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Supporting Informations

Diversity oriented synthesis of tri-substituted methanes containing aminouracil, hydroxynaphthaquinone/ hydroxycoumarin moiety using organocatalysed multicomponent reactions in aqueous medium

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Experimental Section

Starting materials and solvents are commercially available and used without further purification. The purity of the synthesized compounds were ascertained by thin layer chromatography on silica gel GF 254 in ethyl acetate using iodine vapours as detecting agent. Melting points were determined by the melting point determination apparatus using capillary tube method. IR spectra were recorded on a Shimadzu FTIR spectrophotometer in KBr pellet. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ and DMSO-d_6 and are expressed in parts per million (δ, ppm) downfield using Me_4Si as internal standard on Bruker Avance II 400 MHz spectrophotometer. Elemental analyses were carried out in a Perkin Elmer 2400 automatic carbon, hydrogen, nitrogen analyzer.

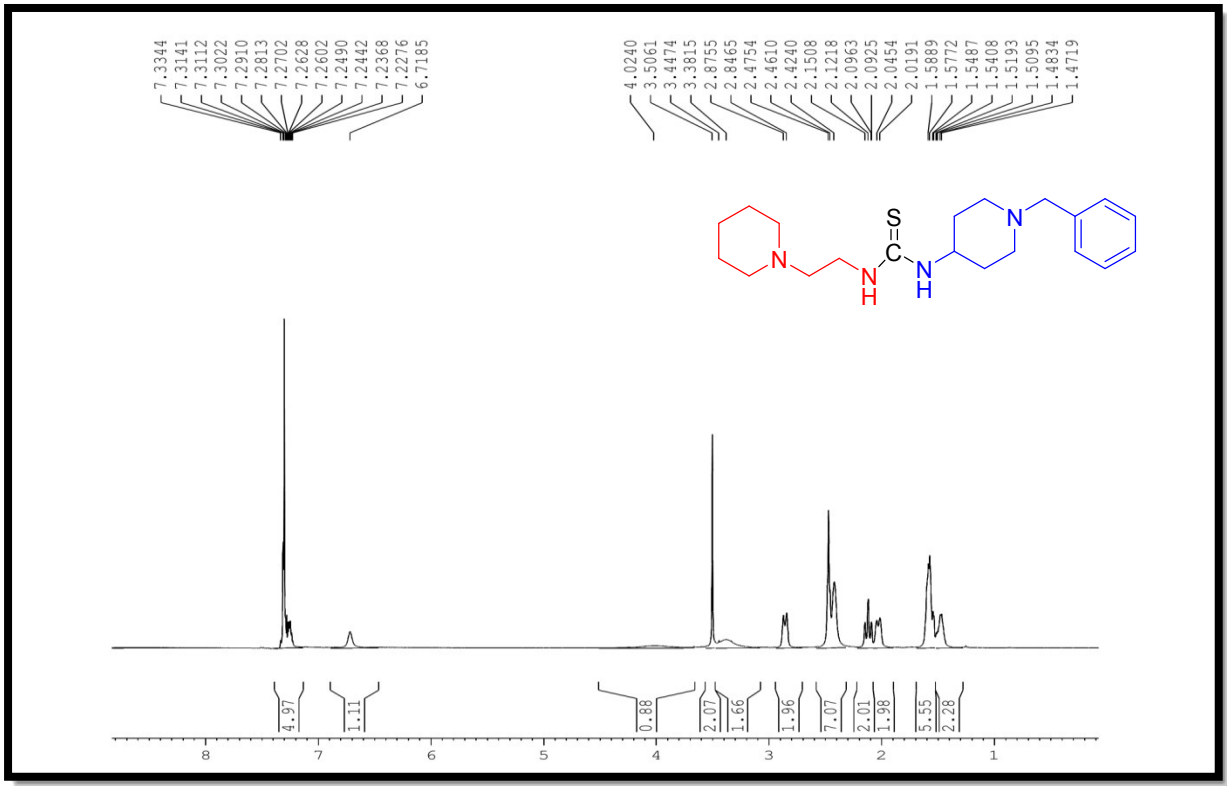
General experimental procedure for the synthesis of bifunctional thiourea based organocatalyst I:

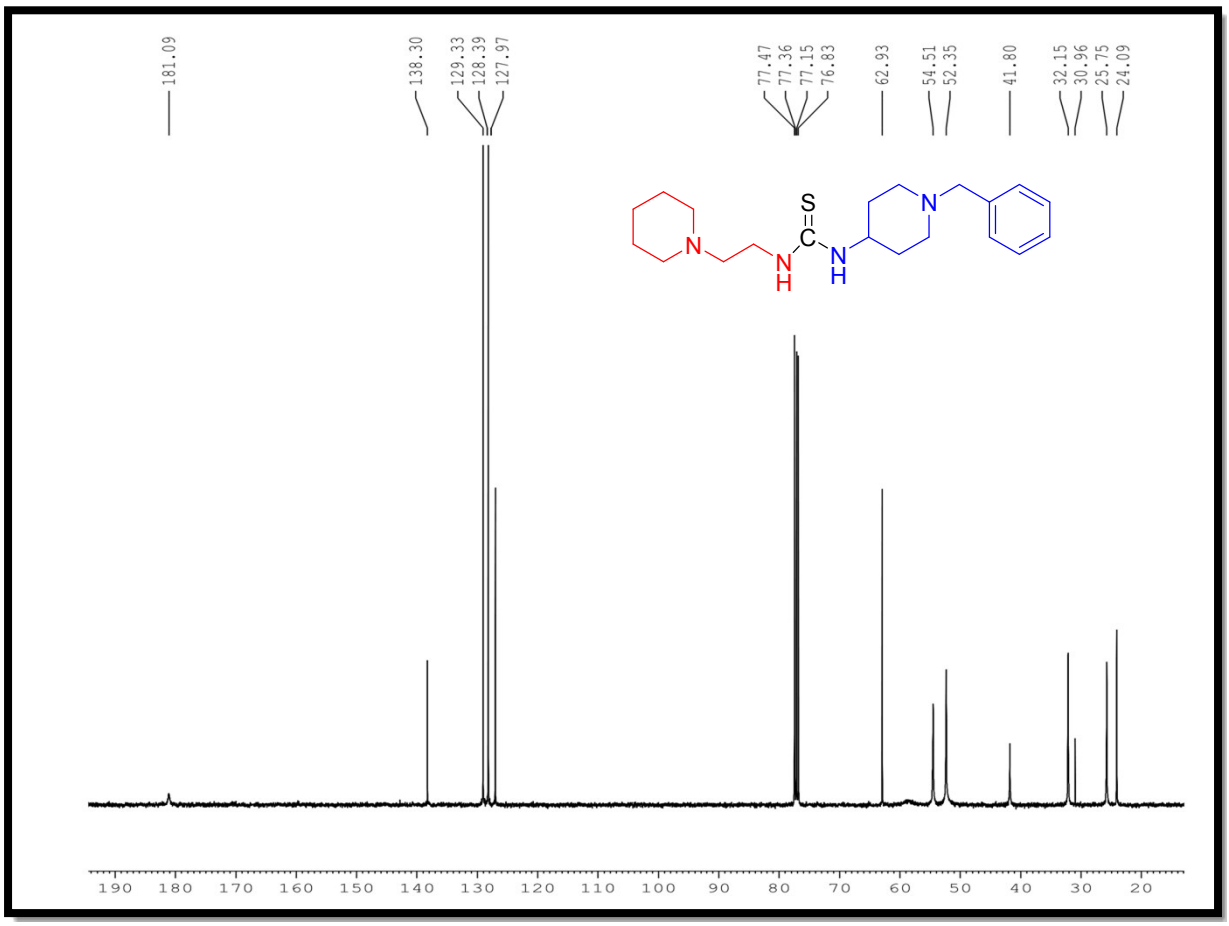
First, 4-amino-1-benzyl piperidine (0.5 mmol) was dissolved in DCM and allowed to cool at 0 C. After ½ an hour, 2-piperidinoethyl isothiocyanate (0.5 mmol) was added in the reaction mixture and allowed to stir at room temperature till the completion of the reaction as checked by TLC. The reaction mixture was cooled, the solid was filtered off and washed with ethanol to afford the desired product.

