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

Supporting information

Synthesis of spirooxindoles fused with pyrazolo-tetrahydropyridinone and coumarin-dihydropyridine-pyrazole tetracycles by reaction medium dependent isatin-based multicomponent reactions

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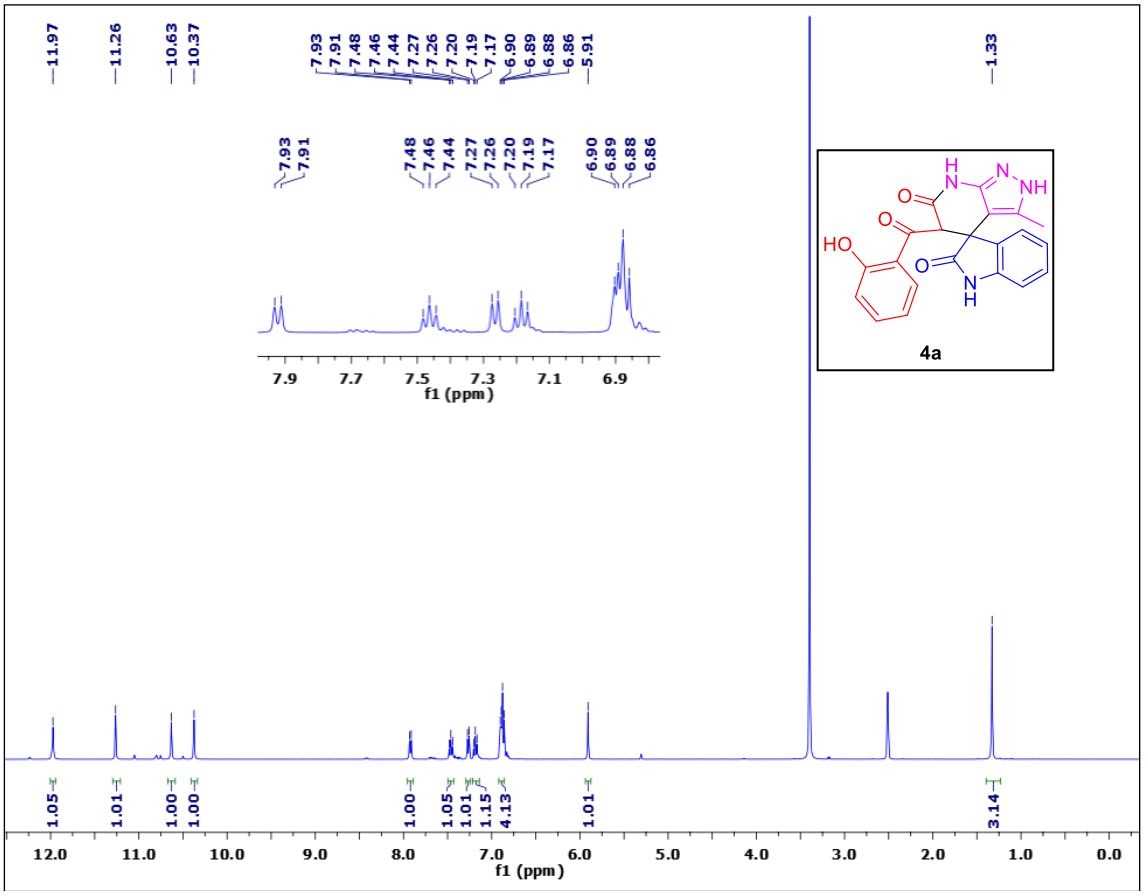
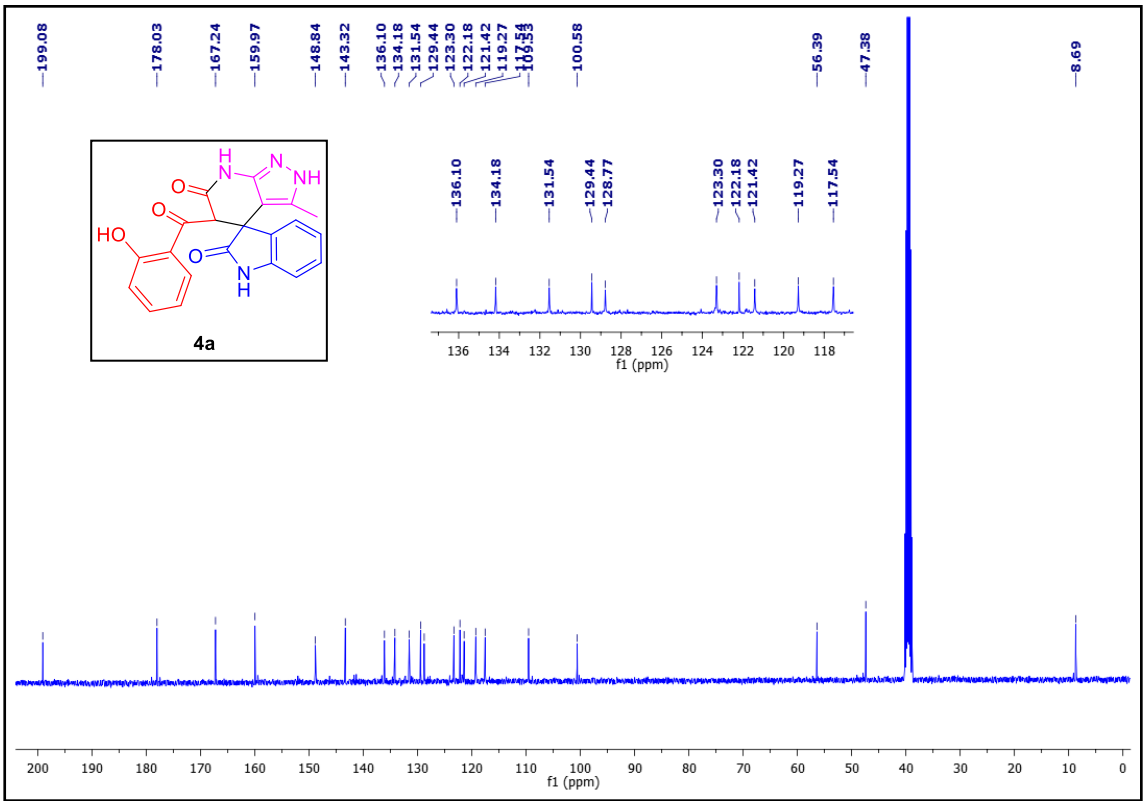
Table of contents:

Copies of ^{1}H and ^{13}C spectrum of compound 4a





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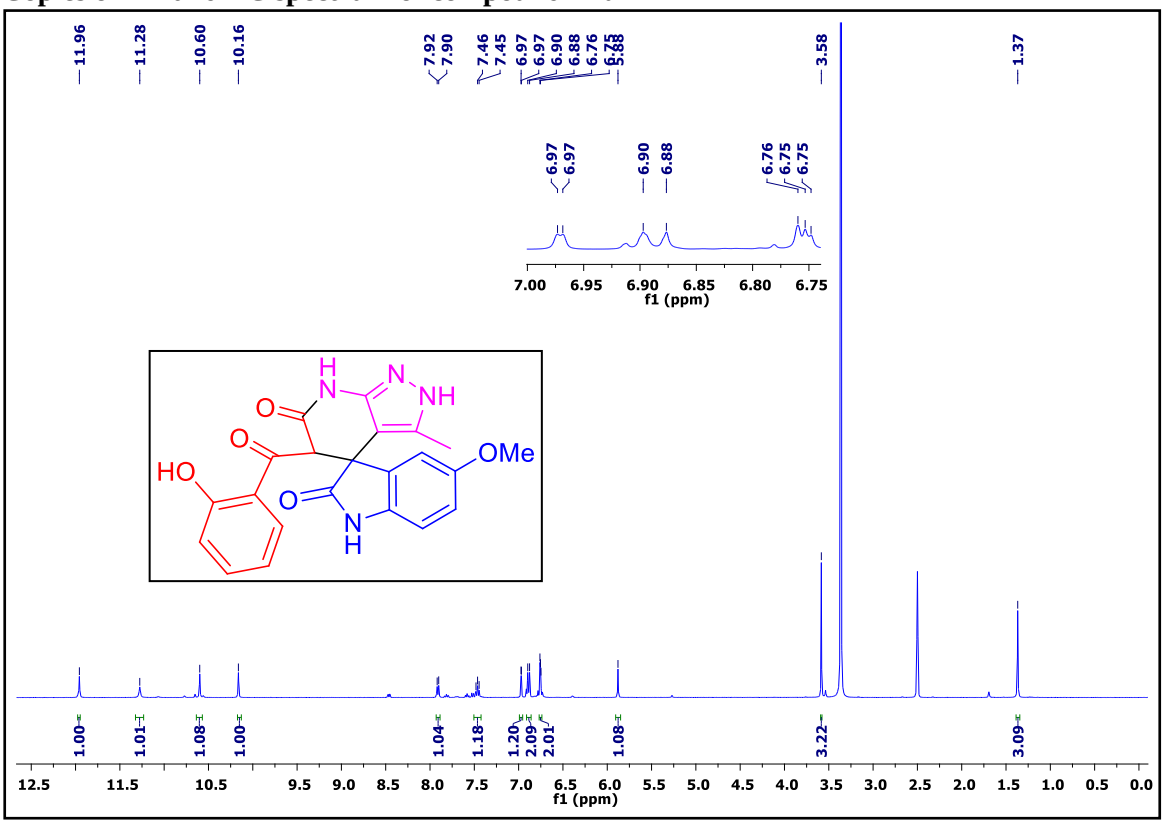

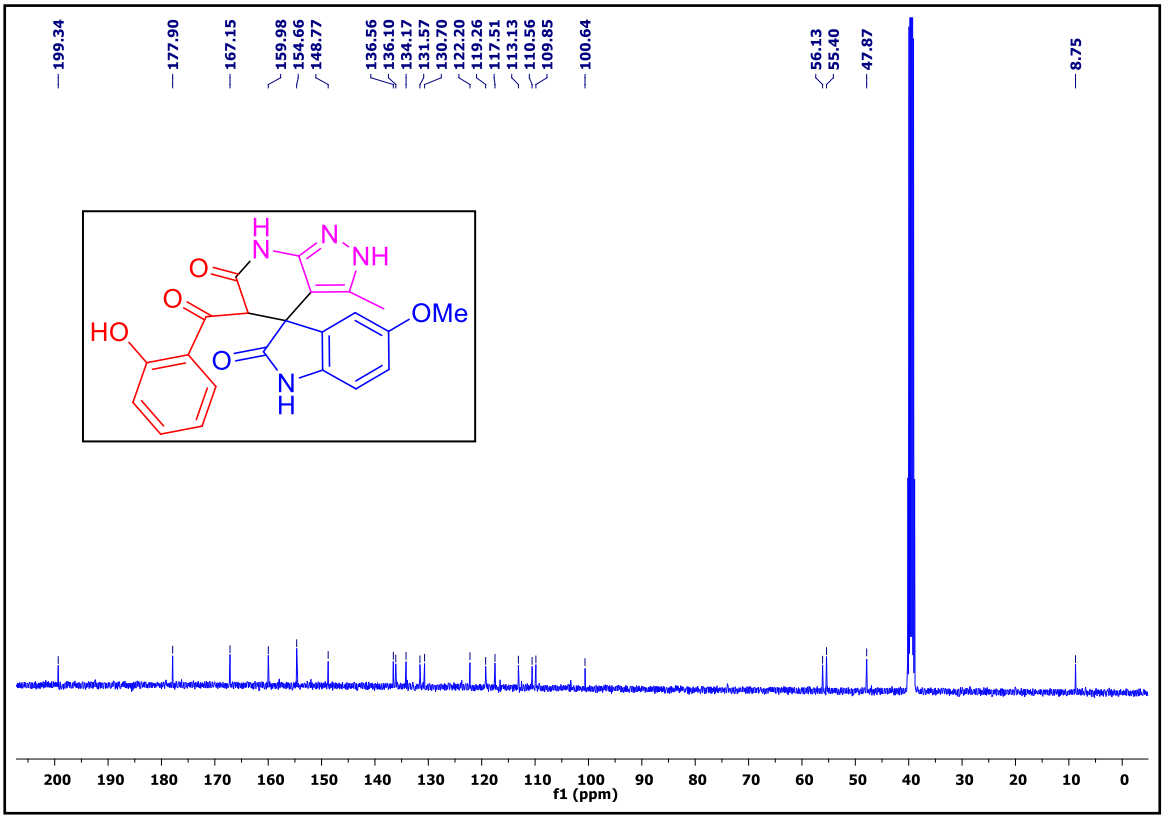

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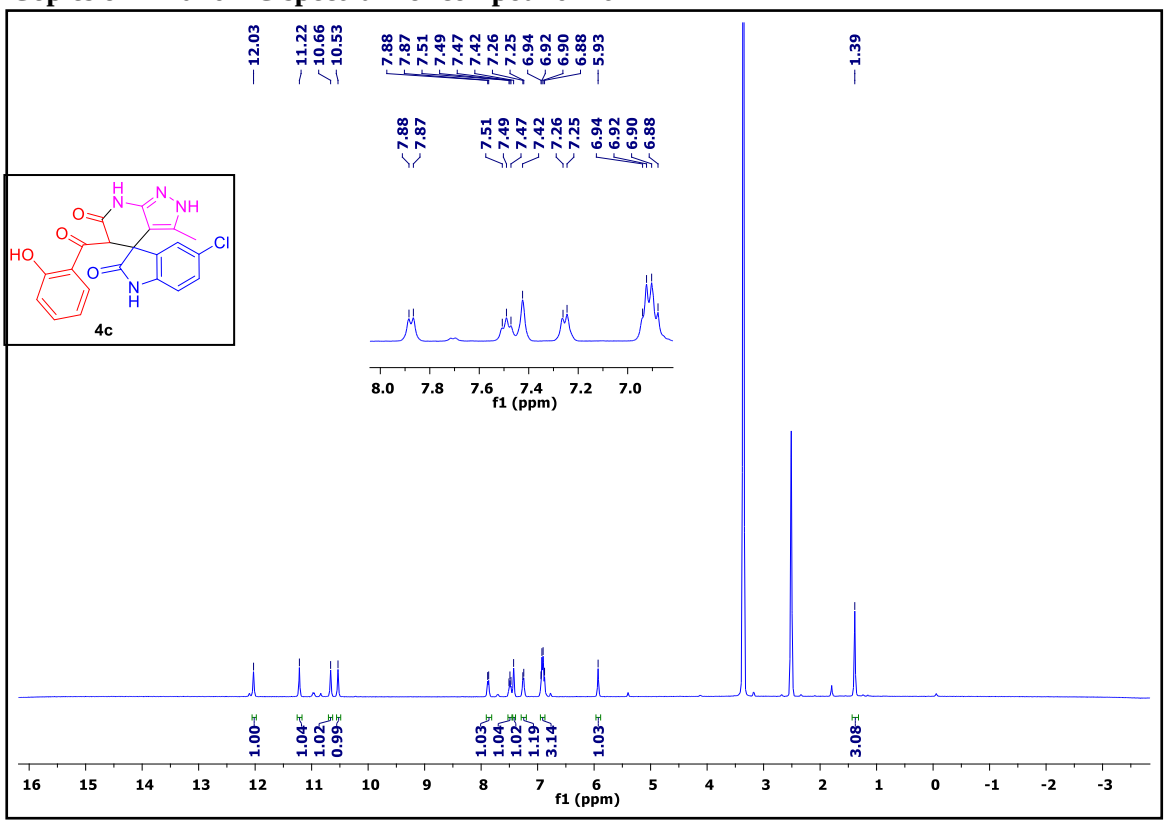

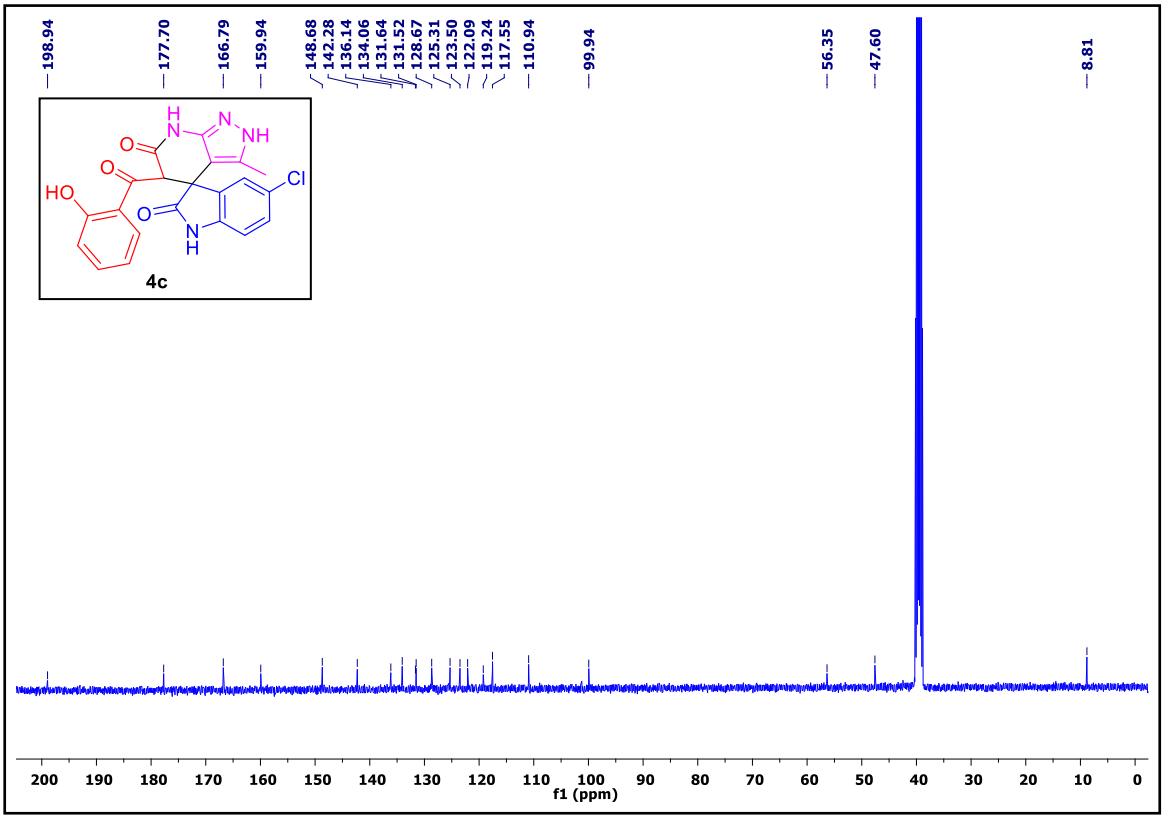

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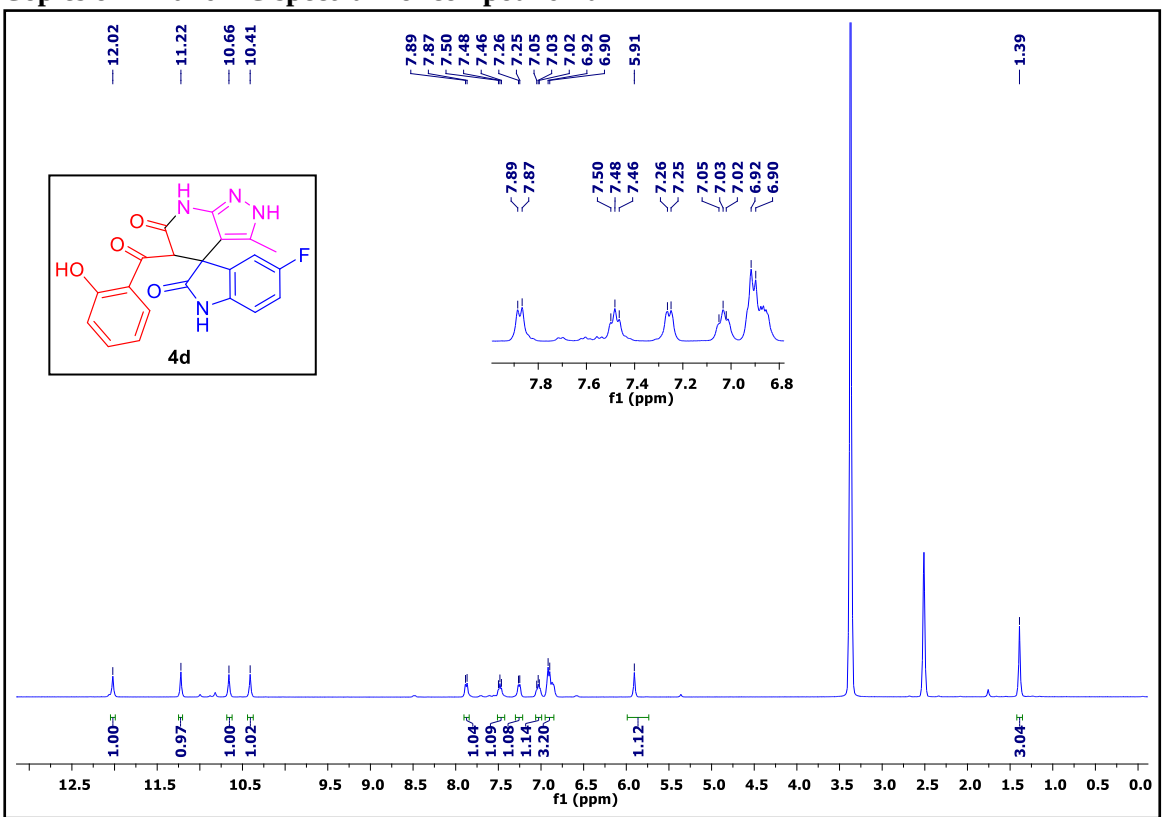

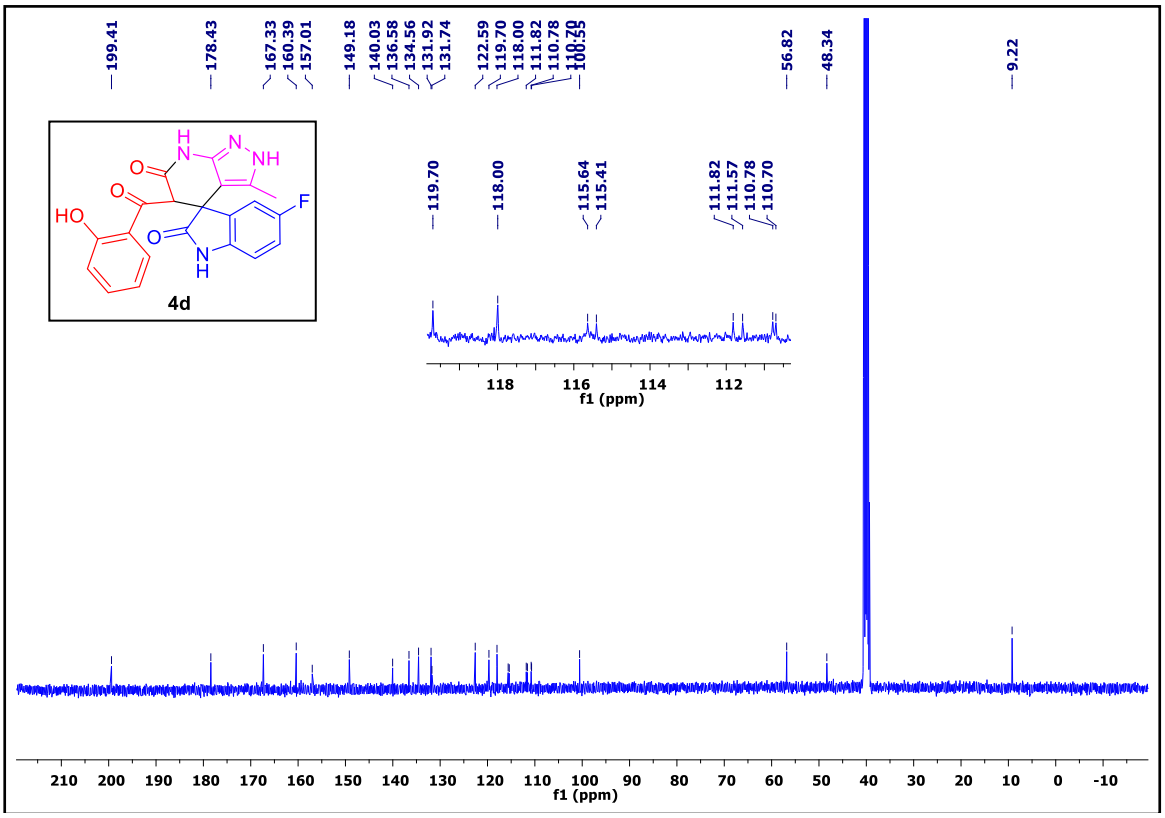

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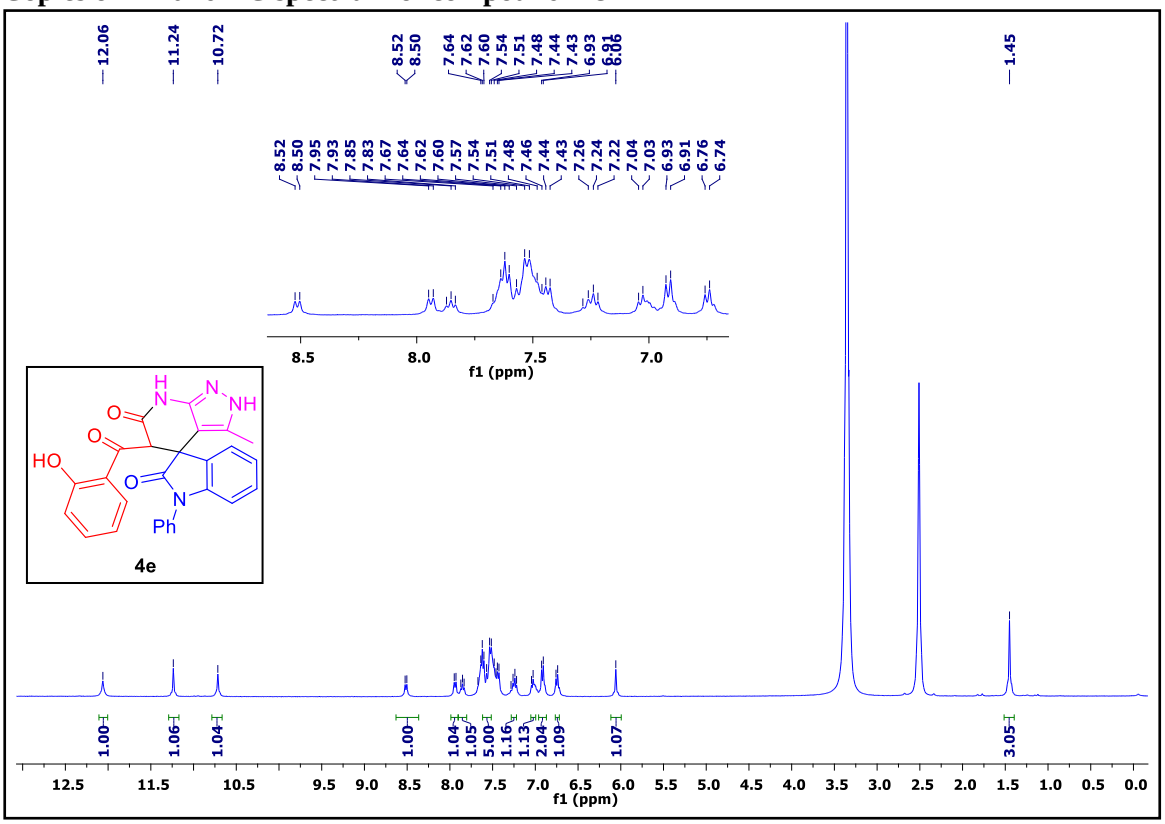

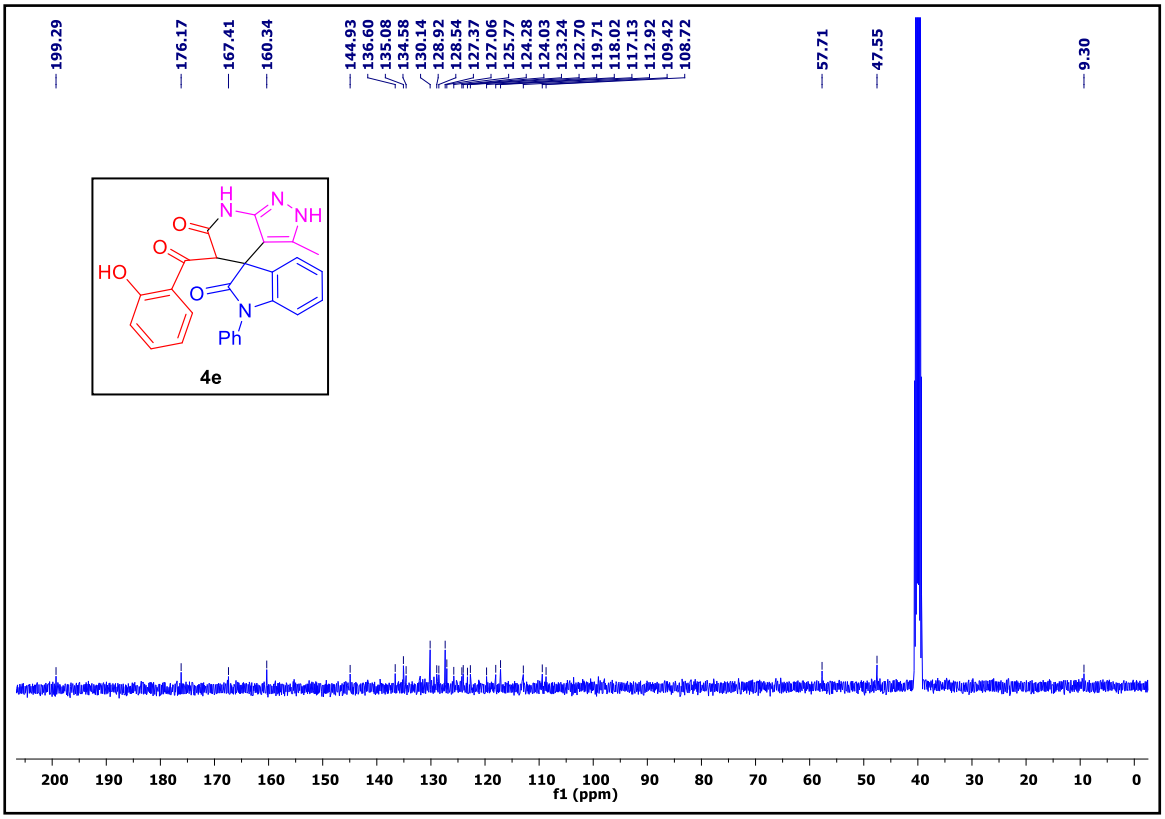

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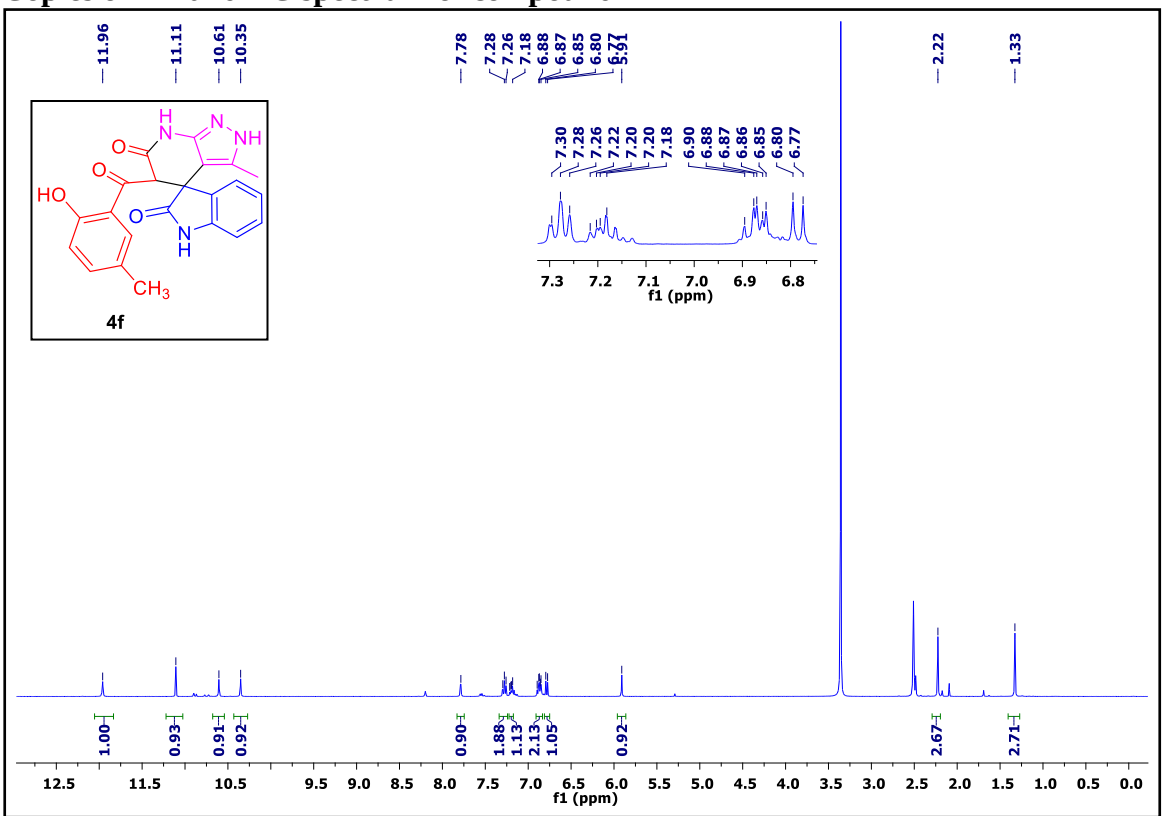

