

A Novel Phenyl and Thiophene Dispiro Indenoquinoxaline Pyrrolidine Quinolones Induced Apoptosis via G1/S and G2/M Phase Cell Cycle Arrest in MCF-7 Cells

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Spectral data

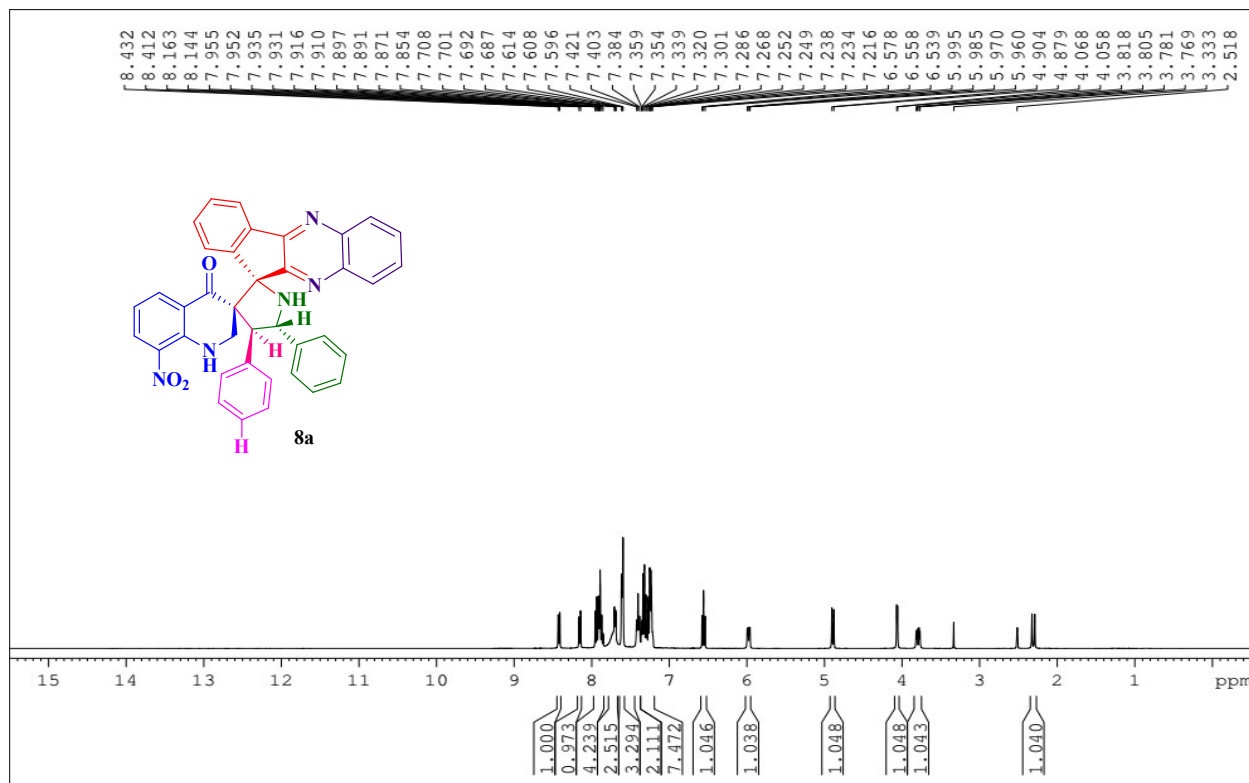


Figure S1. ¹H NMR spectrum of compound 8a

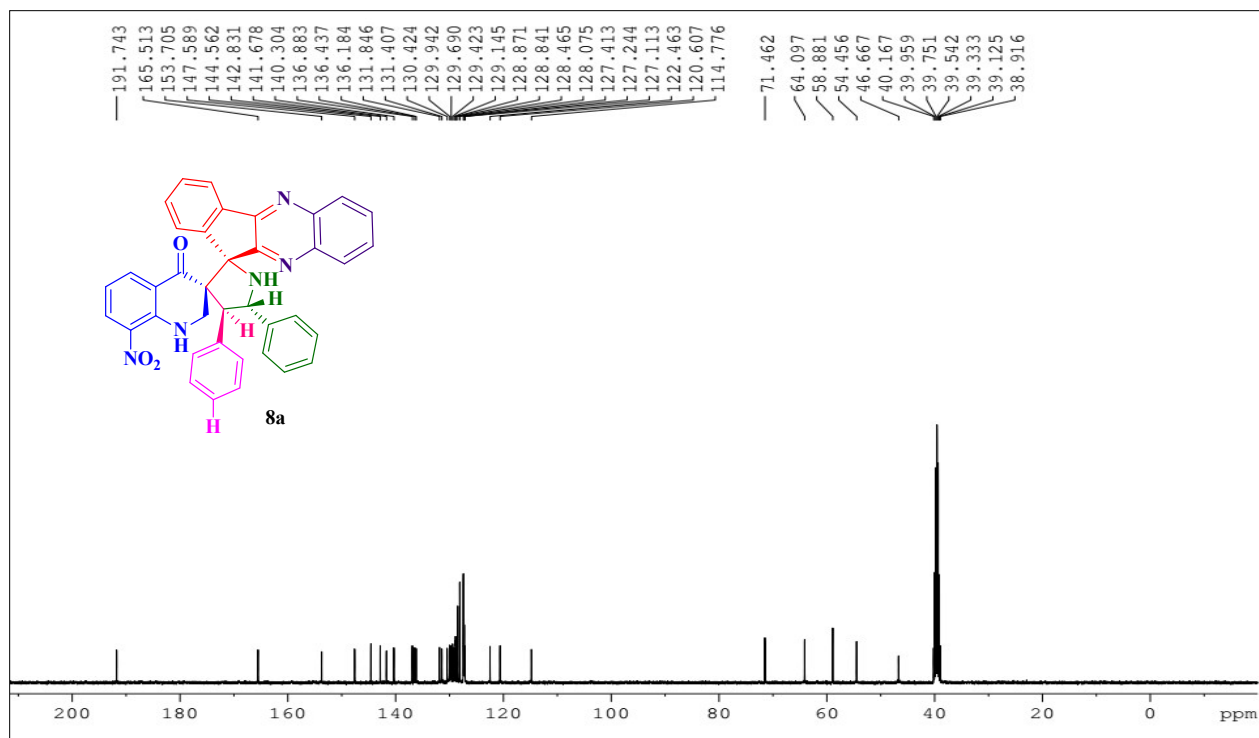


Figure S2. ^{13}C NMR spectrum of compound 8a