Typical experimental procedure for the synthesis of 4c: To a solution of 2-hydroxy-1,4-naphthaquinone 0.174 g (1 mmol) and 4-chlorobenzaldehydes 0.14 g (1 mmol) in 1 ml water, 20 mol% thiourea-based organocatalyst I was added and stirred under reflux condition for 15 minutes. Afterwards, 1,3-dimethyl-6-aminouracil 0.155g (1 mmol) was introduced and stirring was continued till the completion of the reaction as checked by TLC. The resulting mixture was cooled at room temperature, the solid was filtered off, washed with water first, then by 5 ml ethanol to afford the pure product.

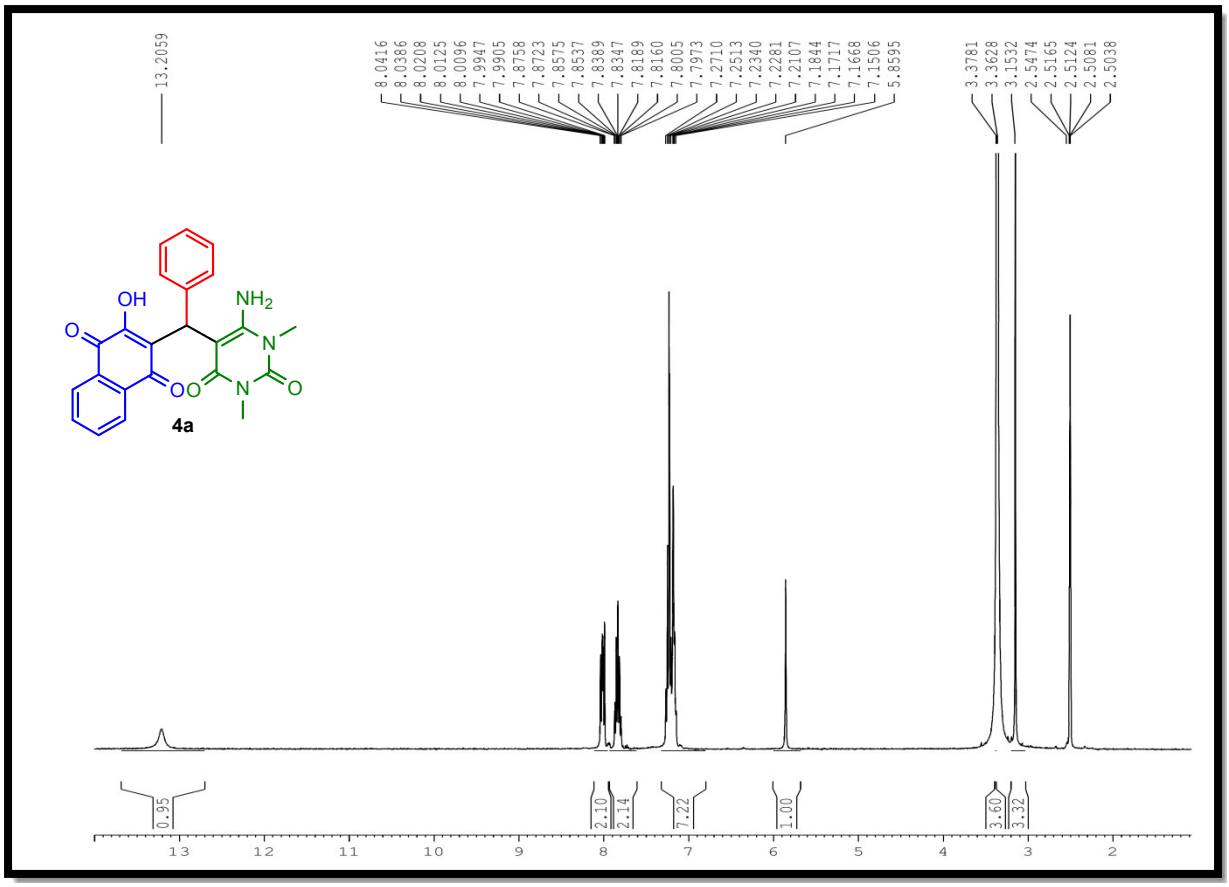
Typical experimental procedure for the synthesis of 6b: To a solution of 4-hydroxycoumarin 0.162 g (1 mmol) and 4-methoxybenzaldehydes 0.136 g (1 mmol) in 1 ml water, 20 mol% thiourea-based organocatalyst I was added and stirred under reflux condition for 15 minutes. Afterwards, 1,3-dimethyl-6-aminouracil 0.155g (1 mmol) was introduced and stirring was continued till the completion of the reaction as checked by TLC. The resulting mixture was cooled at room temperature, the solid was filtered off, washed with water first, then by 5 ml ethanol to afford the pure product.