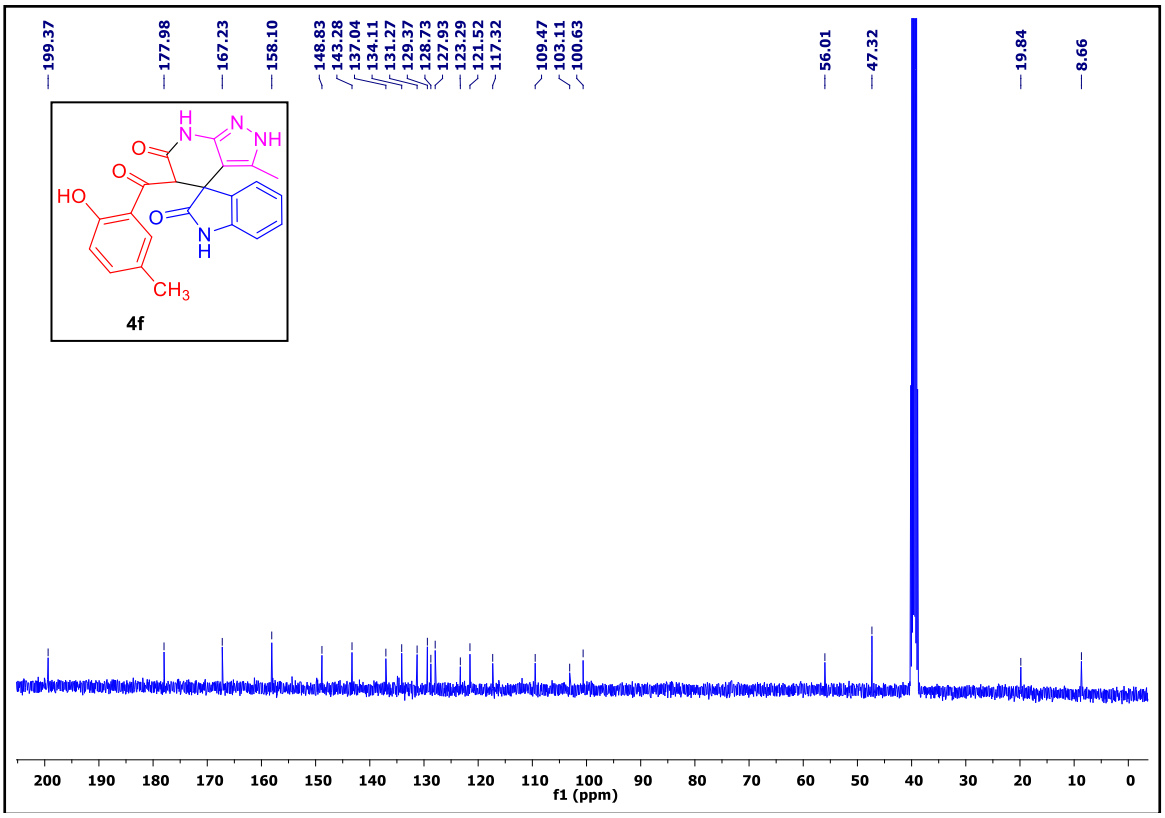

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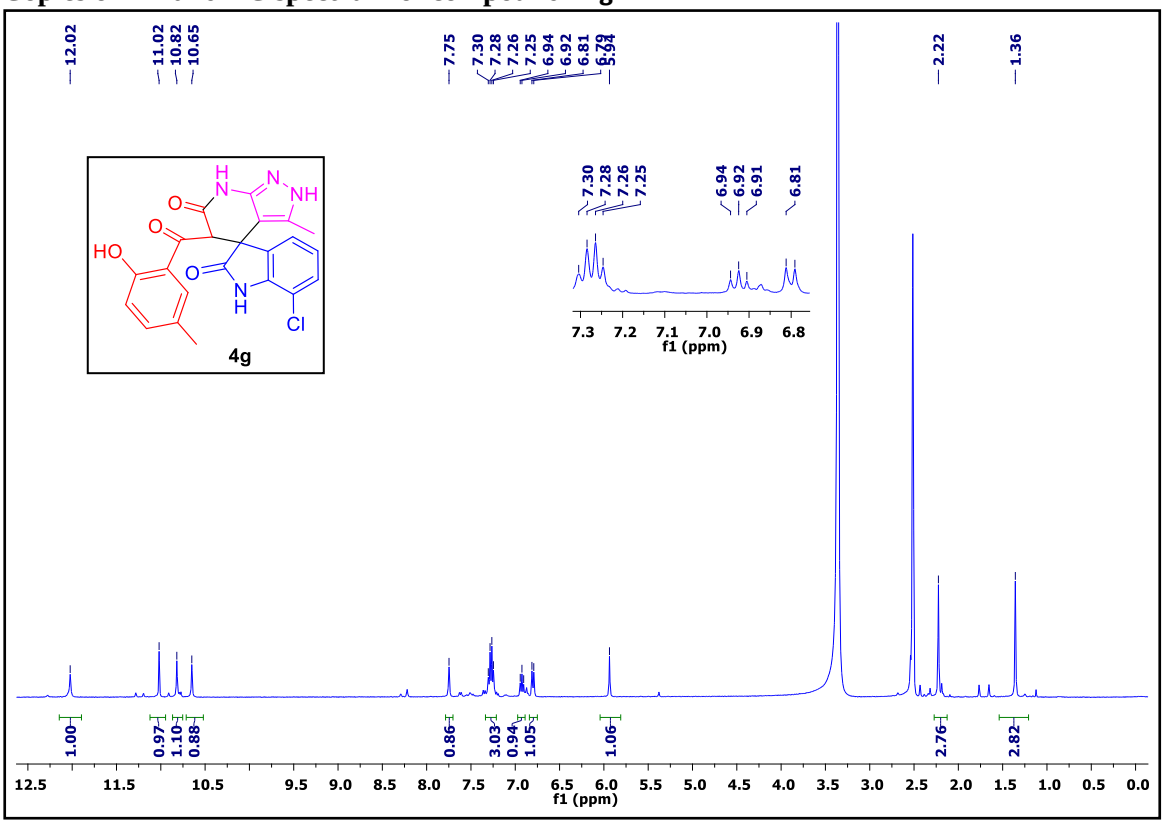

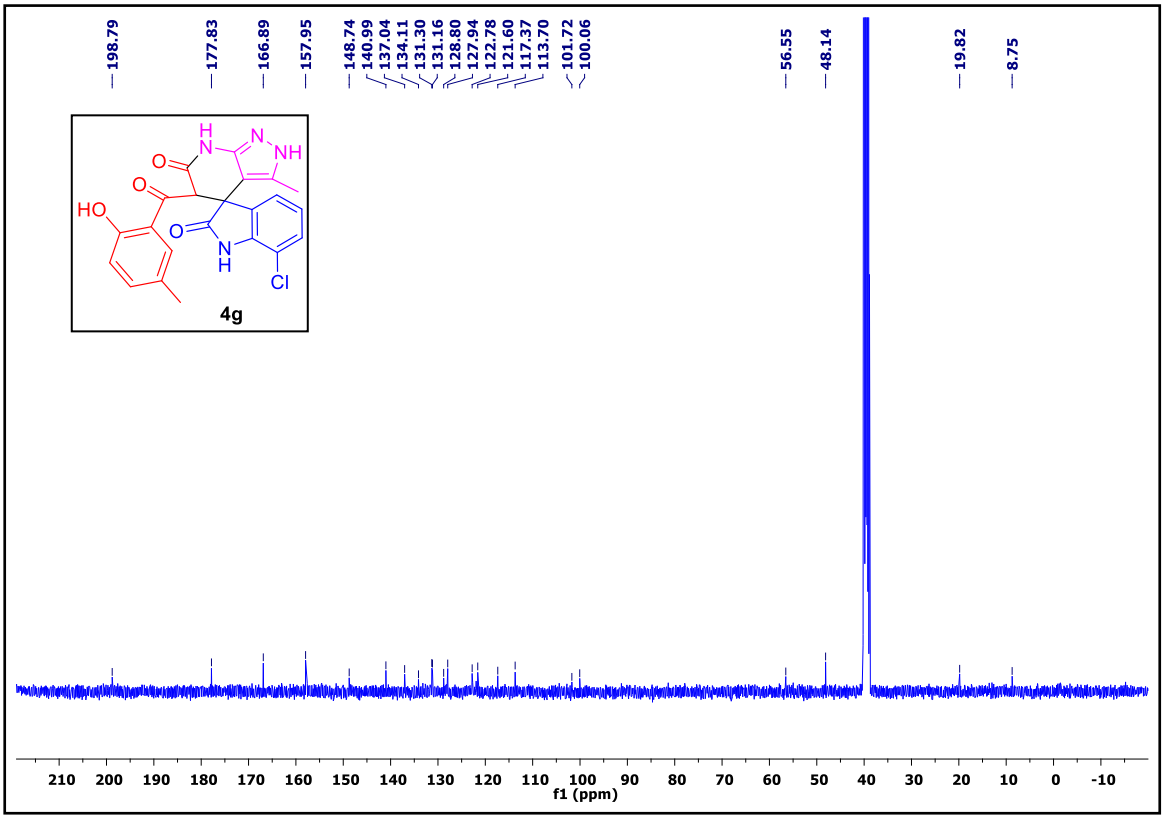

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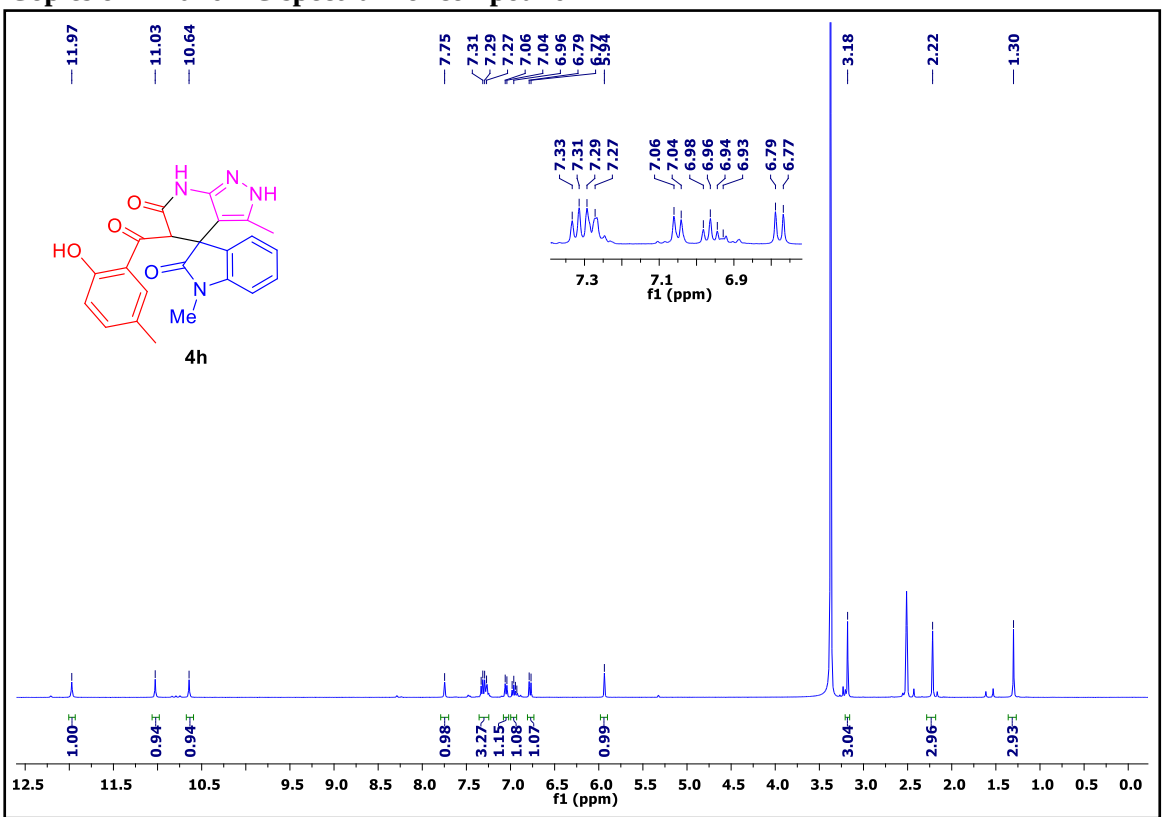

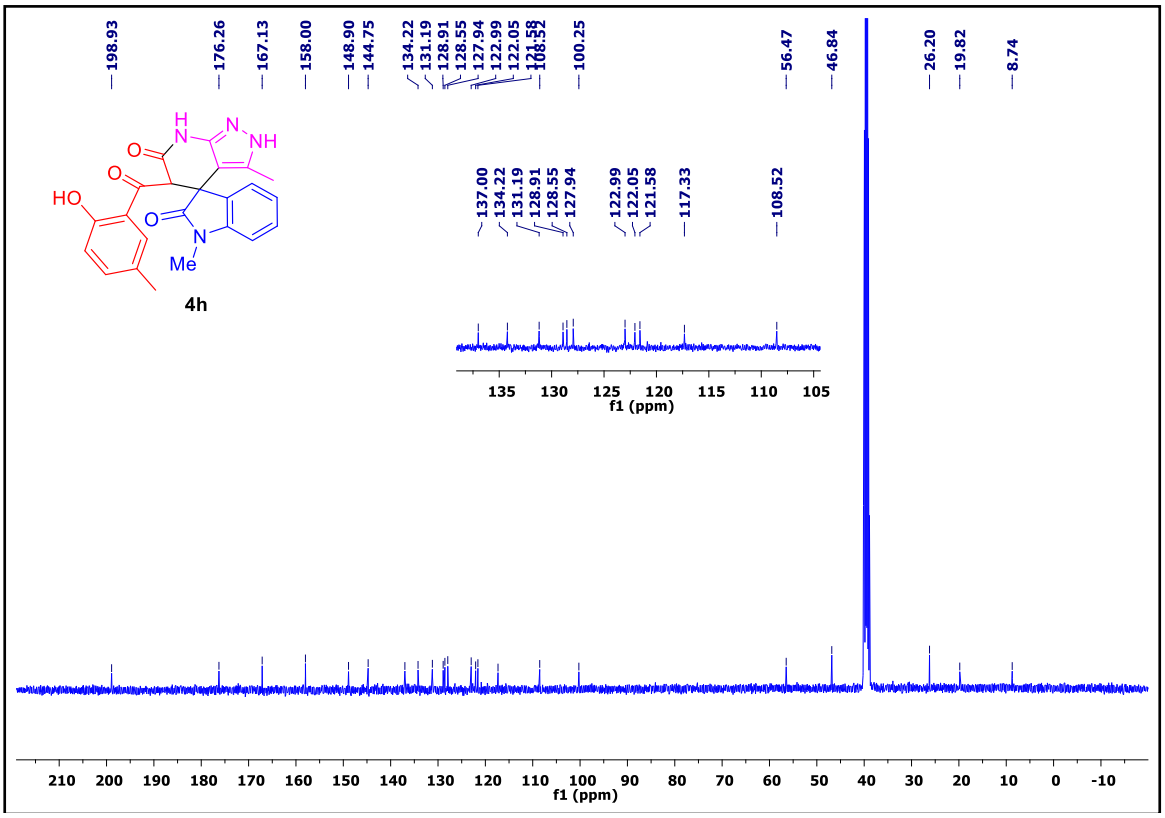

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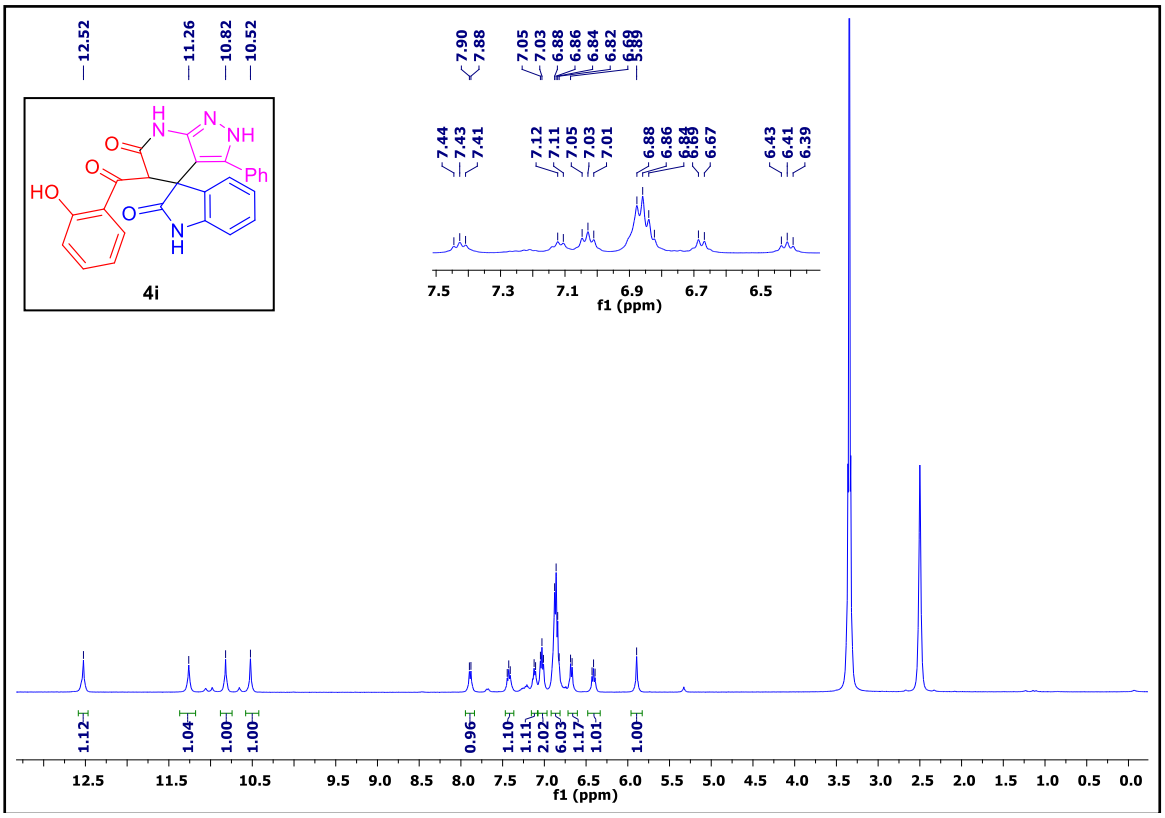

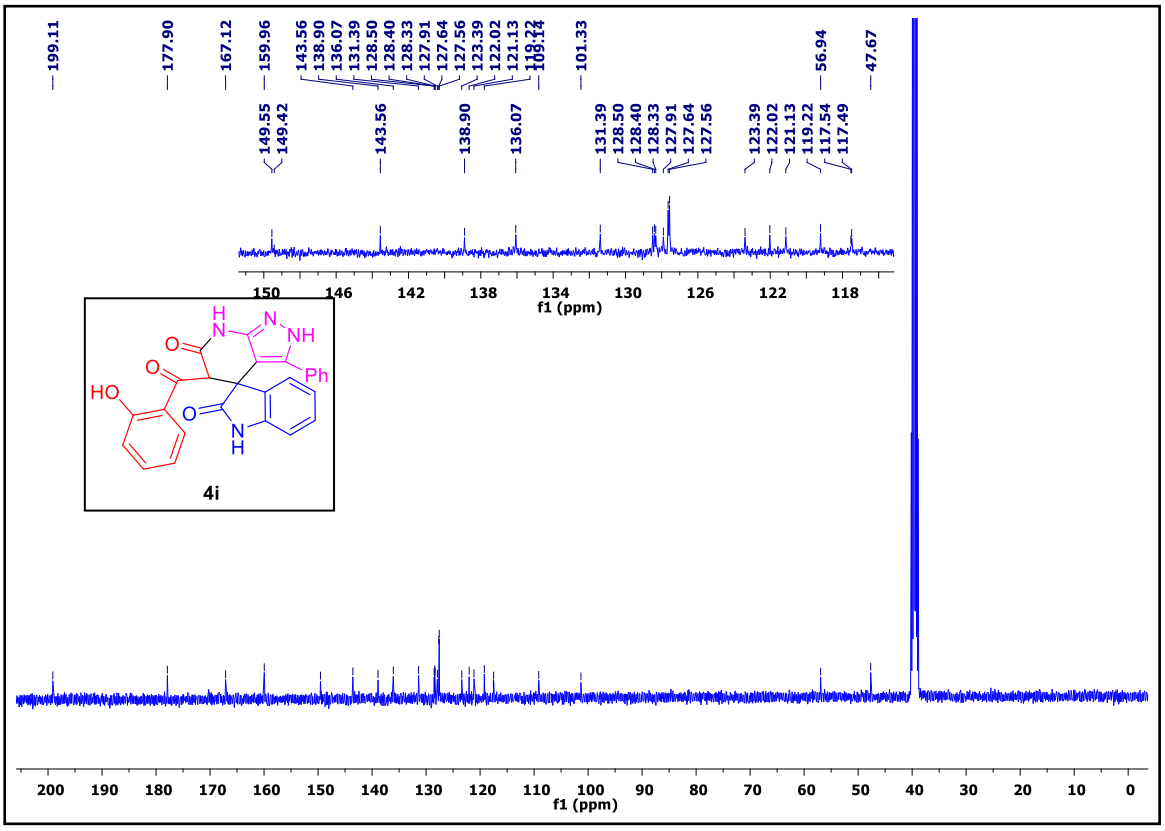

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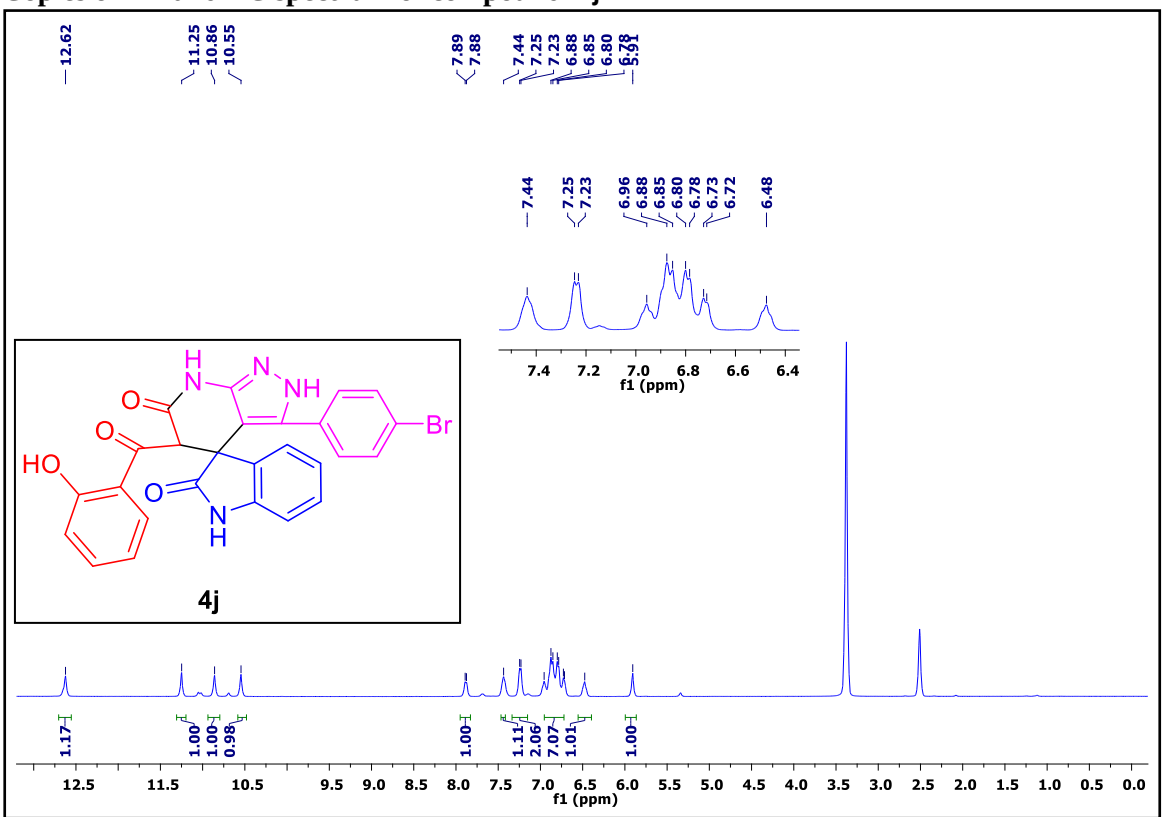

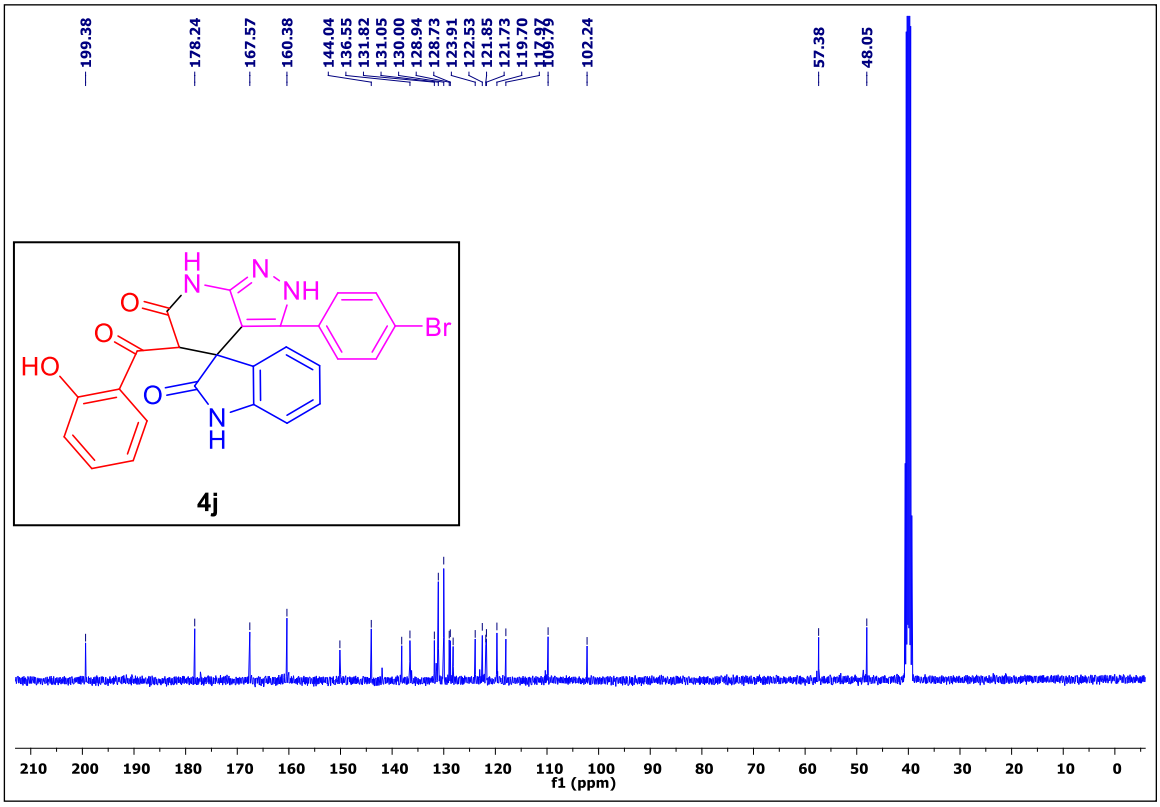

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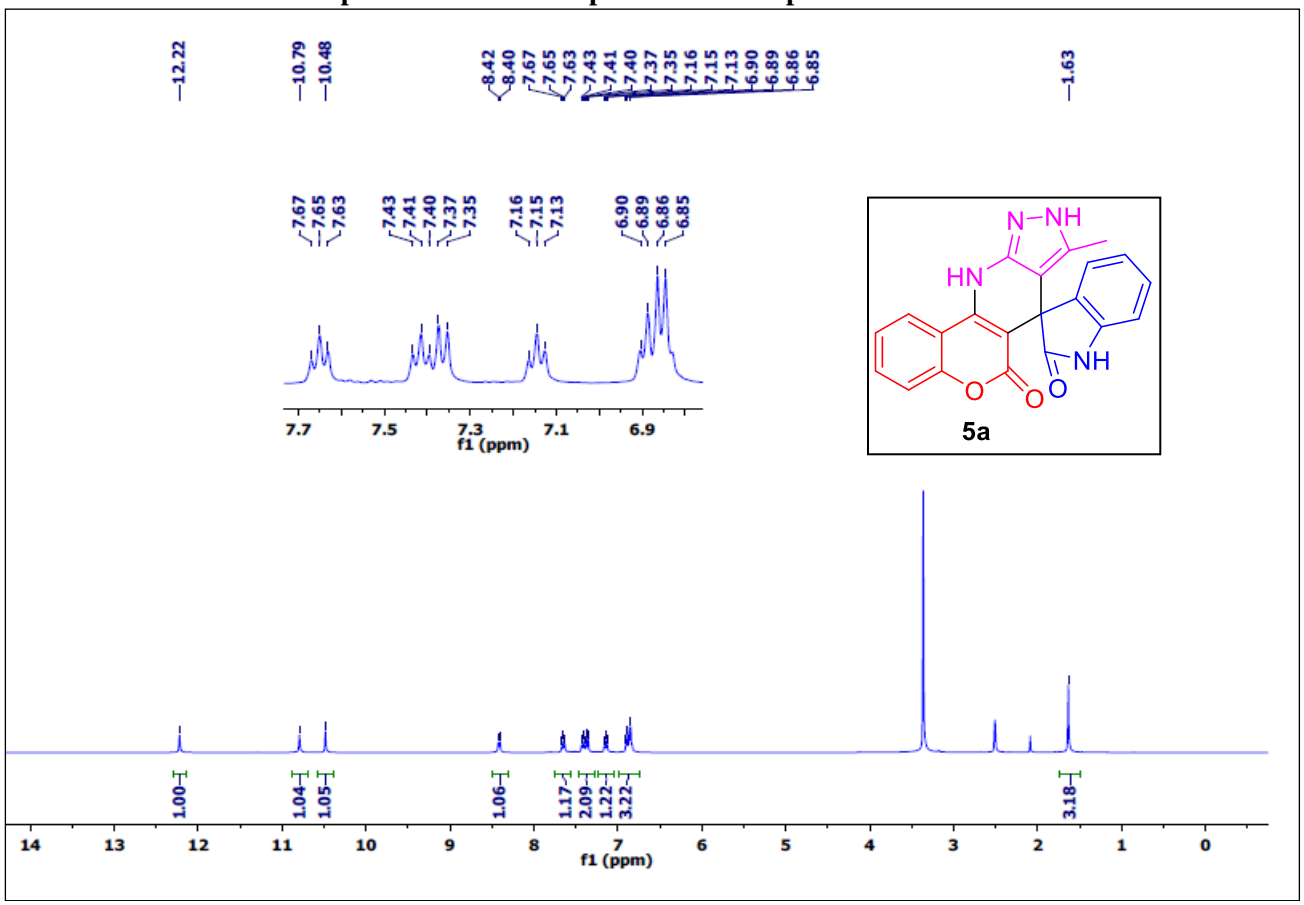

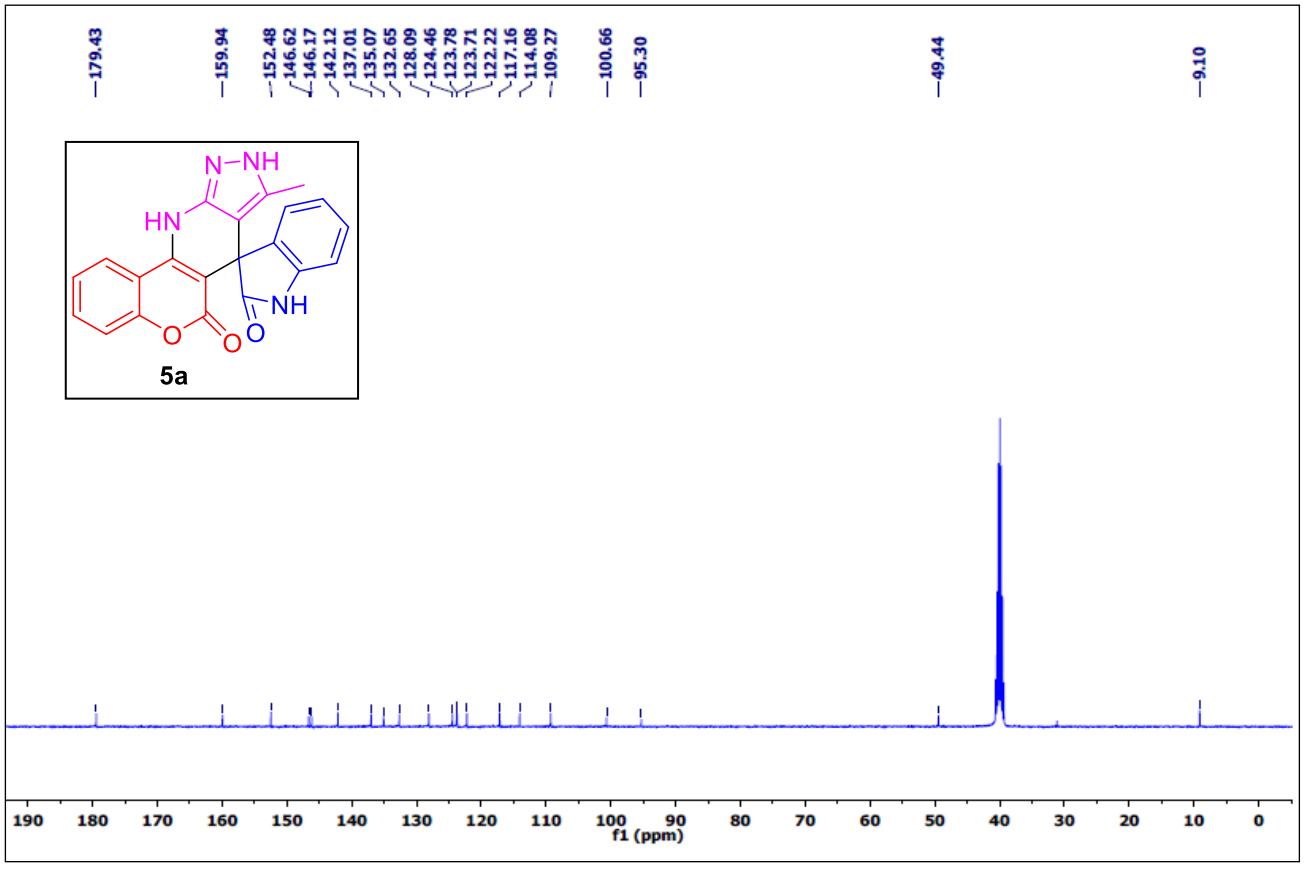

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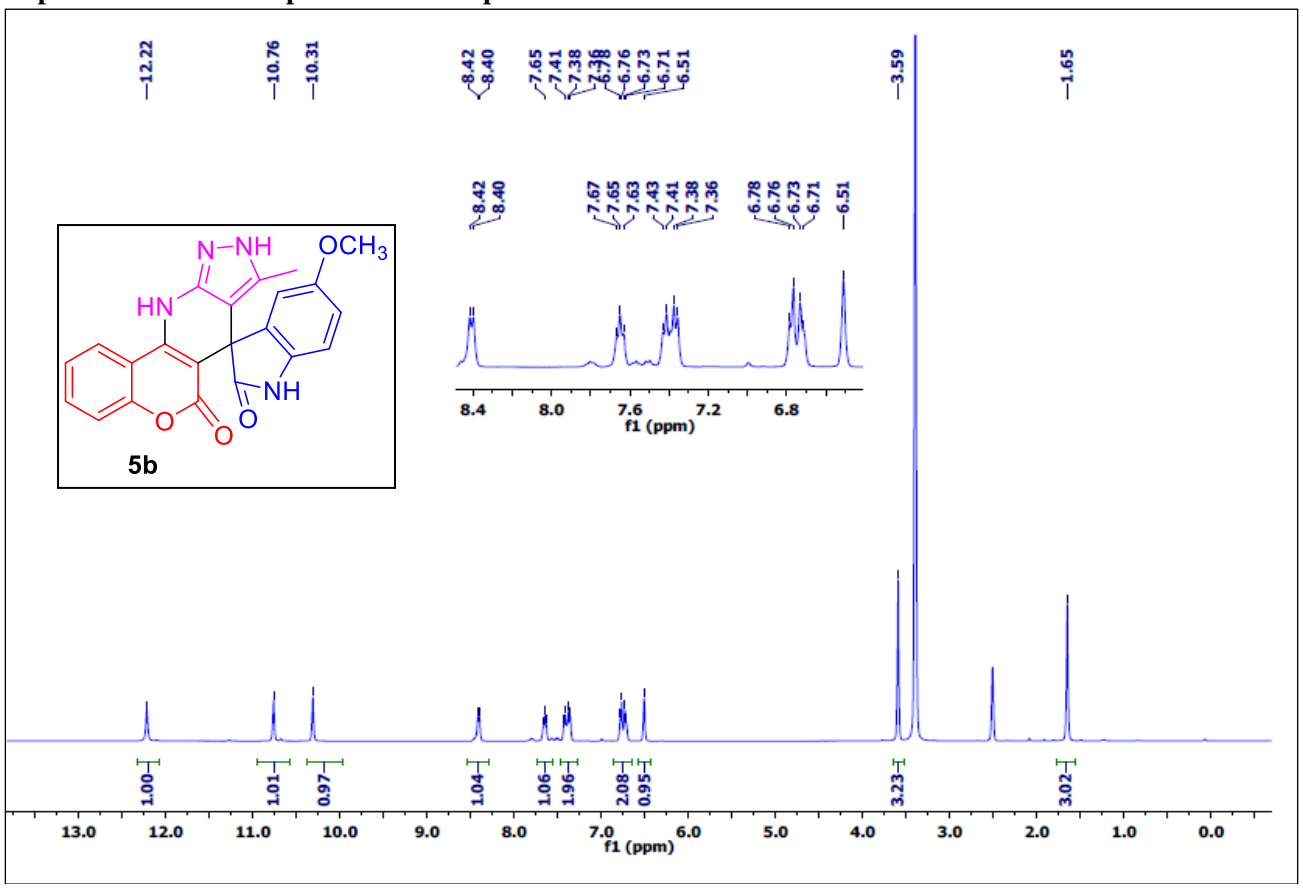

