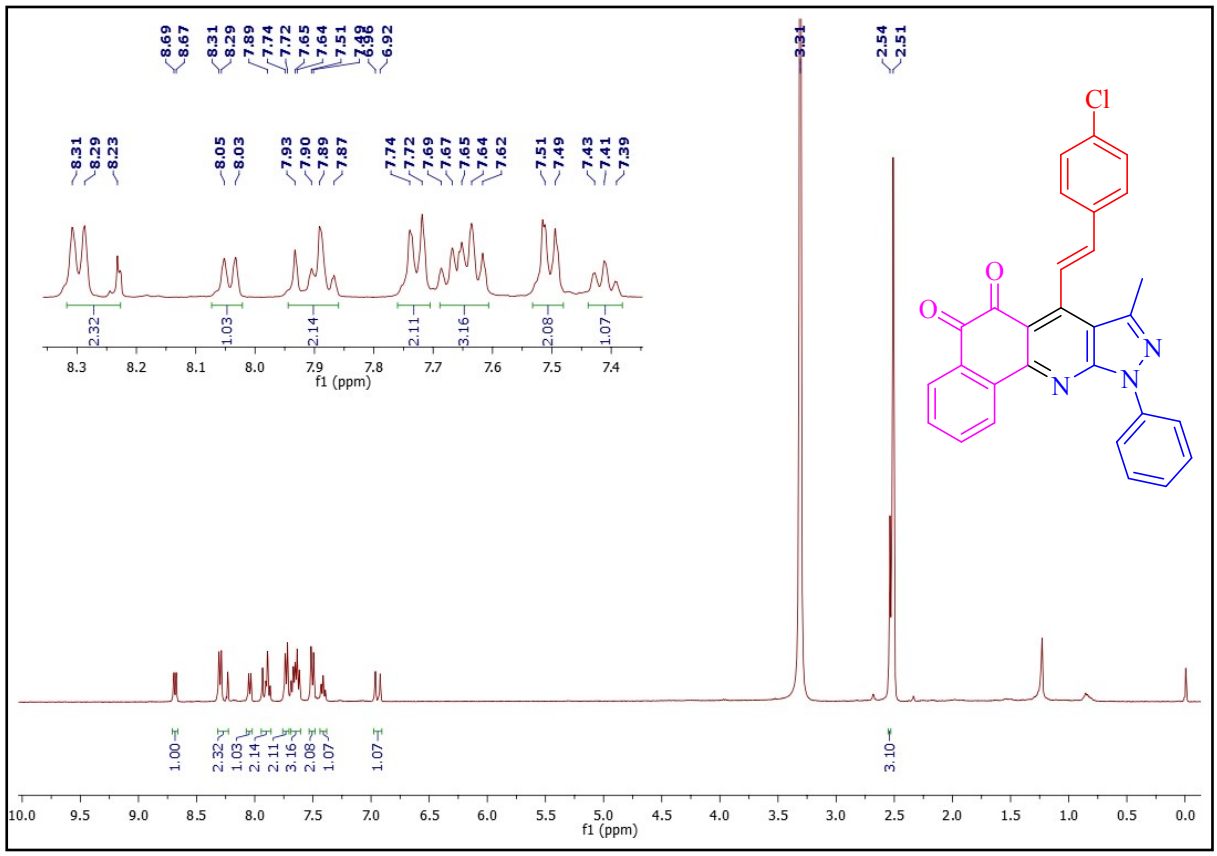
^{1}H NMR Spectra of Compound 4c



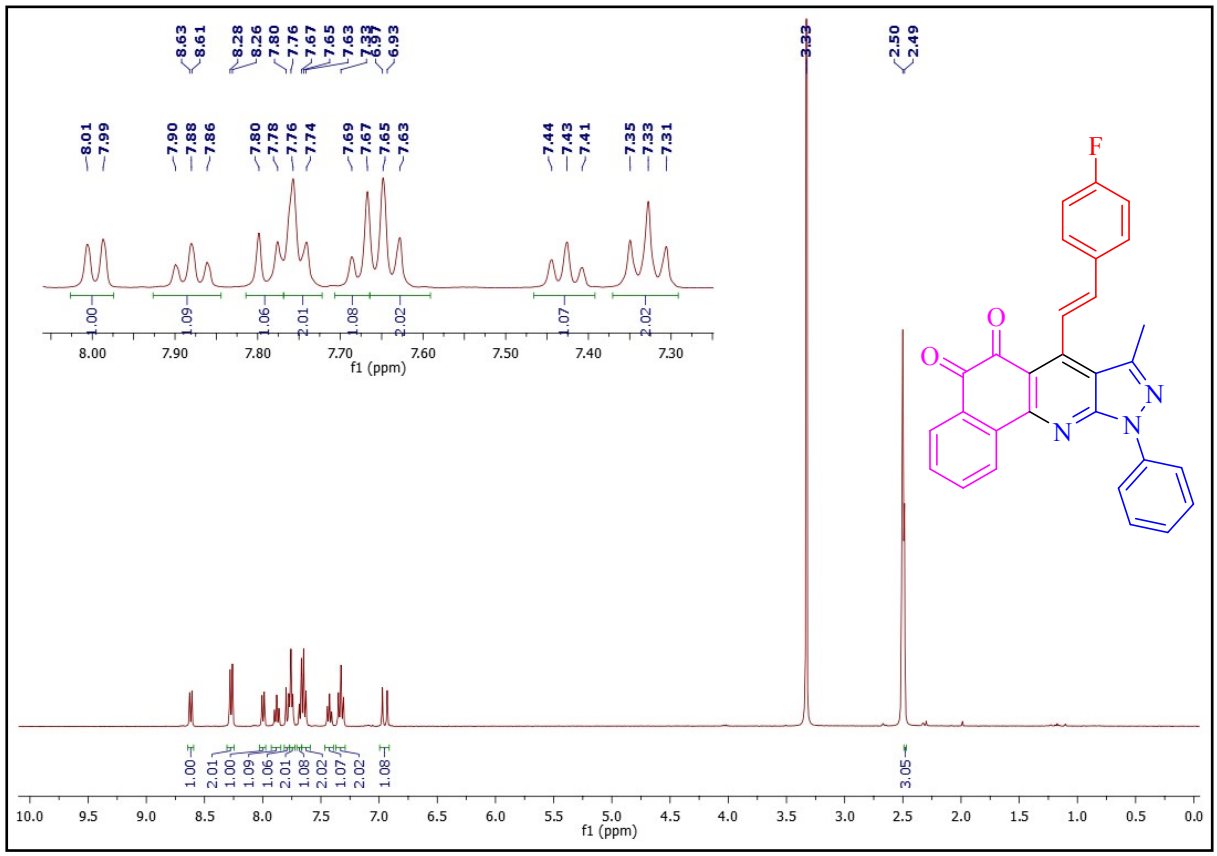
^{1}H NMR Spectra of Compound 4d



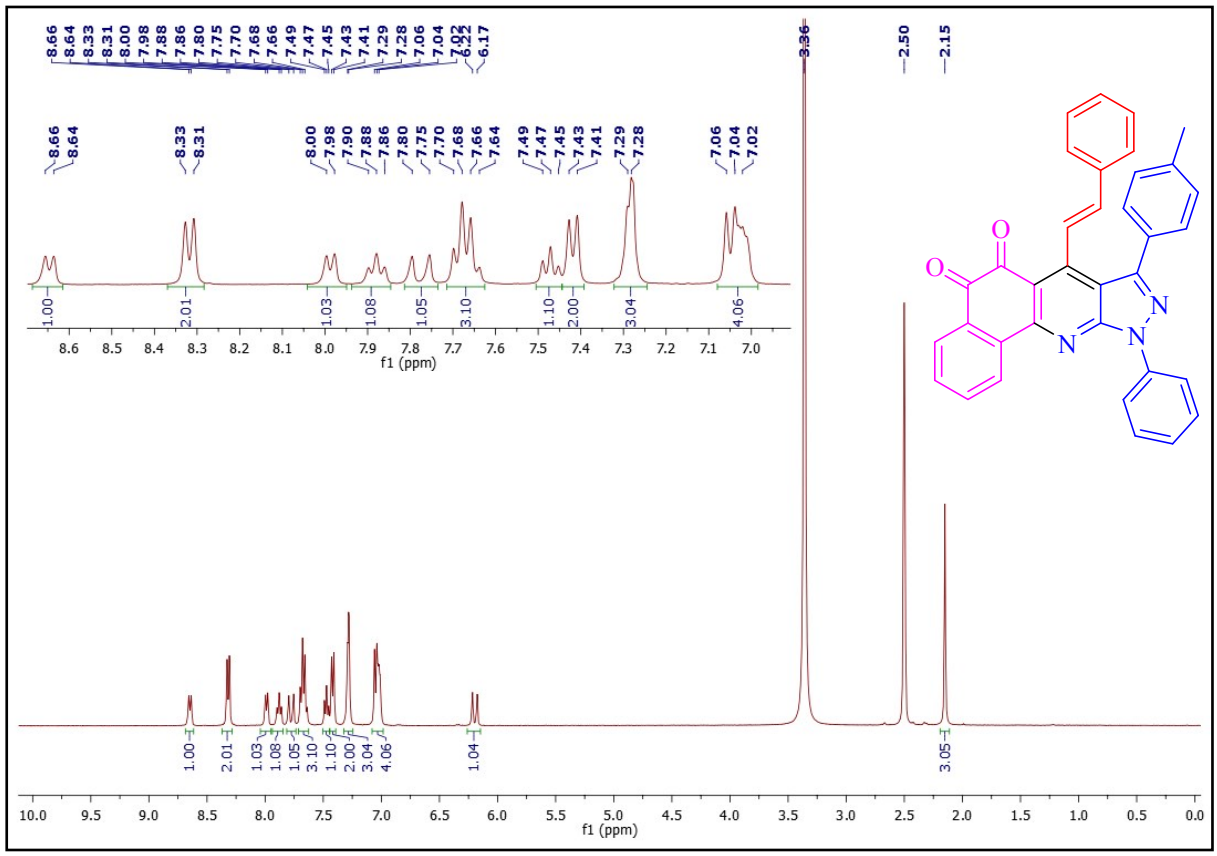
^{1}H NMR Spectra of Compound 4e



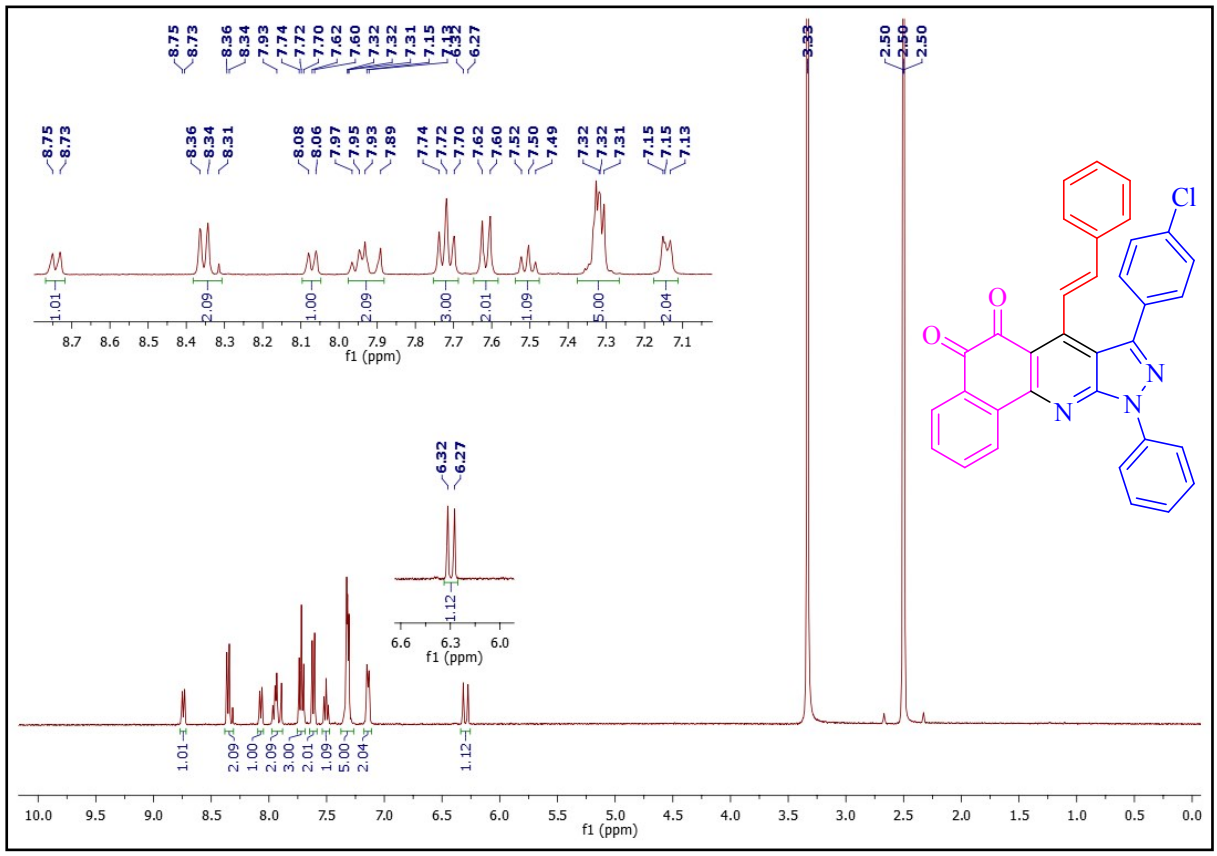
^{1}H NMR Spectra of Compound 4f



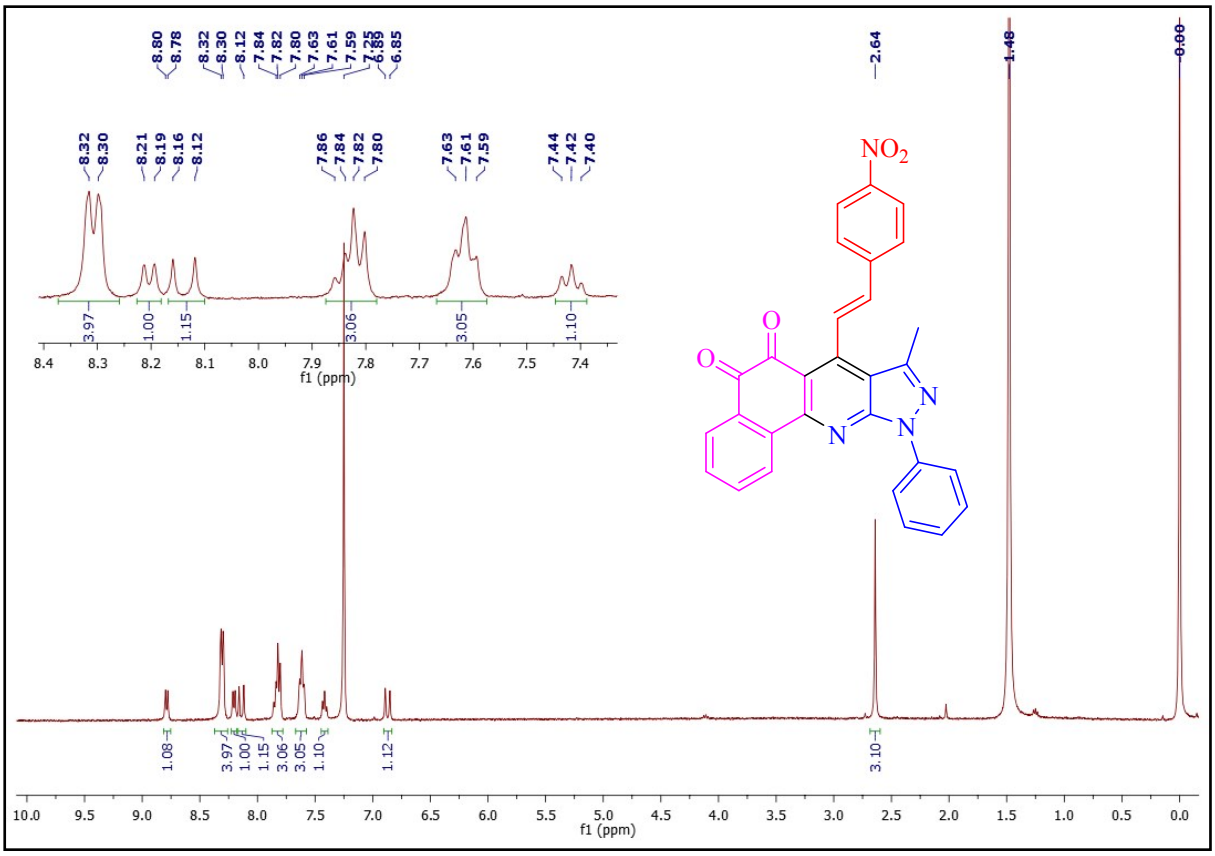
^{1}H NMR Spectra of Compound 4g



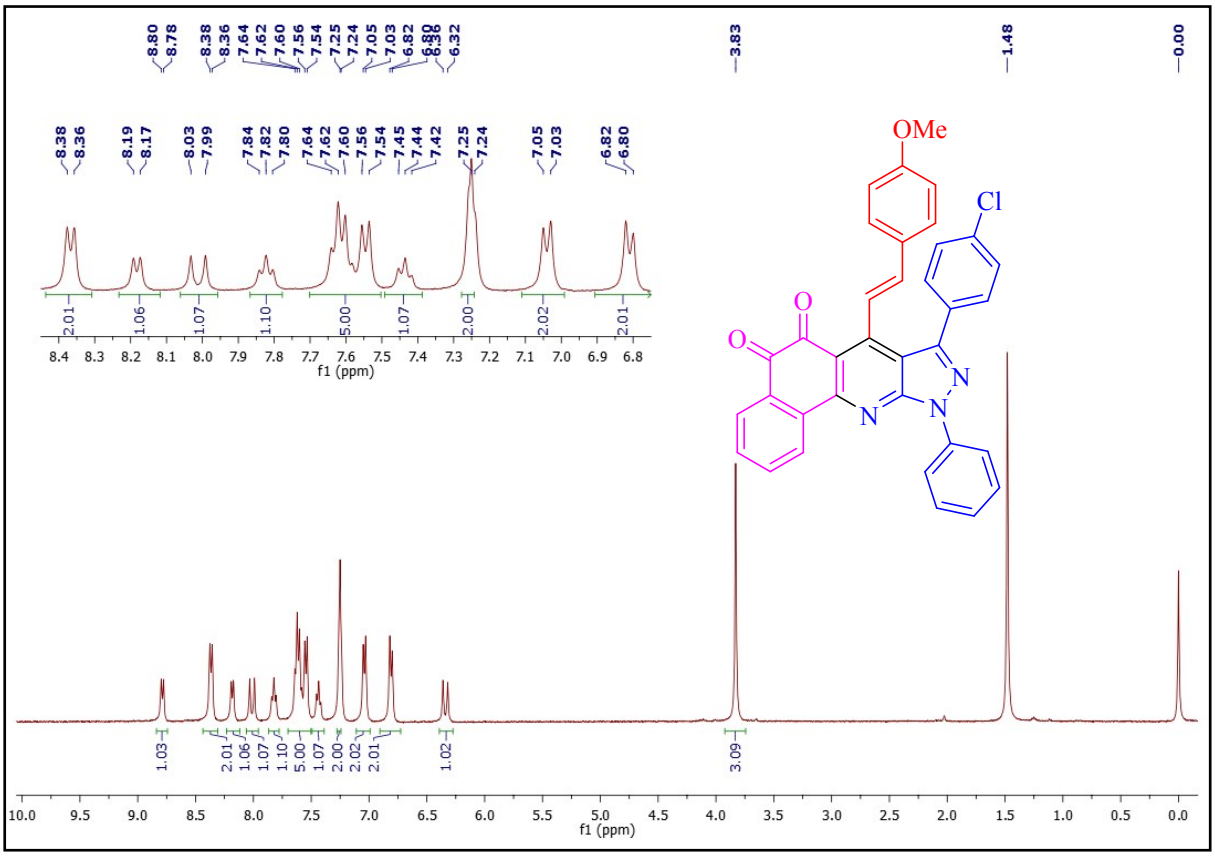