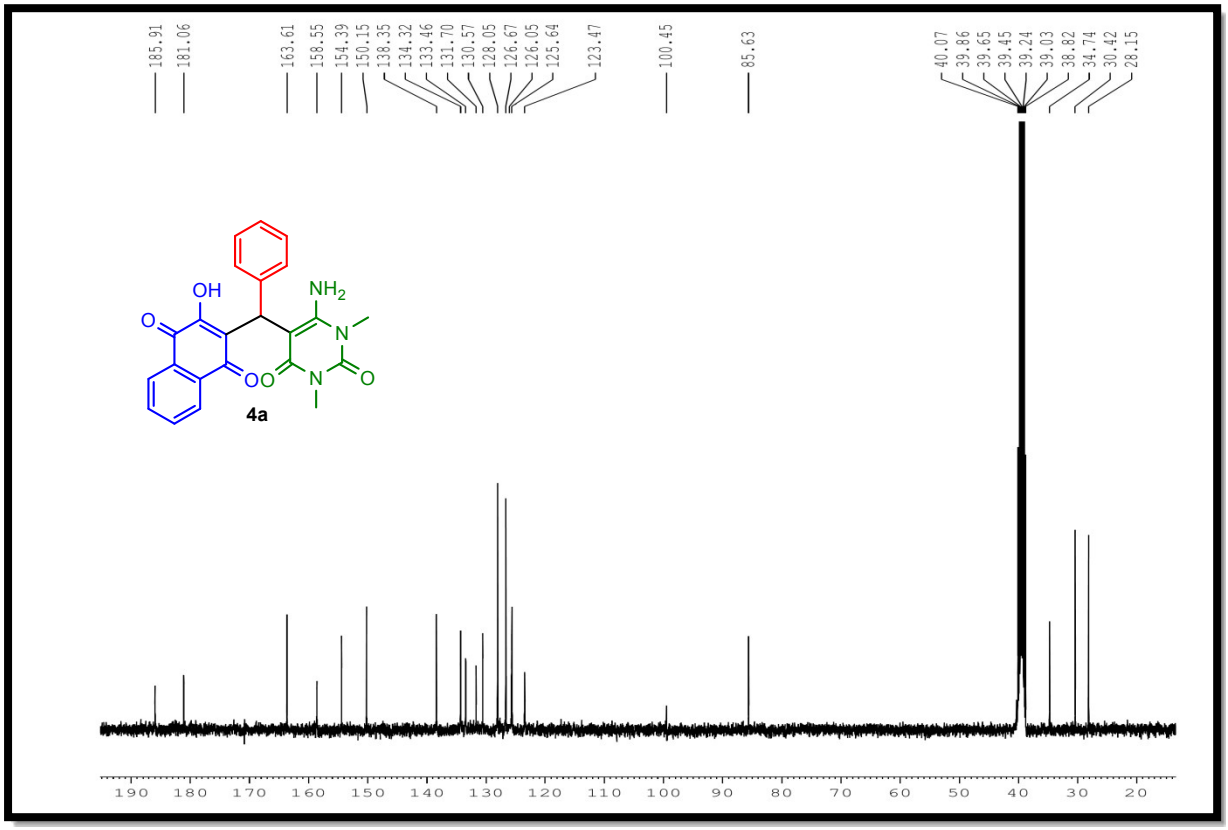
^{1}H & ^{13}C NMR of thiourea-based organocatalyst I





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





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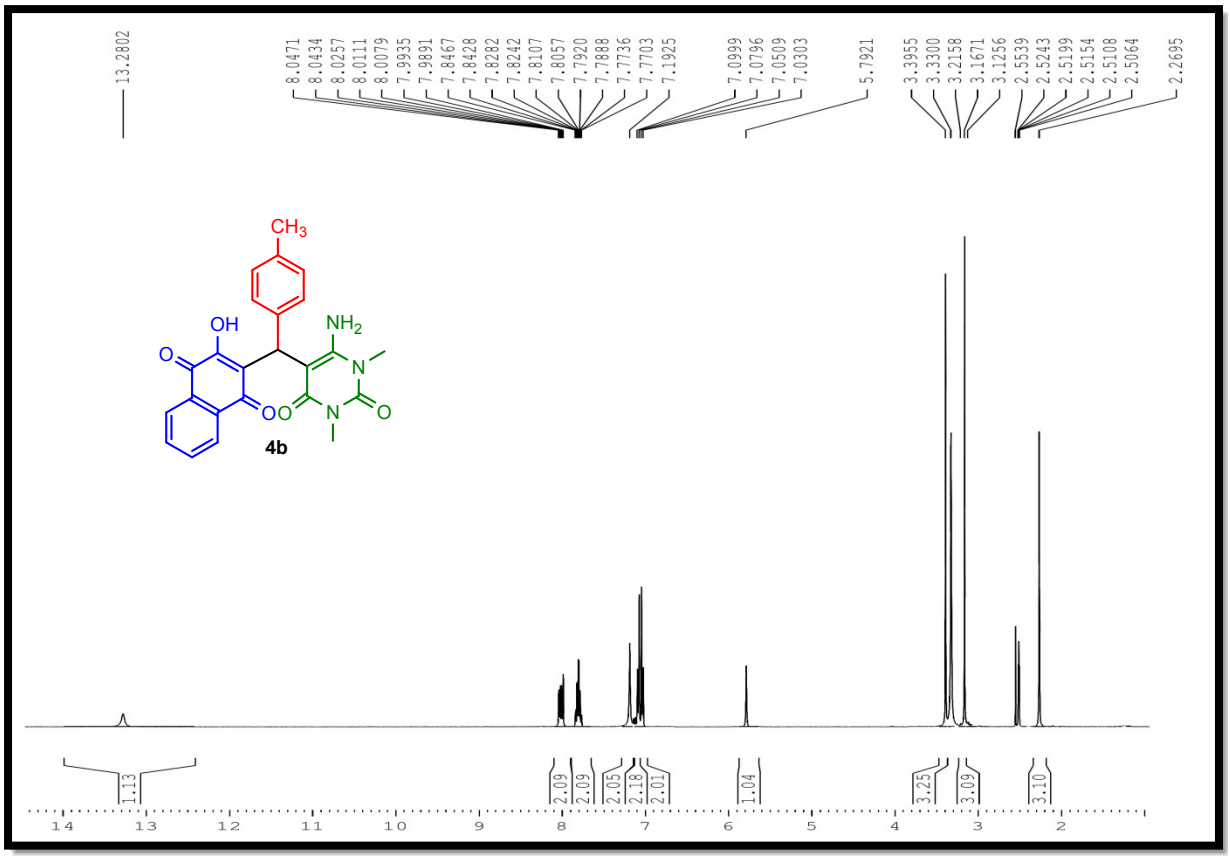