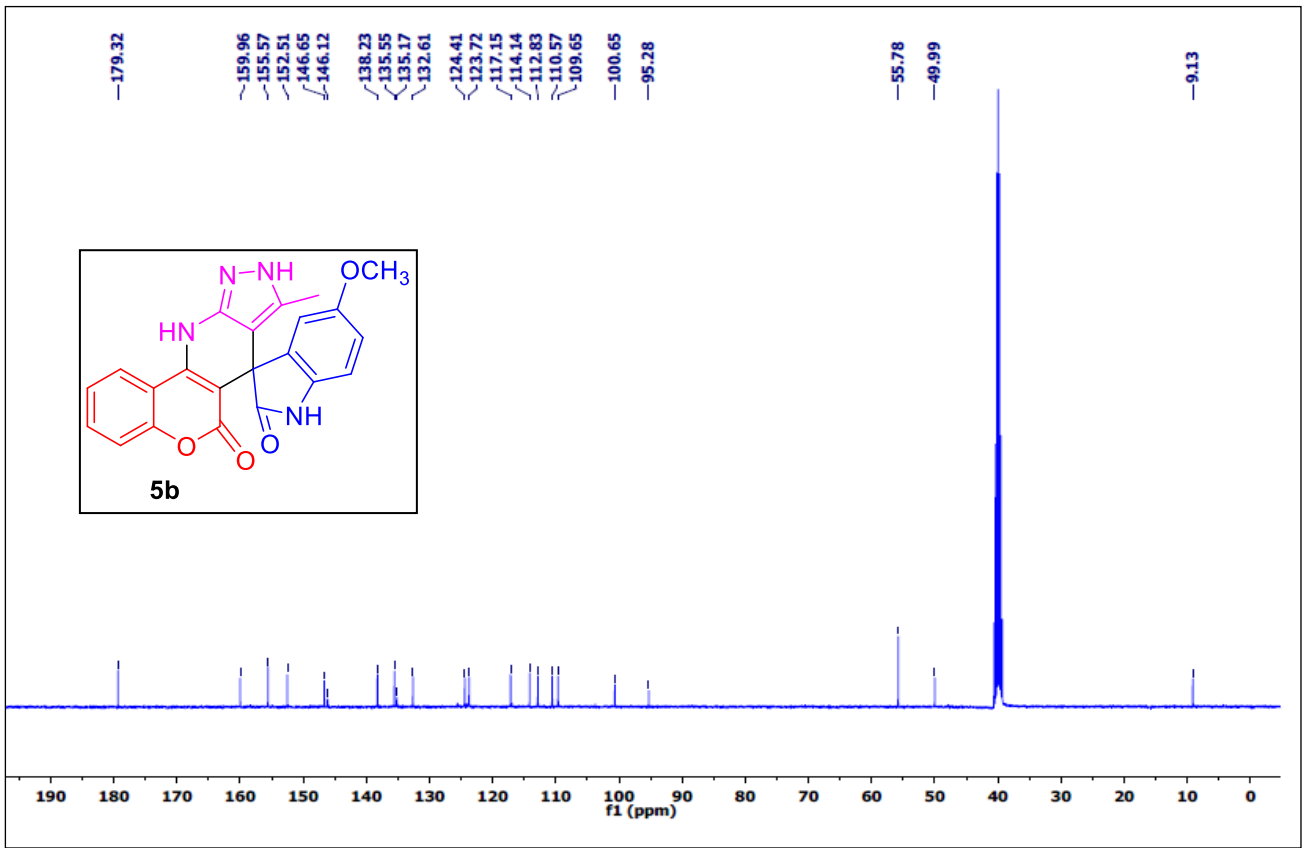

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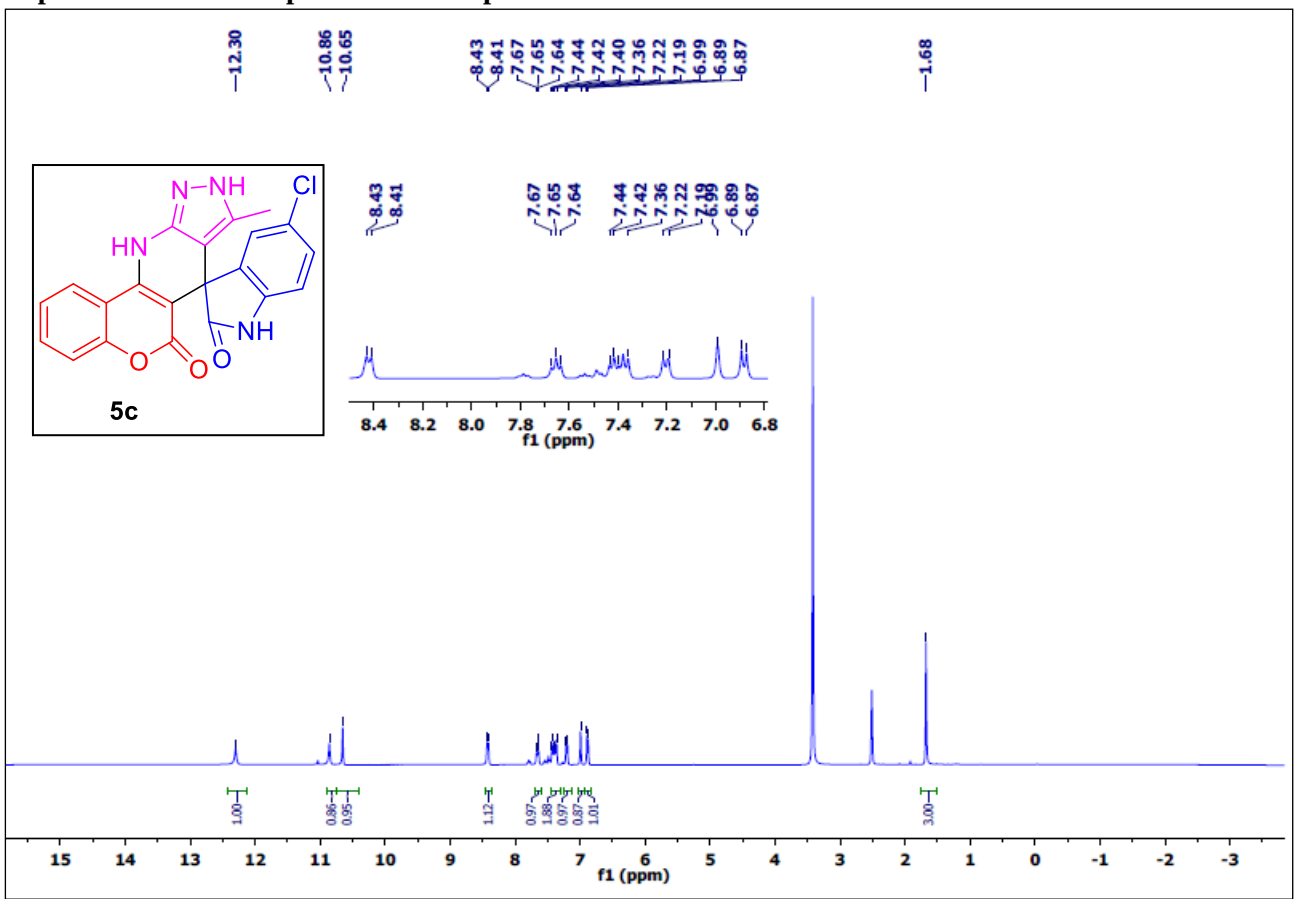

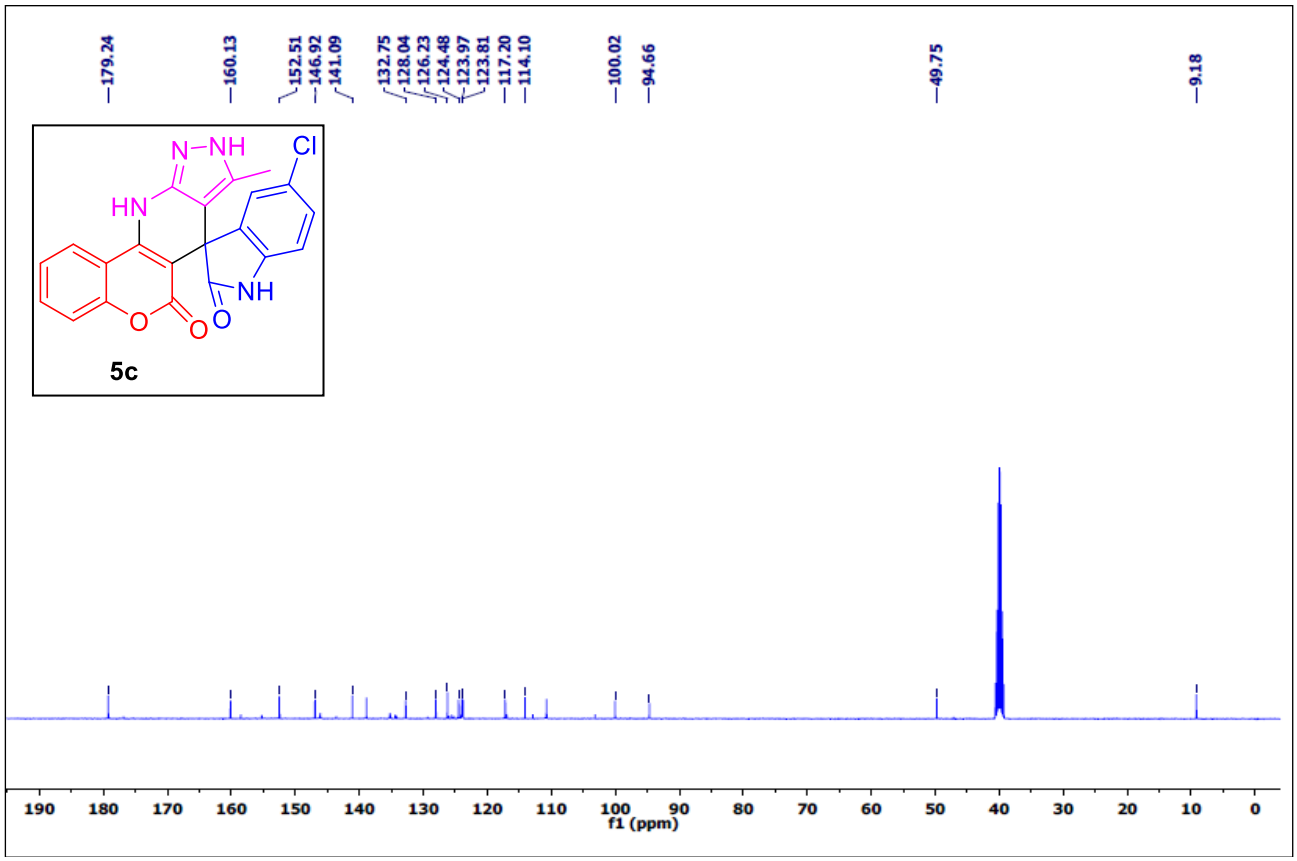

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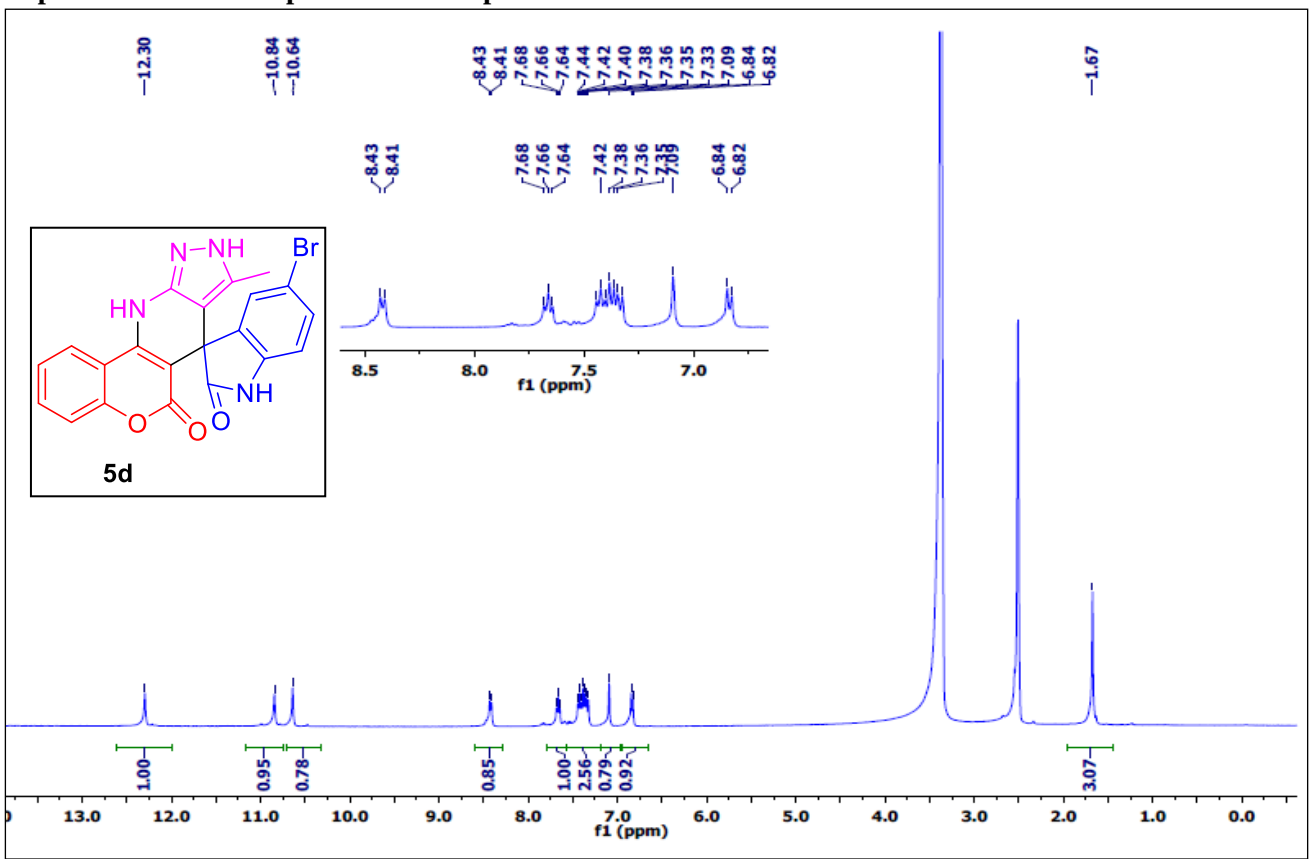

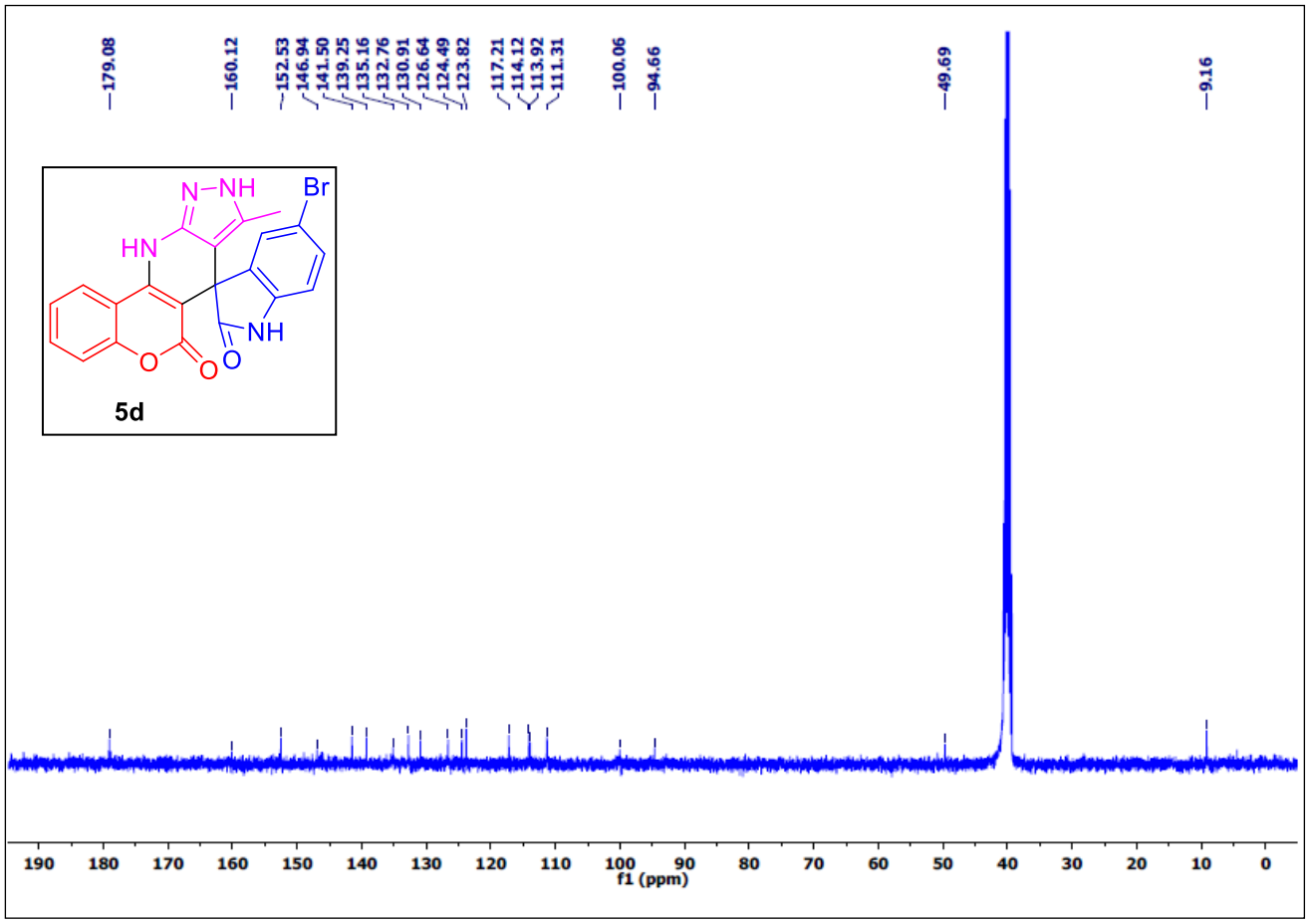

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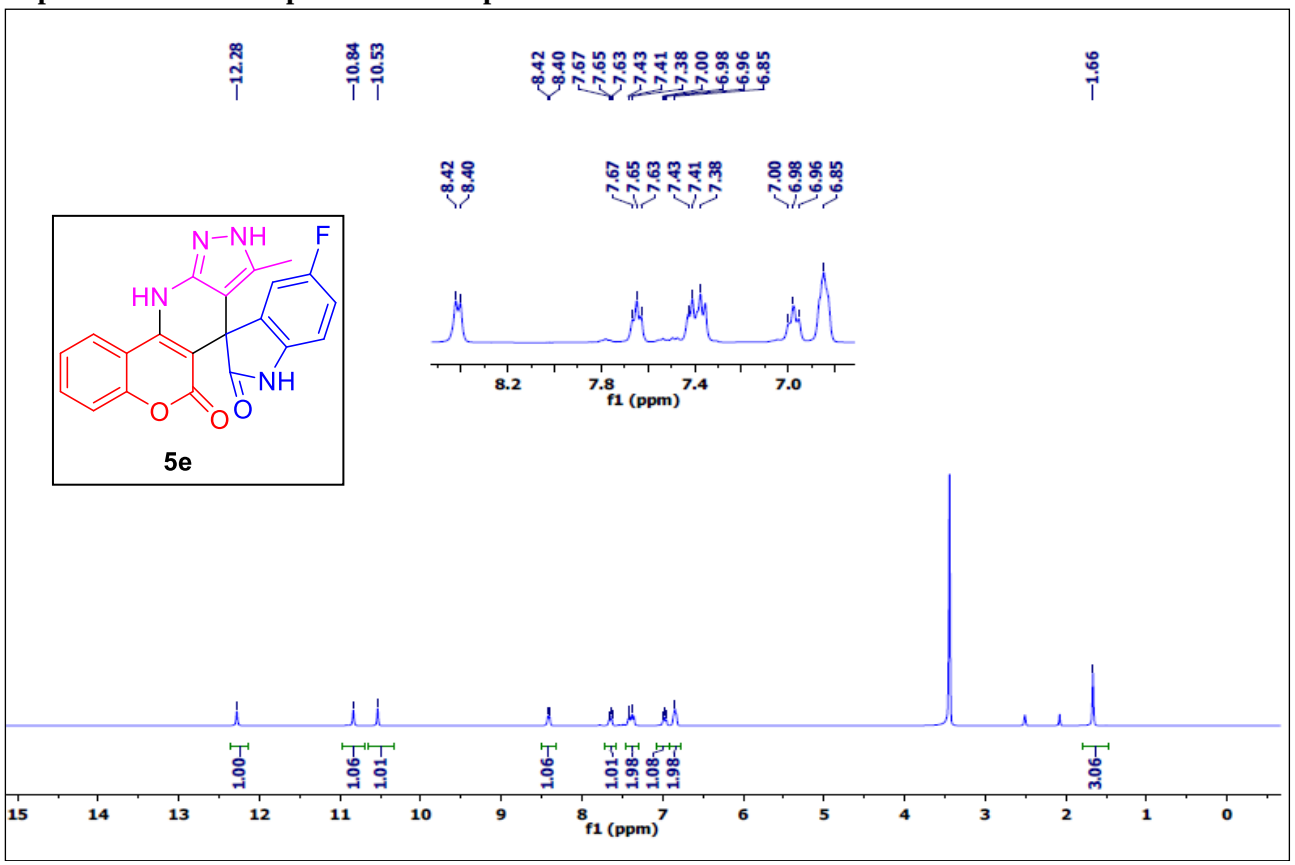

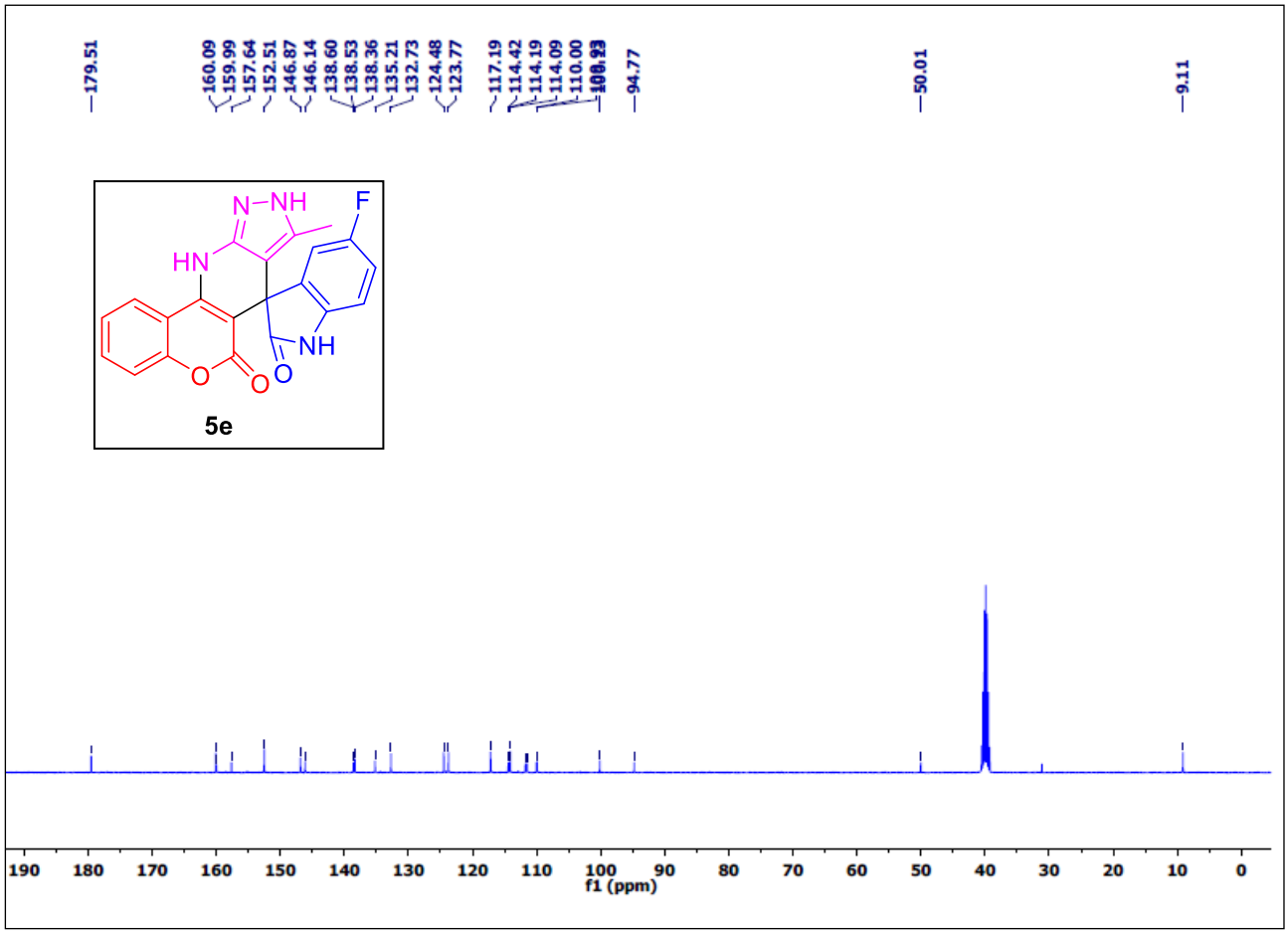

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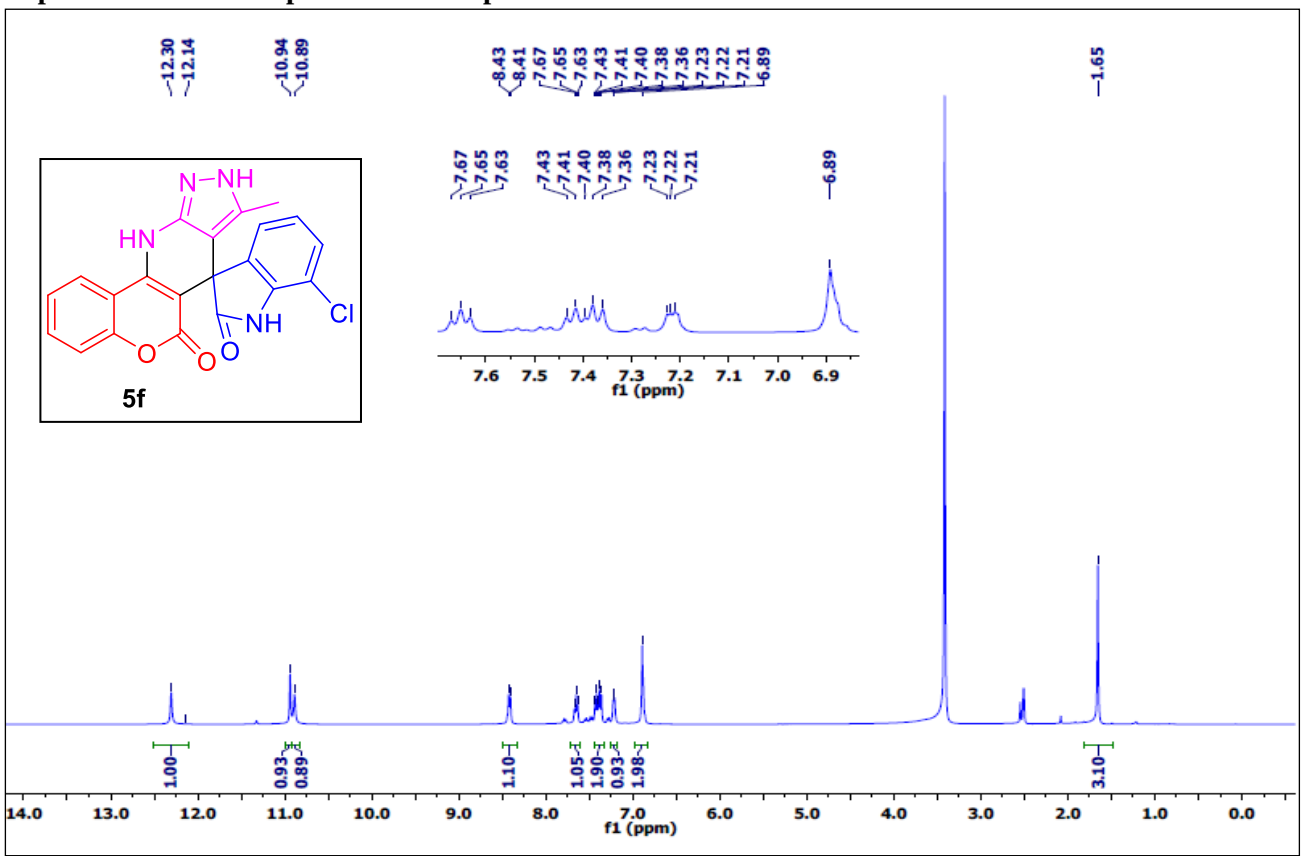

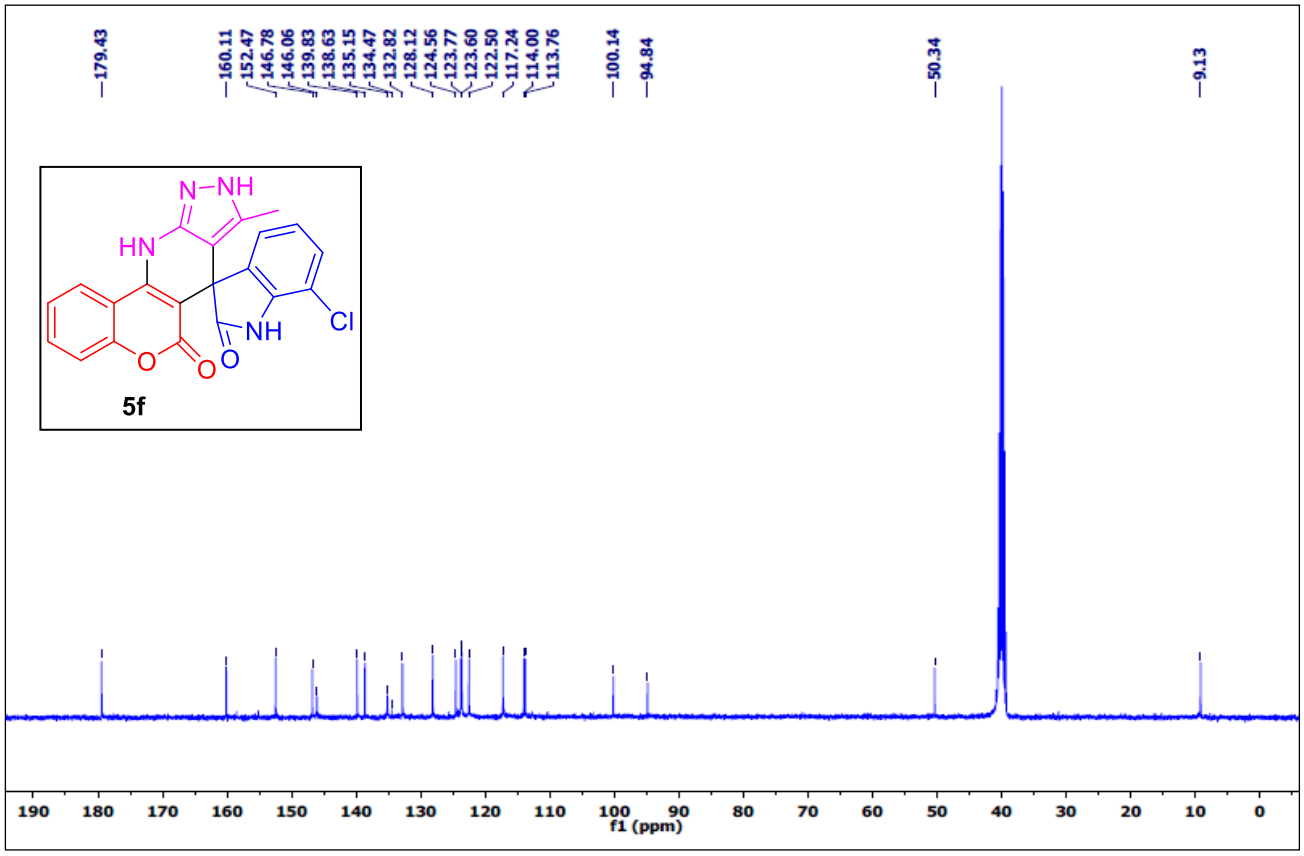

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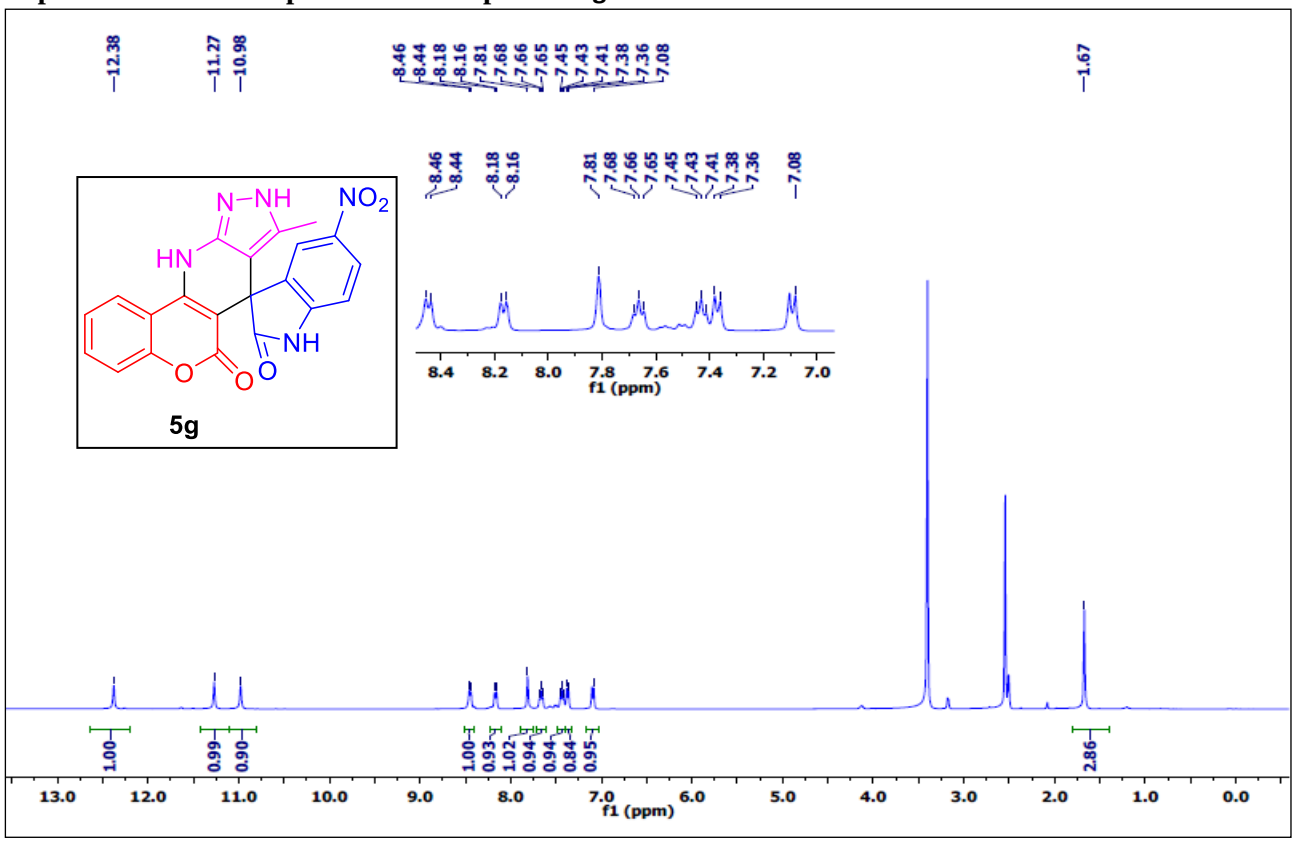