^{1}H NMR Spectra of Compound 4h



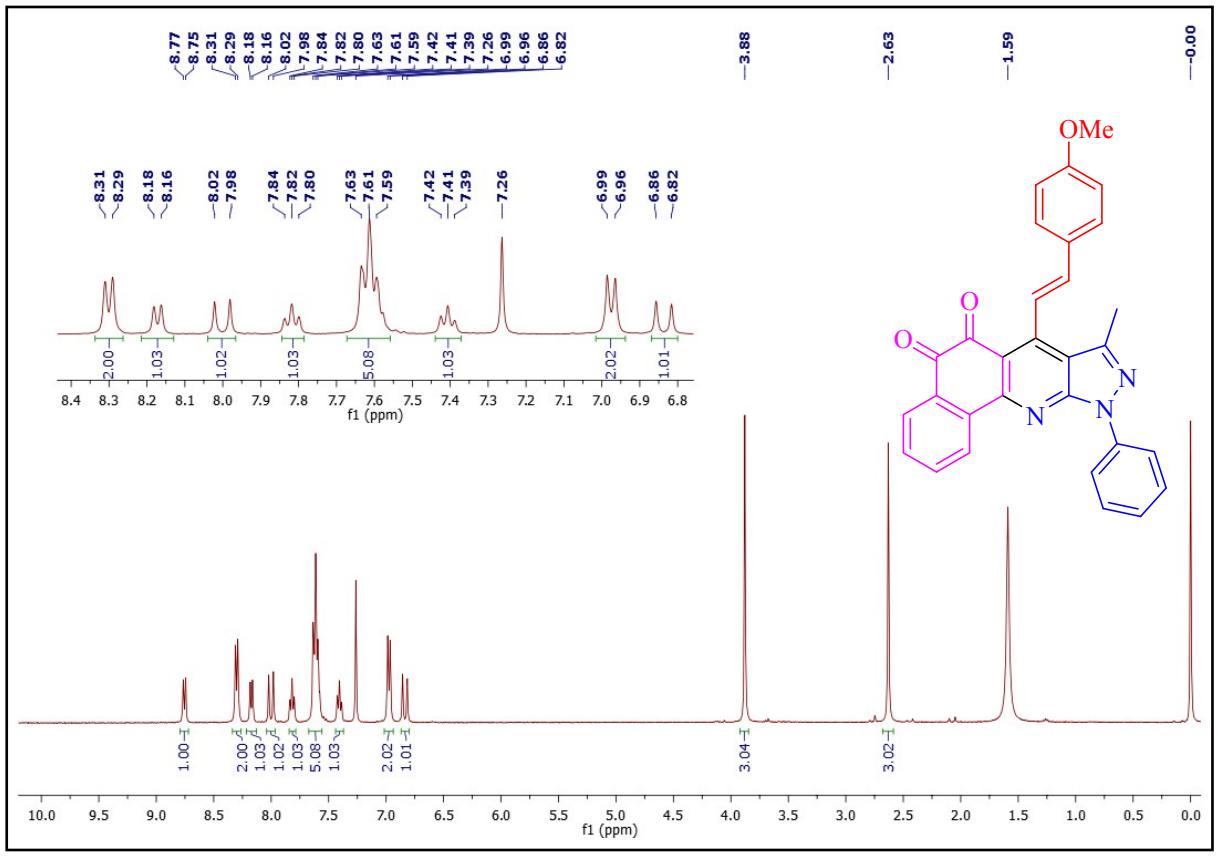
^{1}H NMR Spectra of Compound 4i



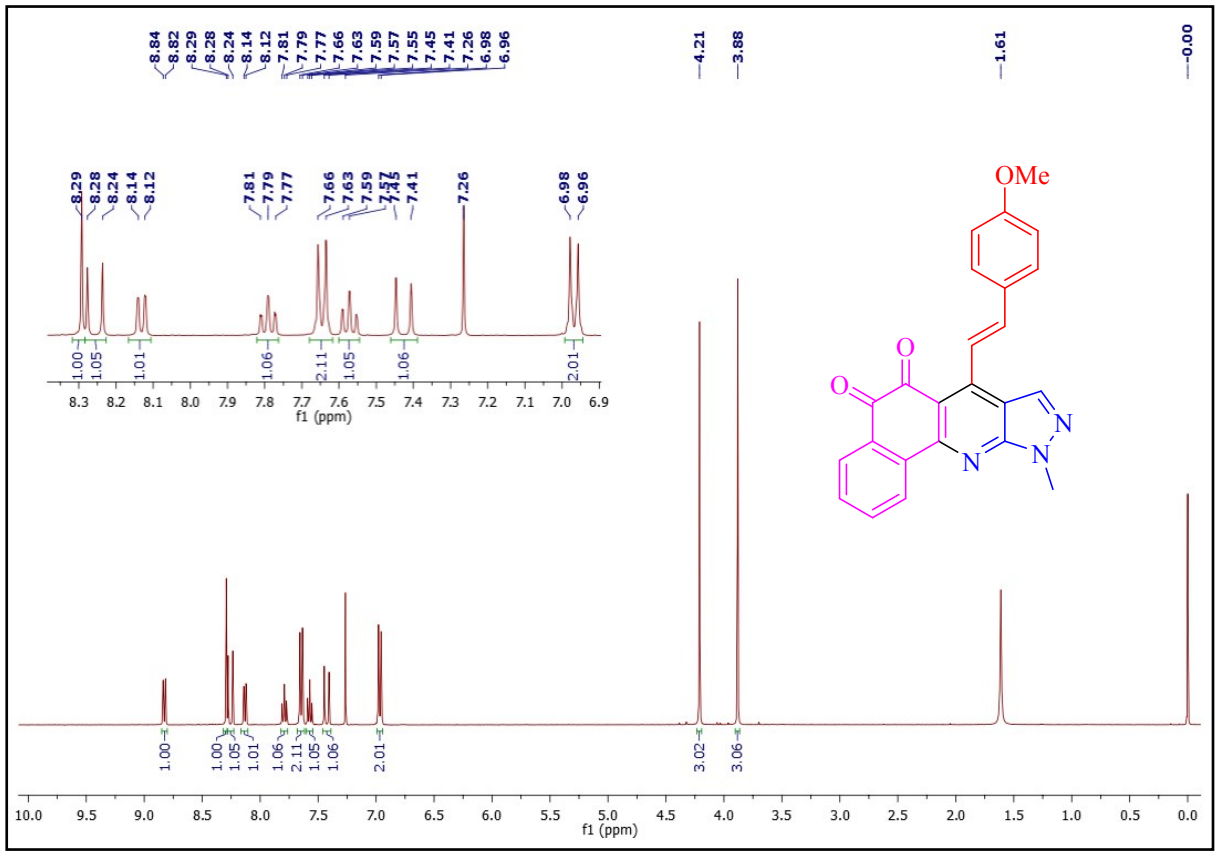
^{1}H NMR Spectra of Compound 4j



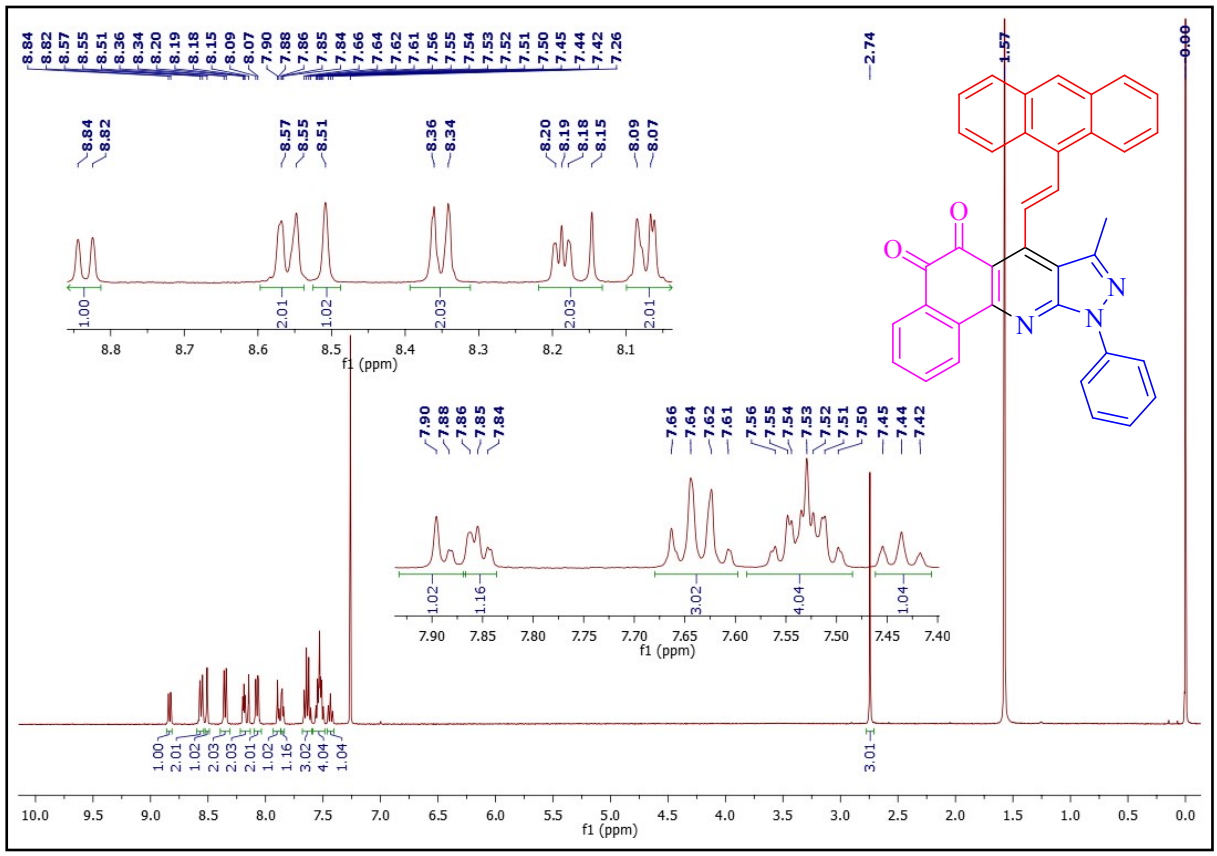
^{1}H NMR Spectra of Compound 4k



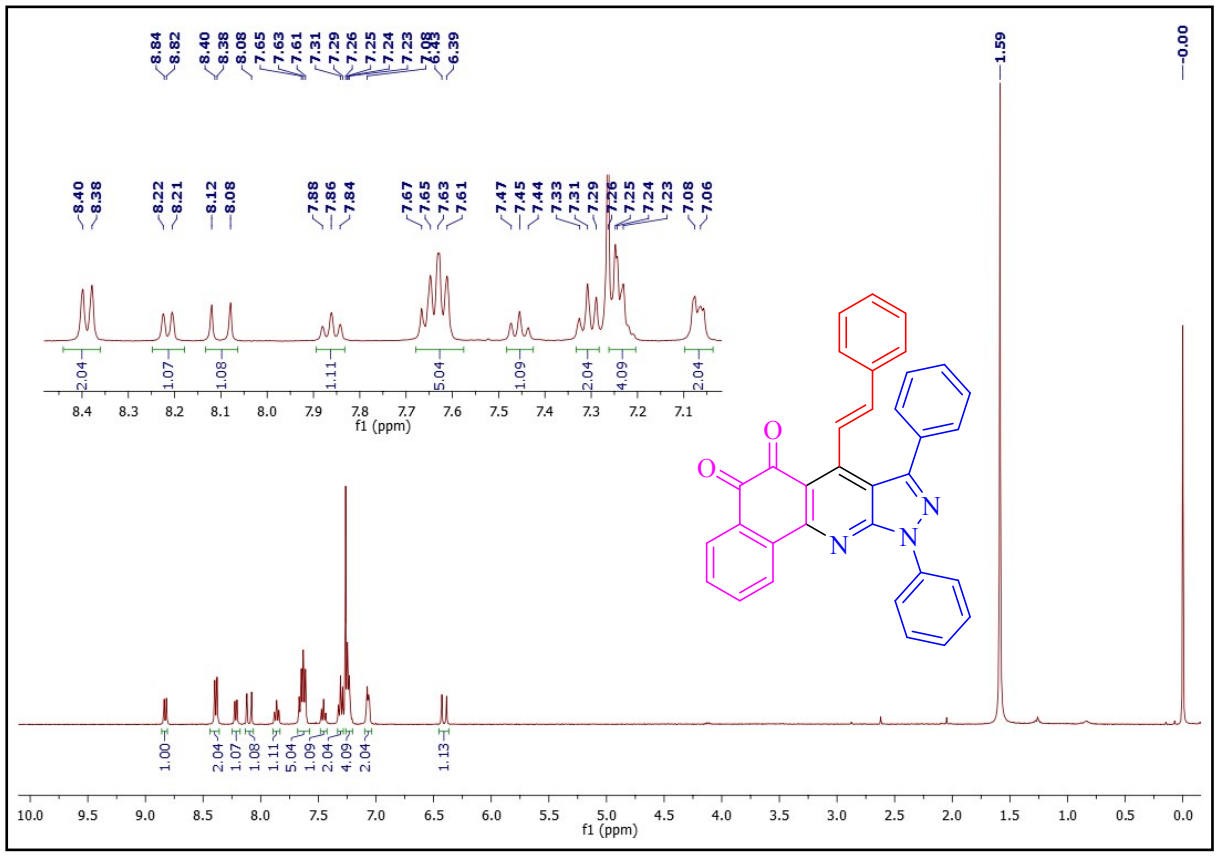
^{1}H NMR Spectra of Compound 4l



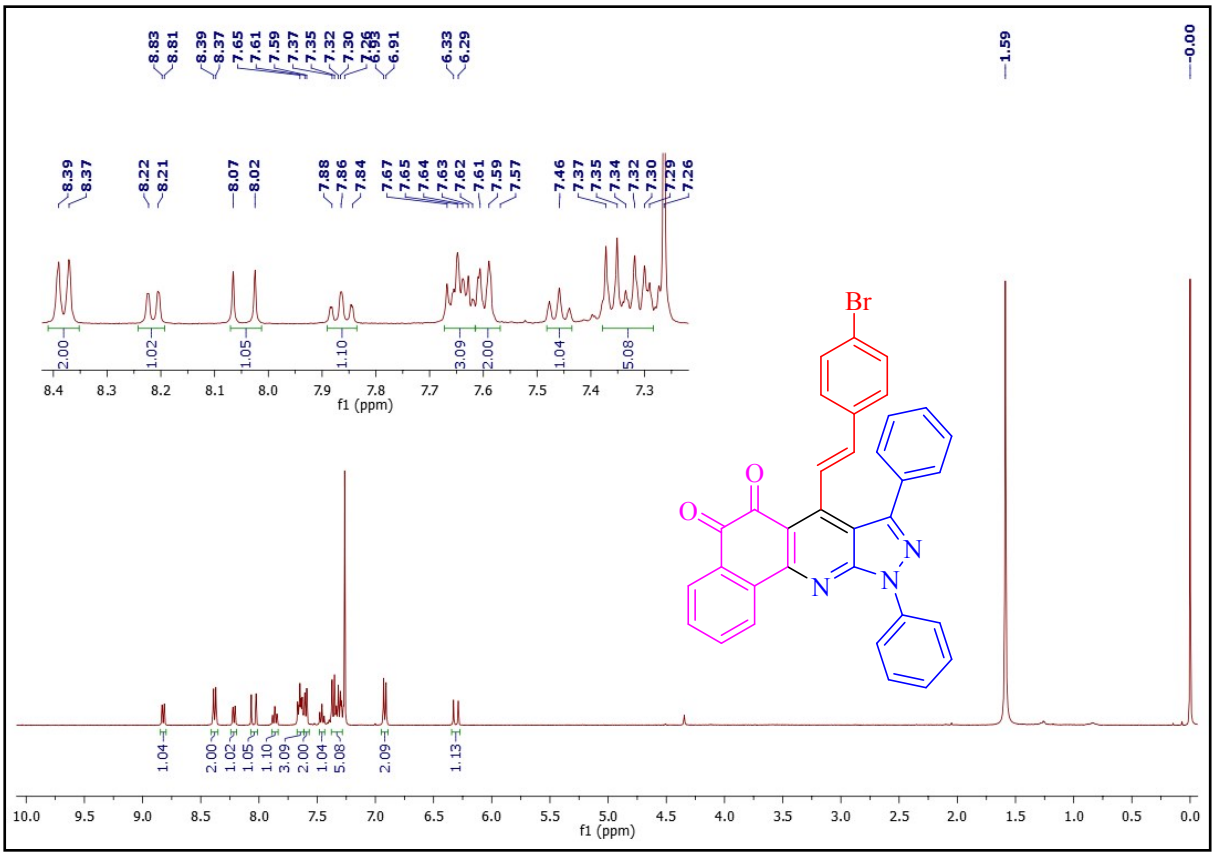
^{1}H NMR Spectra of Compound 4m



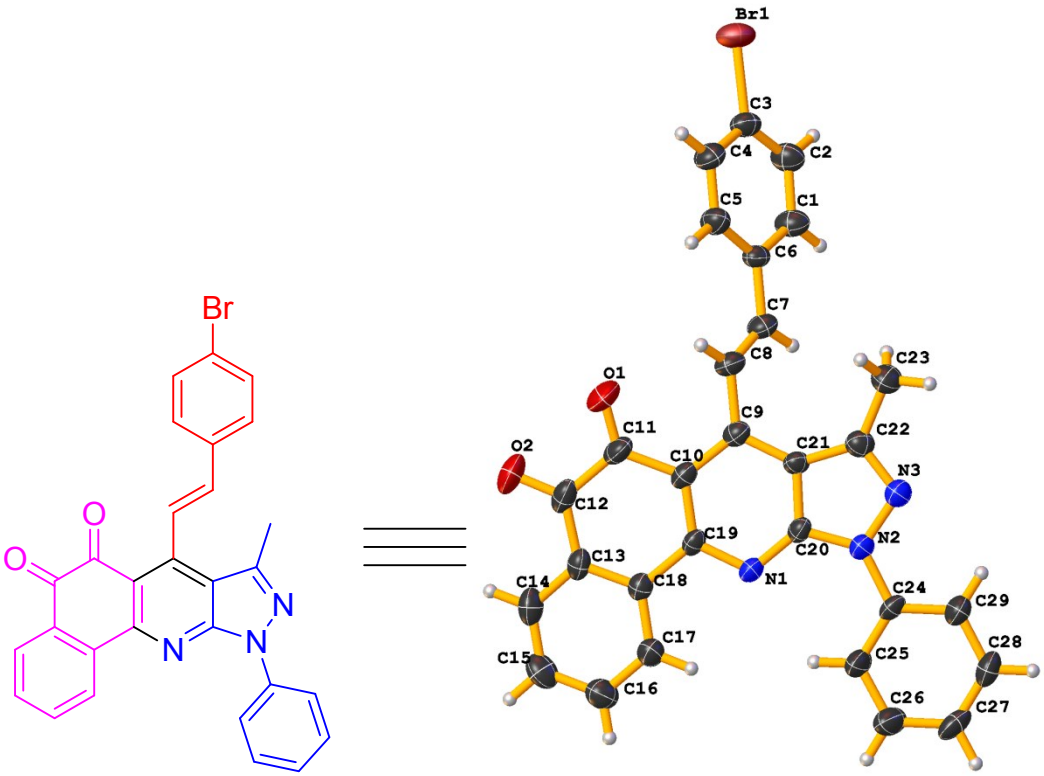