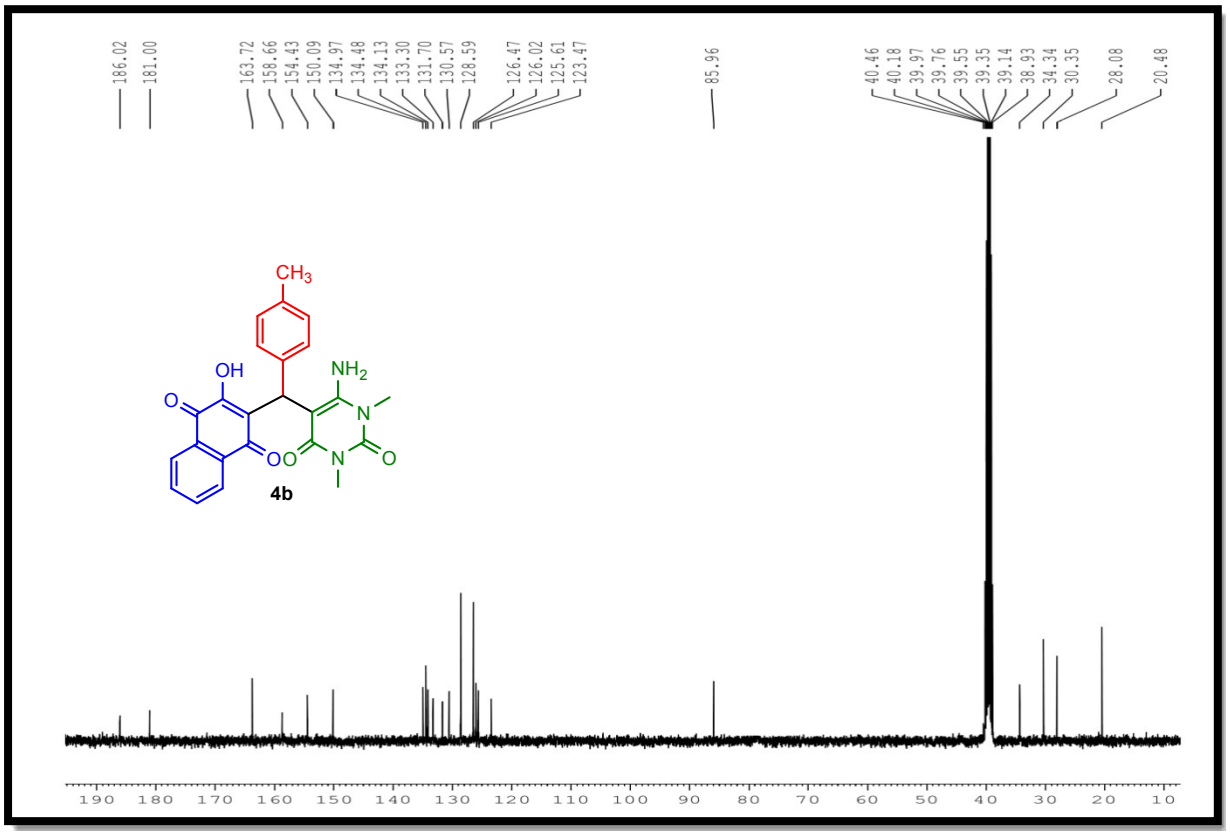

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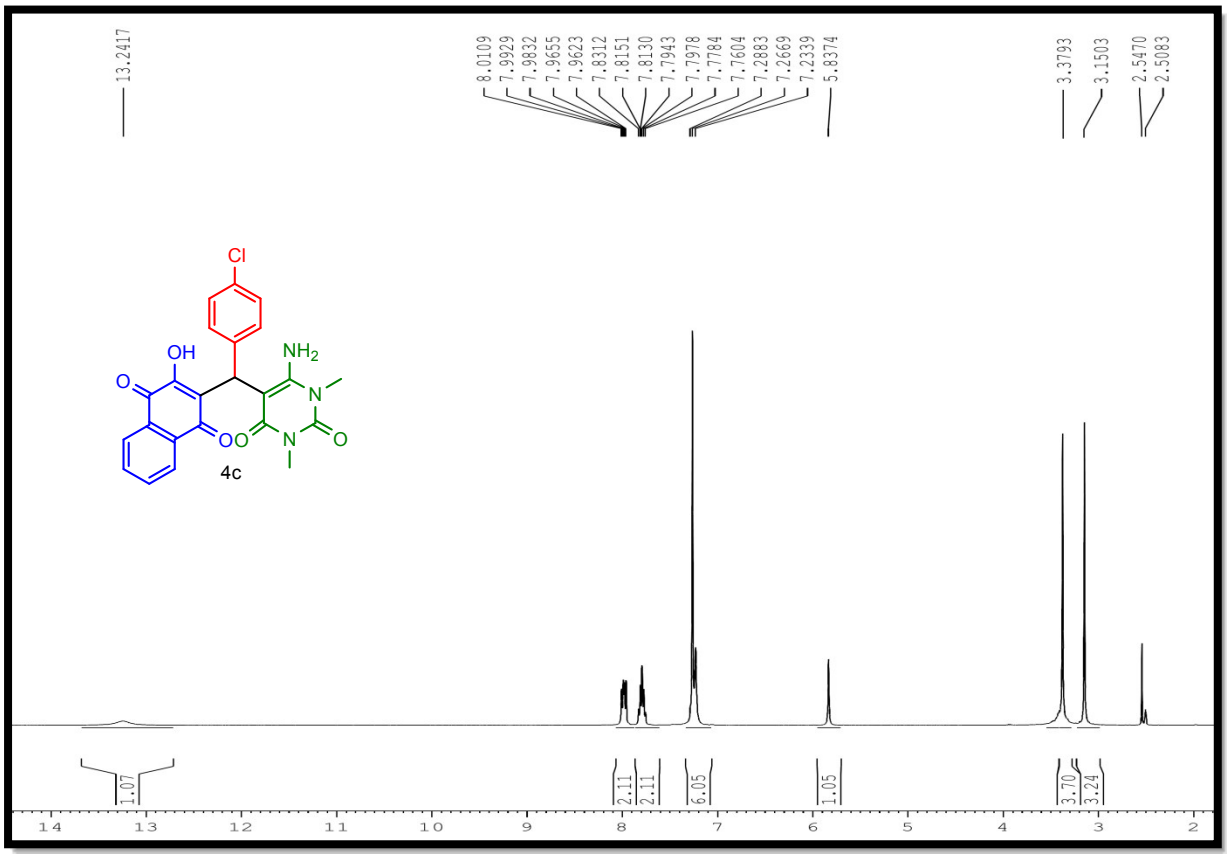