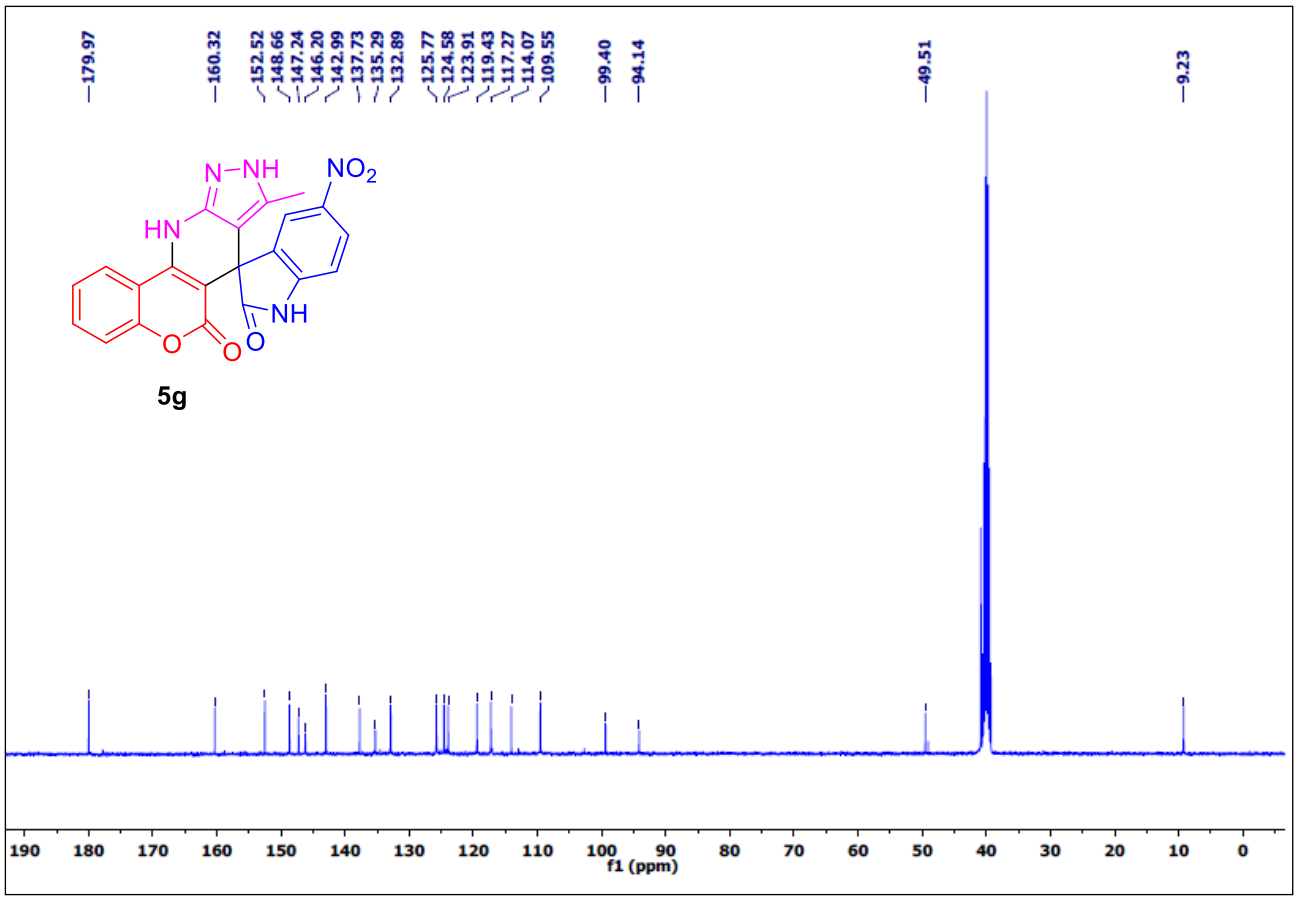

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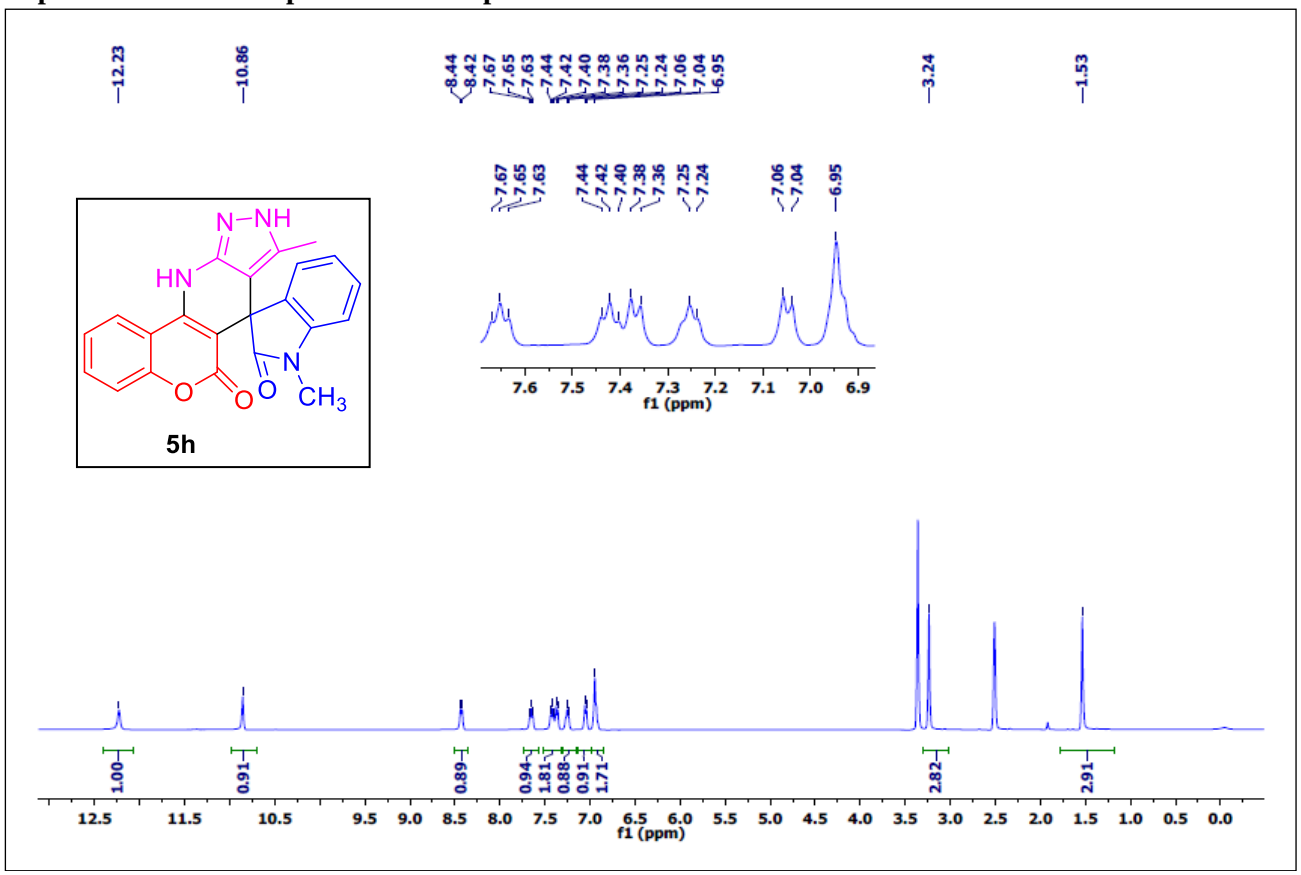

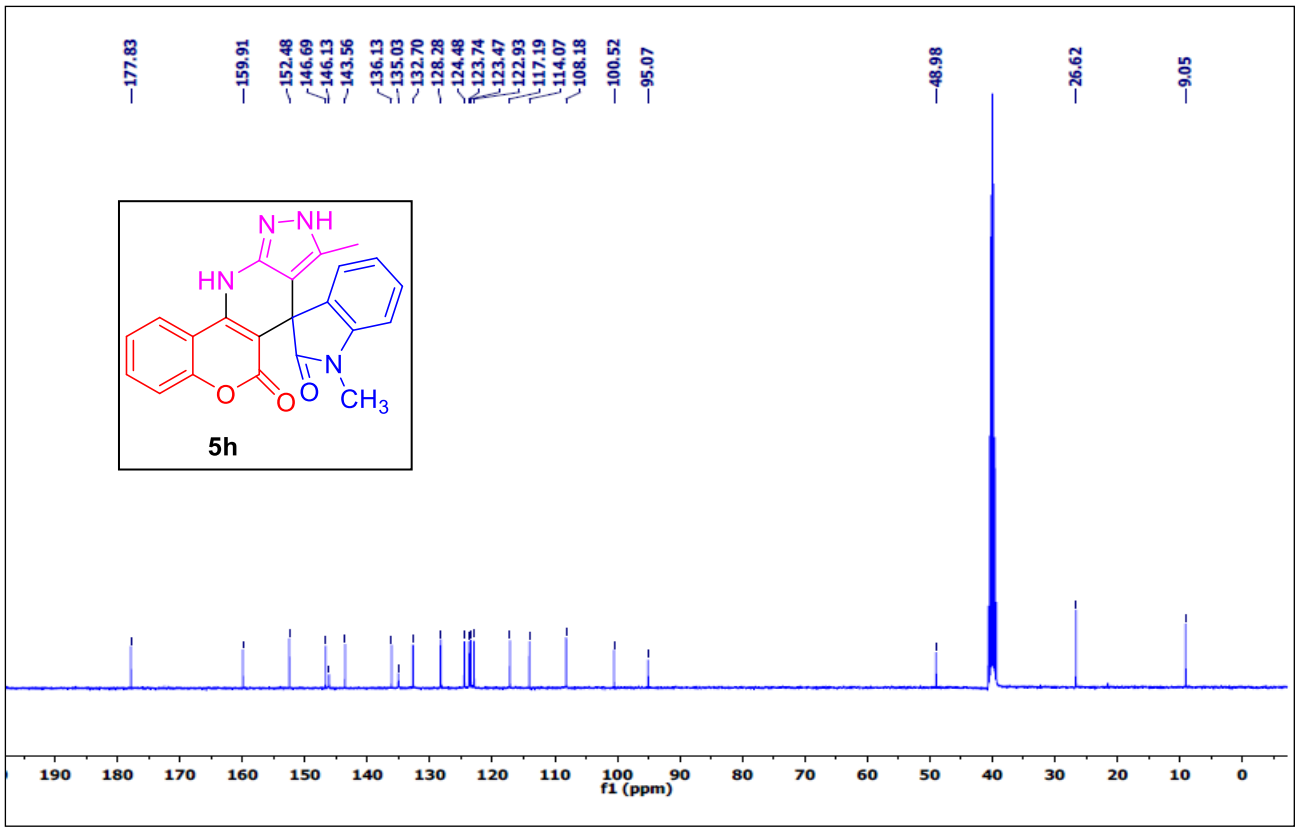

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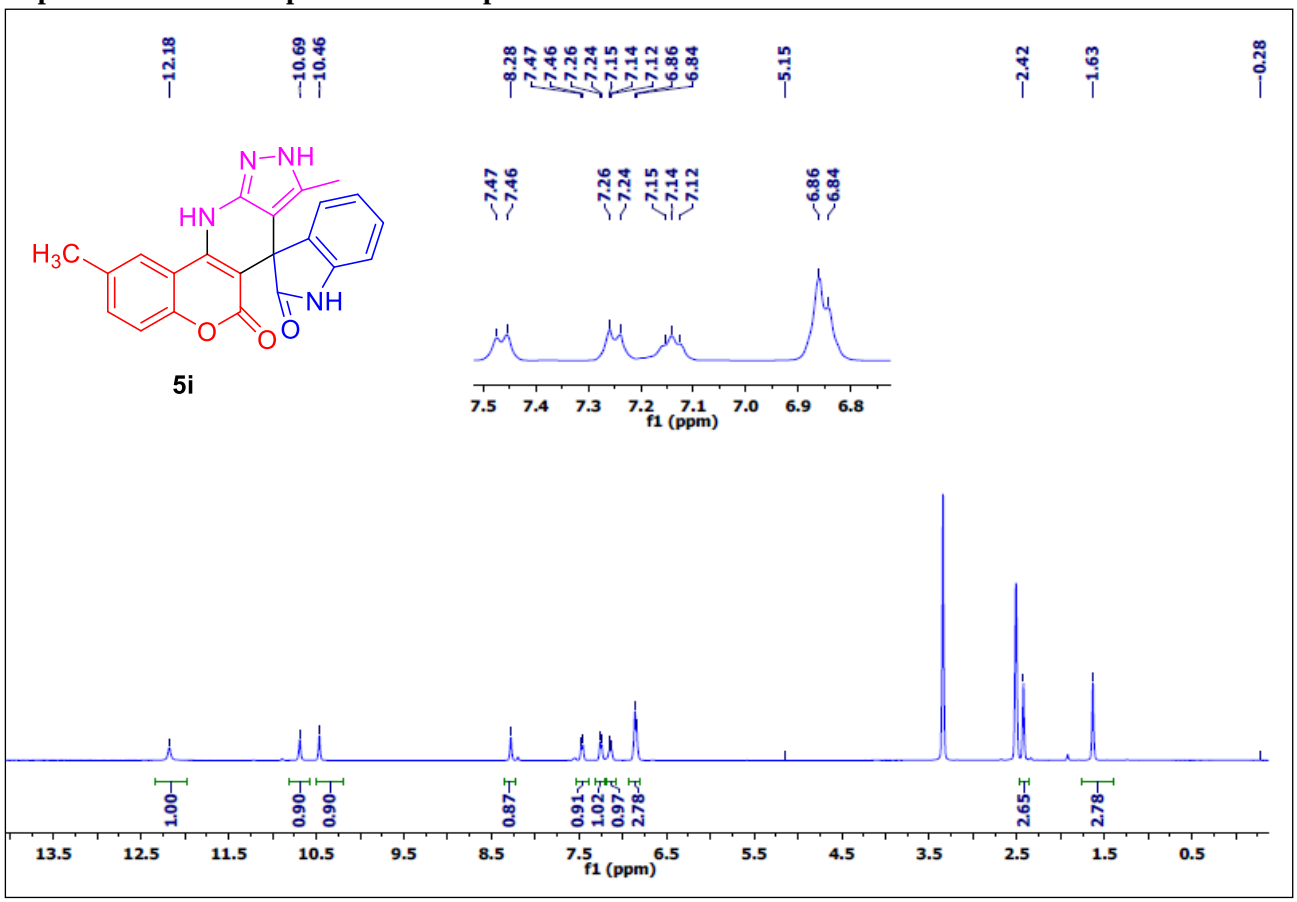

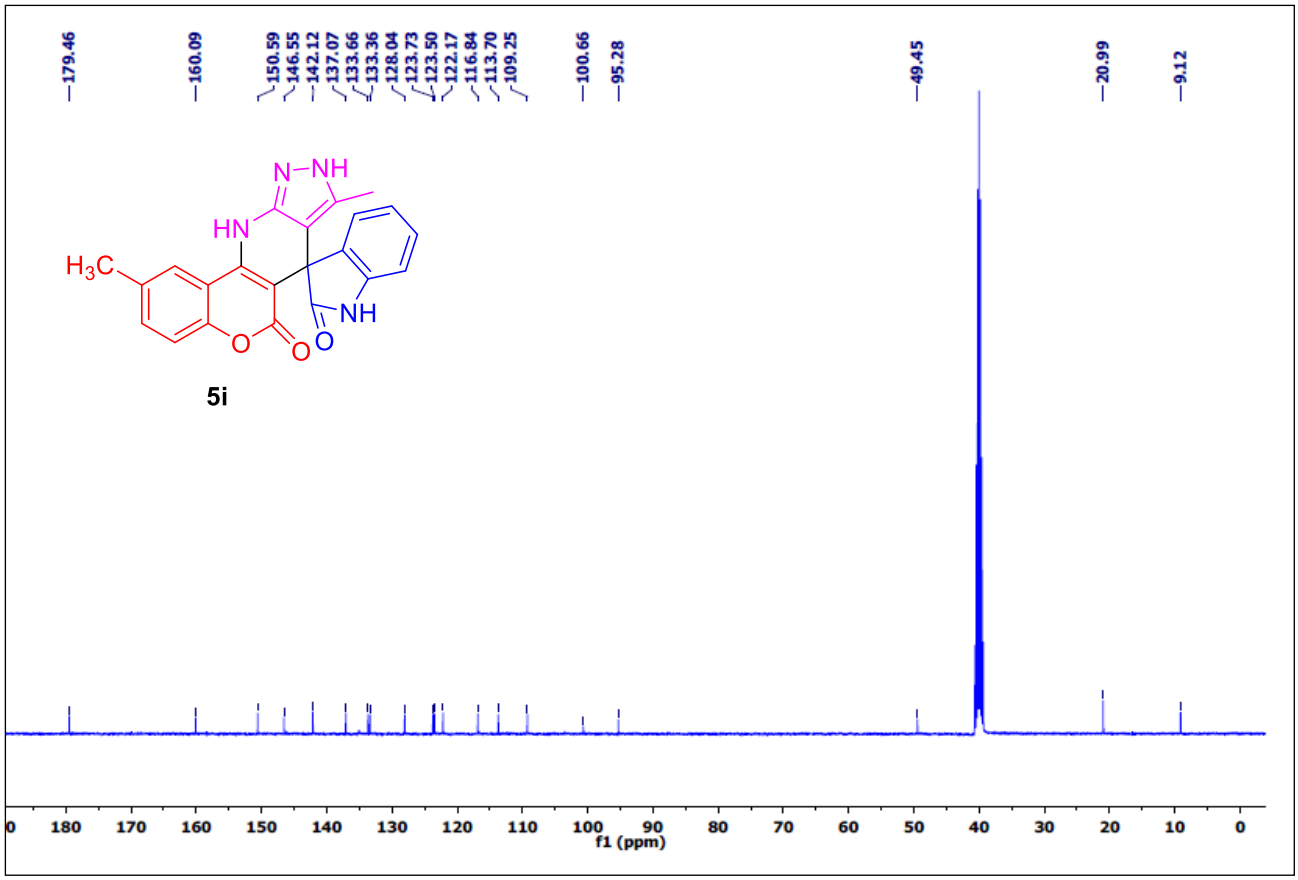

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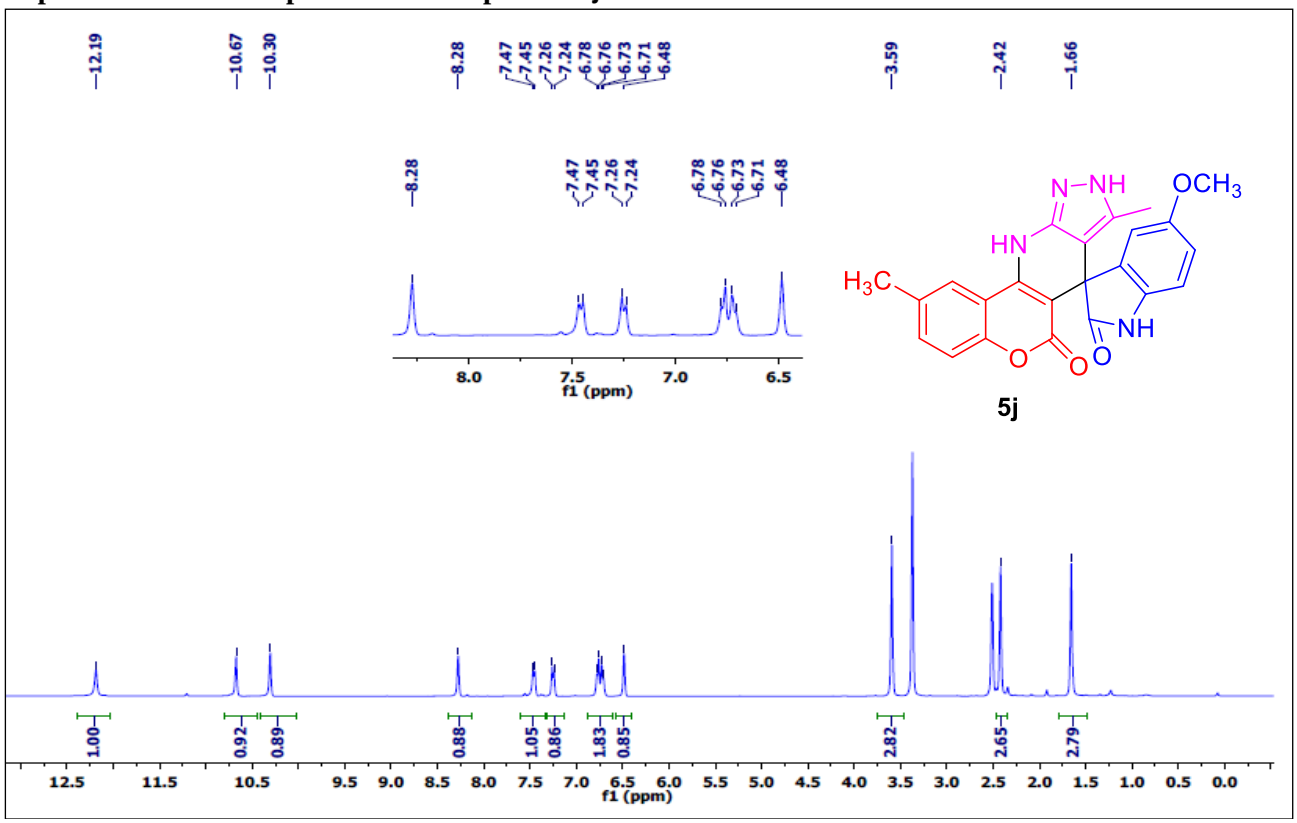

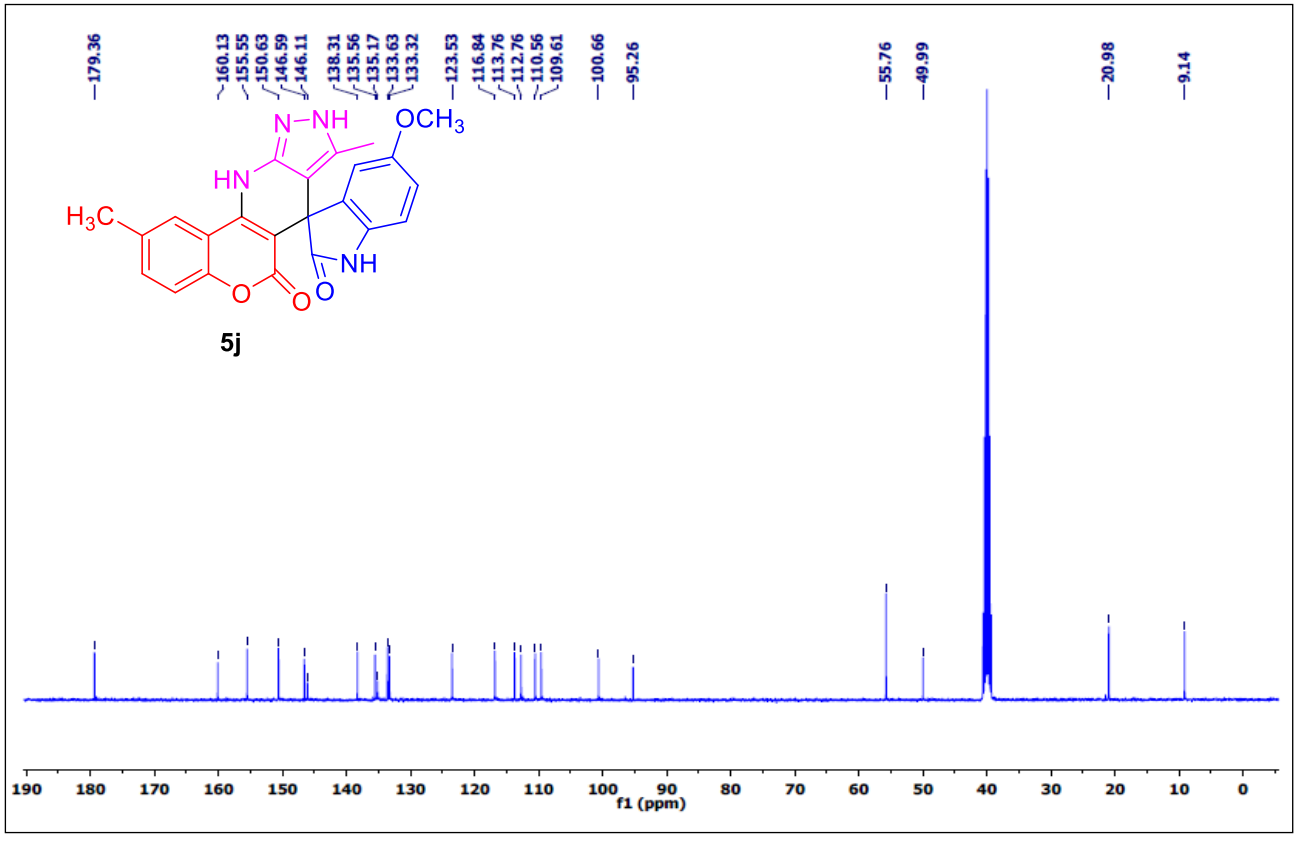

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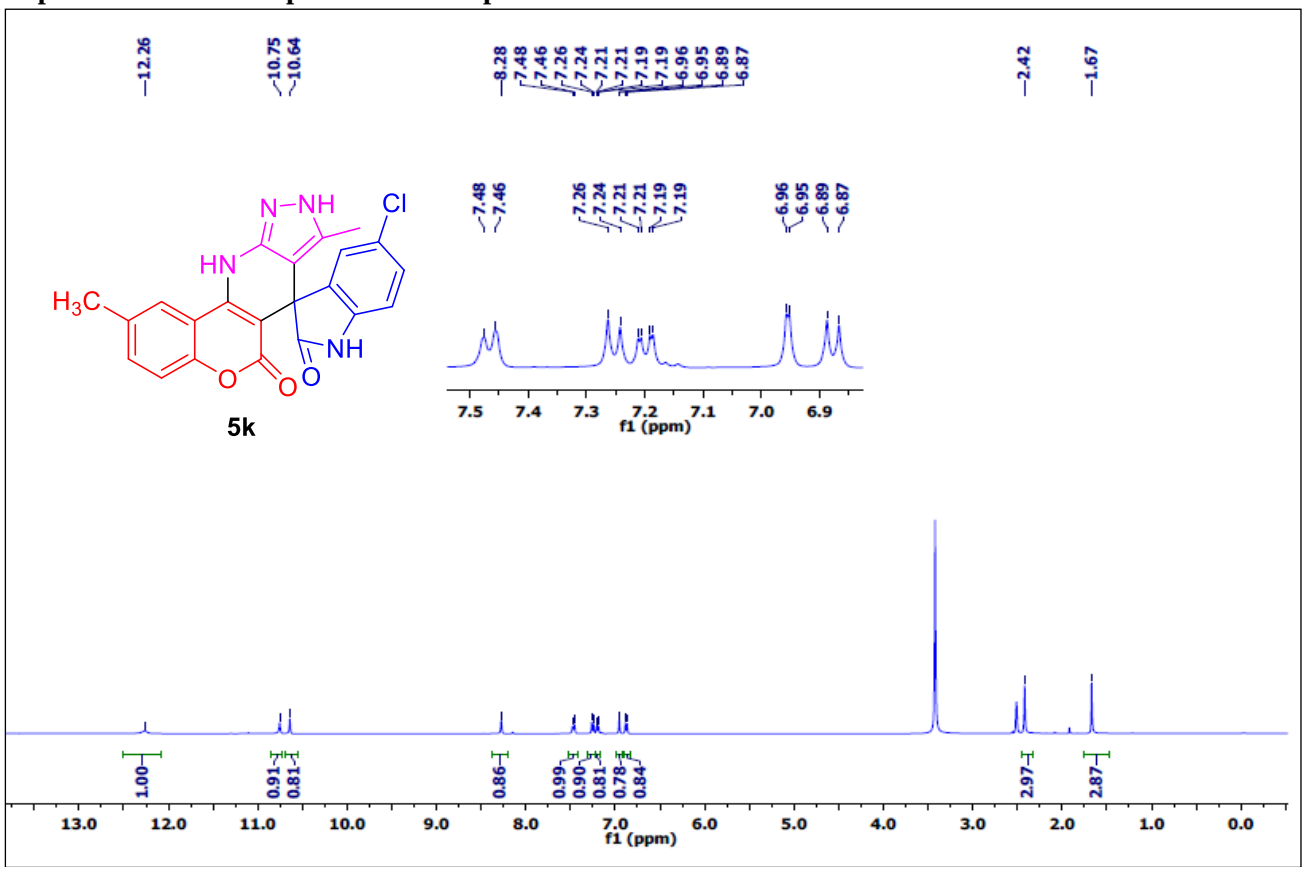

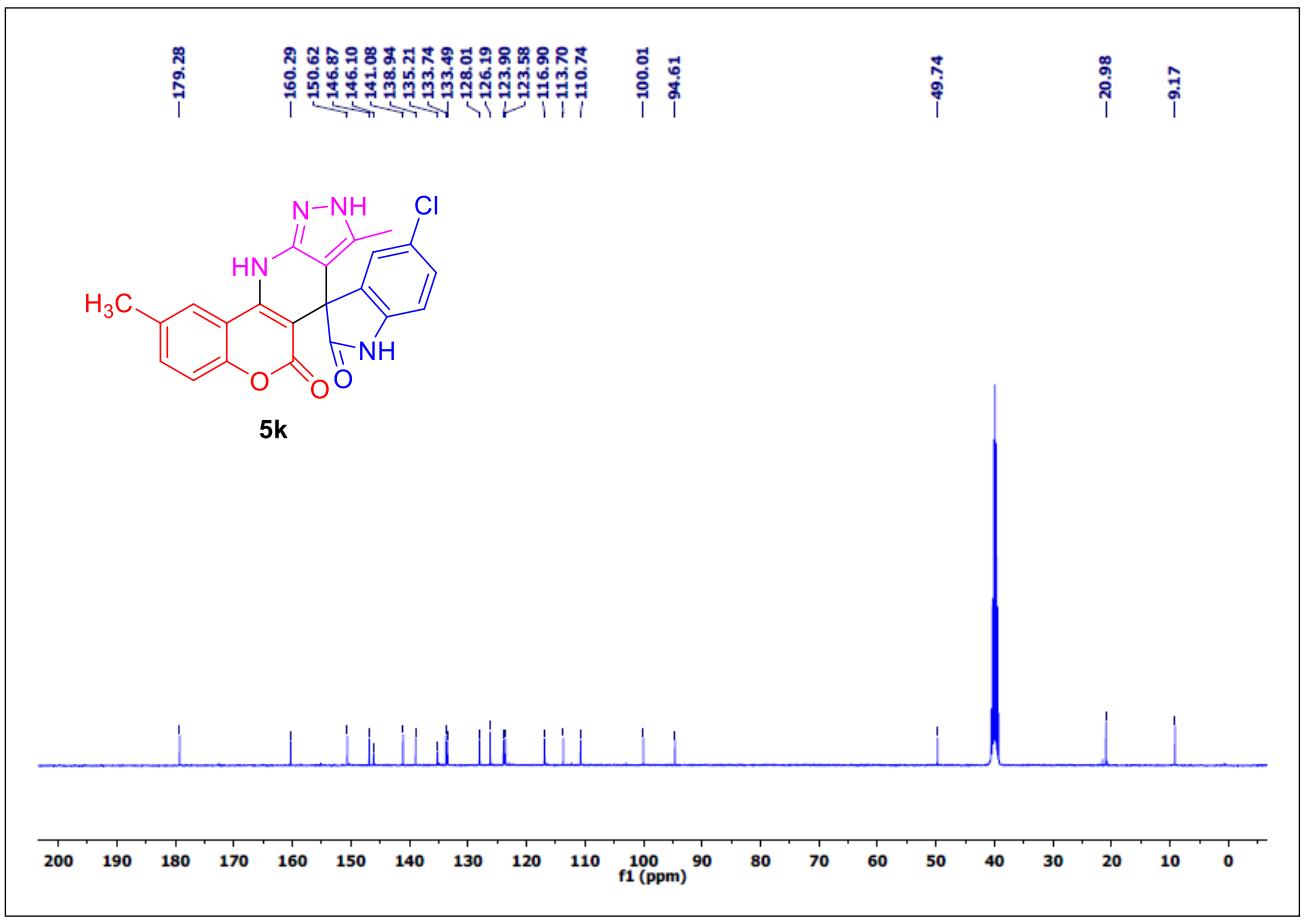

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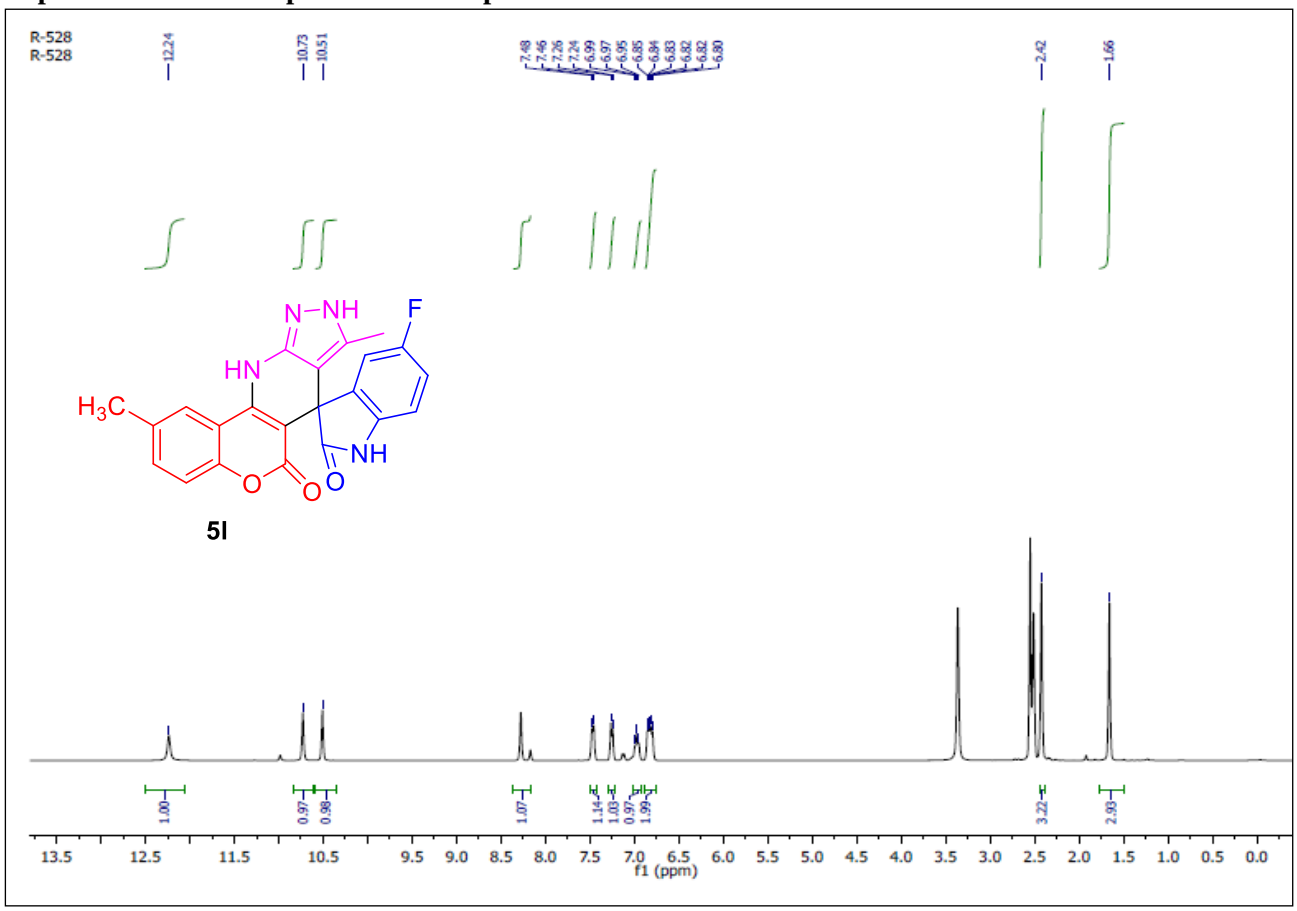