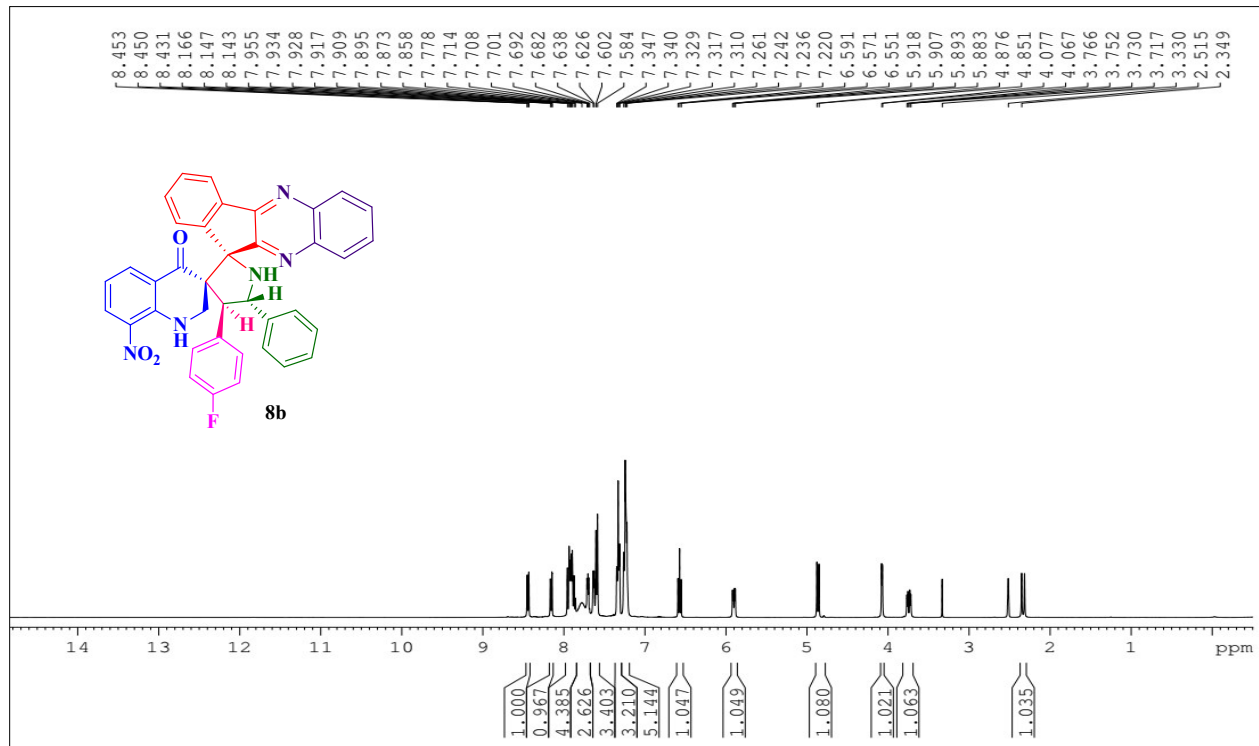


Figure S3. ^1H NMR spectrum of compound 8b

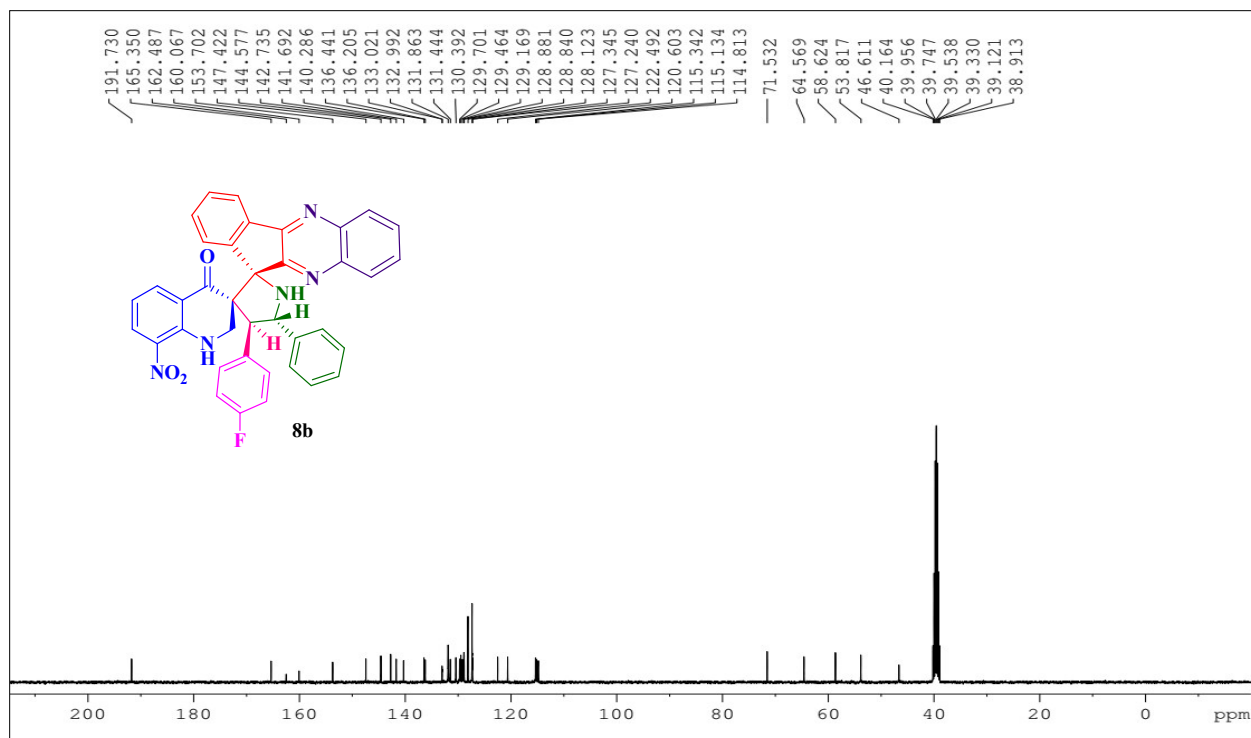


Figure S4. ¹³C NMR spectrum of compound 8b

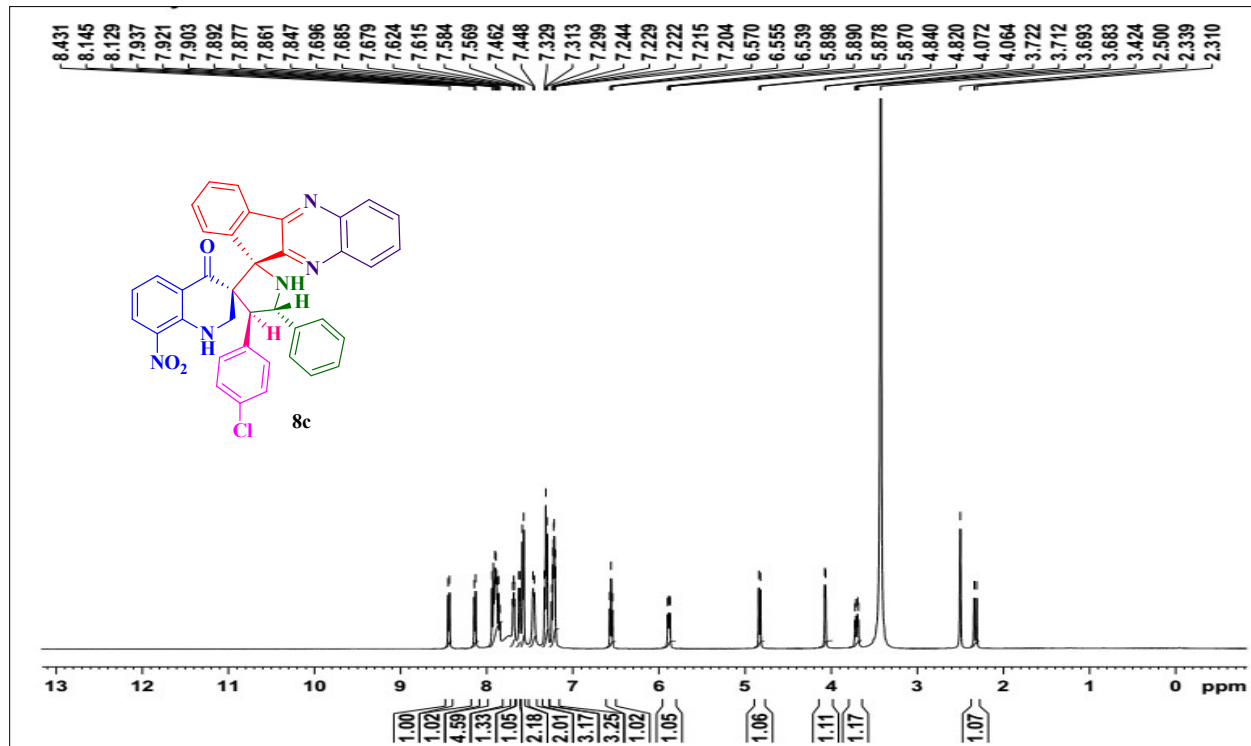


Figure S5. ¹H NMR spectrum of compound 8c

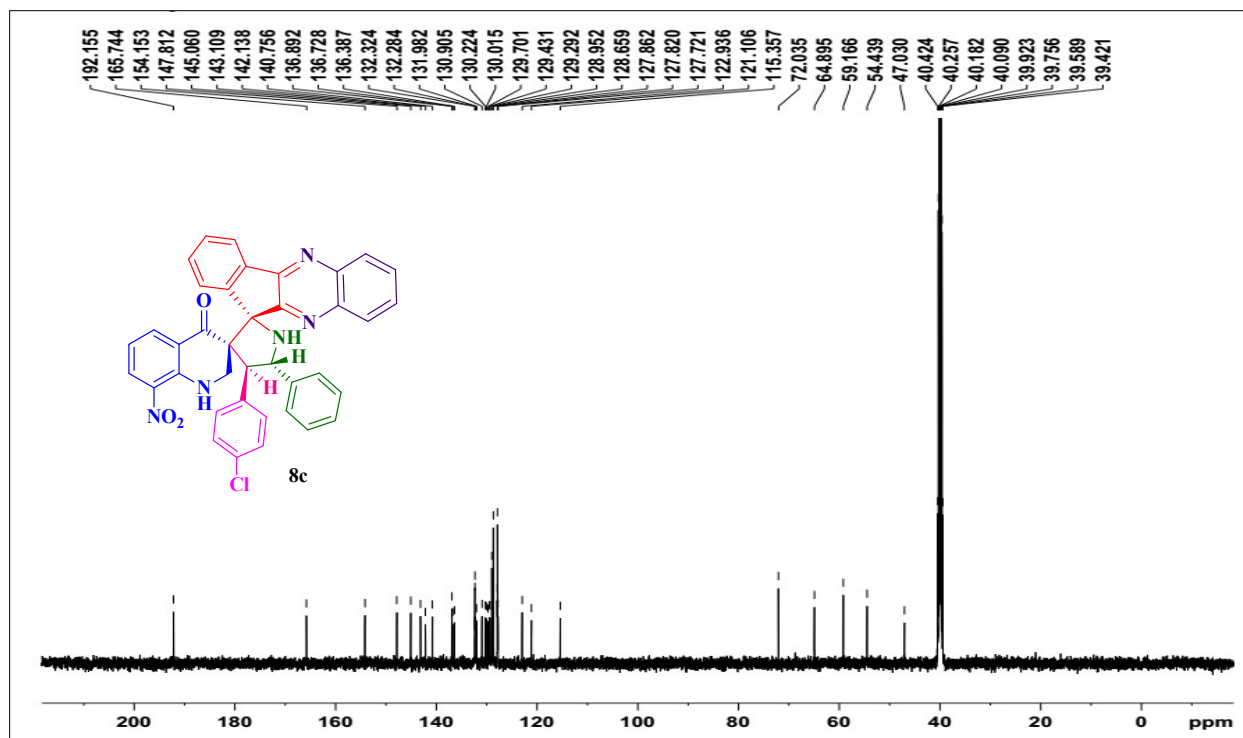


Figure S6. ^{13}C NMR spectrum of compound 8c

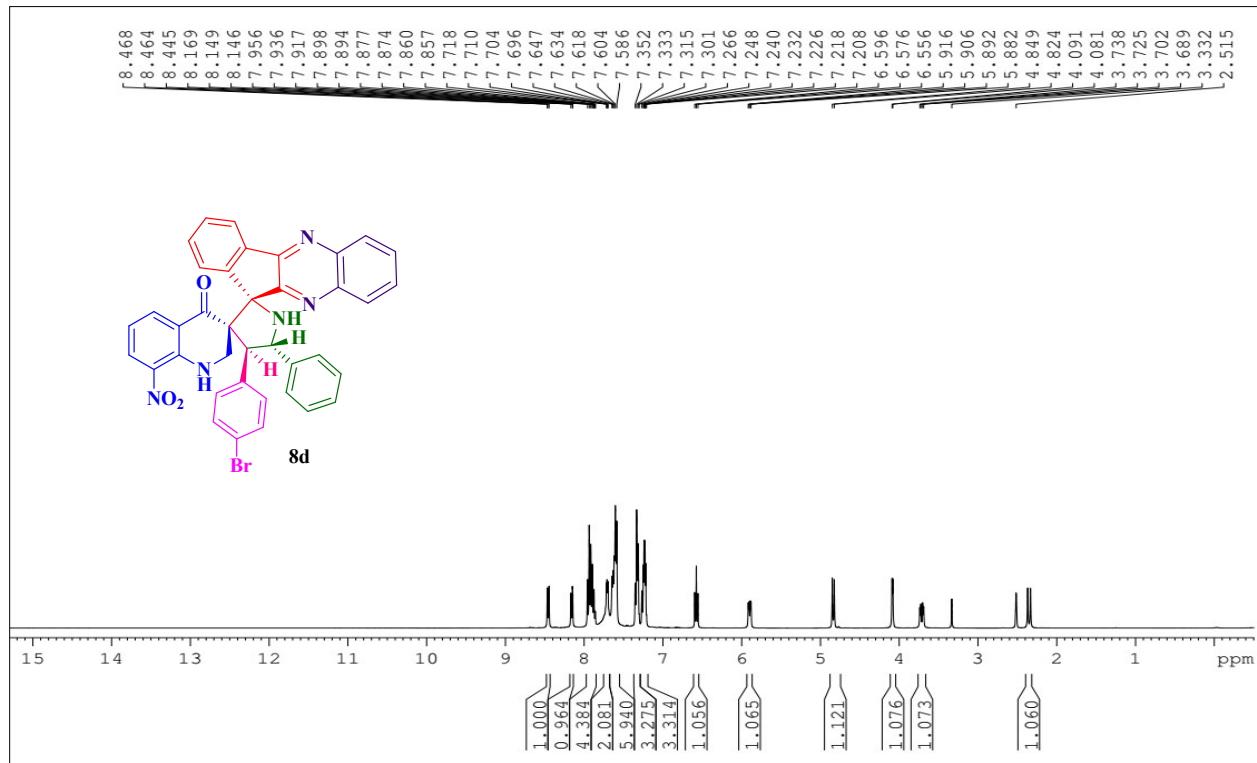