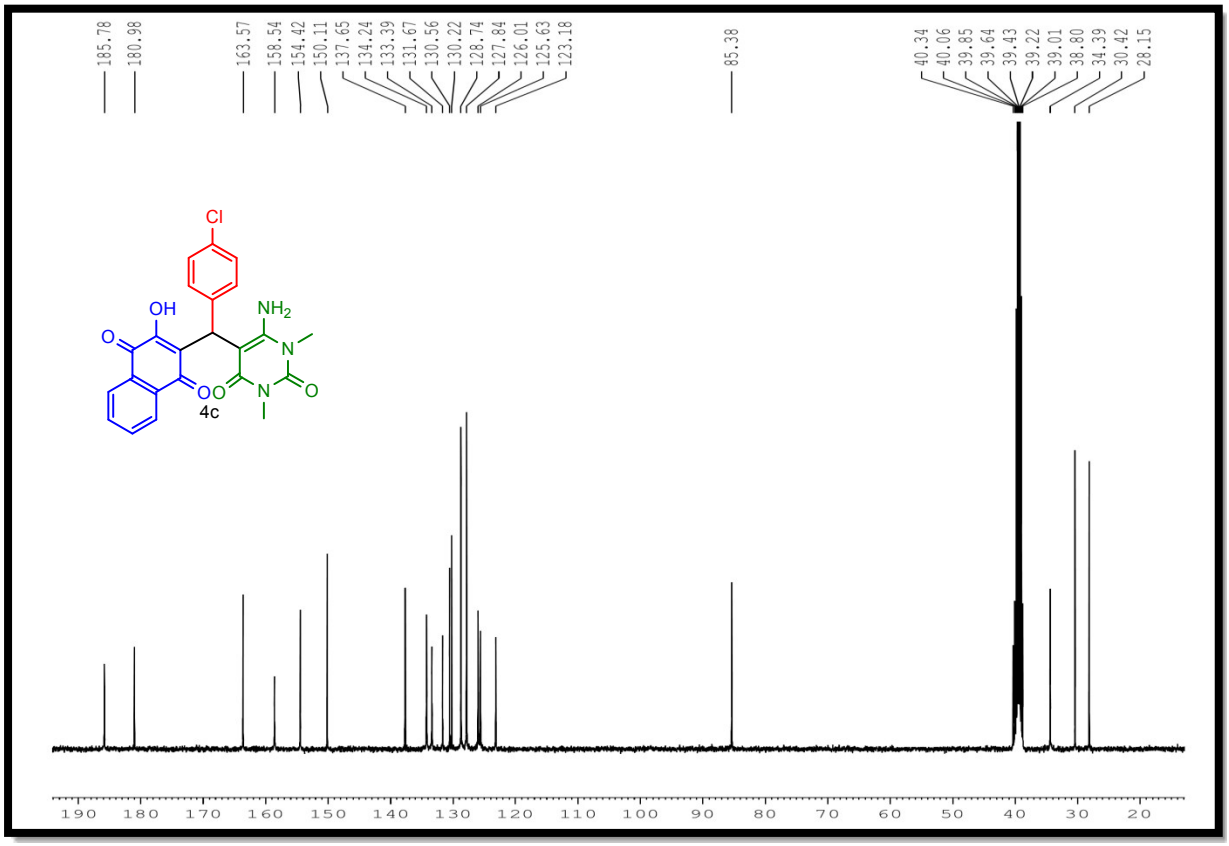

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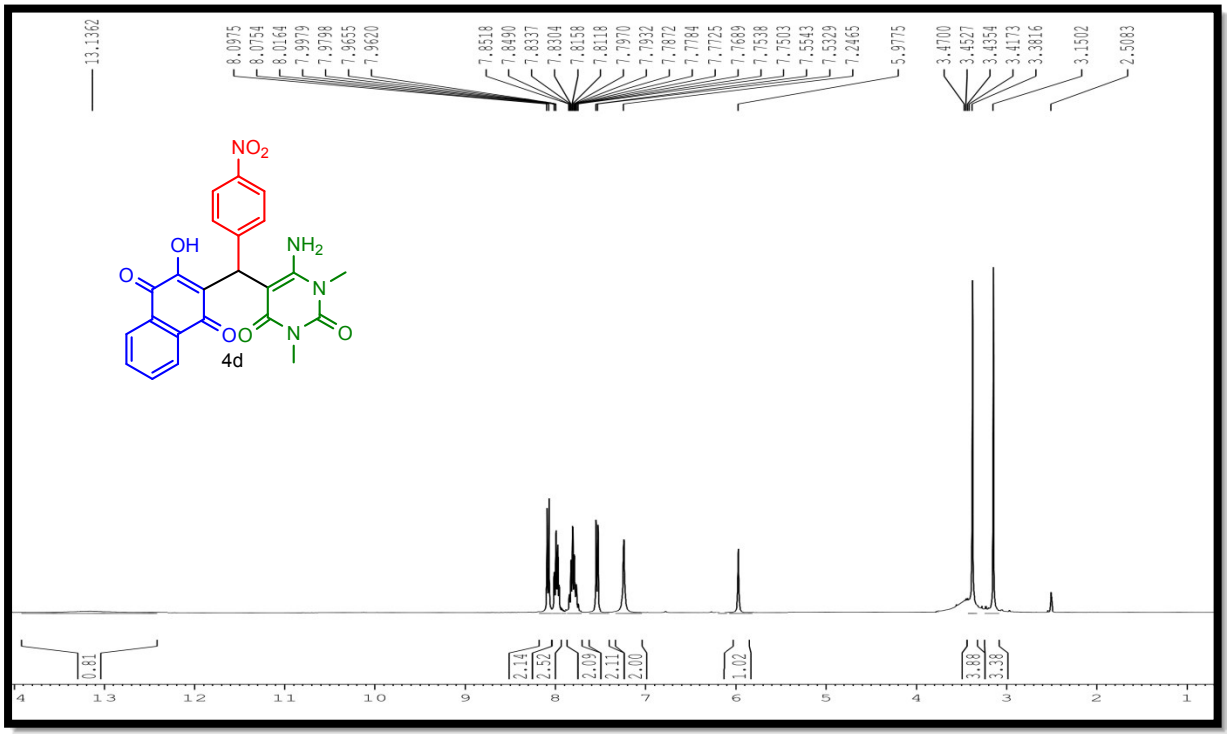