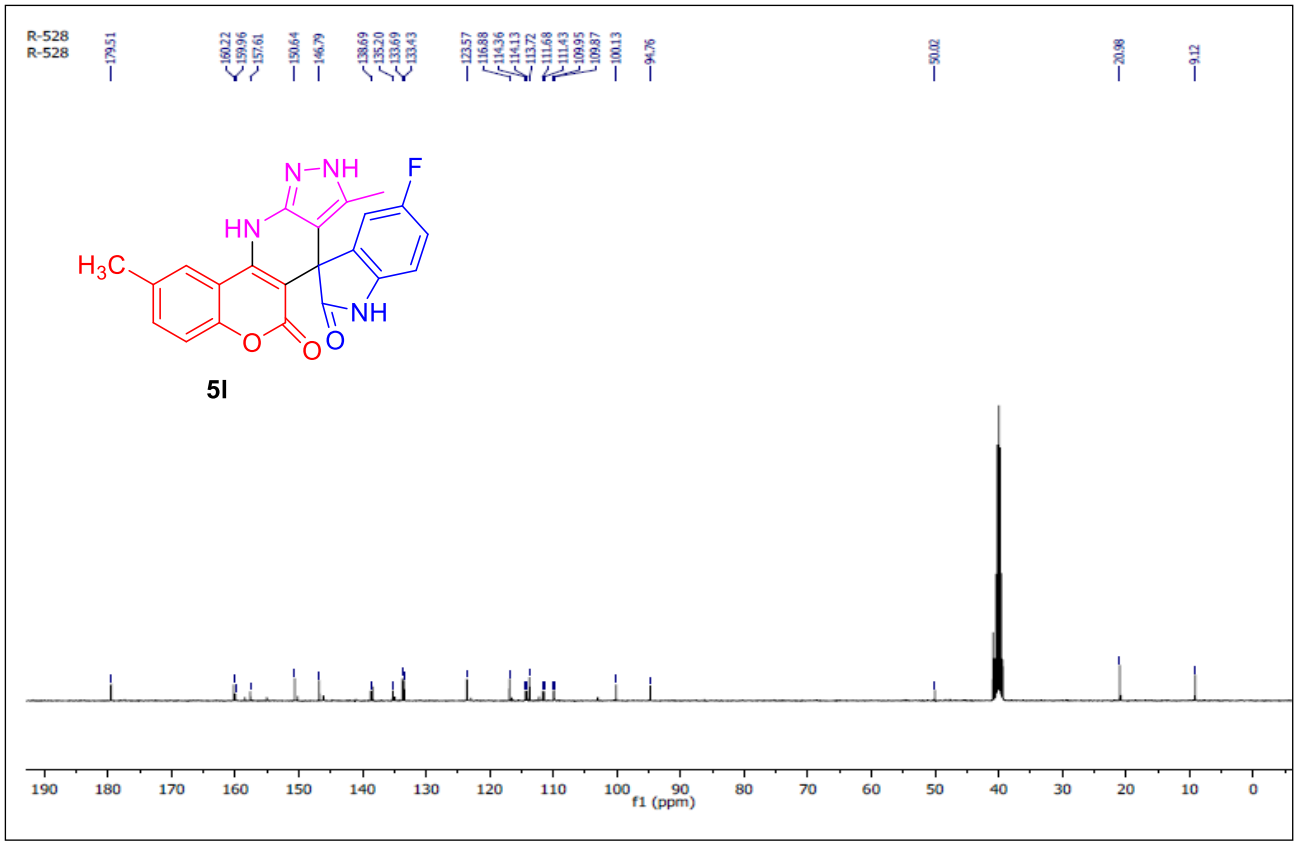

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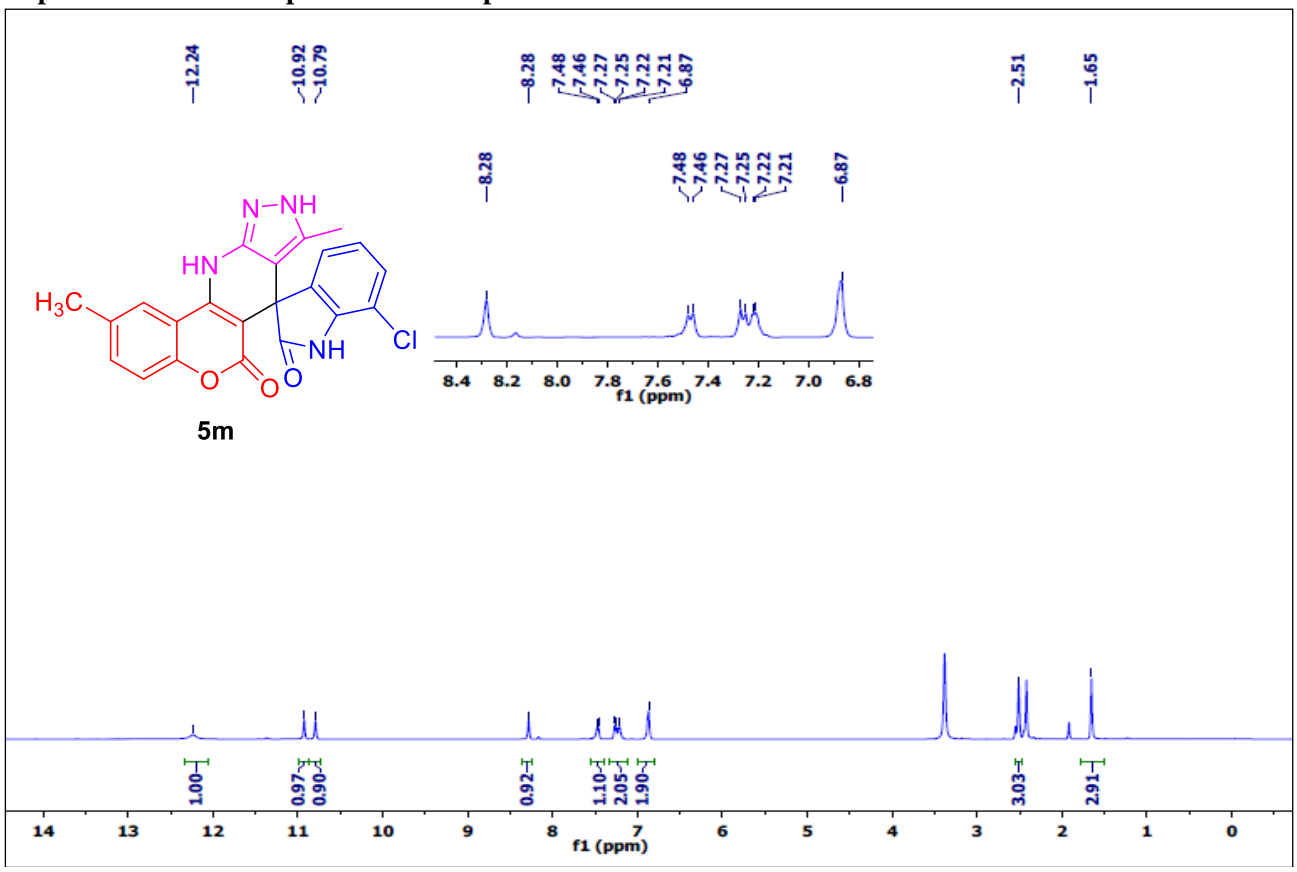

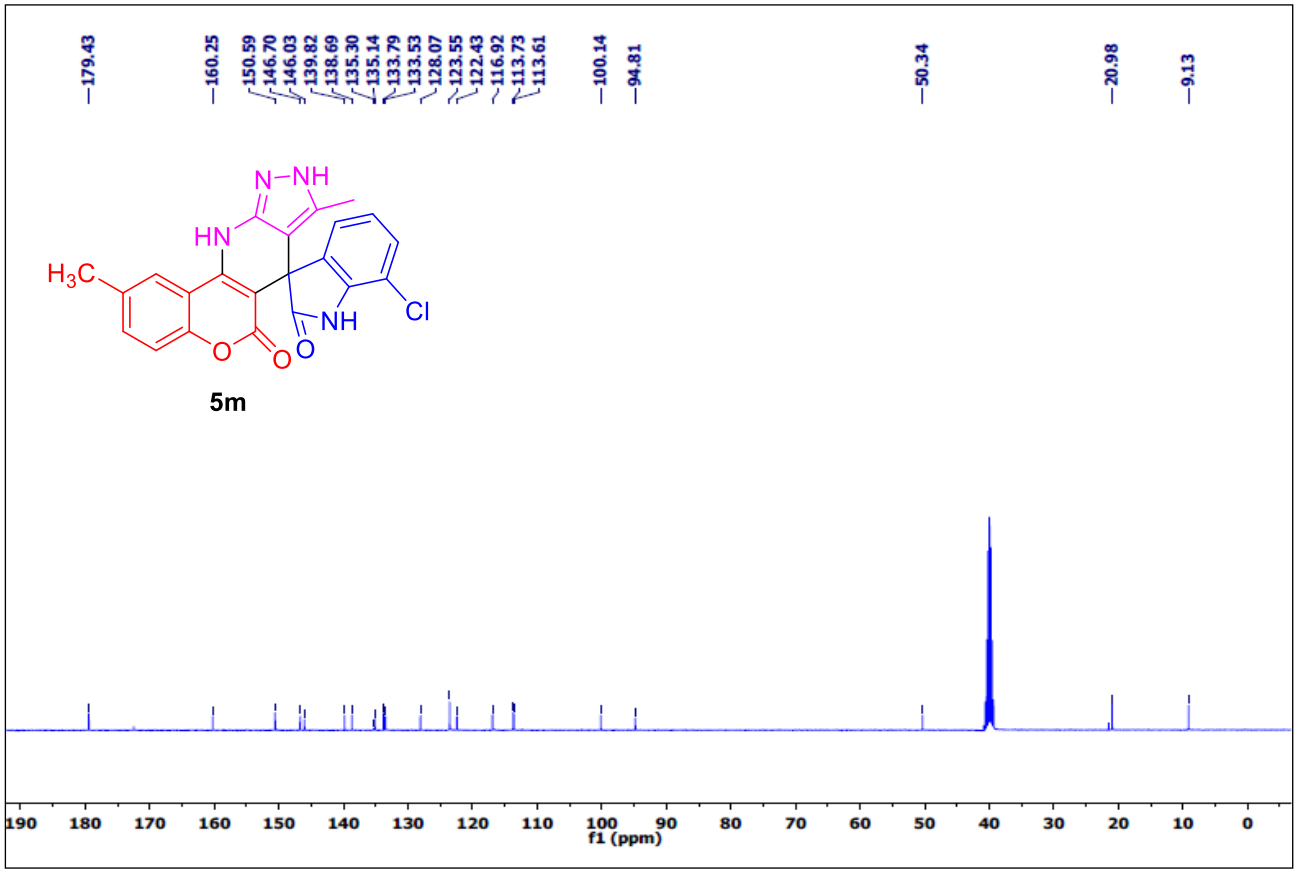

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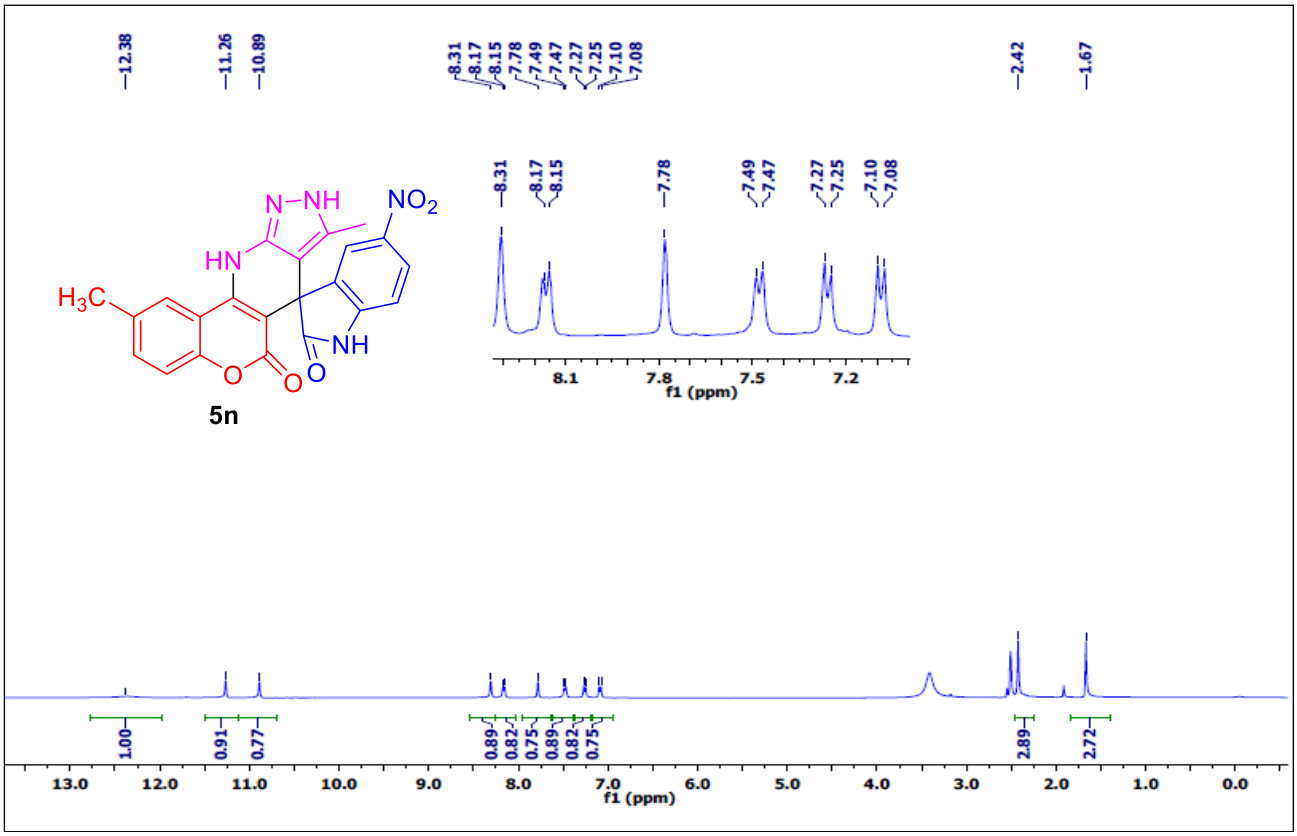

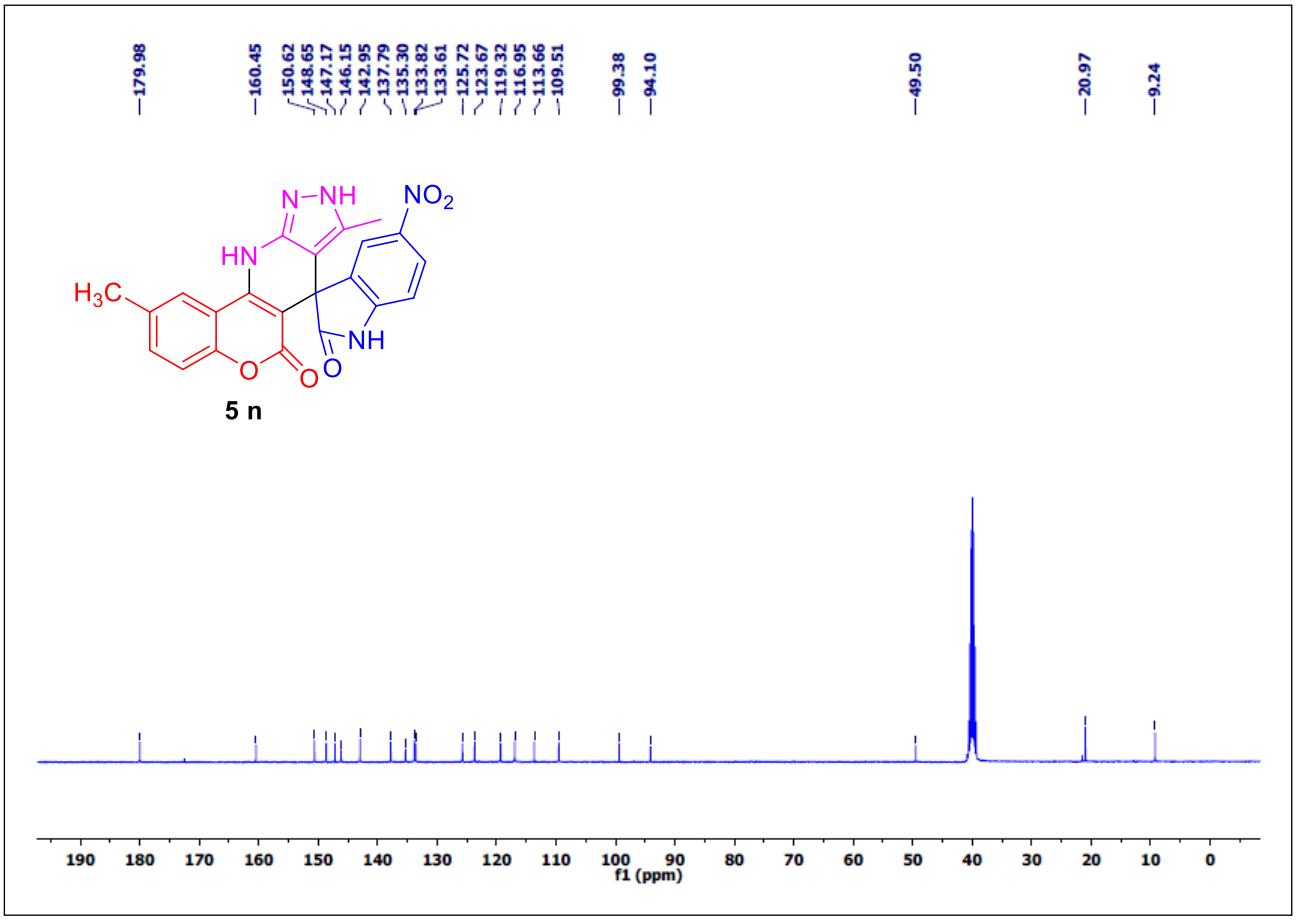

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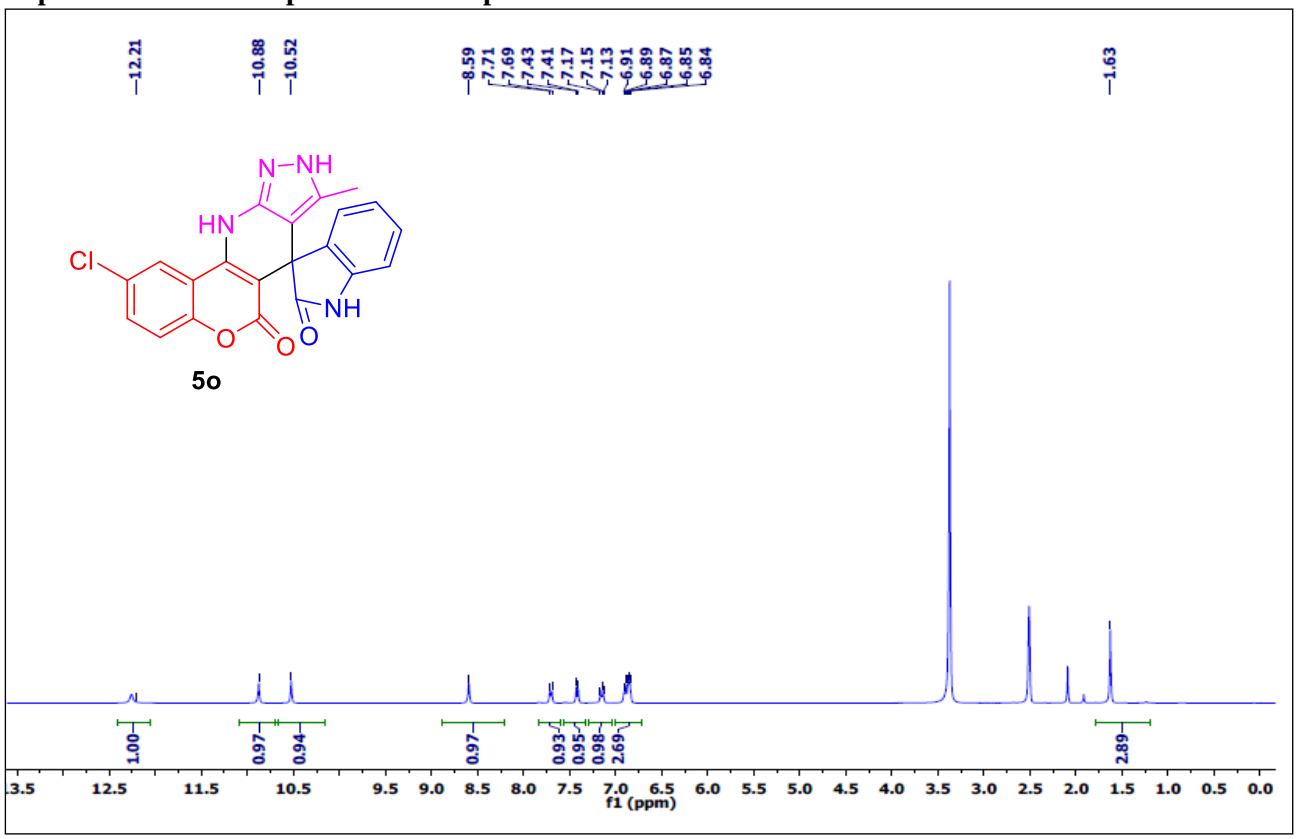

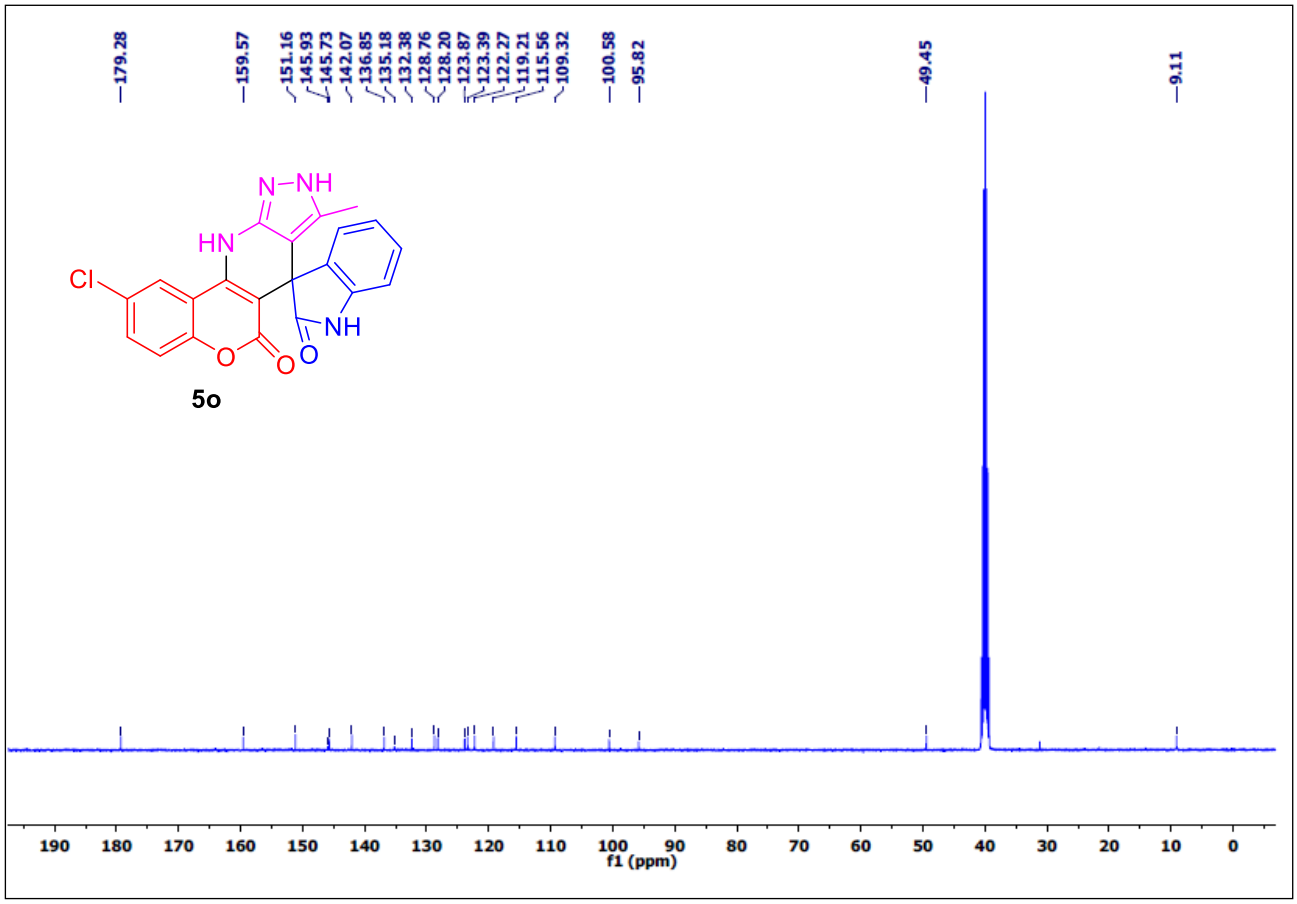

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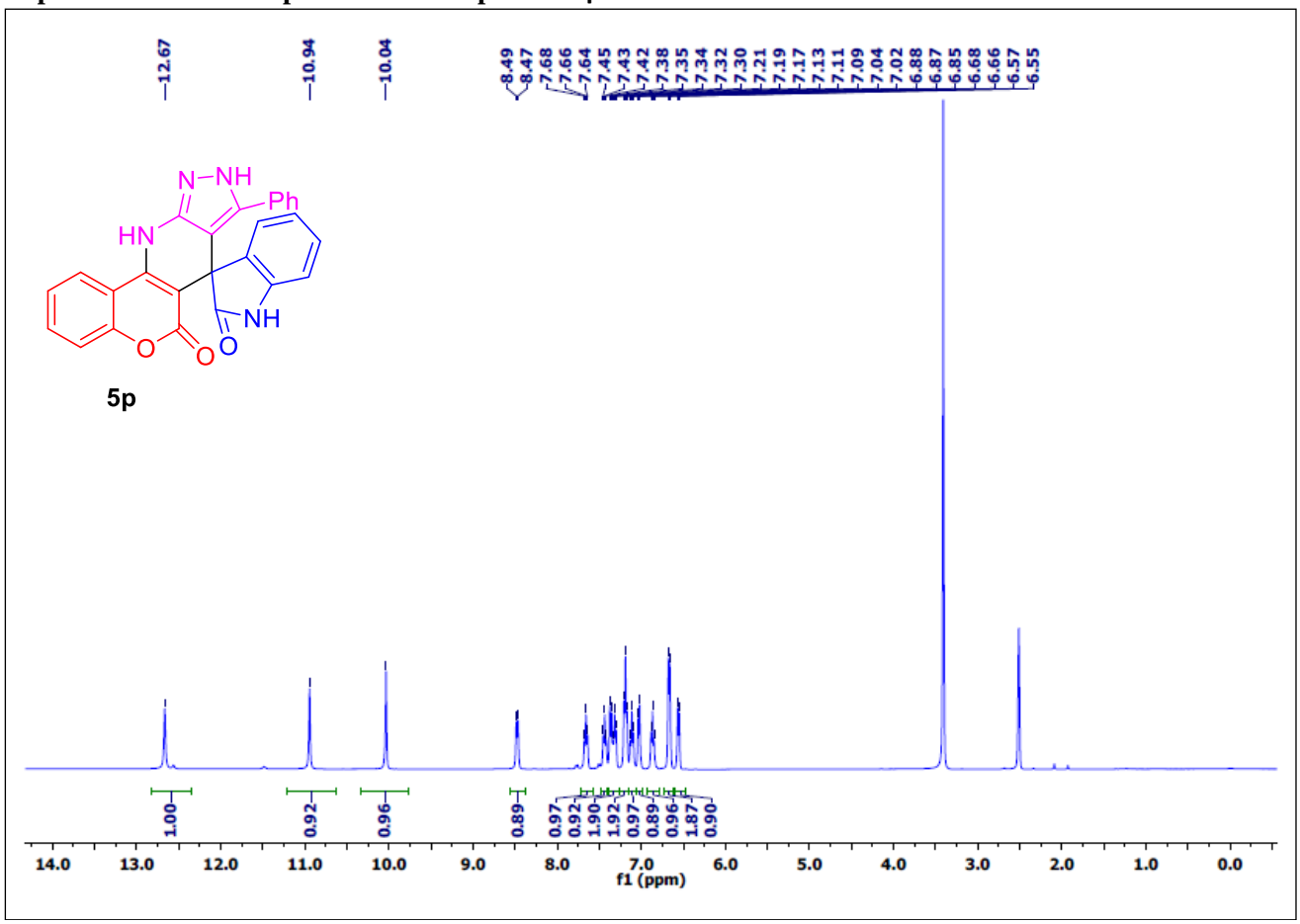

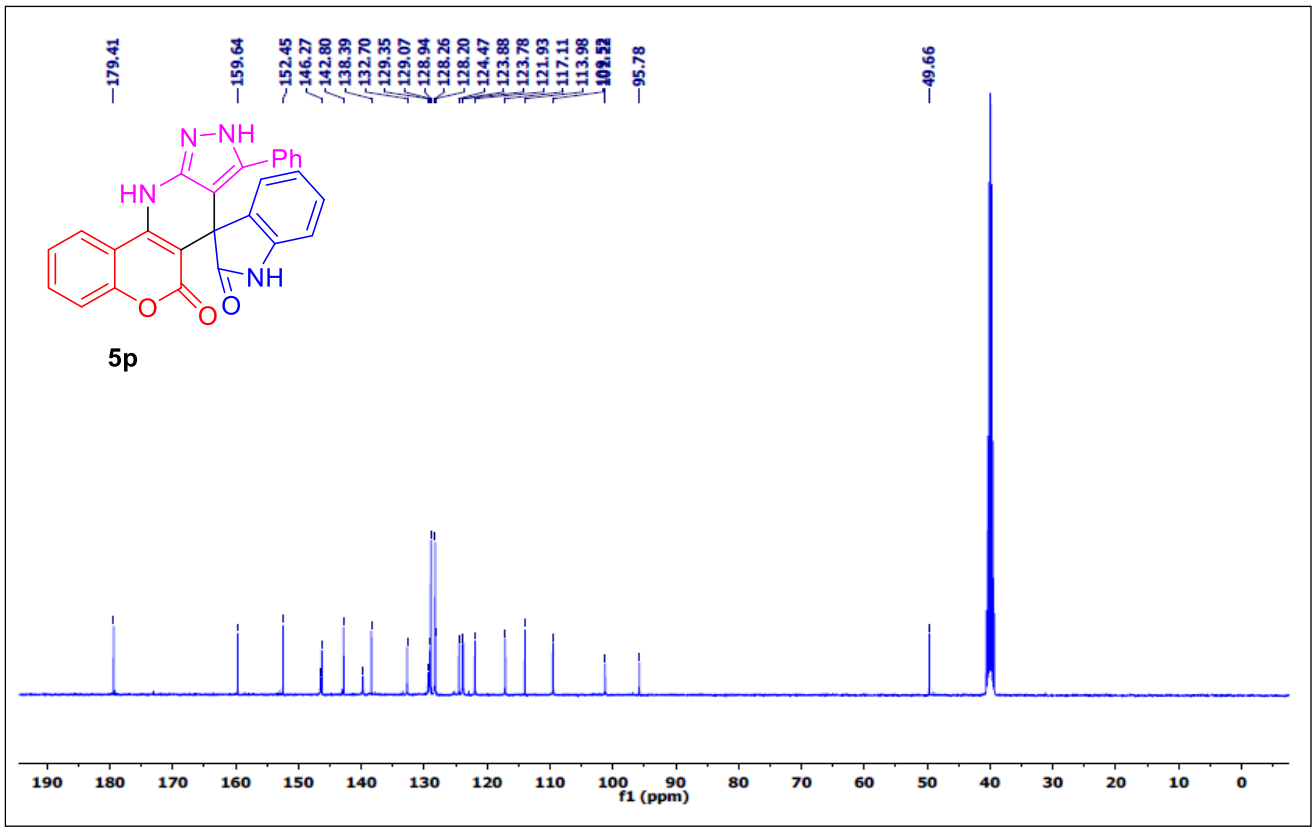

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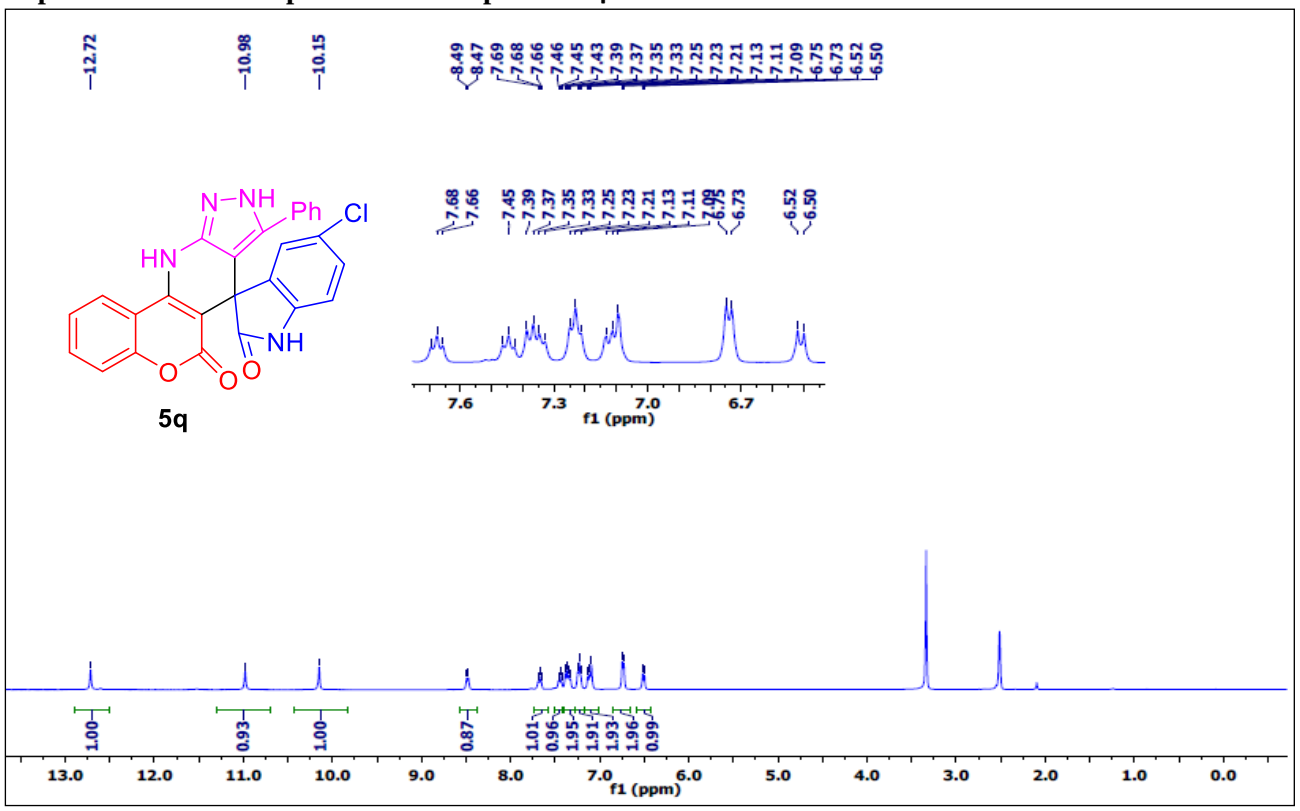