Figure S7. ^1H NMR spectrum of compound 8d

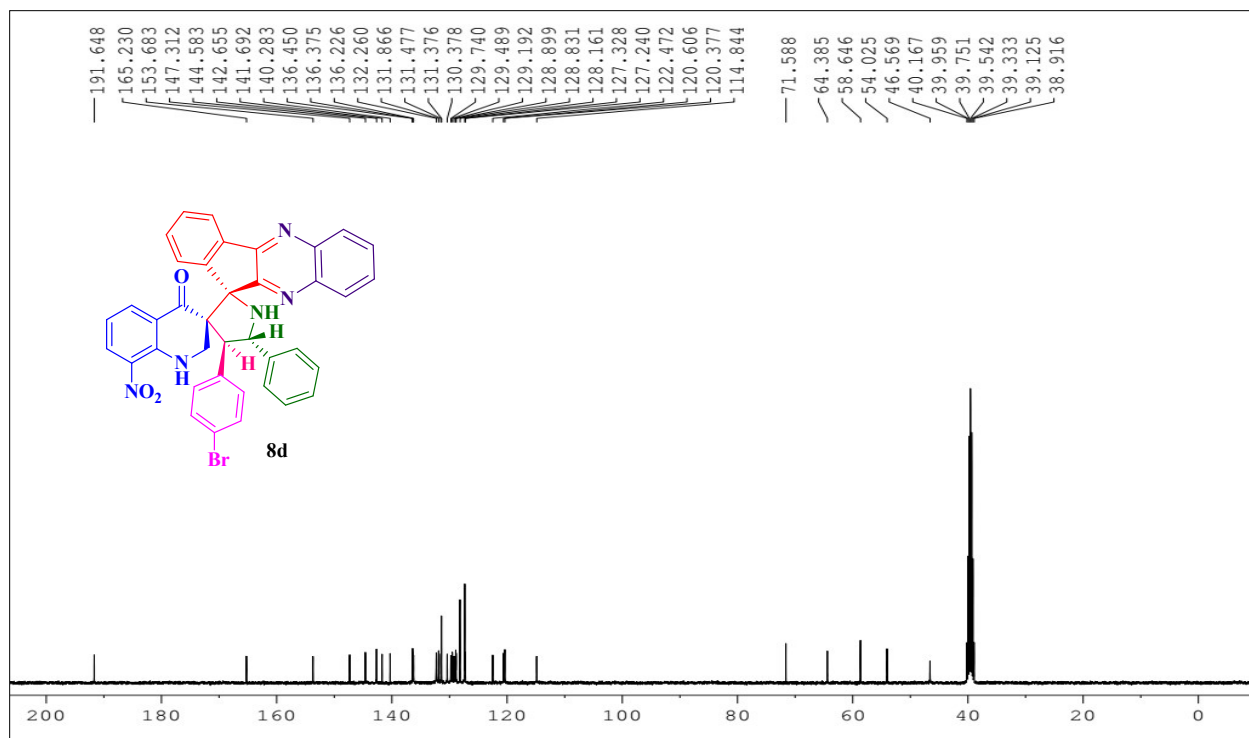


Figure S8. ¹³C NMR spectrum of compound 8d

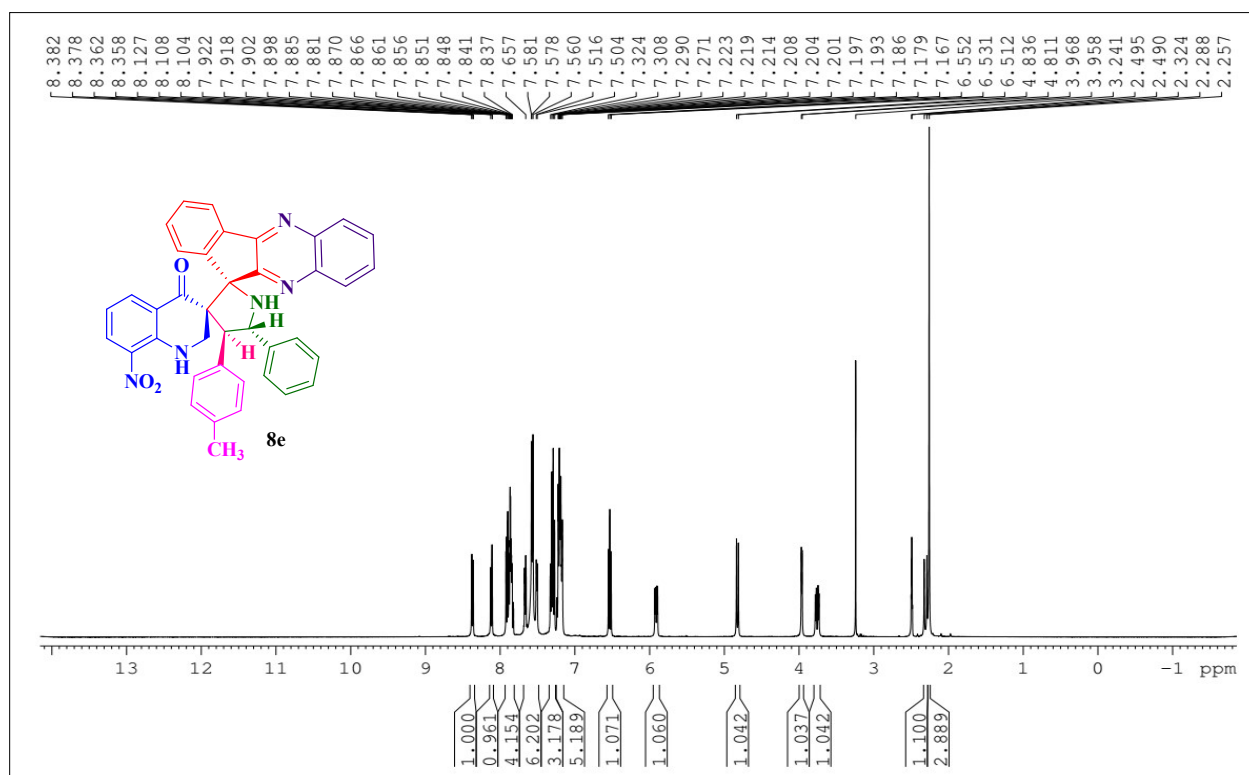


Figure S9. ¹H NMR spectrum of compound 8e

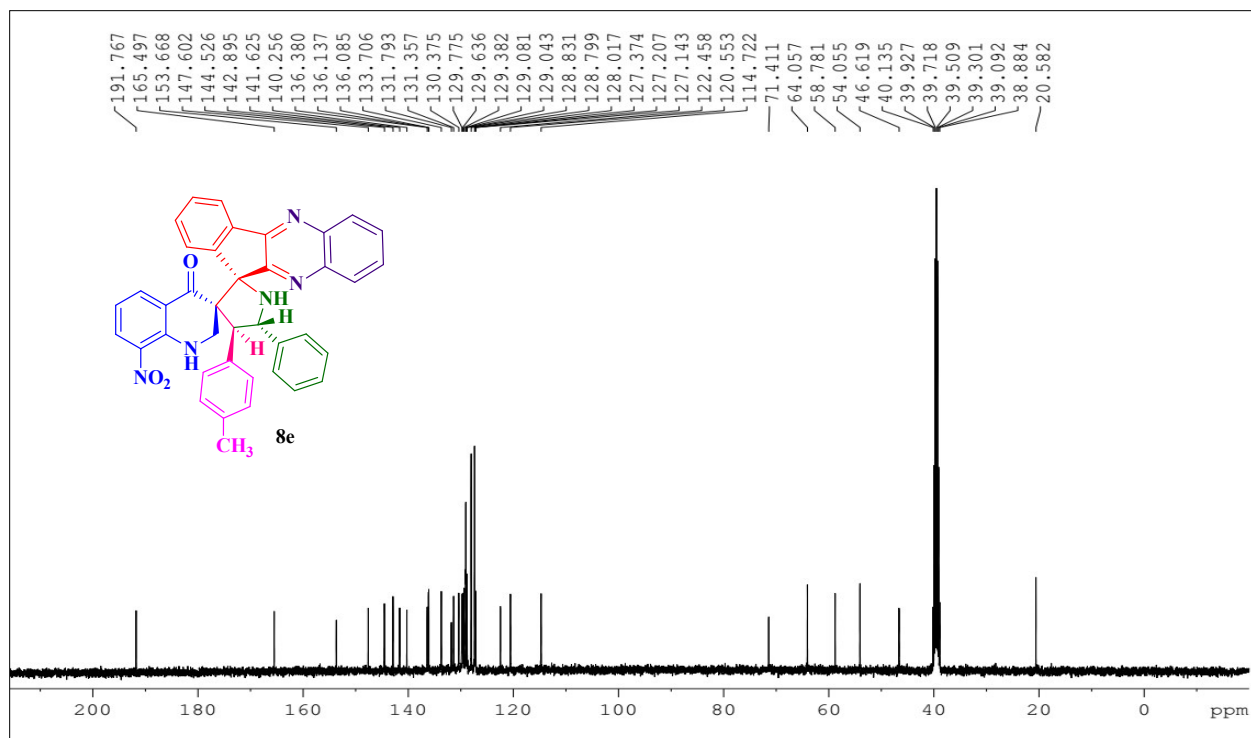


Figure S10. ¹³C NMR spectrum of compound 8e

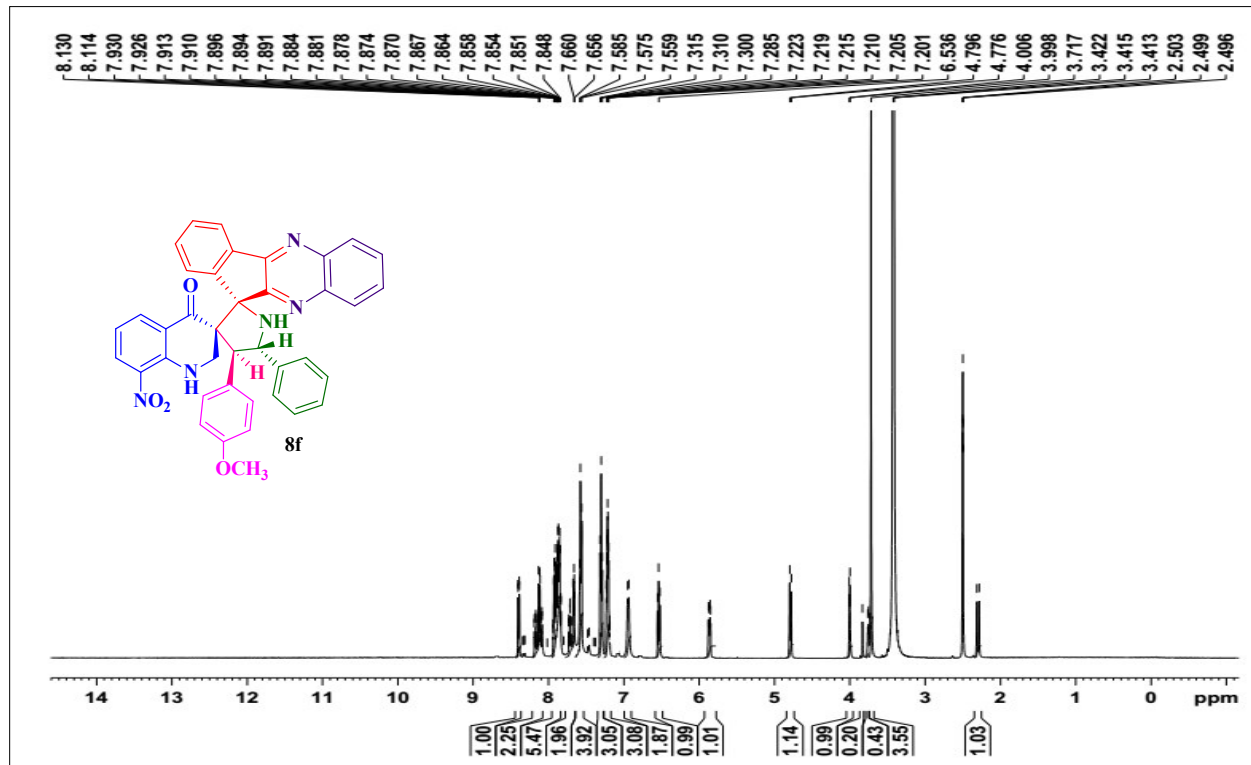


Figure S11. ¹H NMR spectrum of compound 8f

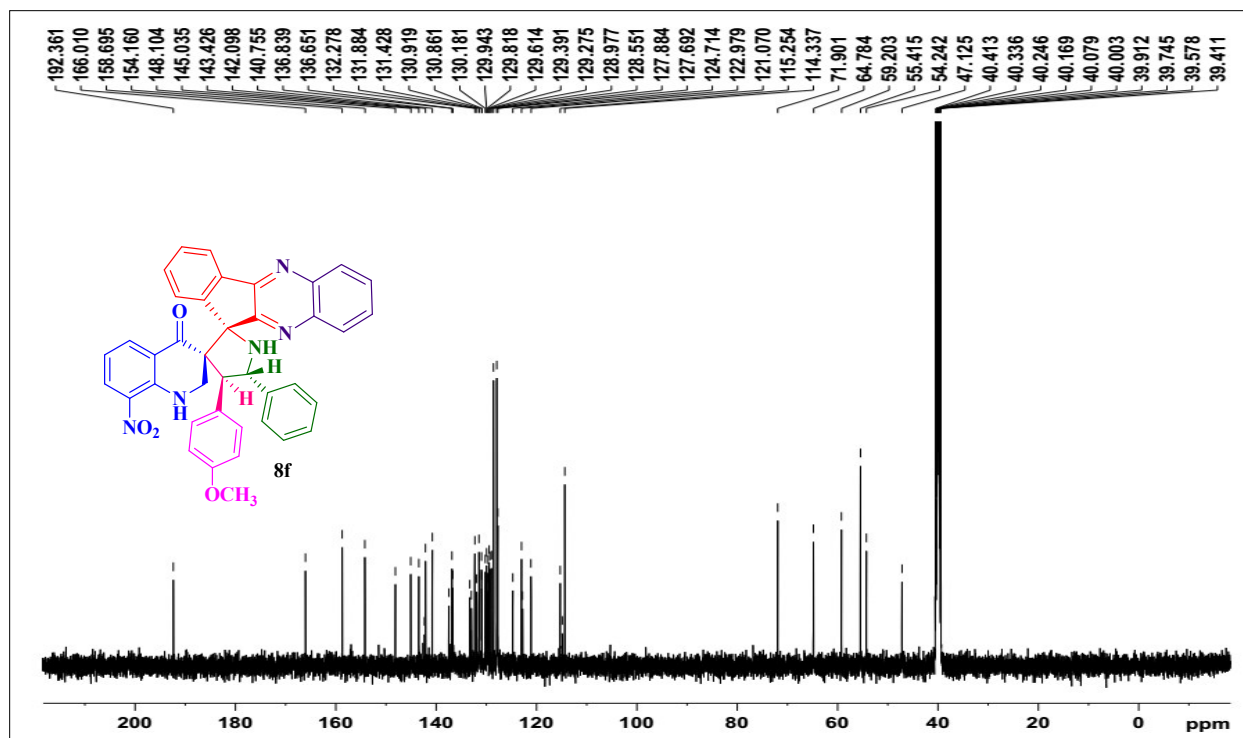