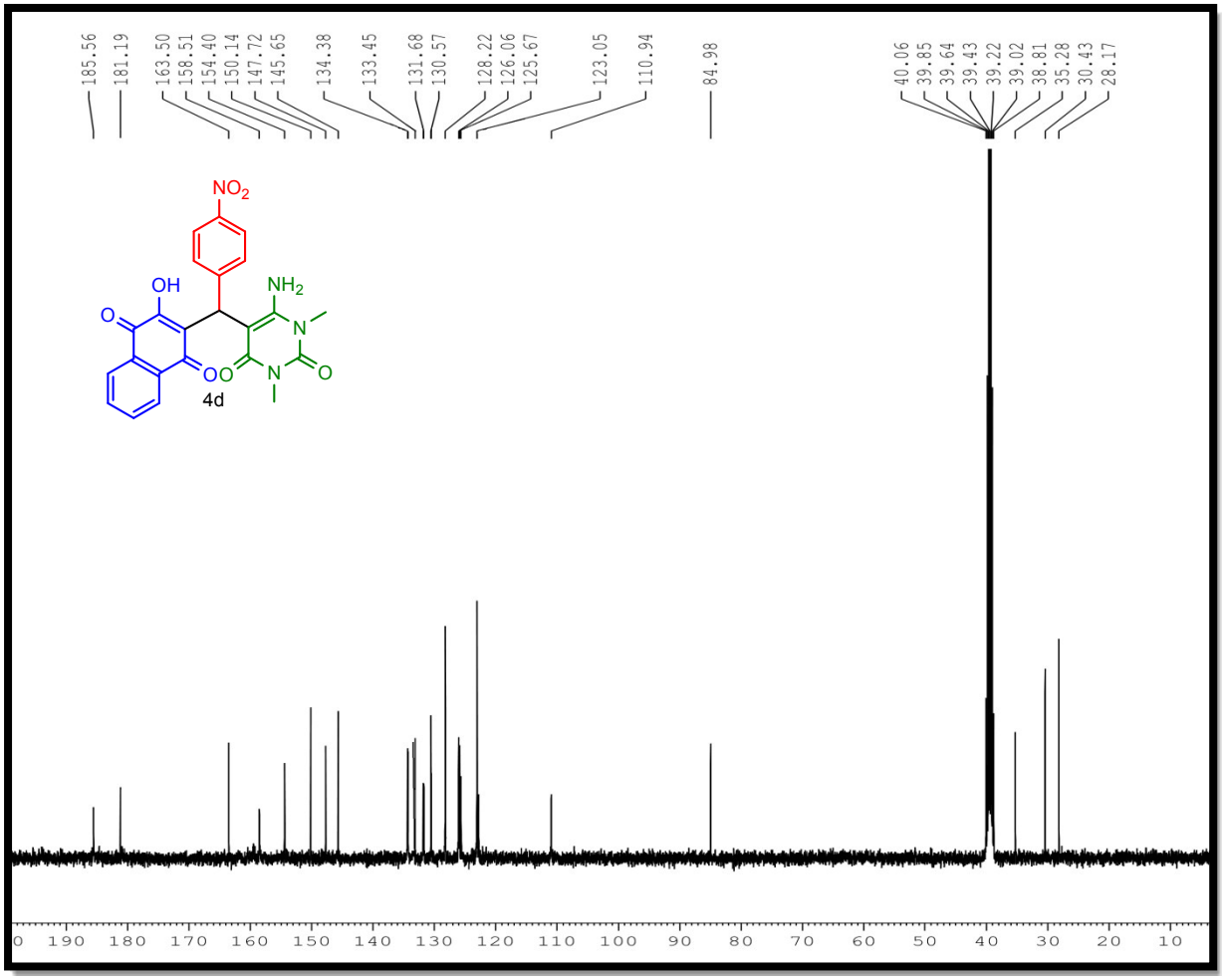

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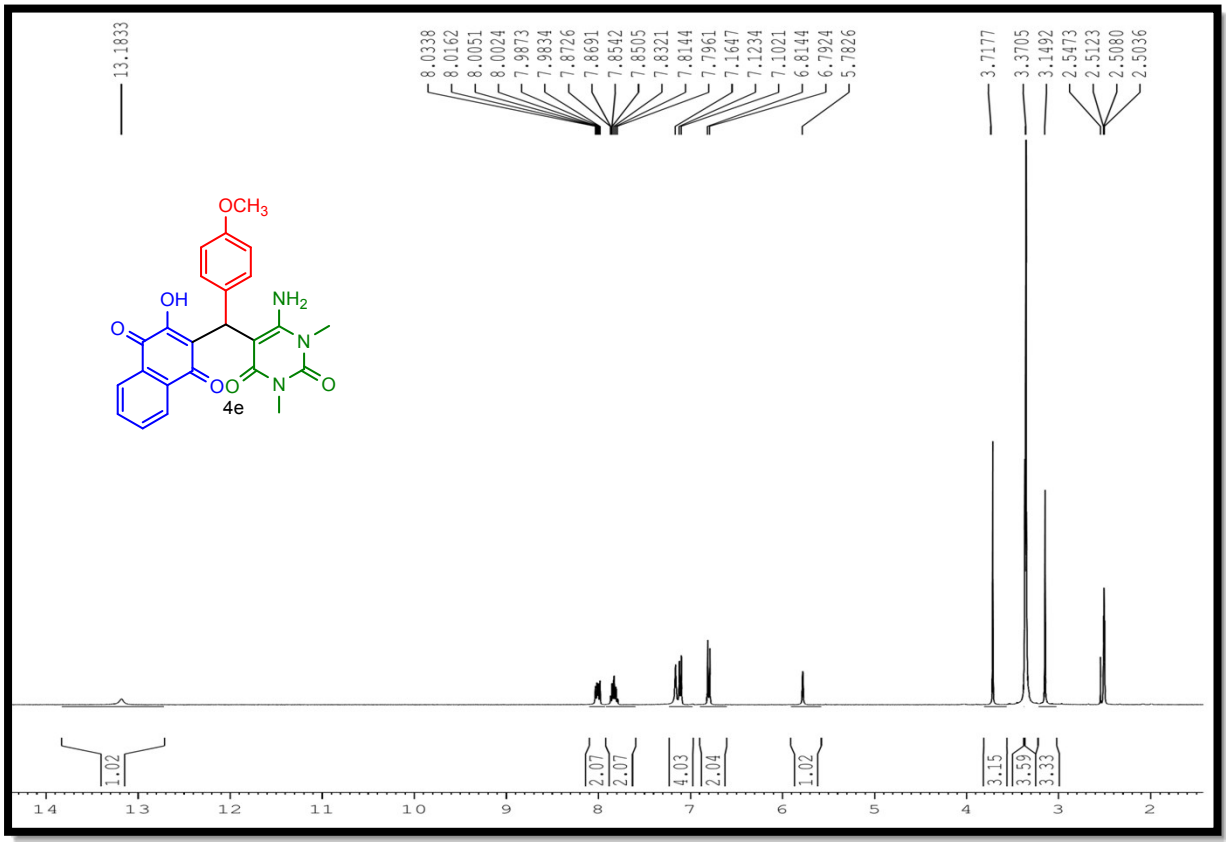