^{1}H NMR Spectra of Compound 4n



^{1}H NMR Spectra of Compound 4o



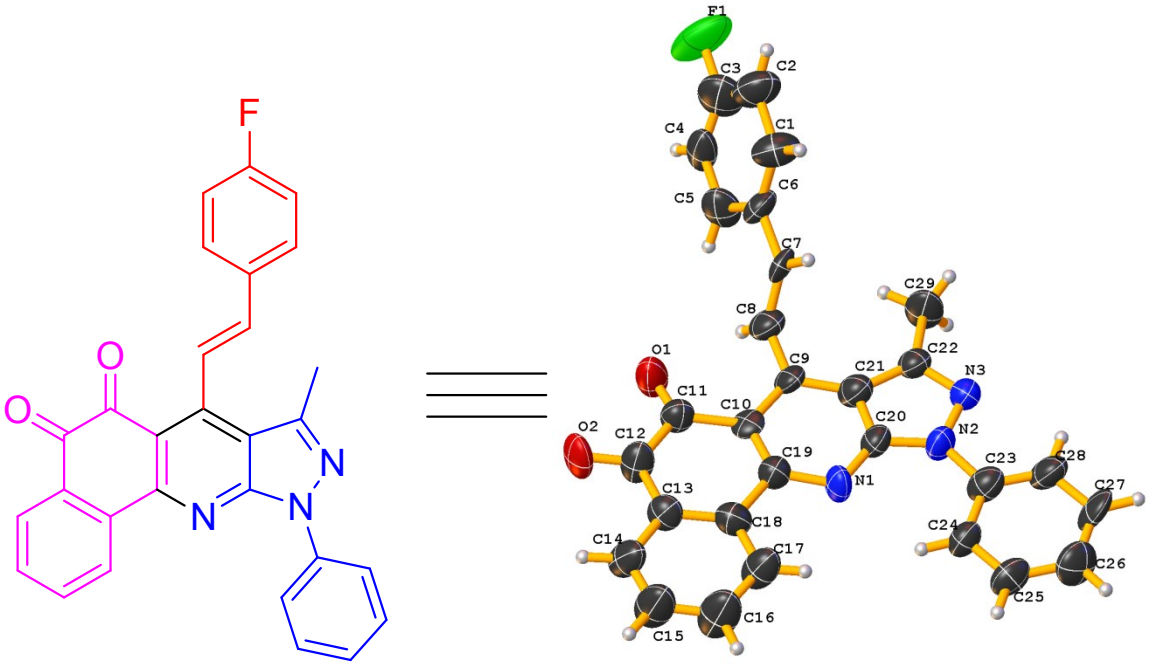
(A) XRD data of 4d with 50% ellipsoidal probability; crystallization: $CHCl_3$ by slow evaporation at room-temperature. (CCDC 1982031).



Identification code	Ra184	
Chemical formula	$C_{29}H_{18}BrN_3O_2$	
Formula weight	520.37 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 = 10.6575(7) Å	α = 110.376(2)°