Figure S12. ^{13}C NMR spectrum of compound 8f

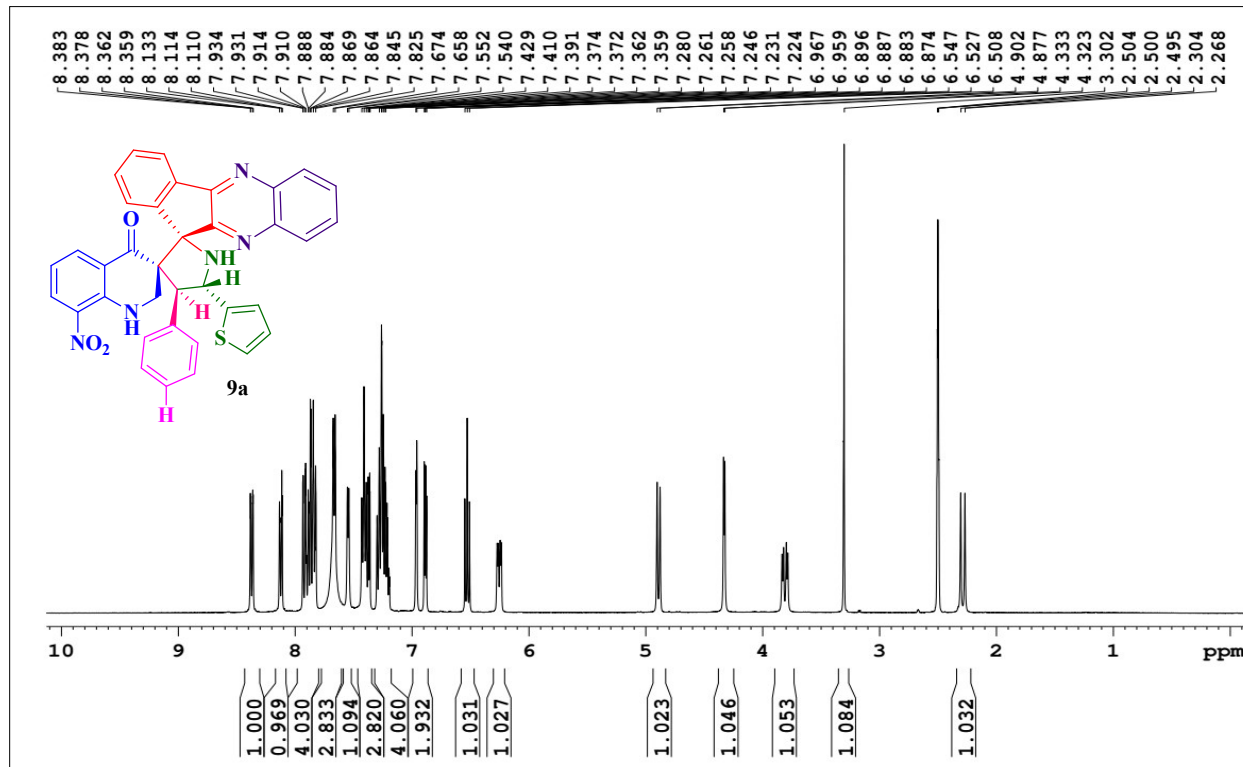


Figure S13. ^1H NMR spectrum of compound 9a

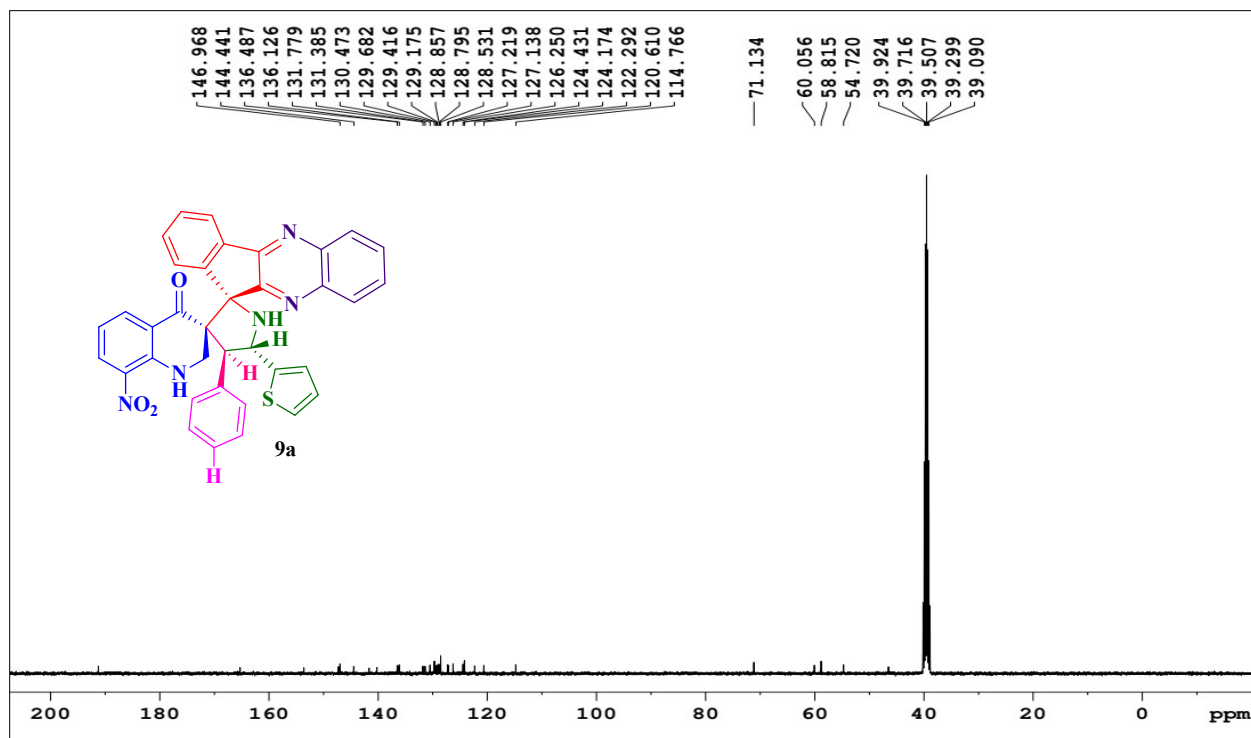


Figure S14. ¹³C NMR spectrum of compound 9a

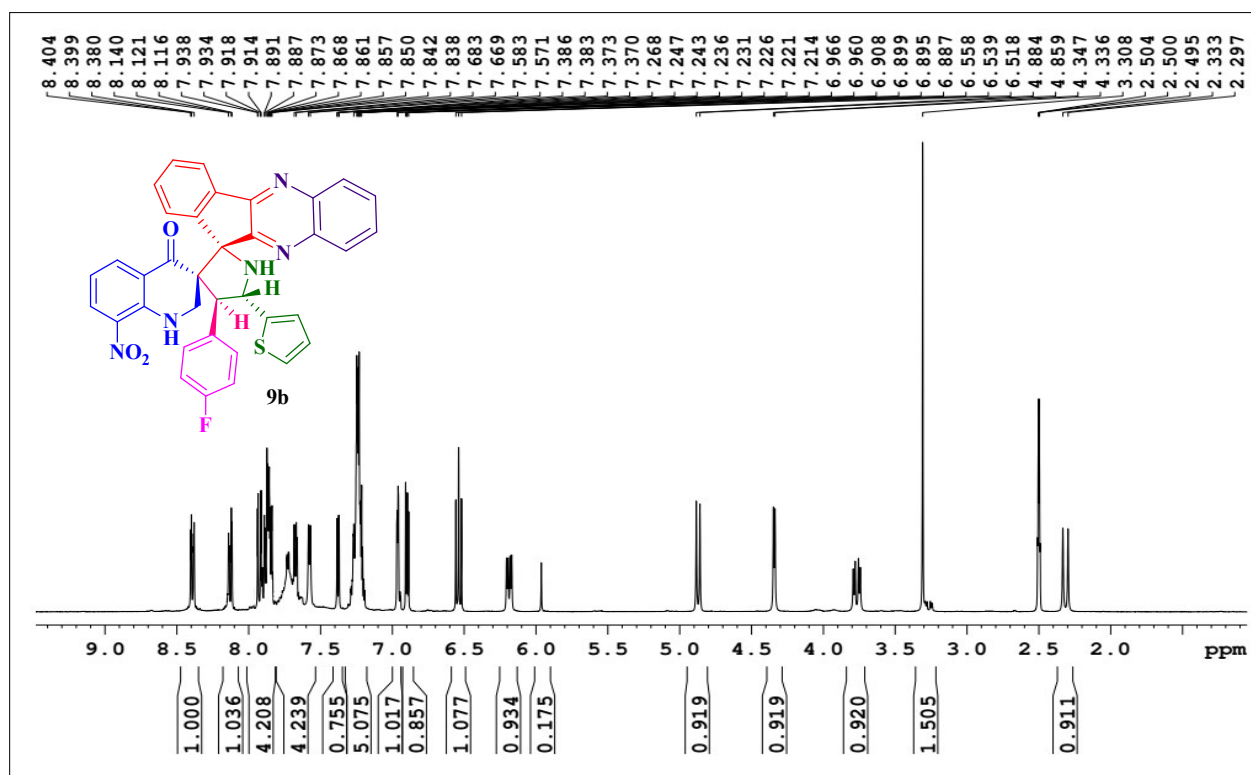


Figure S15. ¹H NMR spectrum of compound 9b

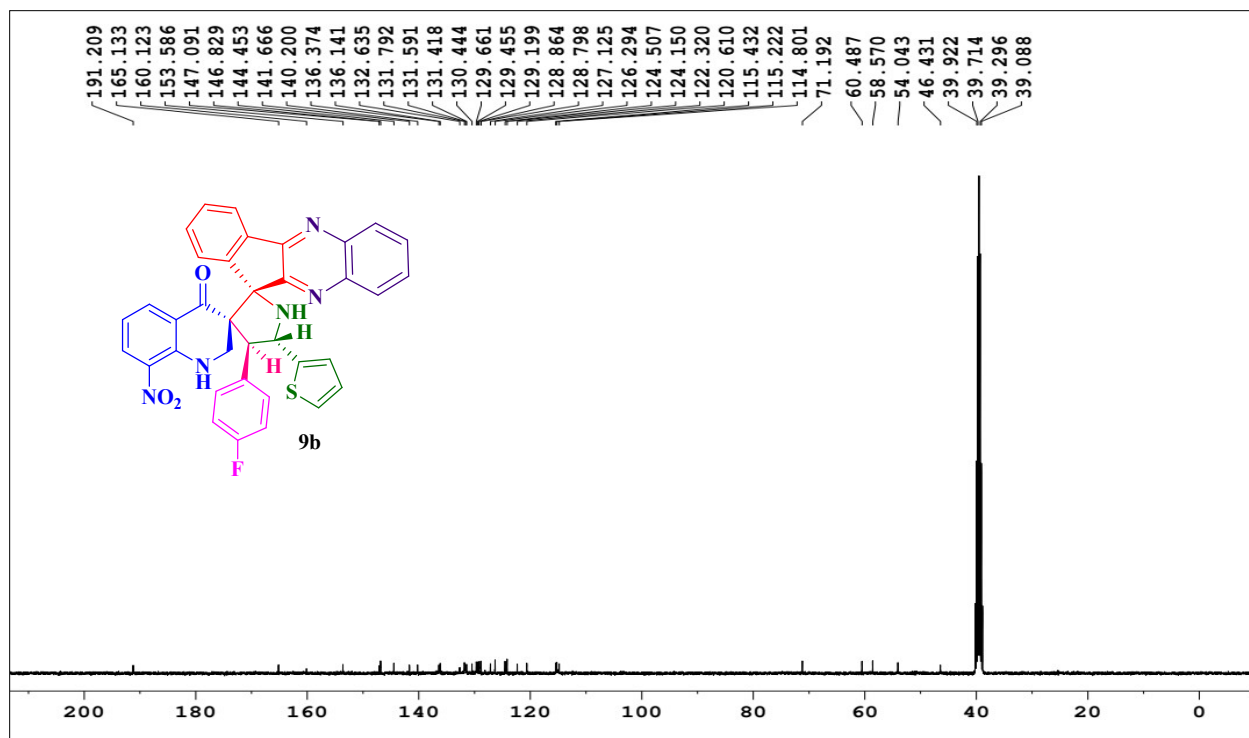


Figure S16. ¹³C NMR spectrum of compound 9b