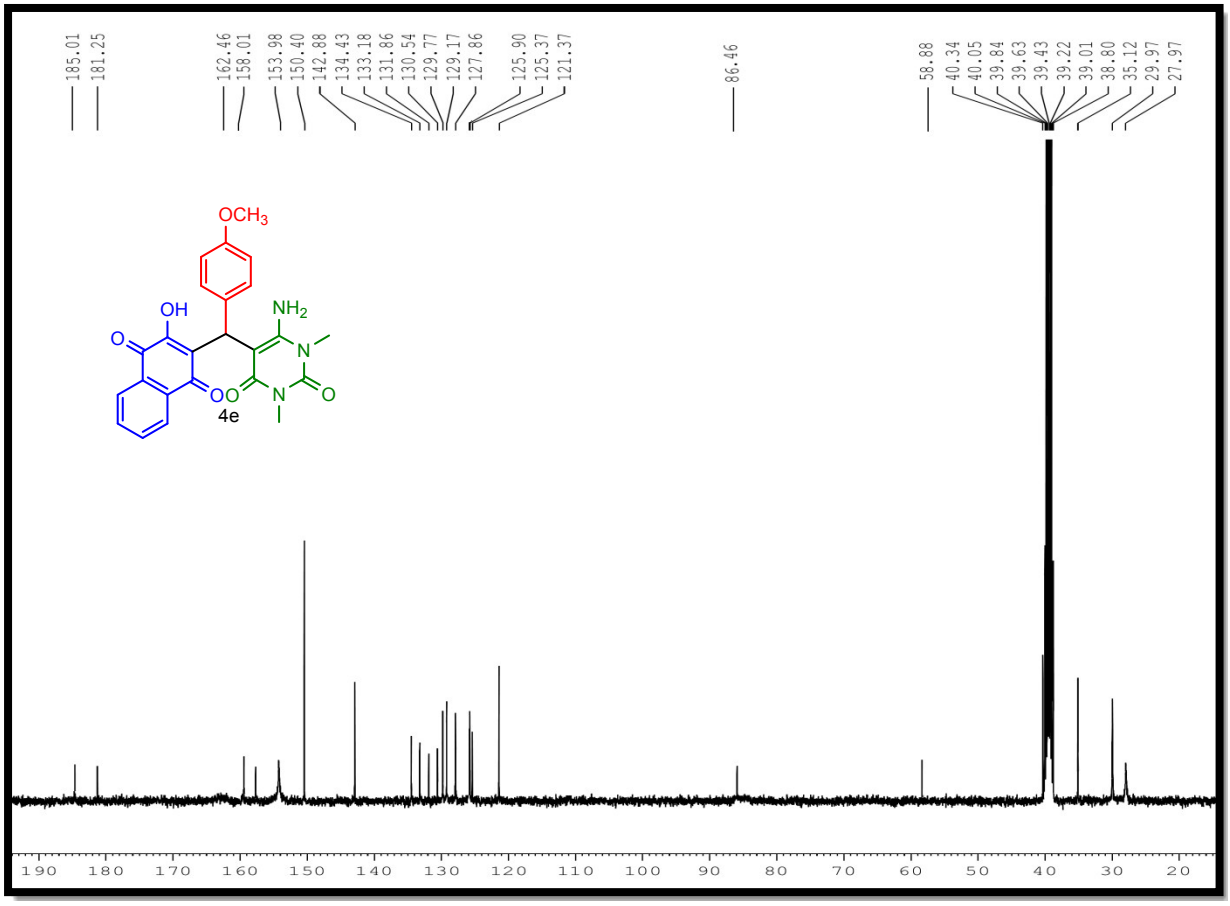

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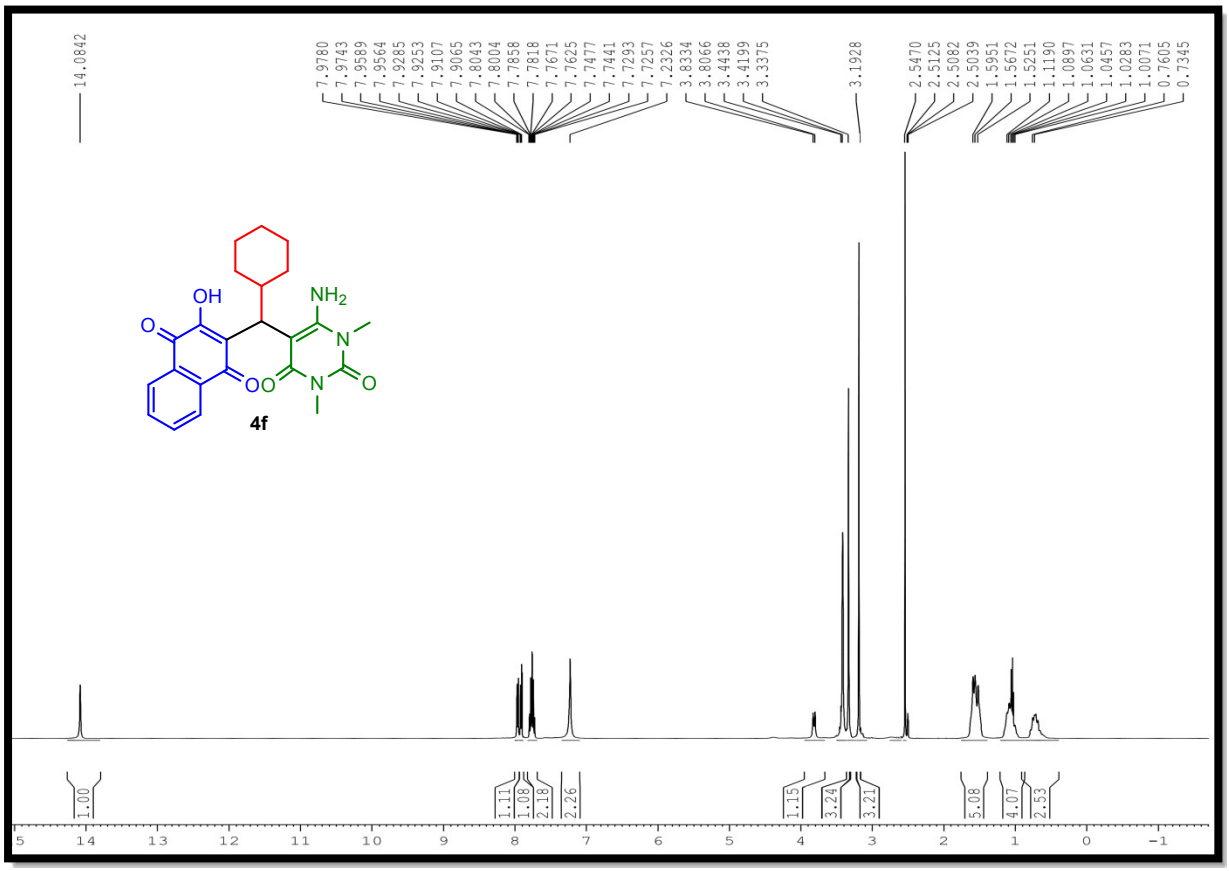
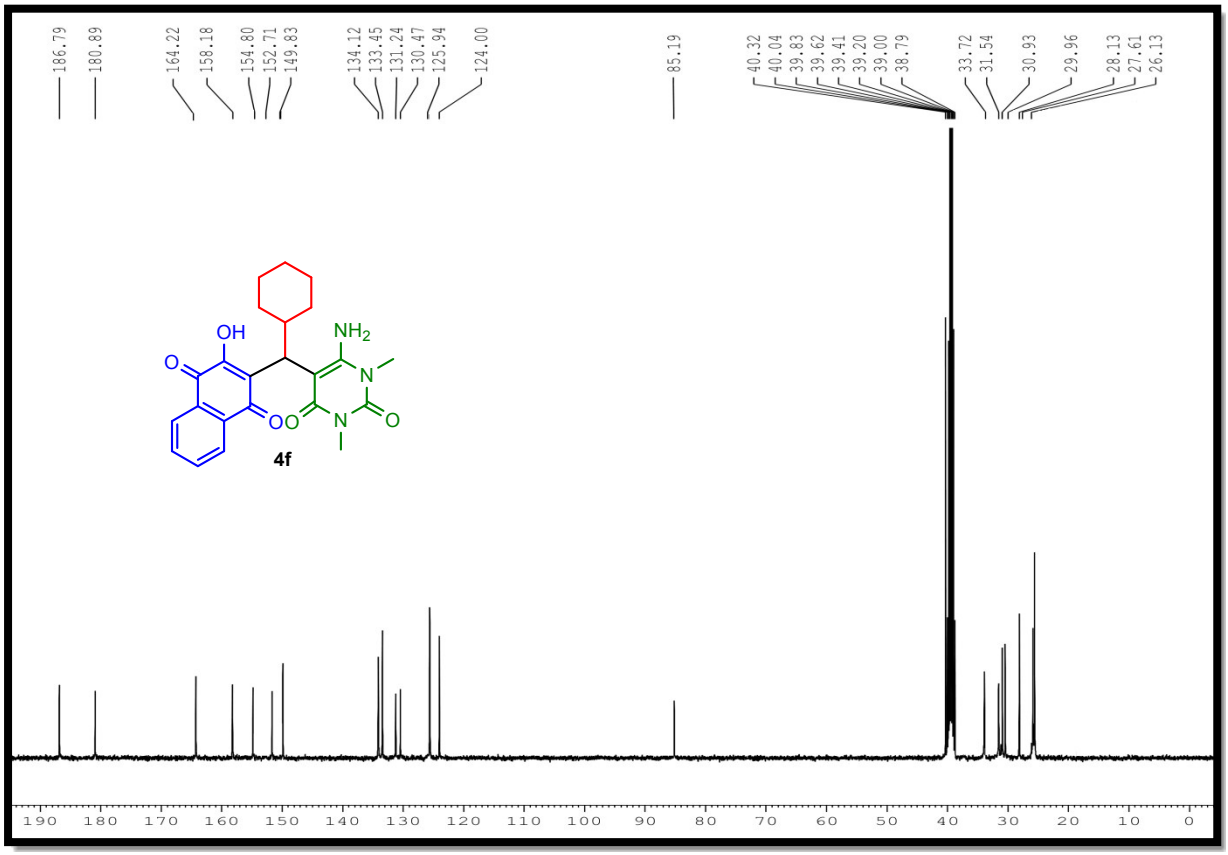