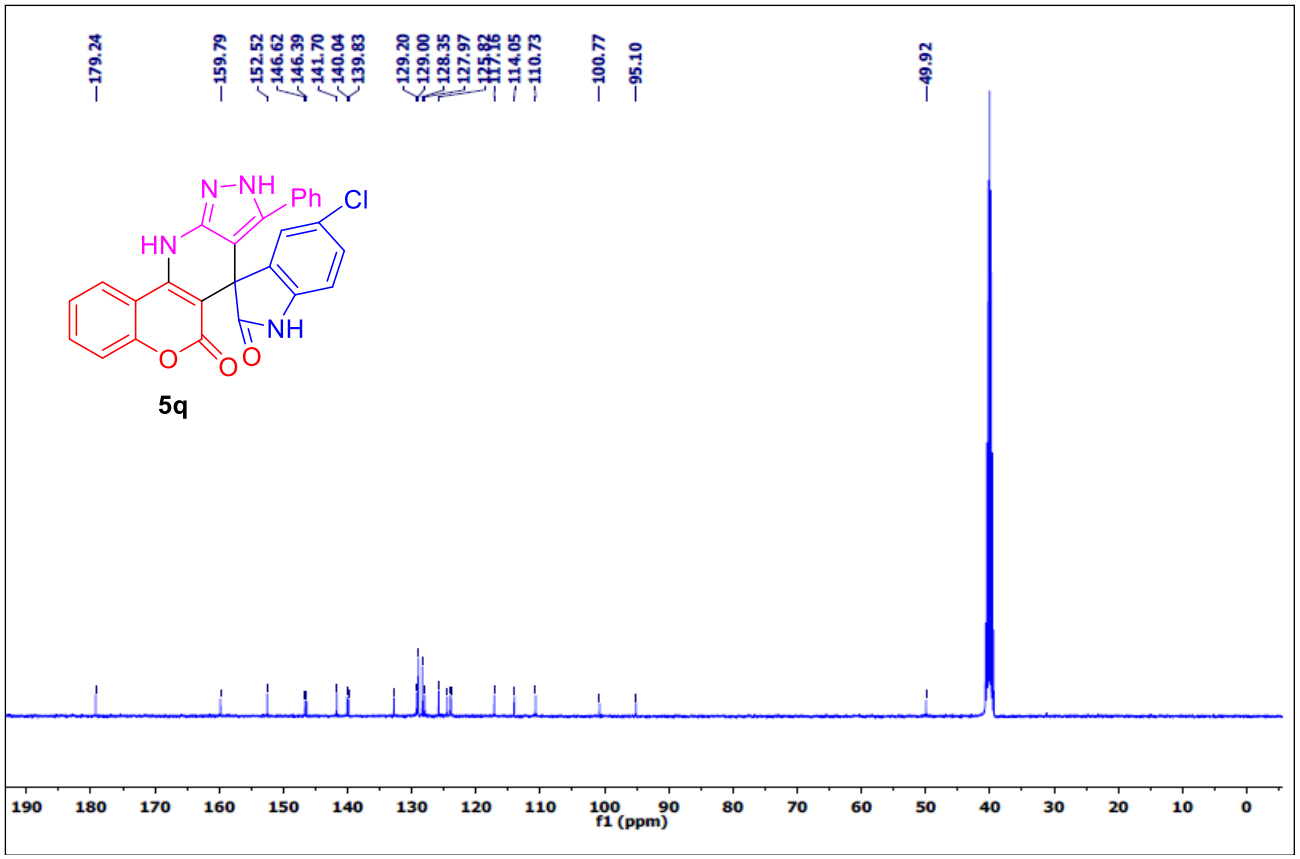

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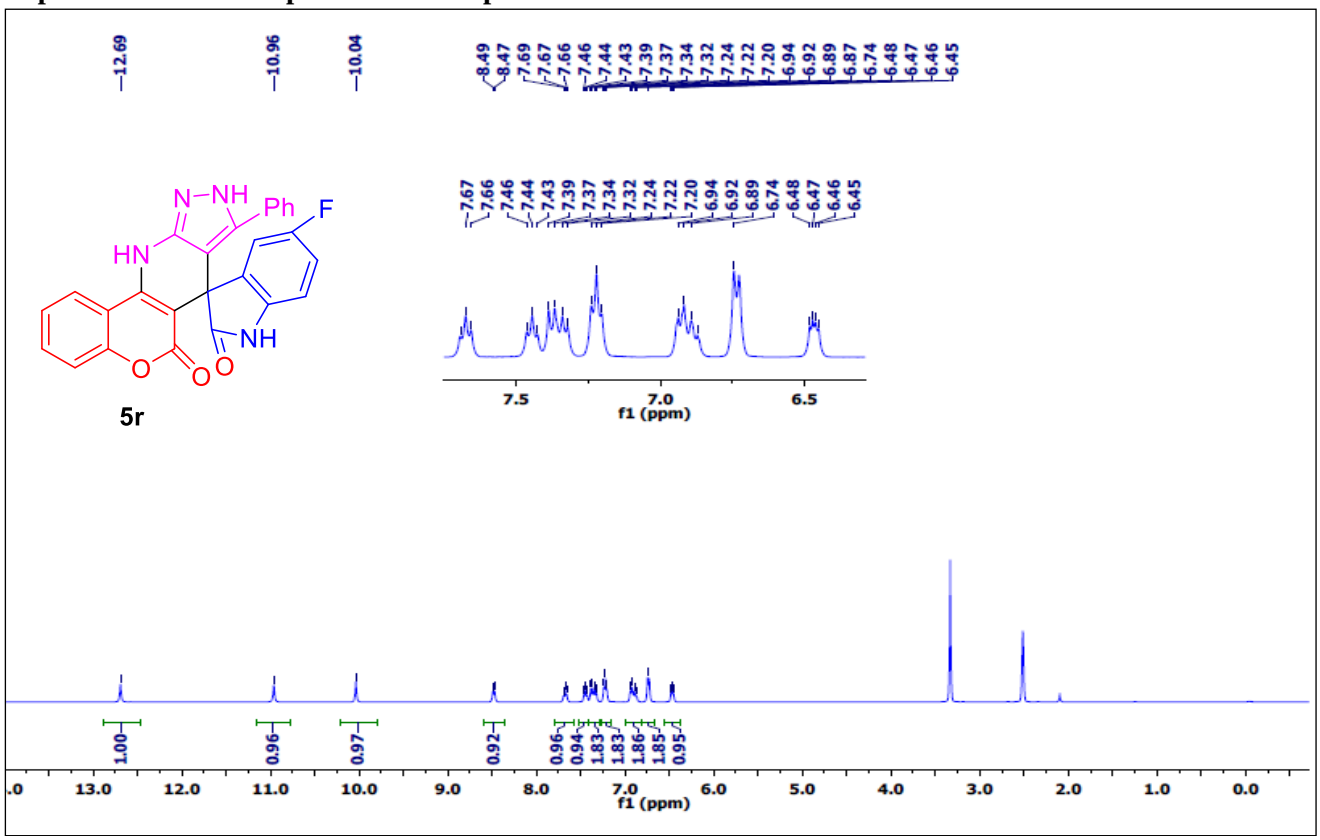
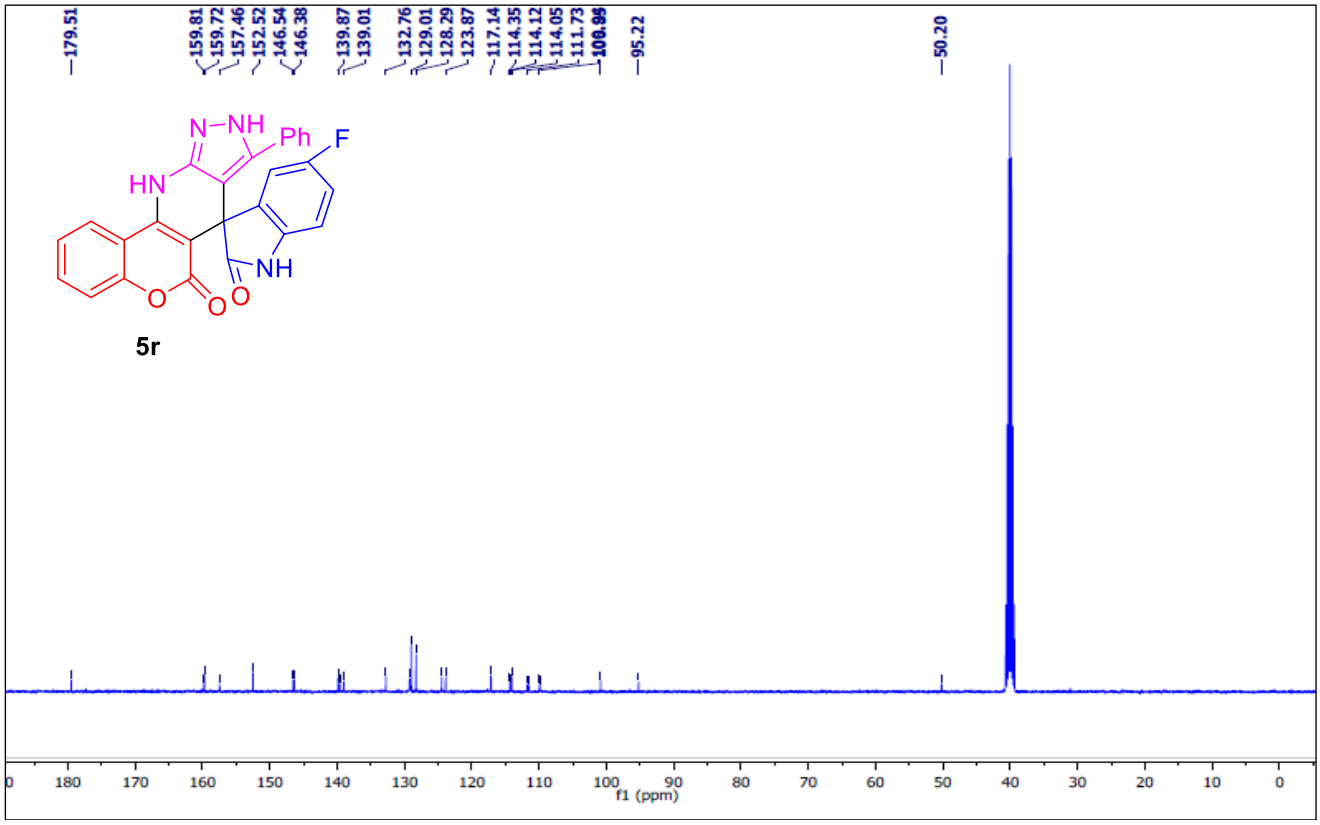
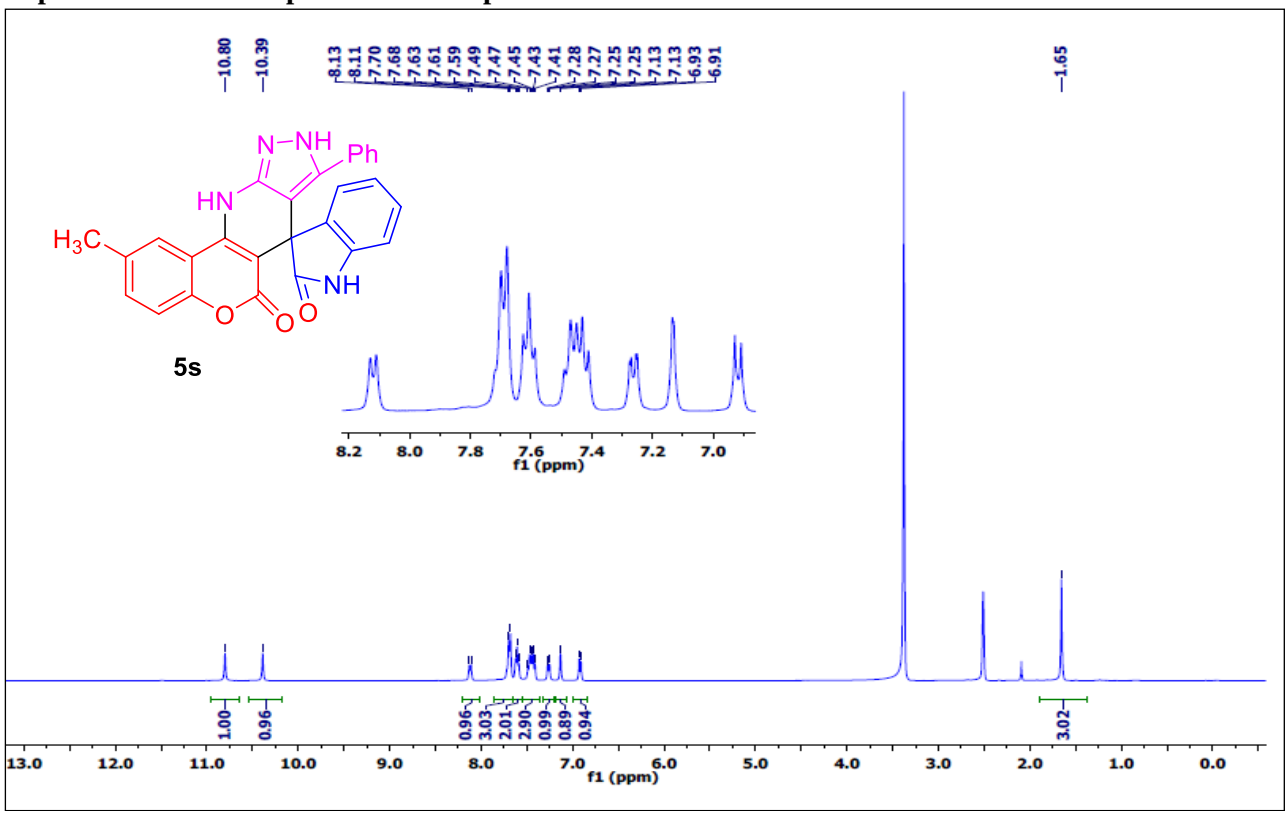
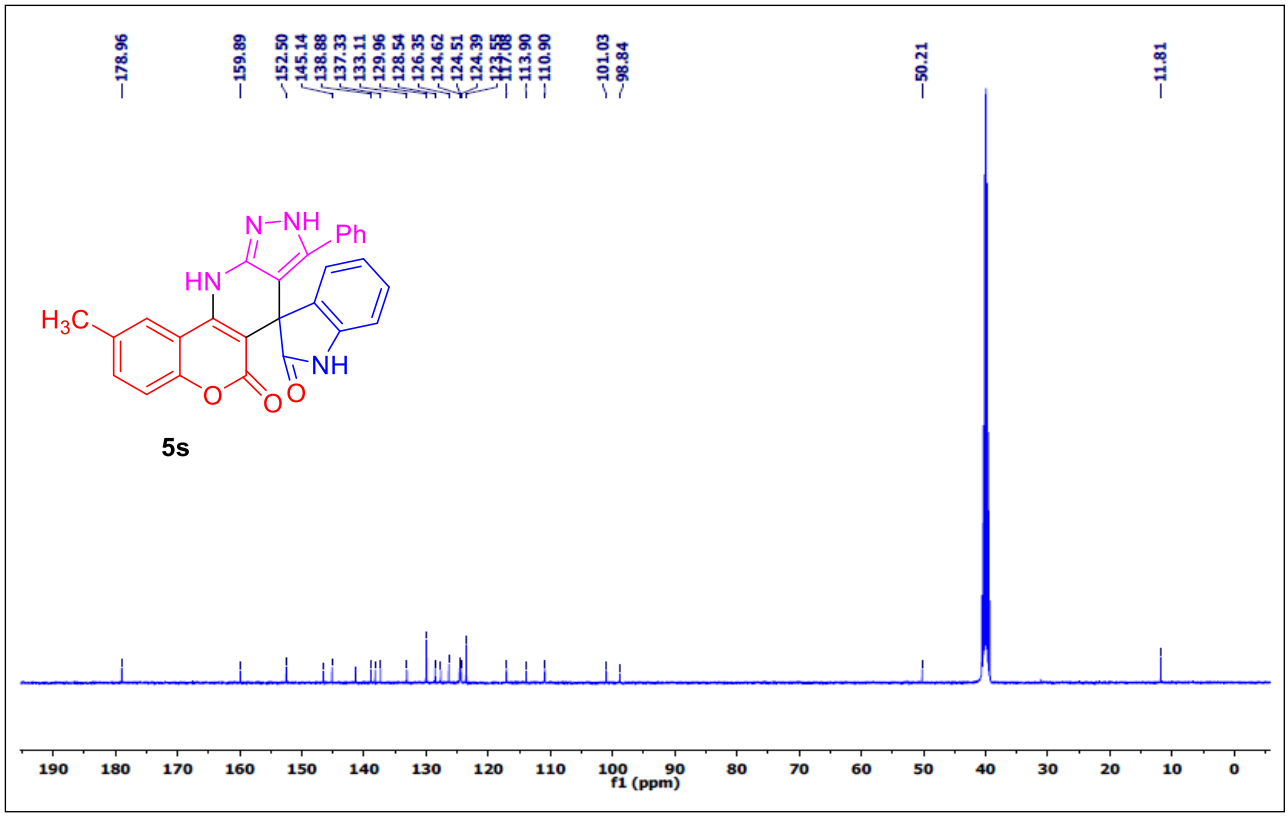


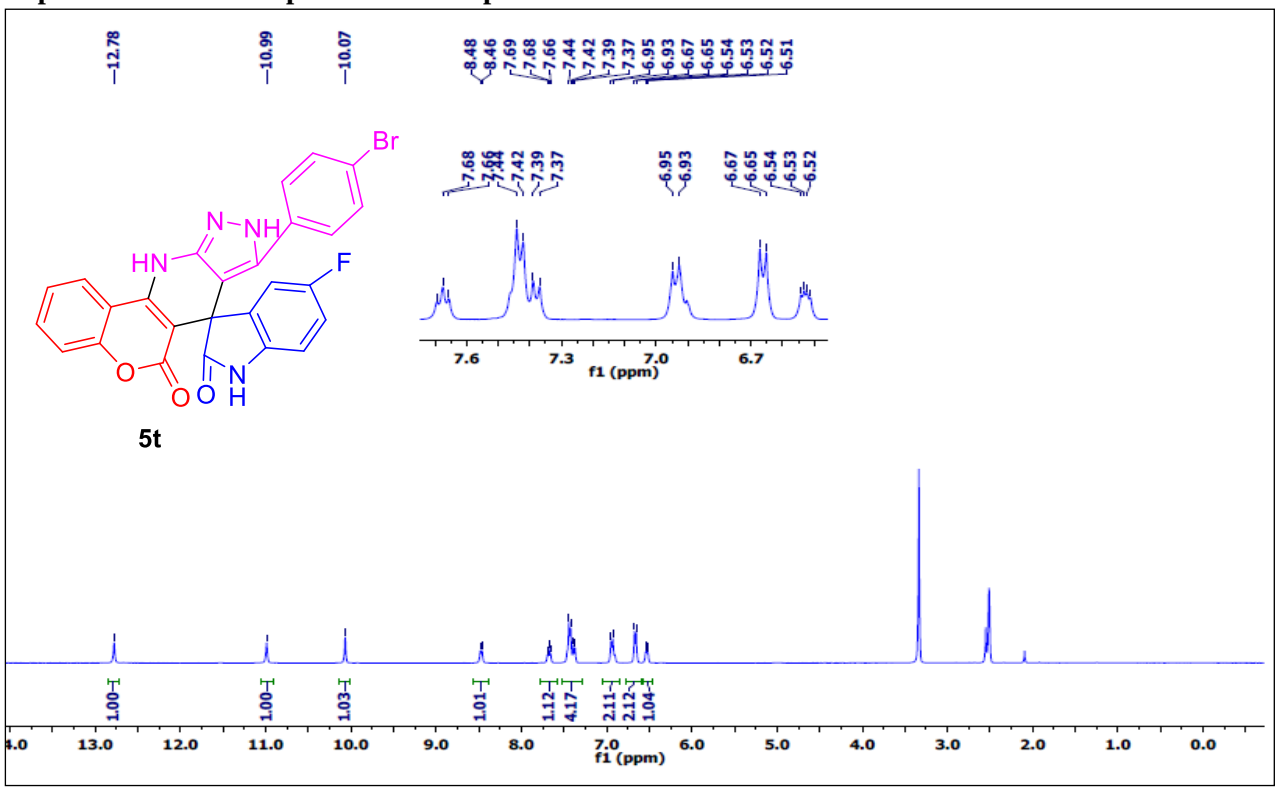


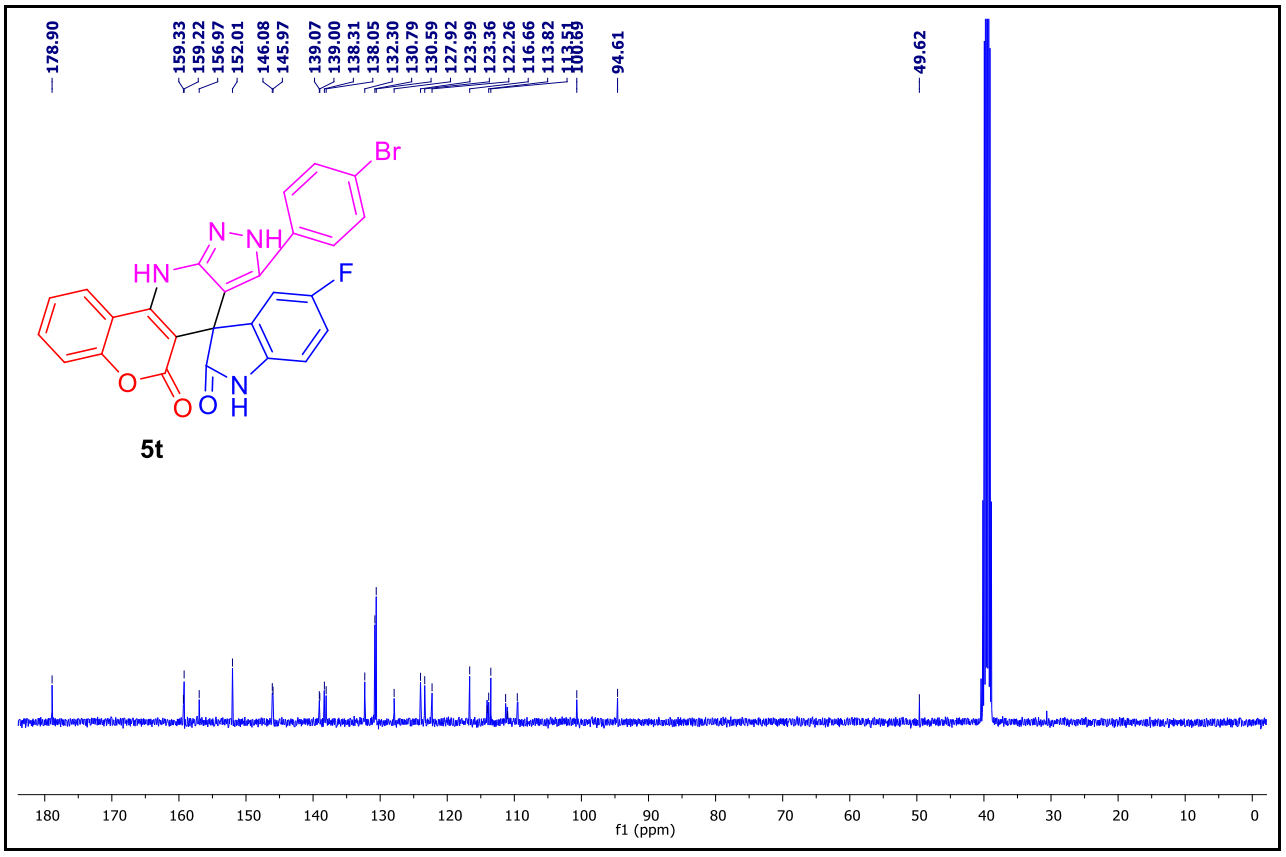
Copies of ^{1}H and ^{13}C spectrum of compound 5s



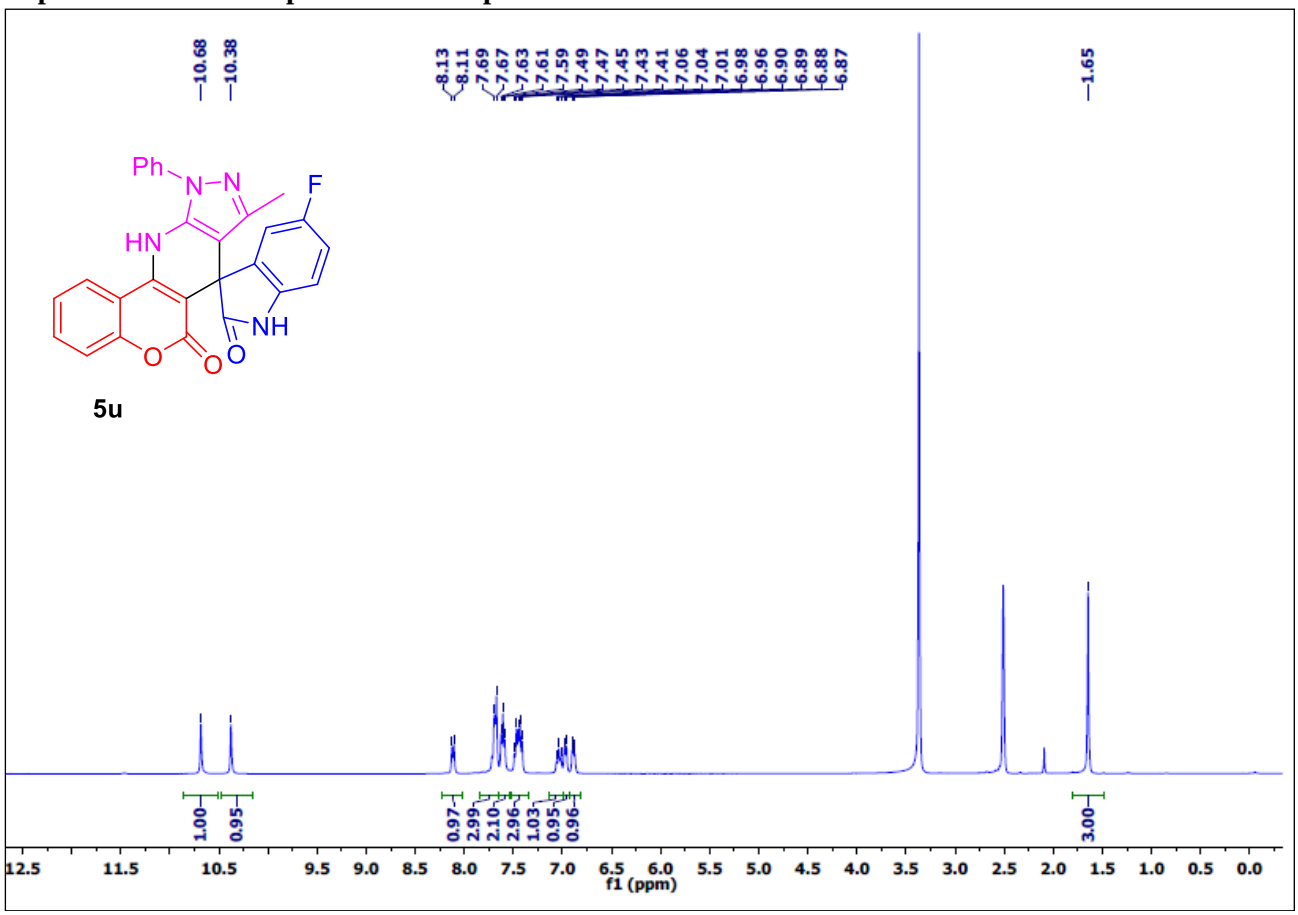


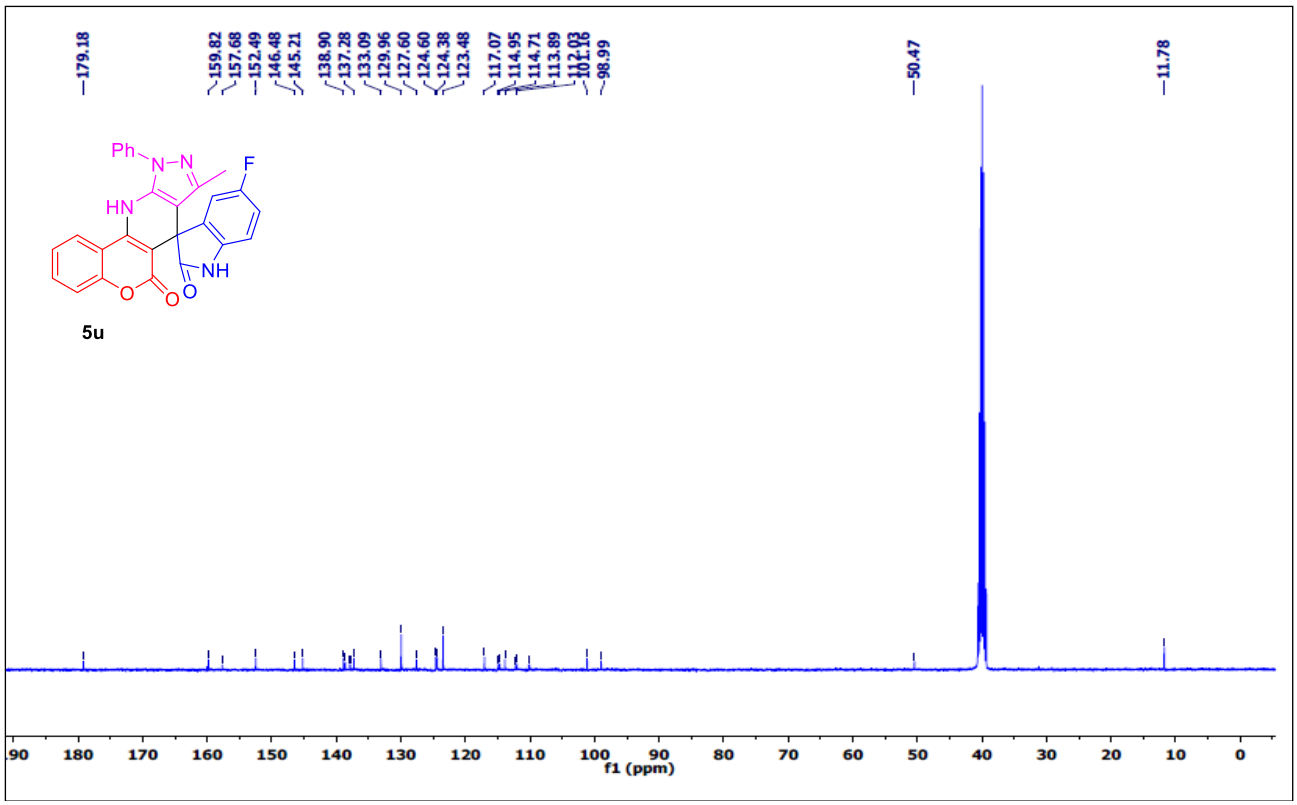
Copies of ^{1}H and ^{13}C spectrum of compound 5t





Copies of ^{1}H and ^{13}C spectrum of compound 5u





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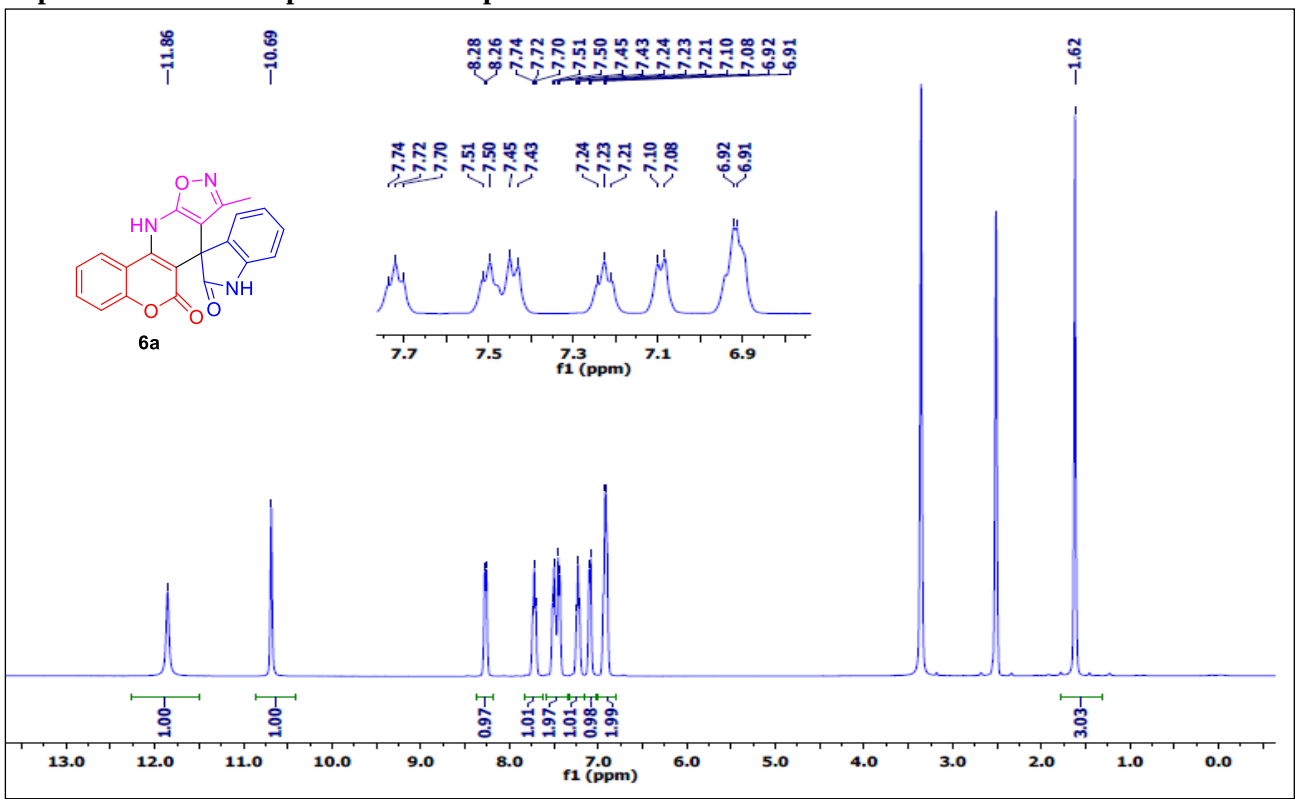
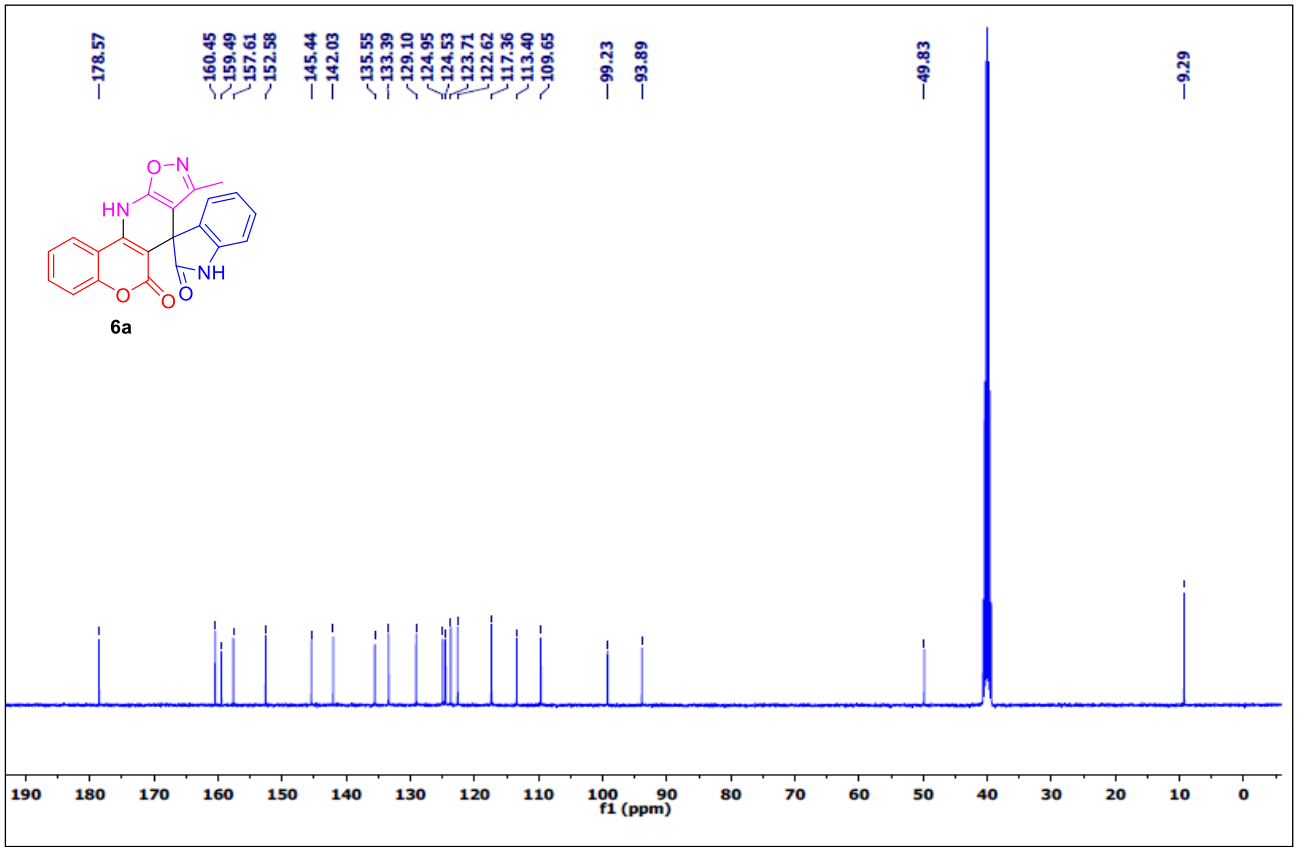
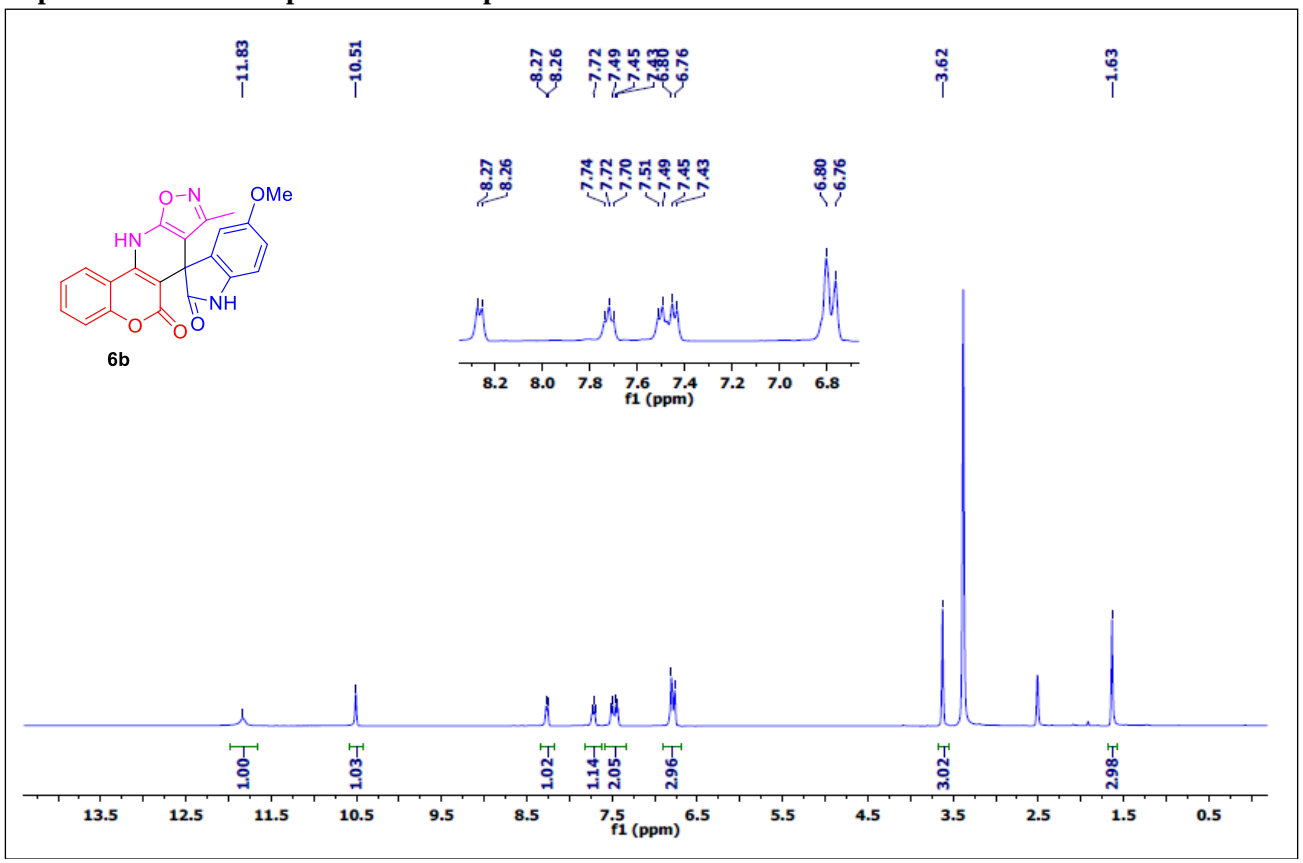
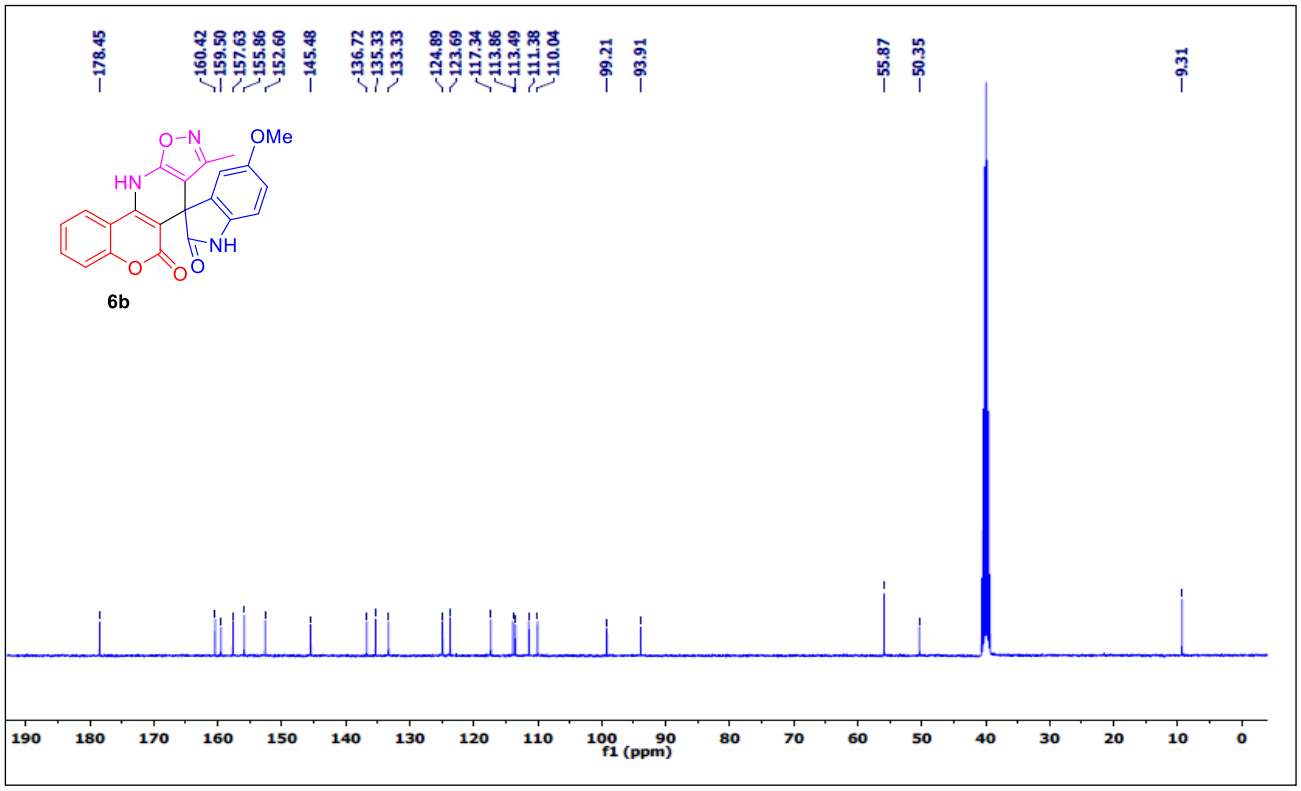