	b = 10.8837(7) Å	β = 102.926(2)°
	c = 11.6850(8) Å	γ = 108.235(2)°
Volume	1119.38(13) $Å^3$	

Z	2
Density (calculated)	1.544 g/cm^3
Absorption coefficient	1.870 mm^{-1}
F(000)	528
Theta range for data collection	2.96 to 26.00°
Index ranges	$-13 \leq h \leq 13$, $-12 \leq k \leq 13$, $-14 \leq l \leq 14$
Reflections collected	14398
Independent reflections	4391 [R(int) = 0.0774]
Coverage of independent reflections	99.8%
Absorption correction	Multi-Scan
Max. and min. transmission	0.5710 and 0.5650
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	4391 / 0 / 318
Goodness-of-fit on F^2	1.010
Final R indices	2306 data; $I>2\sigma(I)$ R1 = 0.0570, wR2 = 0.0735 all data R1 = 0.1500, wR2 = 0.0932
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0211P)^2+0.6426P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0024(5)
Largest diff. peak and hole	0.270 and -0.390 eÅ^{-3}
R.M.S. deviation from mean	0.066 eÅ^{-3}

(B) **XRD data of 4f with 50% ellipsoidal probability; crystallization: $CHCl_3$ by slow evaporation at room-temperature. (CCDC 1982028).**



Identification code	Ra-151r	
Chemical formula	$C_{29}H_{18}FN_3O_2$	
Formula weight	459.46 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal size	0.100 x 0.200 x 0.200 mm	
Crystal system	Monoclinic	
Space group	Pc	
Unit cell dimensions	a = 9.177(4) Å	α = 90°
	b = 12.753(5) Å	β = 123.03(2)°
	c = 11.653(4) Å	γ = 90°
Volume	1143.4(8) $Å^3$	
Z	2	

Density (calculated)	1.335 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	476	
Theta range for data collection	2.65 to 20.00°	
Index ranges	$-8 \leq h \leq 8$, $-12 \leq k \leq 12$, $-11 \leq l \leq 11$	
Reflections collected	10931	
Independent reflections	2133 [R(int) = 0.2956]	
Coverage of independent reflections	99.8 %	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.7465 and 0.6325	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	2133 / 196 / 316	
Goodness-of-fit on F^2	1.026	
Final R indices	833 data; $I>2\sigma(I)$	R1 = 0.0817, wR2 = 0.1479
	all data	R1 = 0.2444, wR2 = 0.2121
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0785P)^2]$, where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.189 and -0.245 $e.Å^{-3}$	
R.M.S. deviation from mean	0.054 $eÅ^{-3}$	