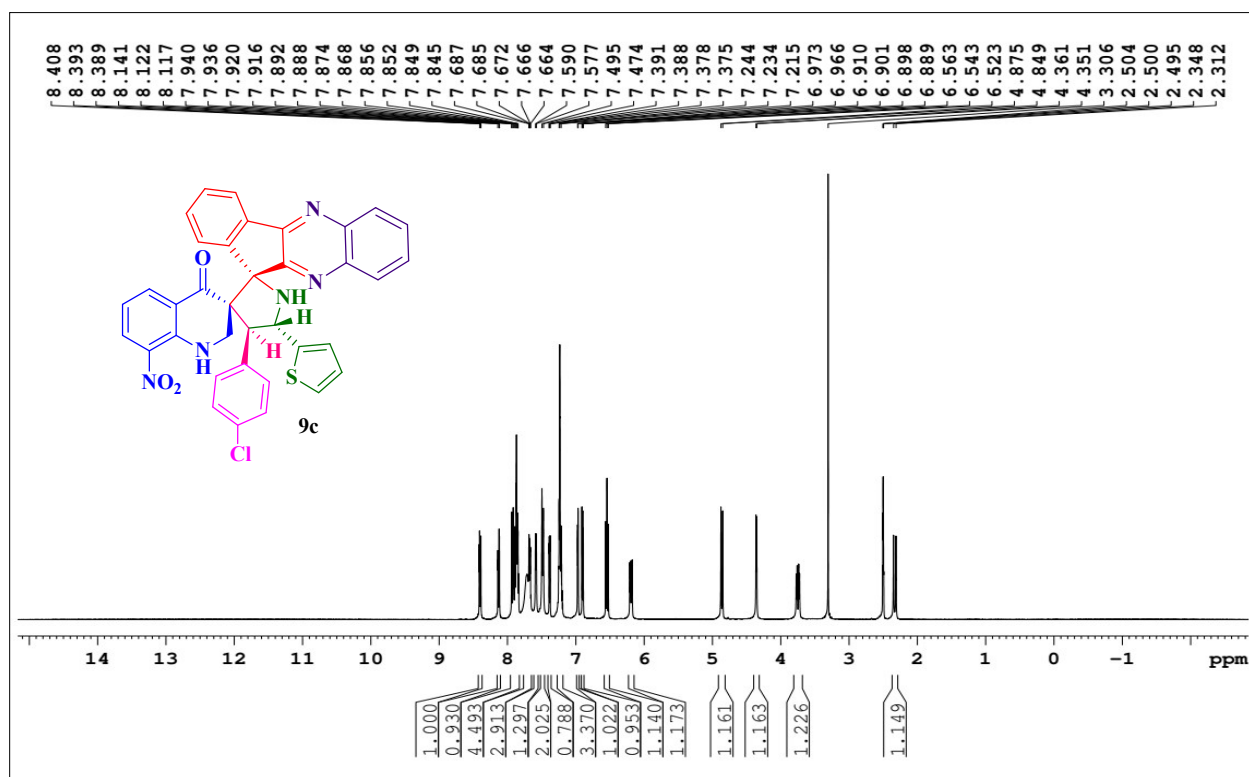


Figure S17. ¹H NMR spectrum of compound 9c

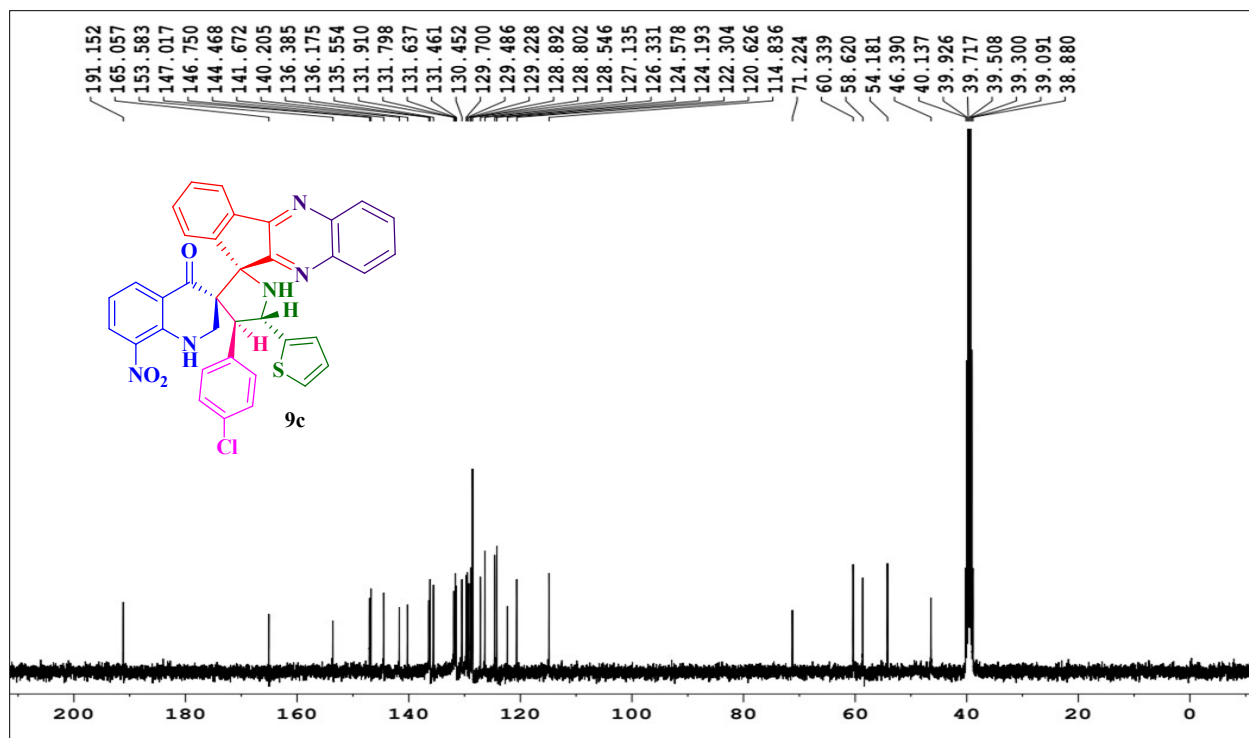


Figure 18. ¹³C NMR spectrum of compound 9c

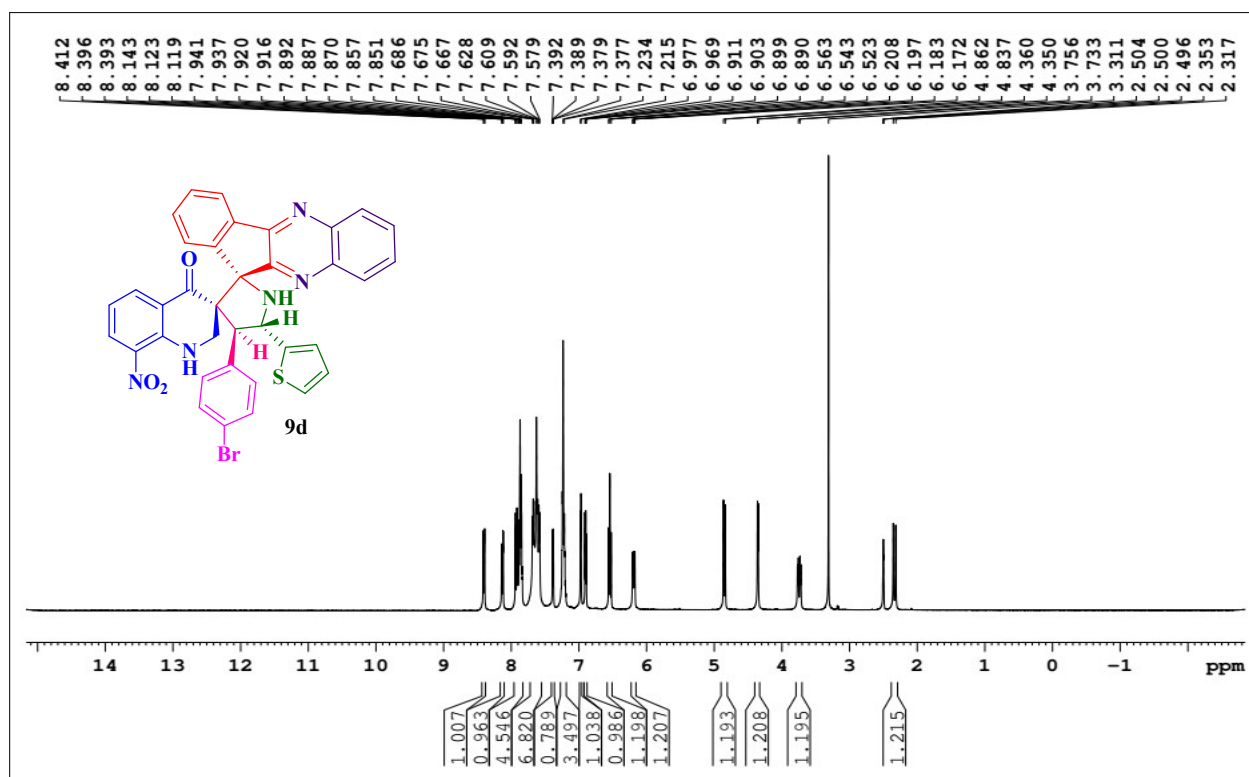


Figure 19. ¹H NMR spectrum of compound 9d

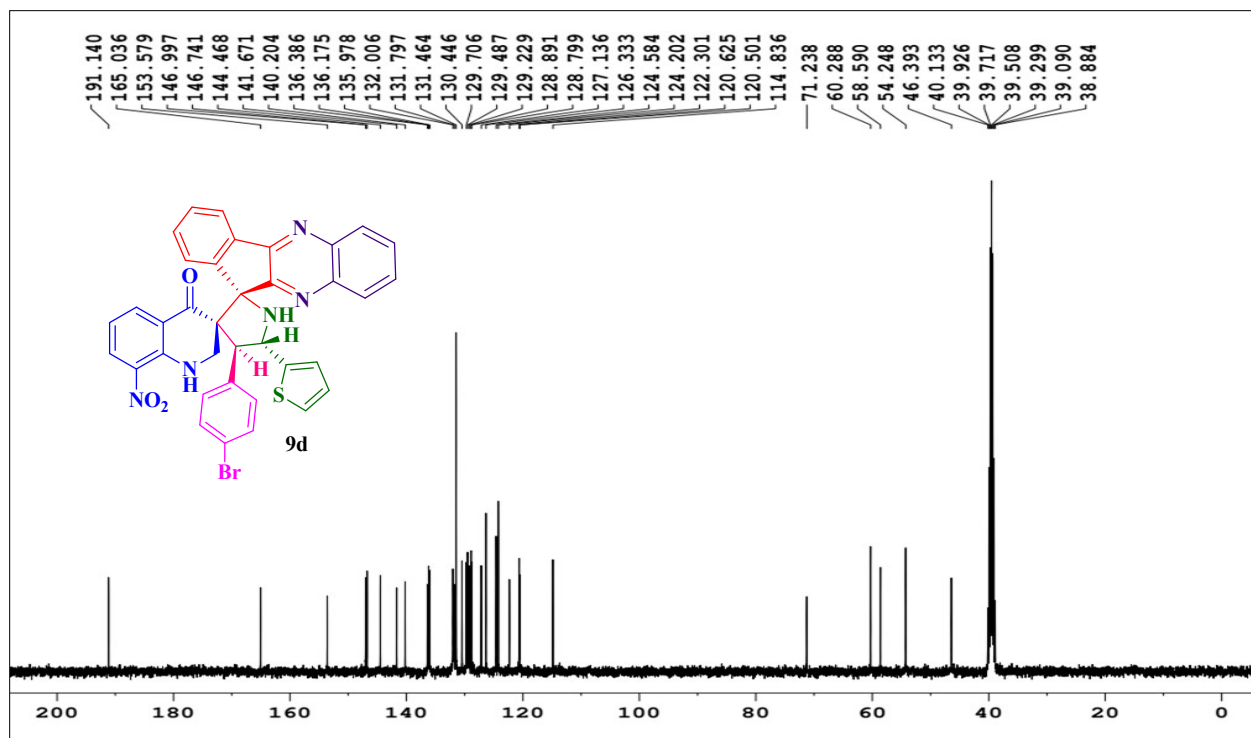


Figure 20. ^{13}C NMR spectrum of compound 9d

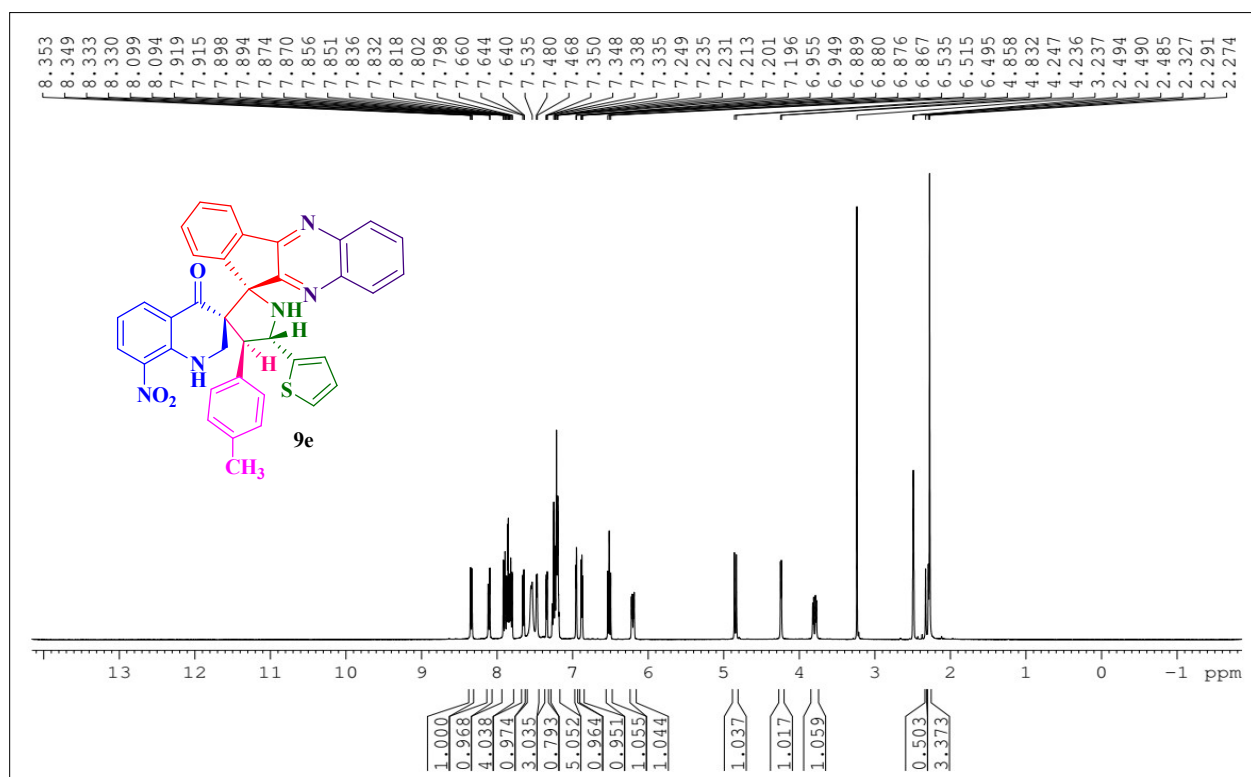