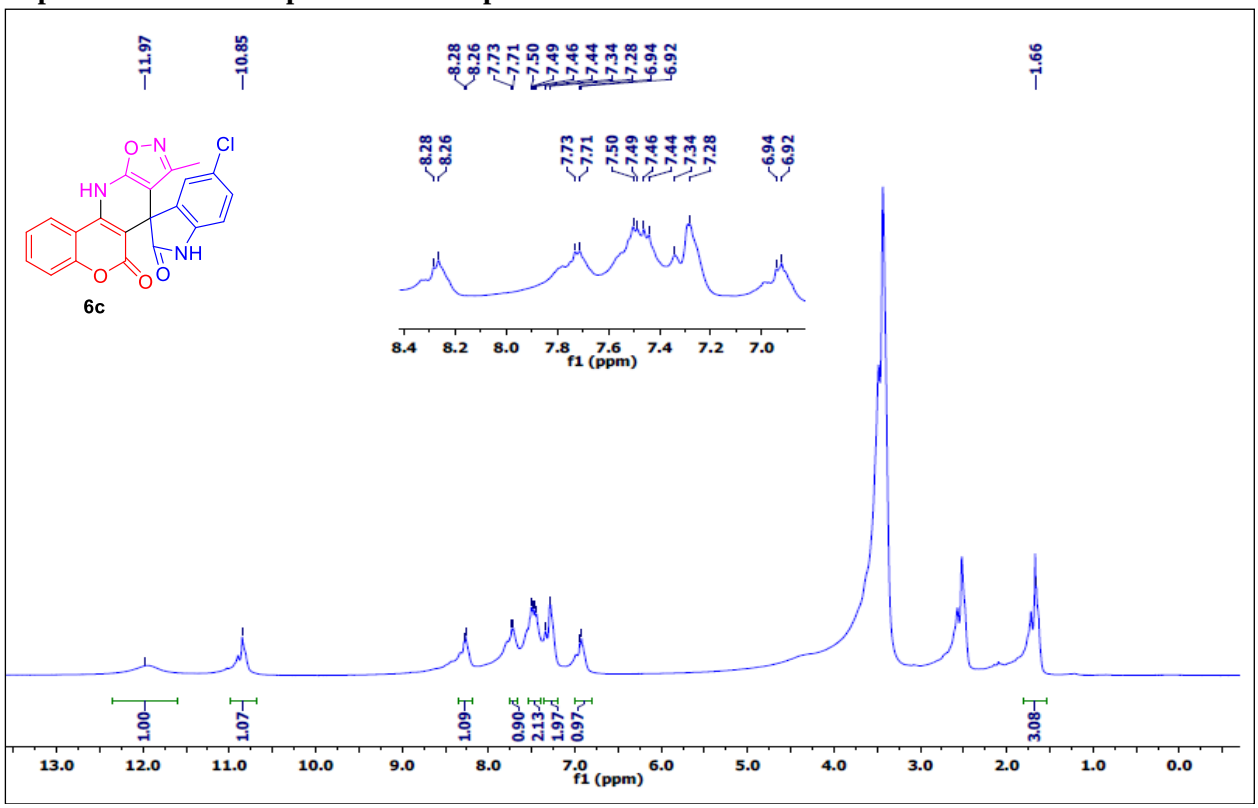


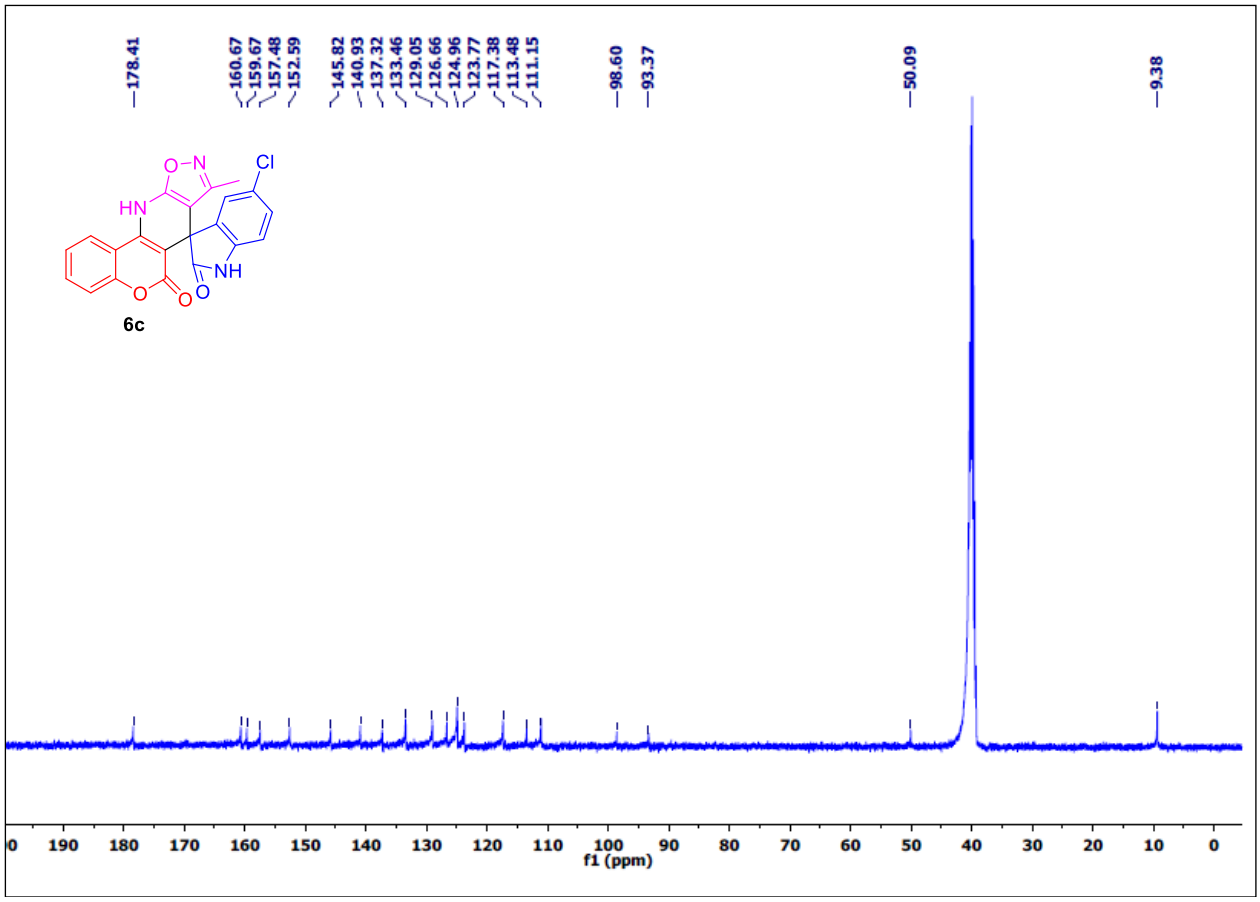
Copies of ^{1}H and ^{13}C spectrum of compound 6b



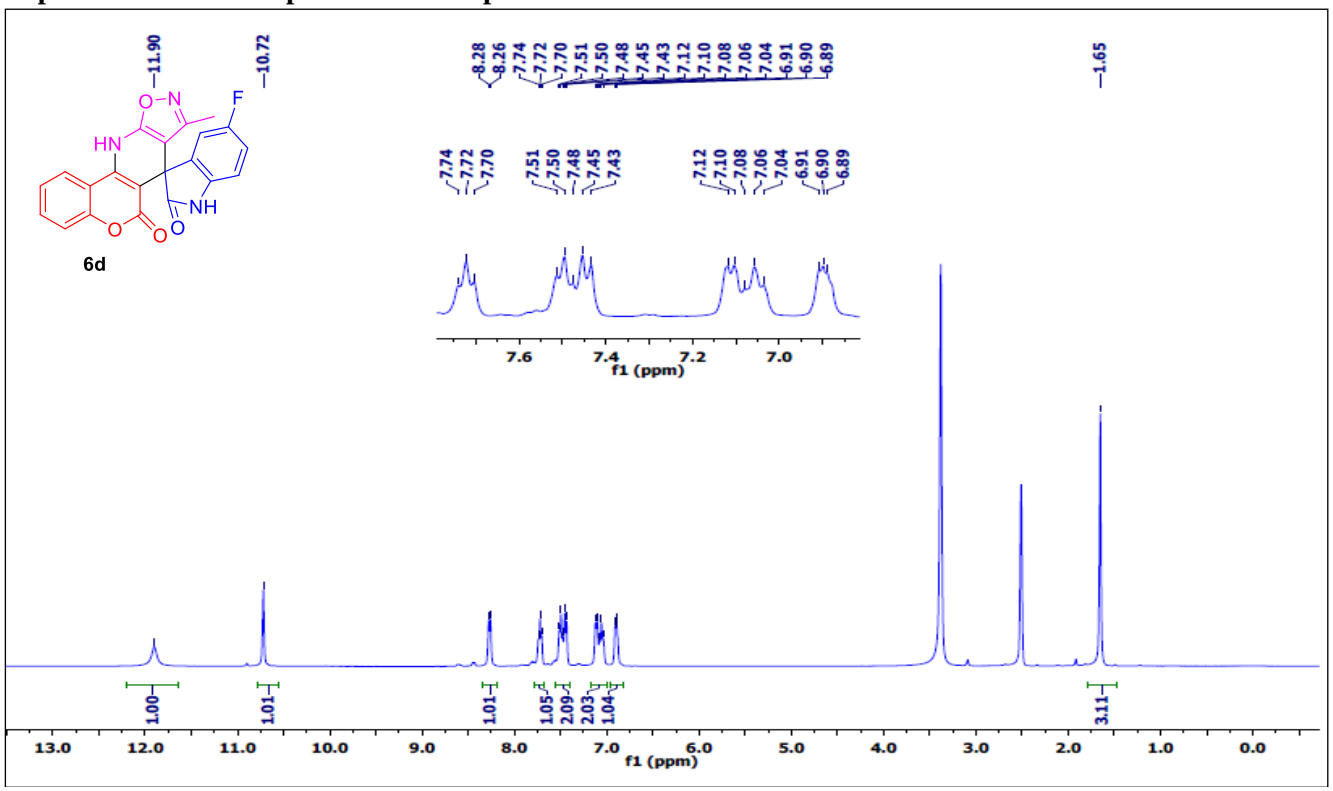


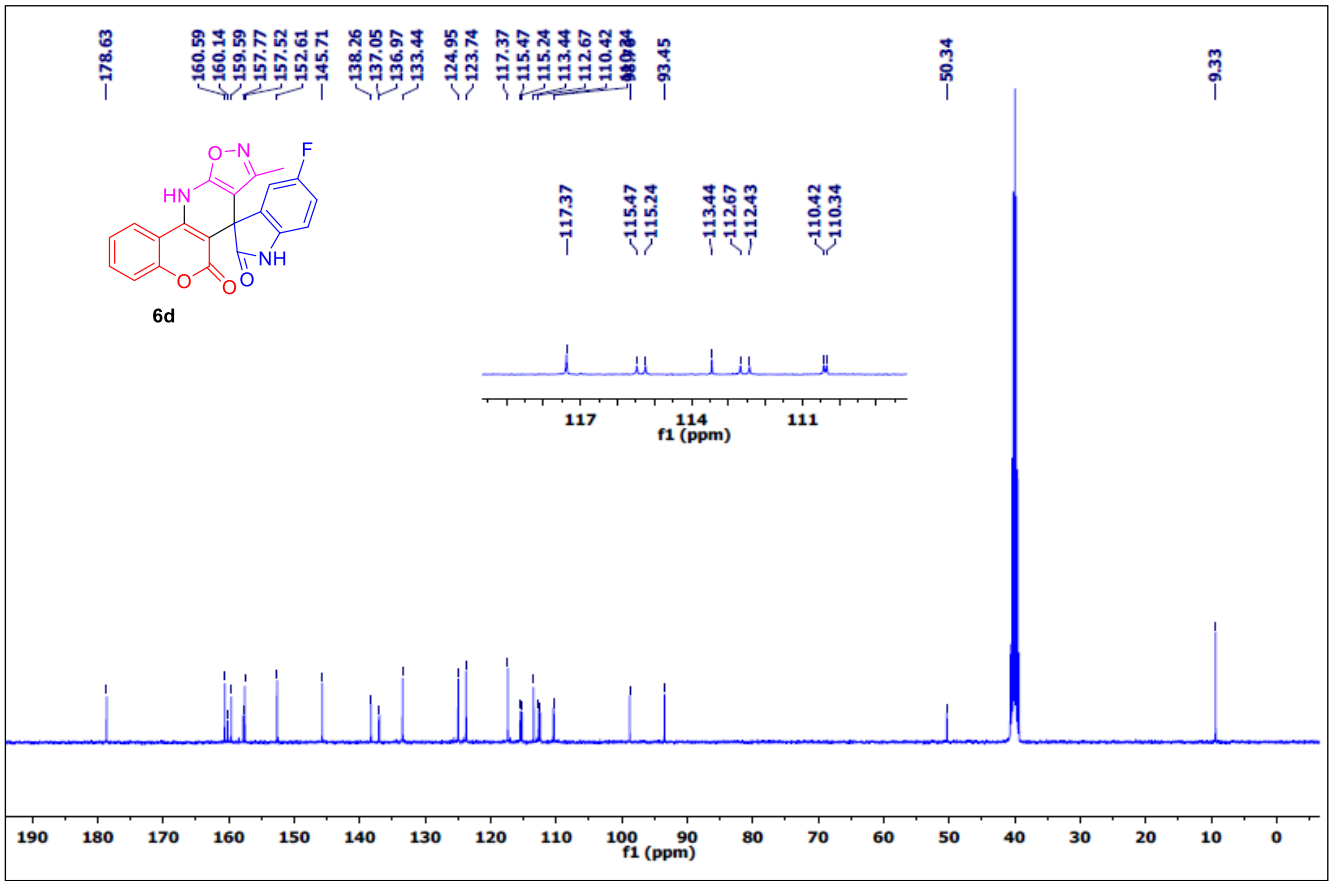
Copies of ^{1}H and ^{13}C spectrum of compound 6c



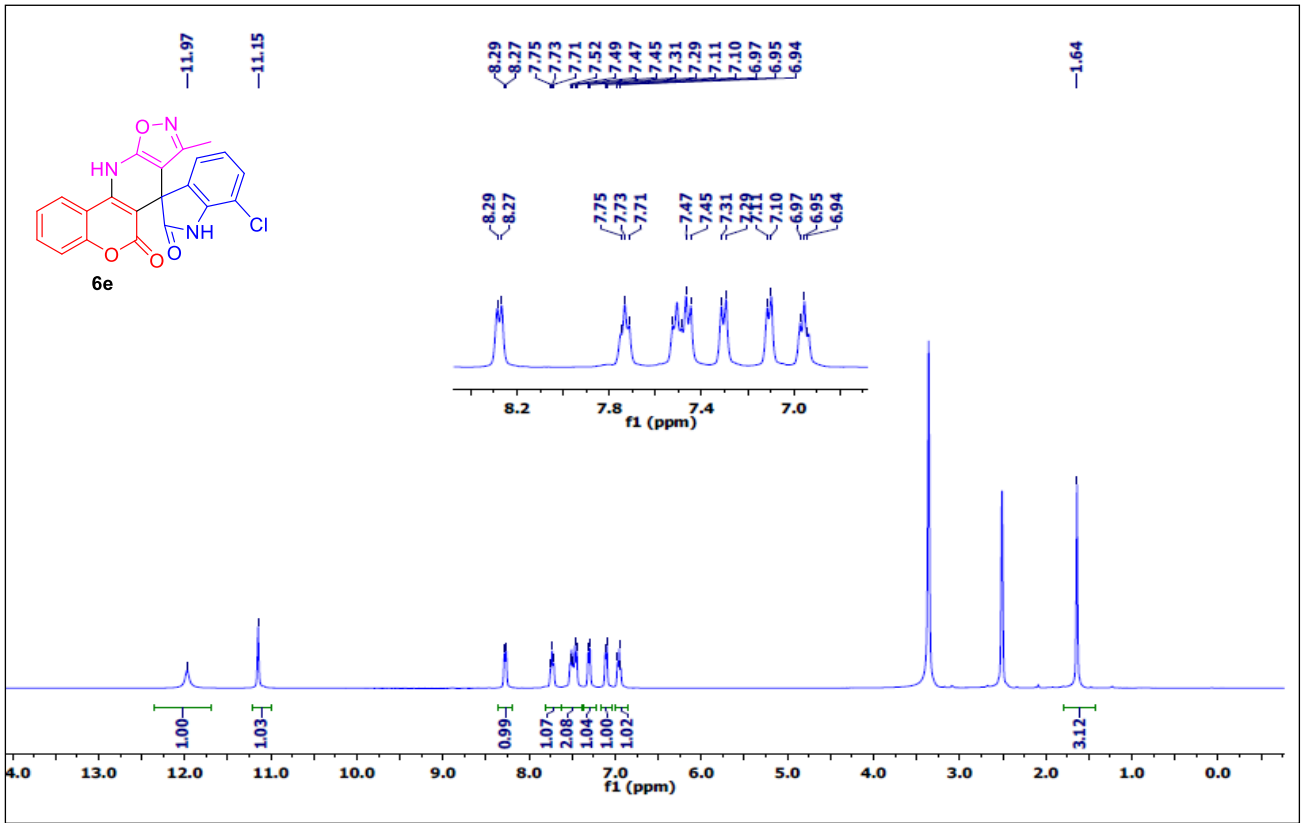


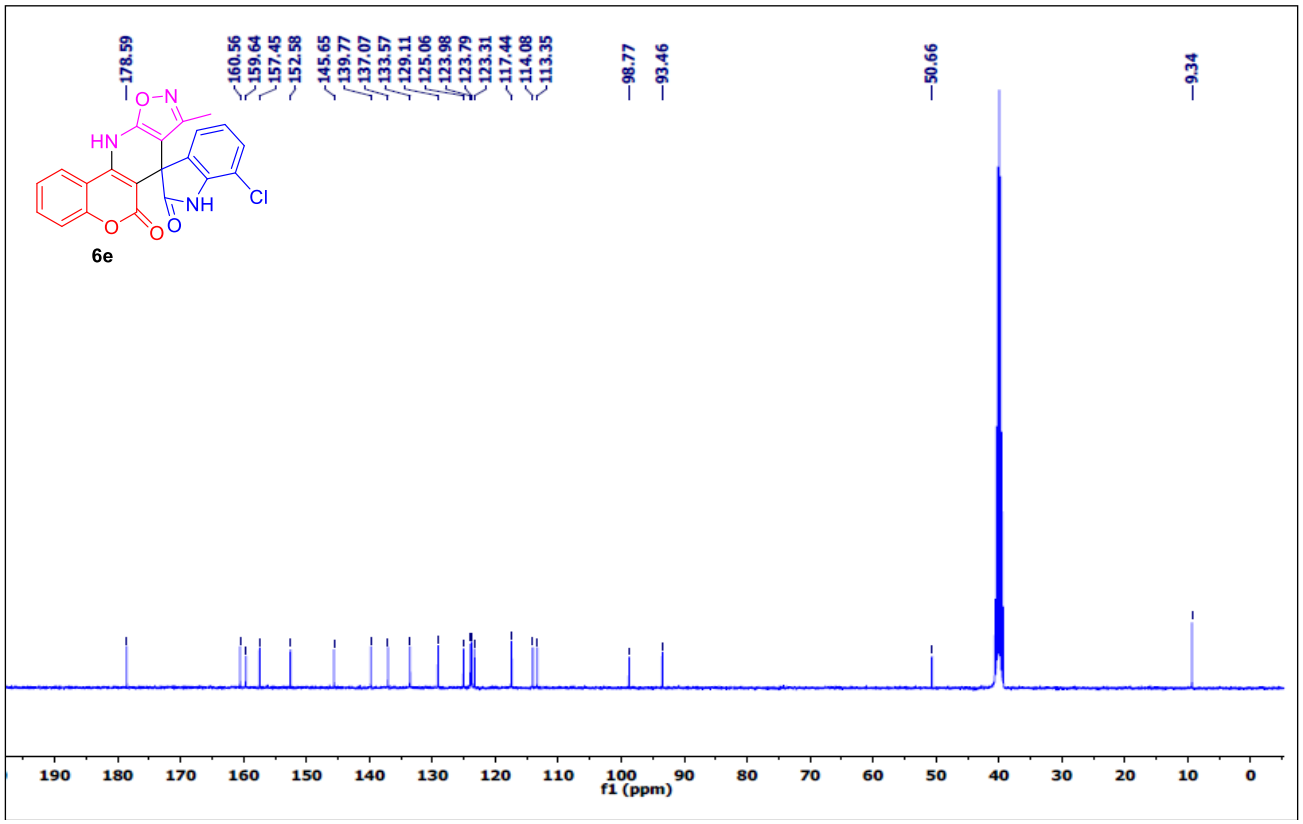
Copies of ^{1}H and ^{13}C spectrum of compound 6d



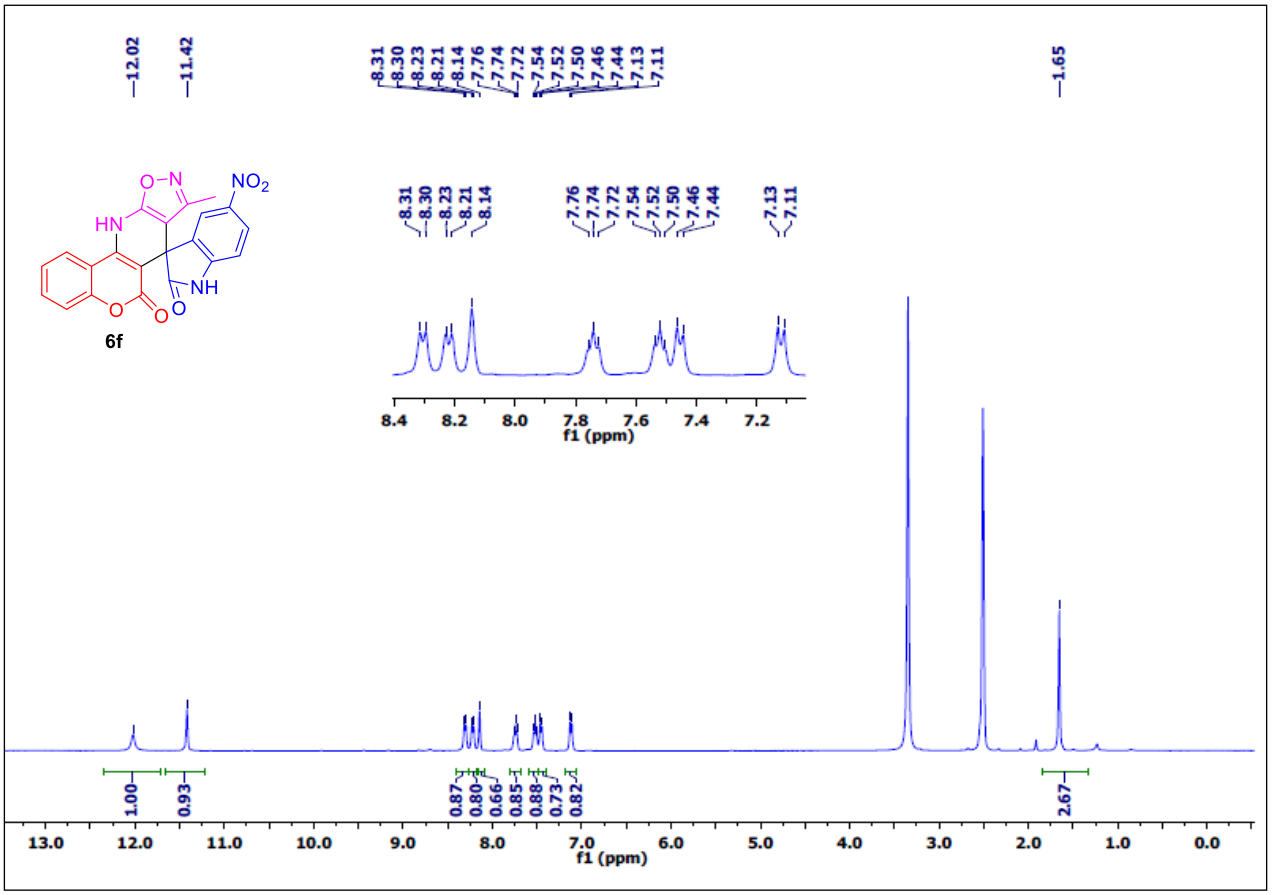


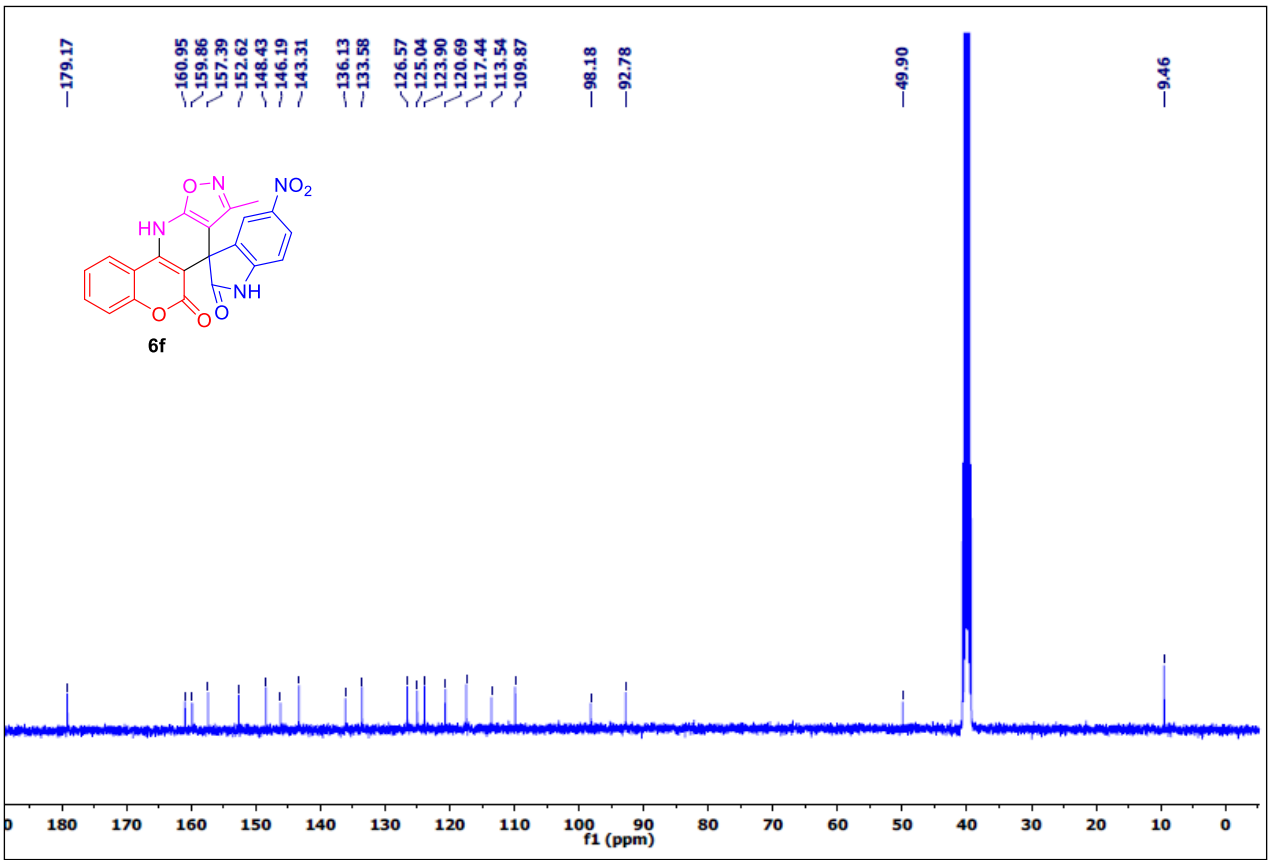
Copies of ^{1}H and ^{13}C spectrum of compound 6e



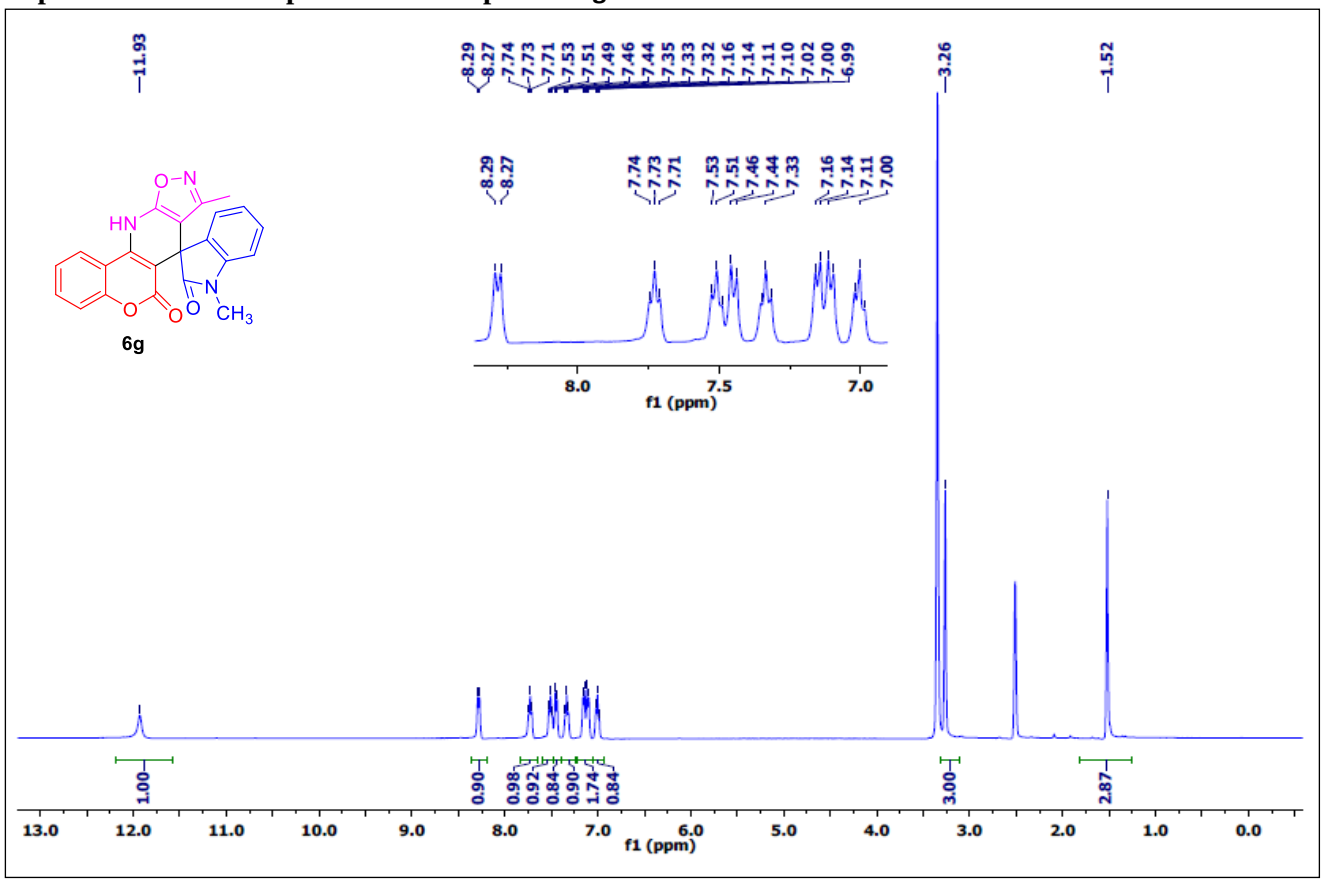


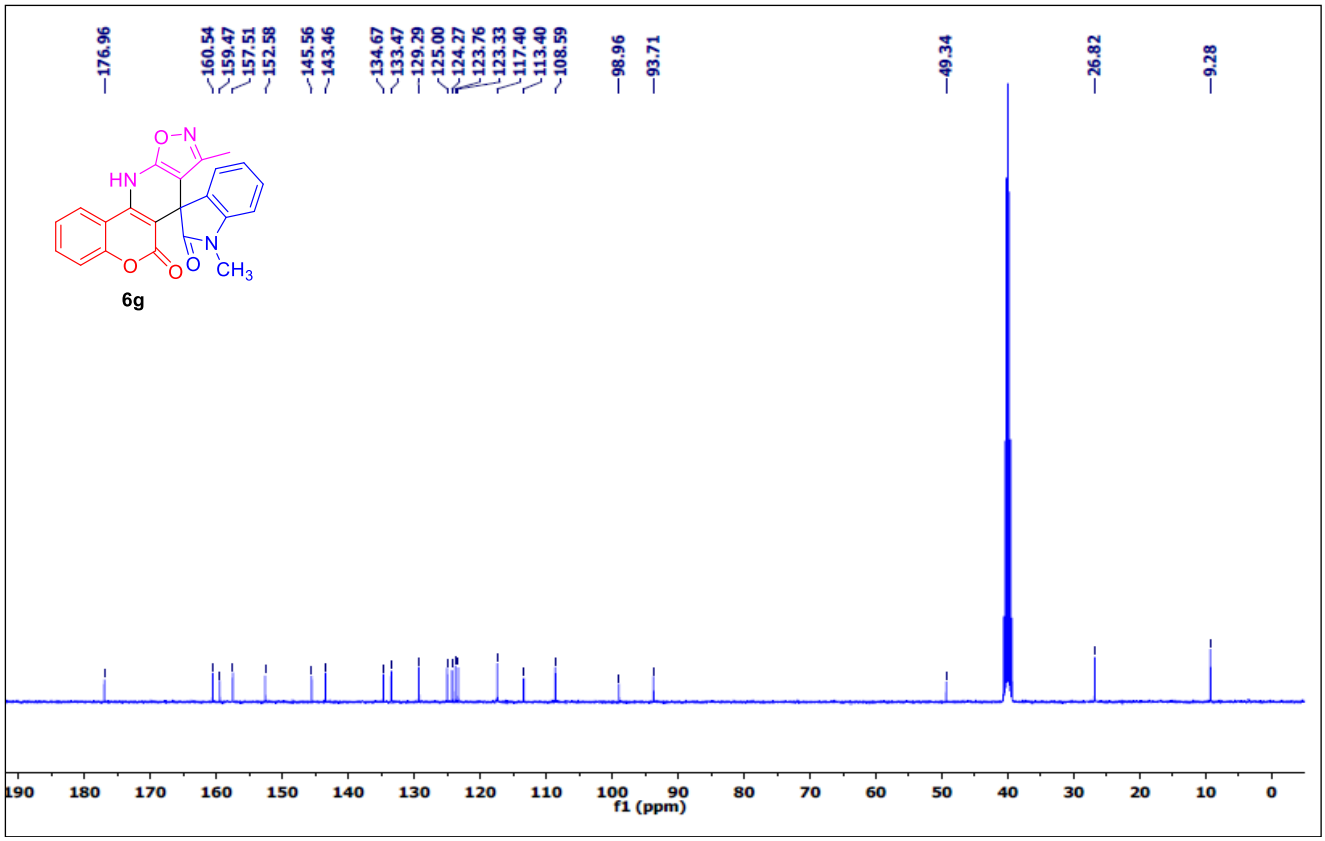
Copies of ^{1}H and ^{13}C spectrum of compound 6f



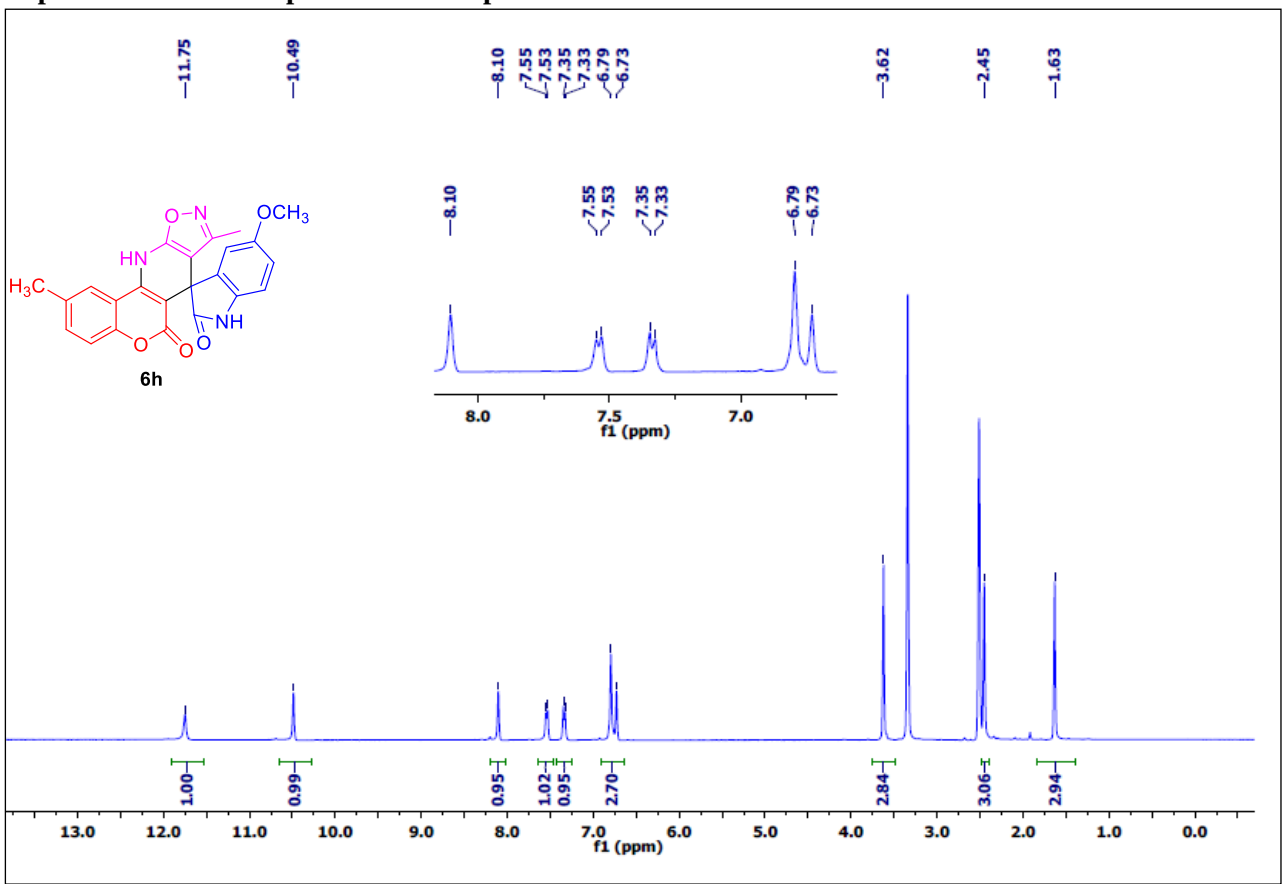


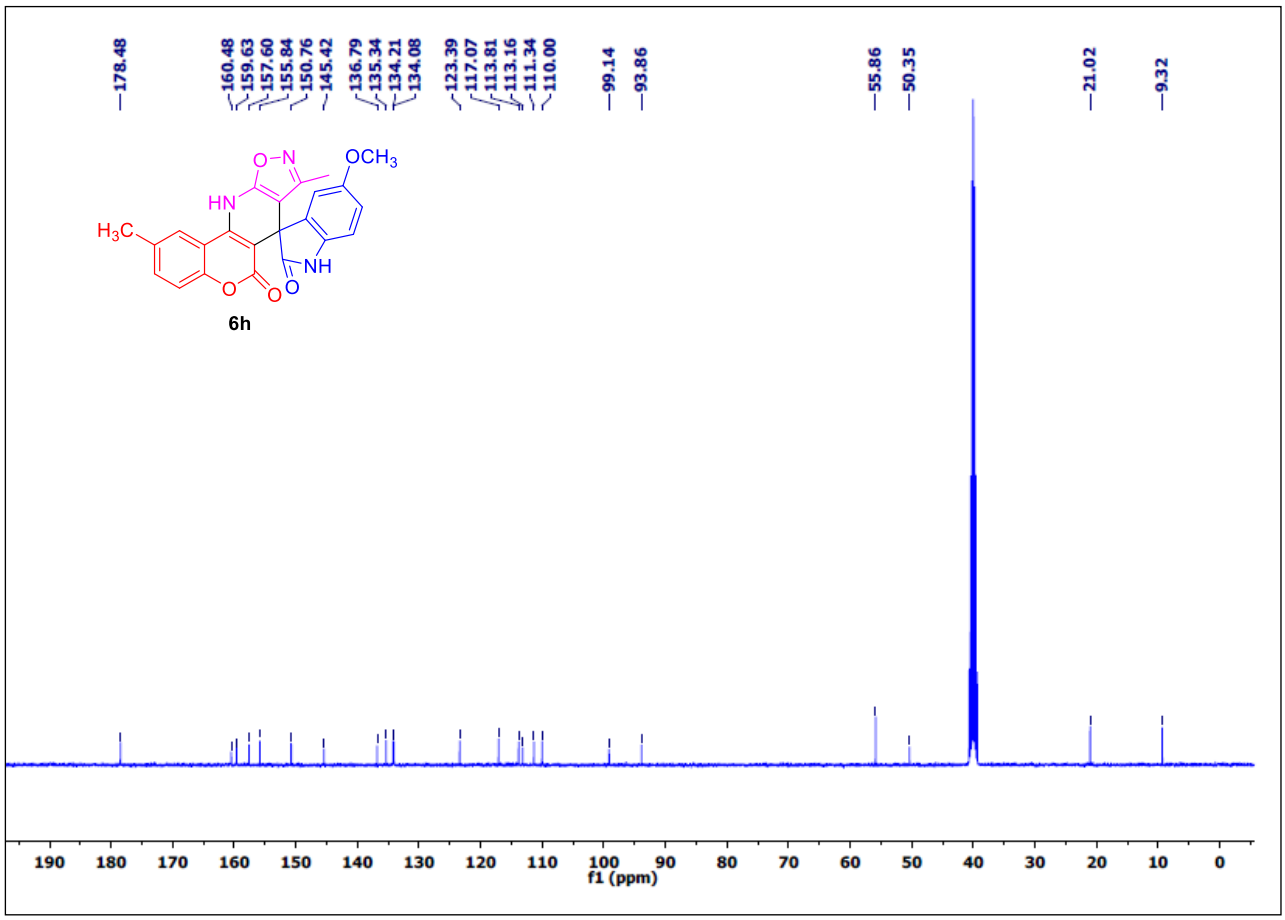
Copies of ^{1}H and ^{13}C spectrum of compound 6g



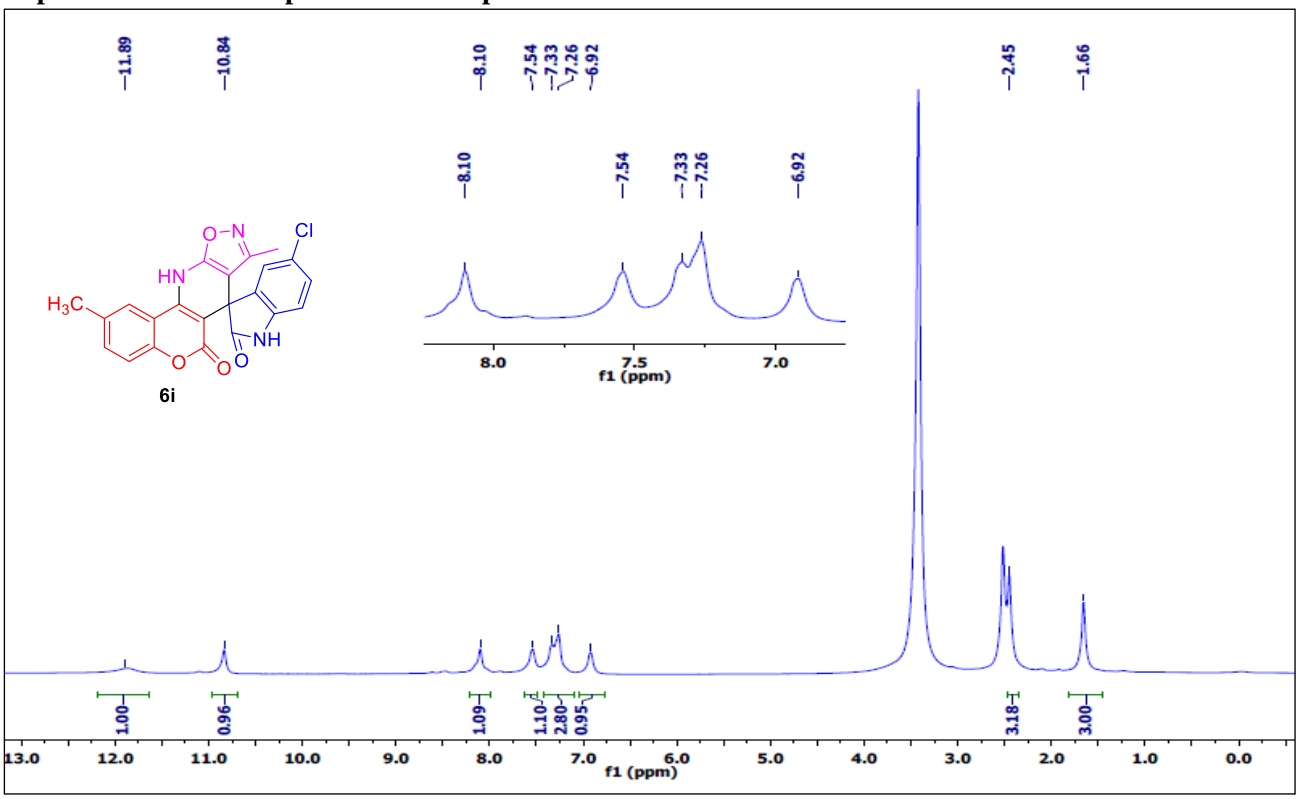


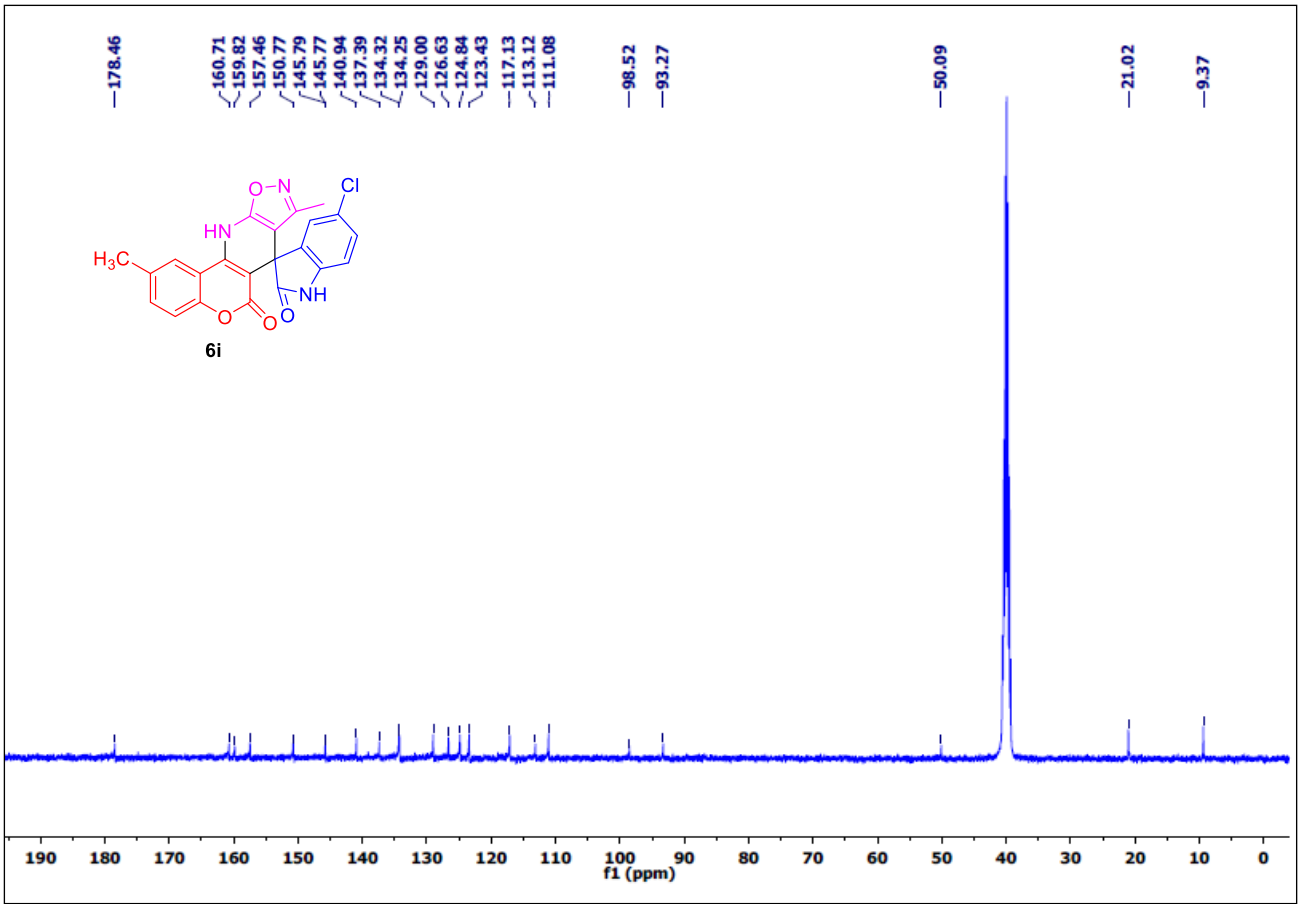
Copies of ^{1}H and ^{13}C spectrum of compound 6h



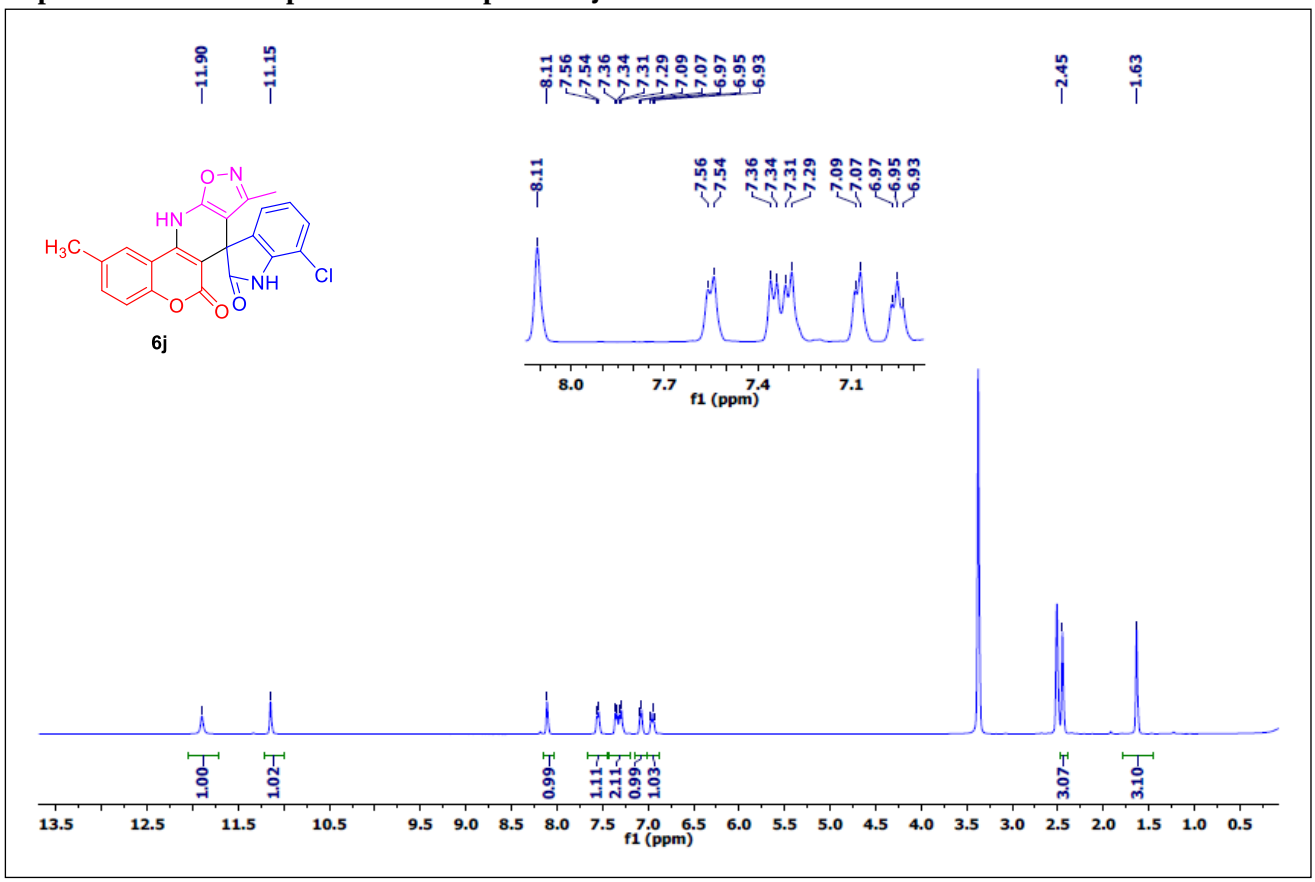


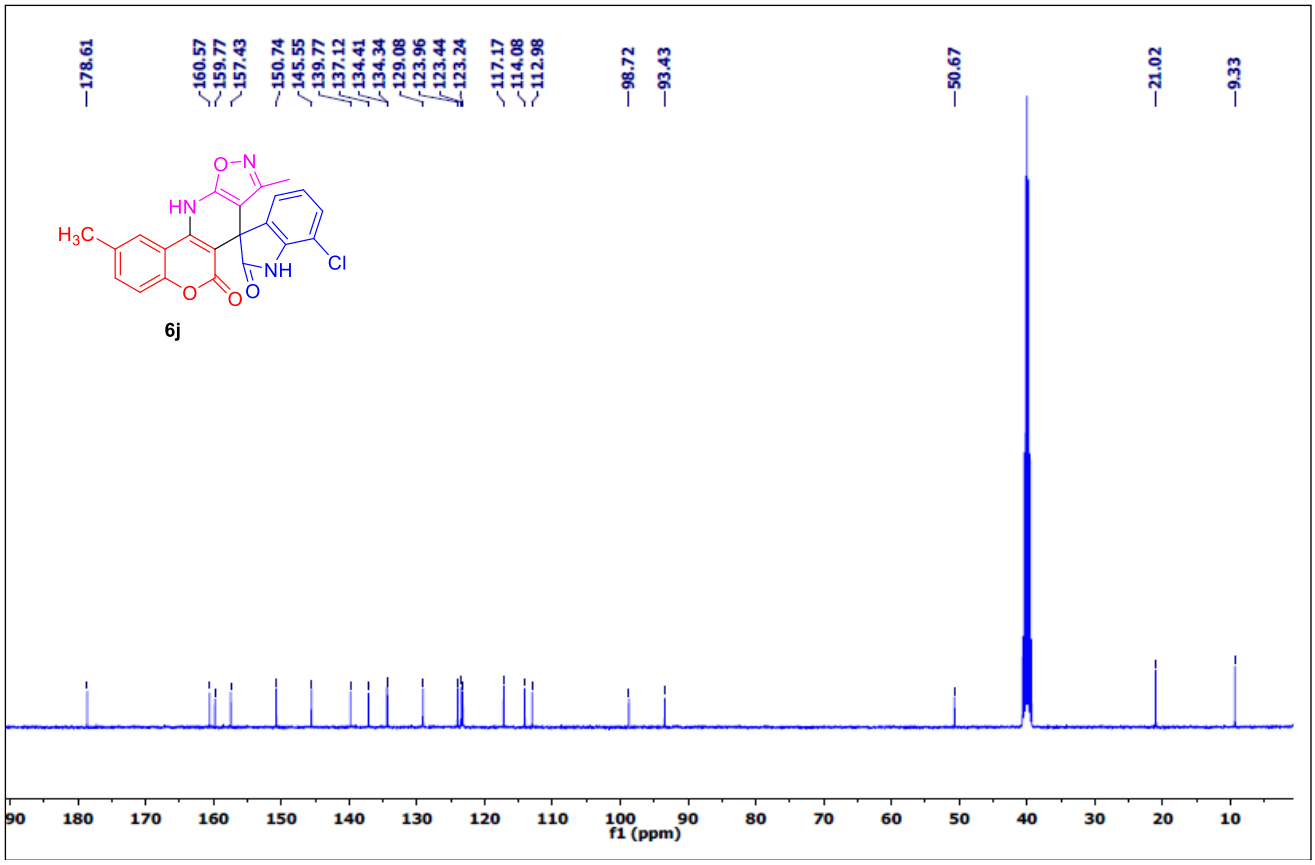
Copies of ^{1}H and ^{13}C spectrum of compound 6i



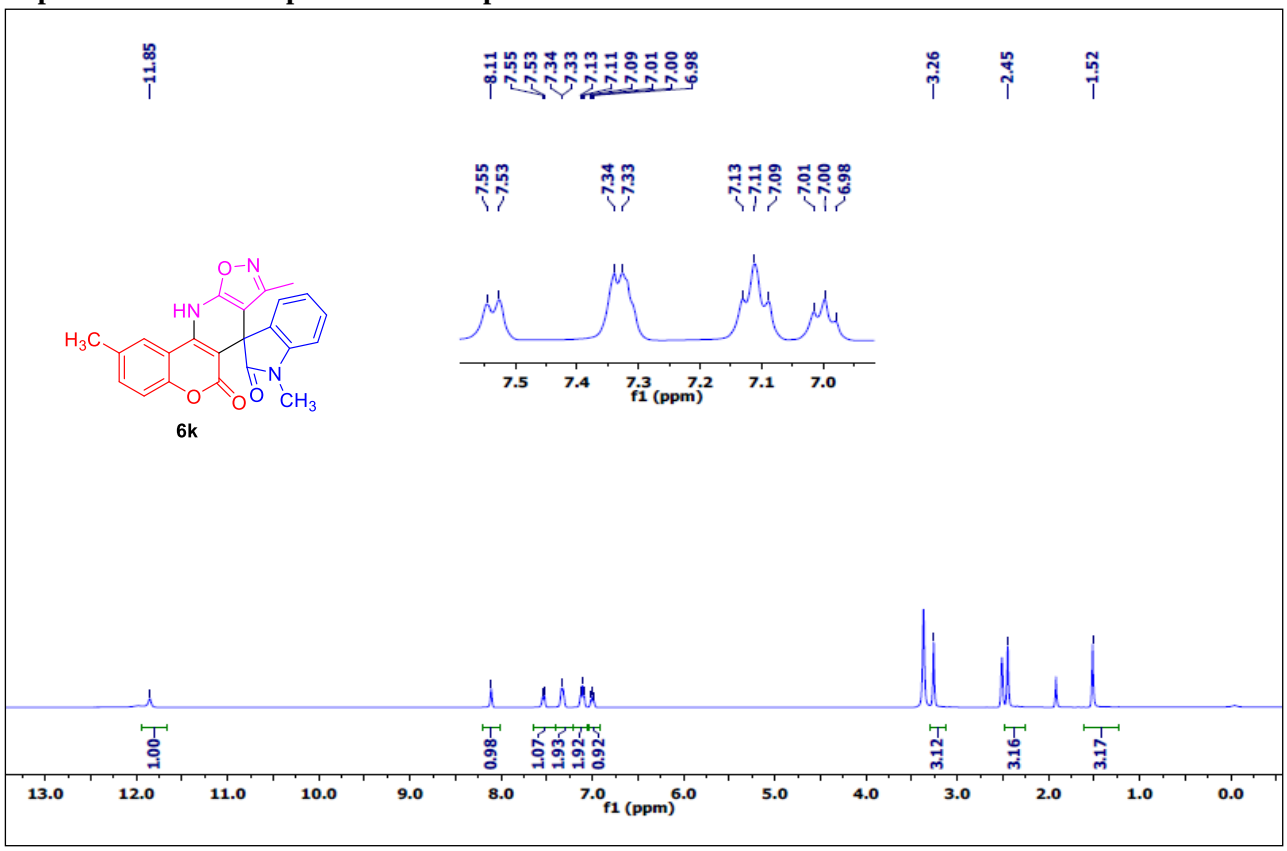


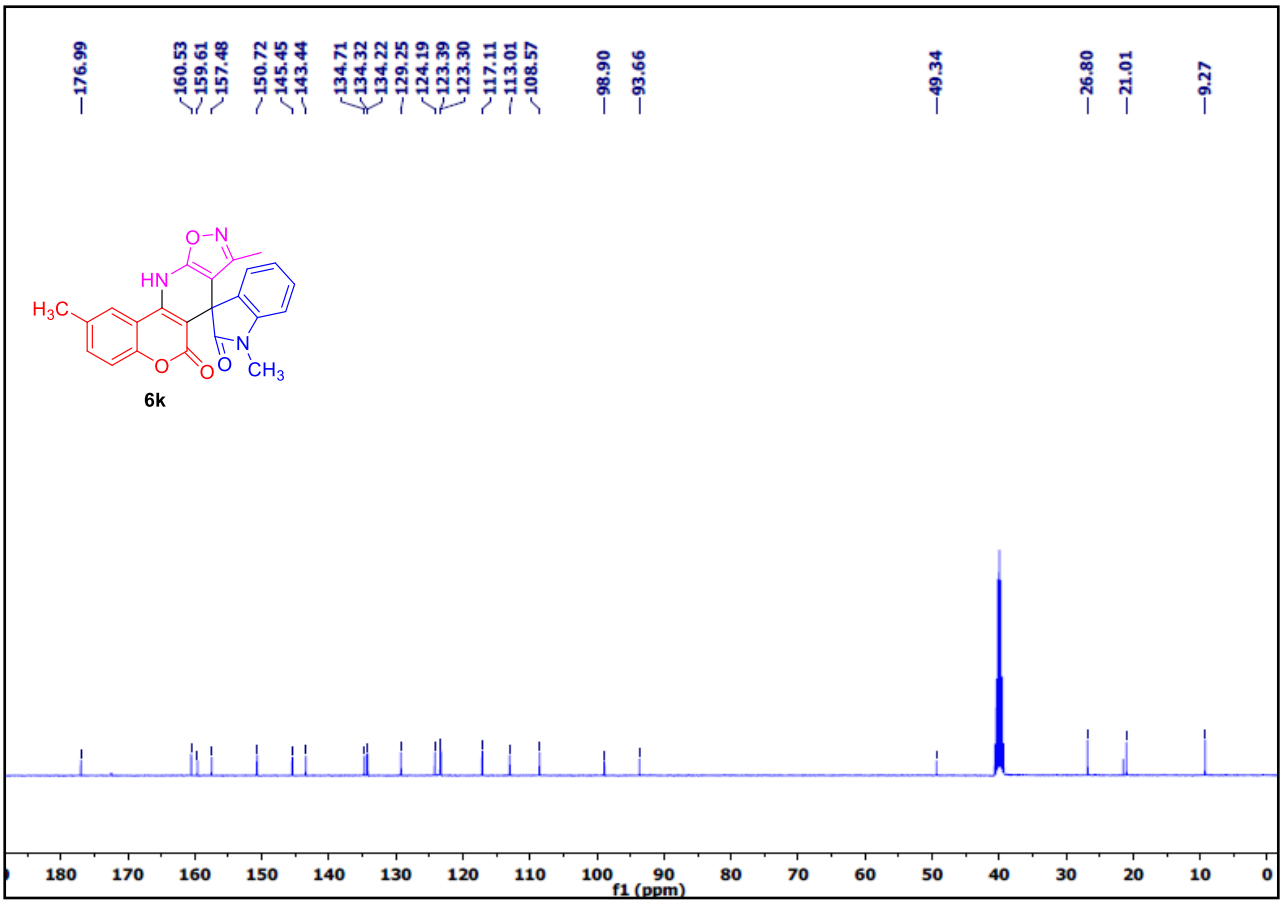
Copies of ^{1}H and ^{13}C spectrum of compound 6j





Copies of ^{1}H and ^{13}C spectrum of compound 6k





Single-Crystal X-Ray Diffraction data

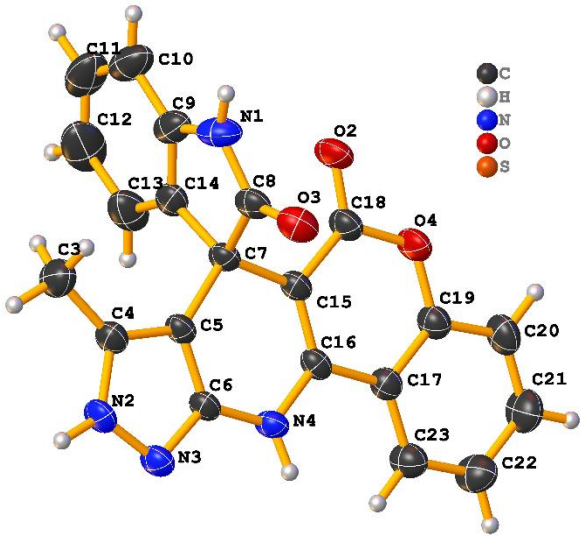


Figure S1. Ortep diagram of **5a** with 50% ellipsoidal probability. (**CCDC 1832278**).

A suitable single crystal of compound **5a** was carefully selected under a polarizing microscope and mounted at the tip of the thin glass fiber using cyanoacrylate (super glue) adhesive. Single crystal structure determination by X-ray diffraction was performed on a Bruker Smart Apex III diffractometer equipped with an Oxford Cryostream low-temperature device and a fine-focus sealed-tube X-ray source (Mo-Kα radiation, λ = 0.71073 Å, graphite monochromated) operating at 50 kV and 30 mA. The structure was solved by direct methods using SHELXS-97. For the final refinement, the hydrogen atoms of the compound was placed geometrically and held in the riding mode. The last cycles of refinement included atomic positions, anisotropic thermal parameters for all the non-hydrogen atoms, and isotropic thermal parameters for all the hydrogen atoms. Details of the structure determination and final refinements for the compound **5a** are given below.

Crystal data and Structure fefinement for 5a

APEX3 software[17] was used for preliminary determination of the unit cell. Crystal structure was solved and refined using SHELXL97,[18] present in the WINGX package of the programs (v 1.63.04a).Data were corrected for absorption effects with SADABS using the multiscan technique.[19] XPREP[17] determined the space to be Pbca, with z = 4 for the formula unit, $C_{23}H_{19}N_4O_4S$. The final anisotropic full-matrix least squares refinement on F_o^2 with 336 variables converged at R_1 = 4.75% for the observed data and wR2 = 11.22% for all data. The standard deviation[20] of an observation of unit weight was 1.068. Unit weights were used (least squares function minimized: (SHELXL-2014/7)[28]: Σ w $(F_o^2 - F_c^2)^2$ where w is the least squares weights. Standard deviation of an observation of unit weight: $[\Sigma \text{ w } (F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$ where N_o is the number of observations, N_v is the number of variables). The largest peak on the final difference electron density synthesis was 0.215 e/Å^{-3}and the deepest hole was -0. 285 e/Å-3. On the basis of the final model, the calculated density is 1.408 g cm^{-3} and F (000) = 933.7. This slightly high R_1 was due to the disordered of DMSO molecule as a solvent. The crystal structure of **5a** has been shown below using OLEX2.[22] The details of the crystallographic data are listed in Table S1.

Table S1. Crystal data and structure refinement for **5a**

CCDC Number	**1832278**
Empirical formula	$C_{23}H_{19}N_4O_4S$
Formula weight	447.92
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 9.3279(6) Å α= 90°.
	b = 21.2988(14) Å β= 113.536(2)°

	c = 11.6031(8) Å γ = 90°
Volume	2113.5(2) Å3
Z	4
Density (calculated)	1.408 Mg/m3
Absorption coefficient	0.192 mm-1
F(000)	933.7
Crystal size	0.4 x 0.1 x 0.1 mm3
Theta range for data collection	2.566 to 25.000°
Index ranges	-11<=h<=11, -25<=k<=25, -13<=l<=13
Reflections collected	49871
Independent reflections	3710 [R(int) = 0.0584]
Completeness to theta = 25.000°	99.7 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	3710 / 102 / 336
Goodness-of-fit on F2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.0983
R indices (all data)	R1 = 0.0873, wR2 = 0.1122
Extinction coefficient	0.0061(8)
Largest diff. peak and hole	0.215 and -0.285 e.Å-3

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