Figure 21. ^1H NMR spectrum of compound 9e

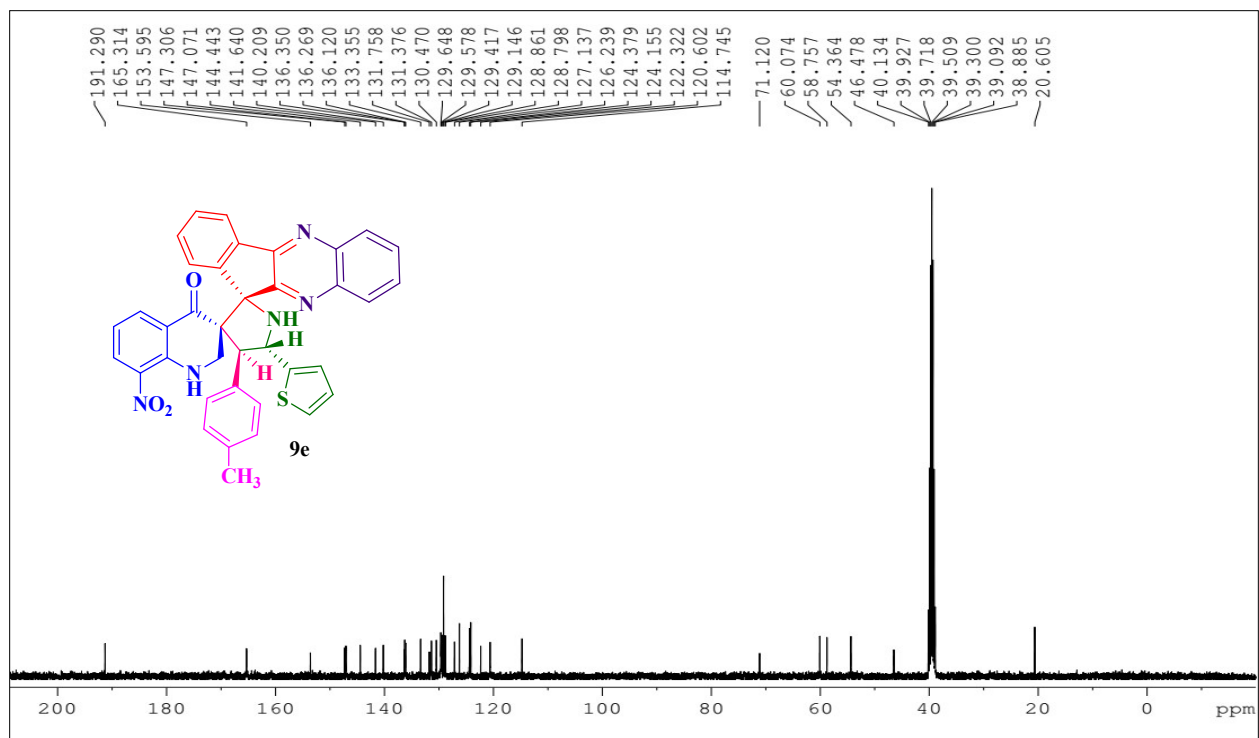


Figure 22. ¹³C NMR spectrum of compound 9e

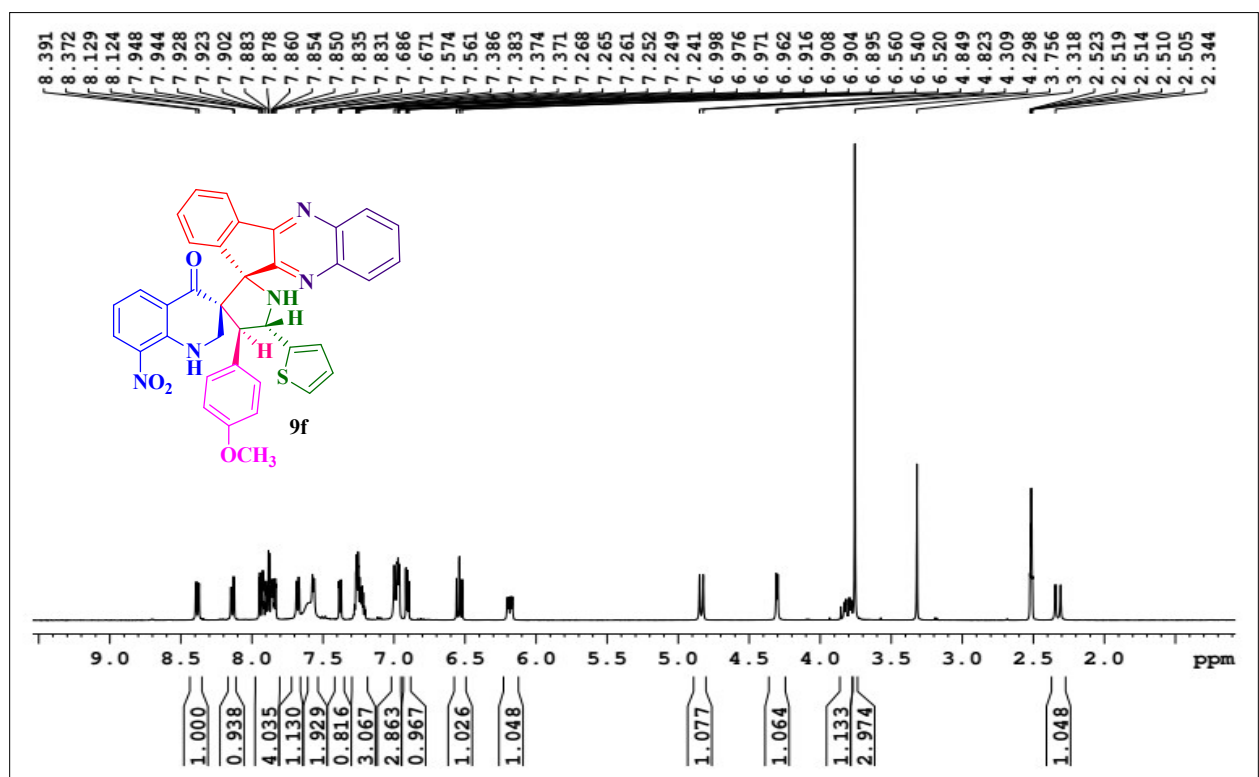


Figure 23. ¹H NMR spectrum of compound 9f

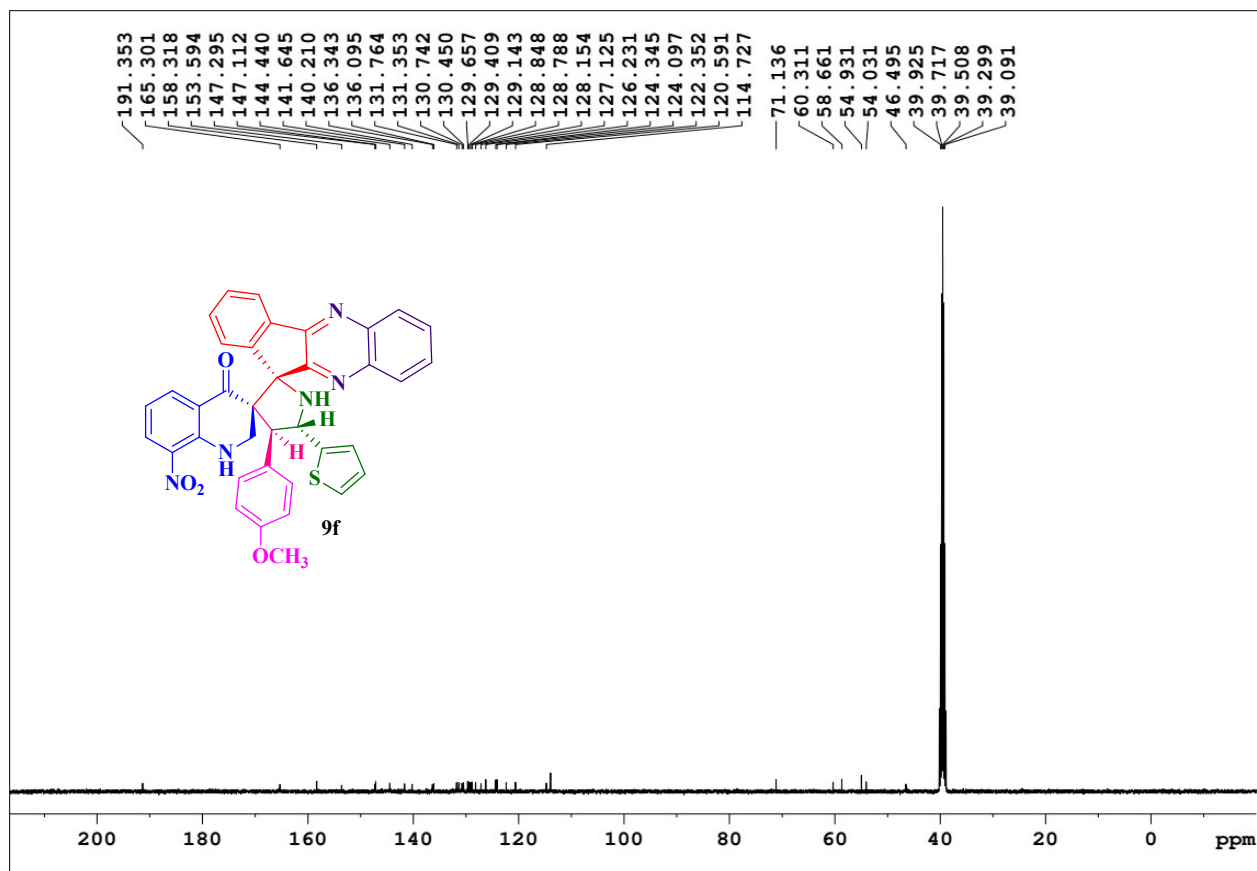


Figure 24. ¹³C NMR spectrum of compound 9f

Table S1 Crystallographic details of the compound 9f

Empirical formula	C ₃₇ H ₂₇ N ₅ O ₄ S
Formula weight	637.69
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2 ₁ /c
Unit cell dimensions	a = 13.472(3) Å; α = 90 b = 16.568(3) Å; β = 93.40(3)° c = 13.524(3) Å; γ = 90
Volume	3013.5(11) Å ³
Z	4

Density (calculated)	1.406 Mg/m ³
Absorption coefficient	0.160 mm ⁻¹
F(000)	1328
Crystal size	0.22 × 0.18 × 0.14 mm ³
Theta range for data collection	2.410 to 23.933°.
Index ranges	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -14 ≤ l ≤ 14
Reflections collected	23334
Independent reflections	3888 [R(int) = 0.0241]
Completeness to theta = 25.242°	71.40%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3888 / 3 / 443
Goodness-of-fit on F ²	1.045
Final R indices [I > 2σ(I)]	R1 = 0.0349, wR2 = 0.0888
R indices (all data)	R1 = 0.0396, wR2 = 0.0948
Largest diff. peak and hole	0.184 and -0.291 e.Å ⁻³