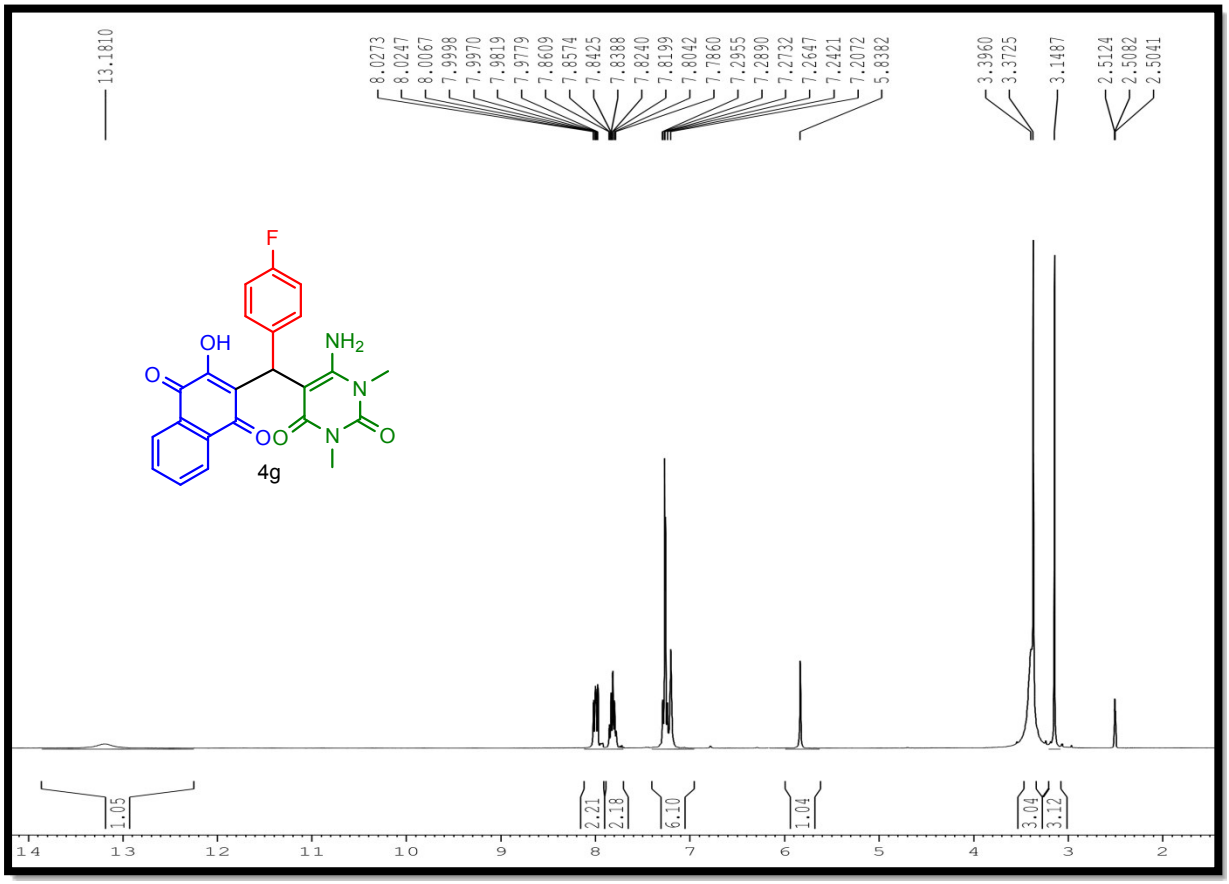
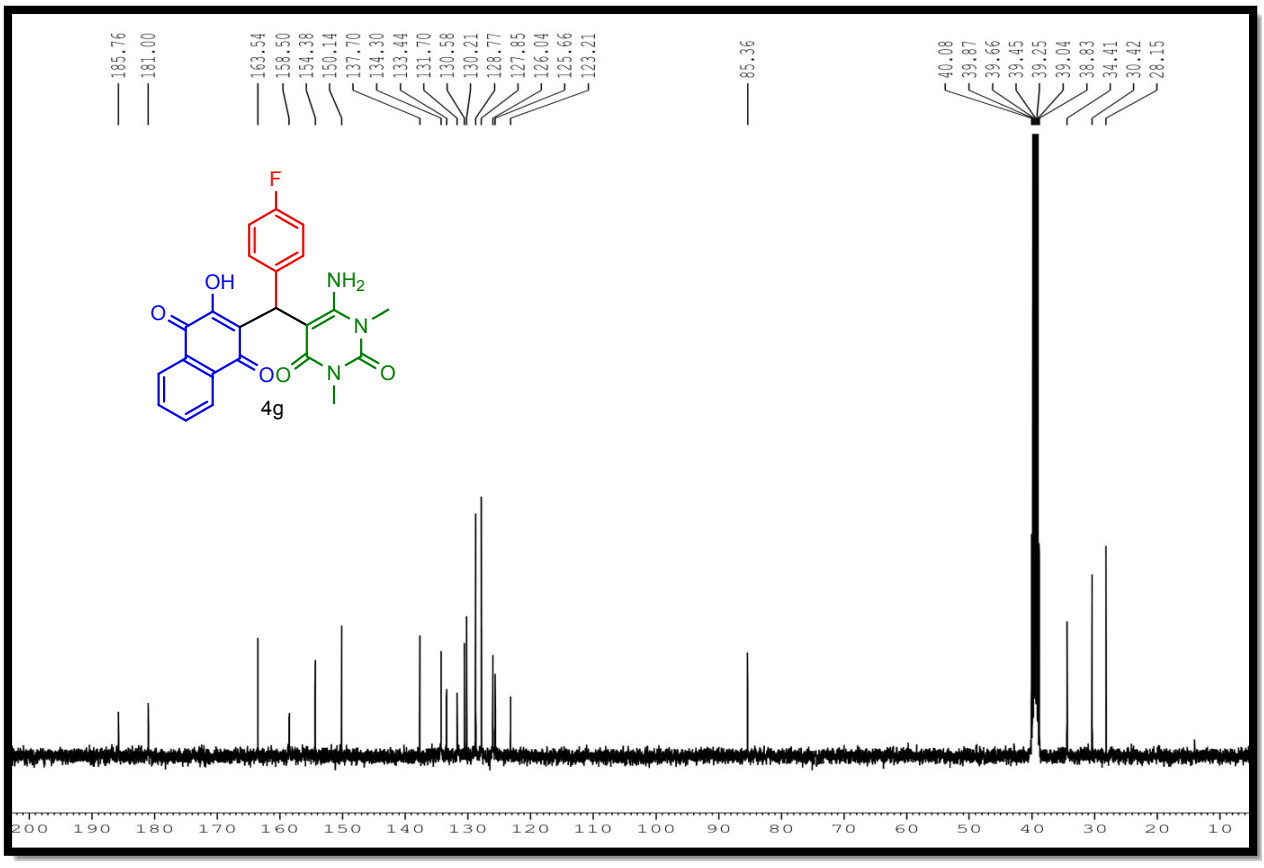




^{1}H & ^{13}C NMR Spectra of 4g





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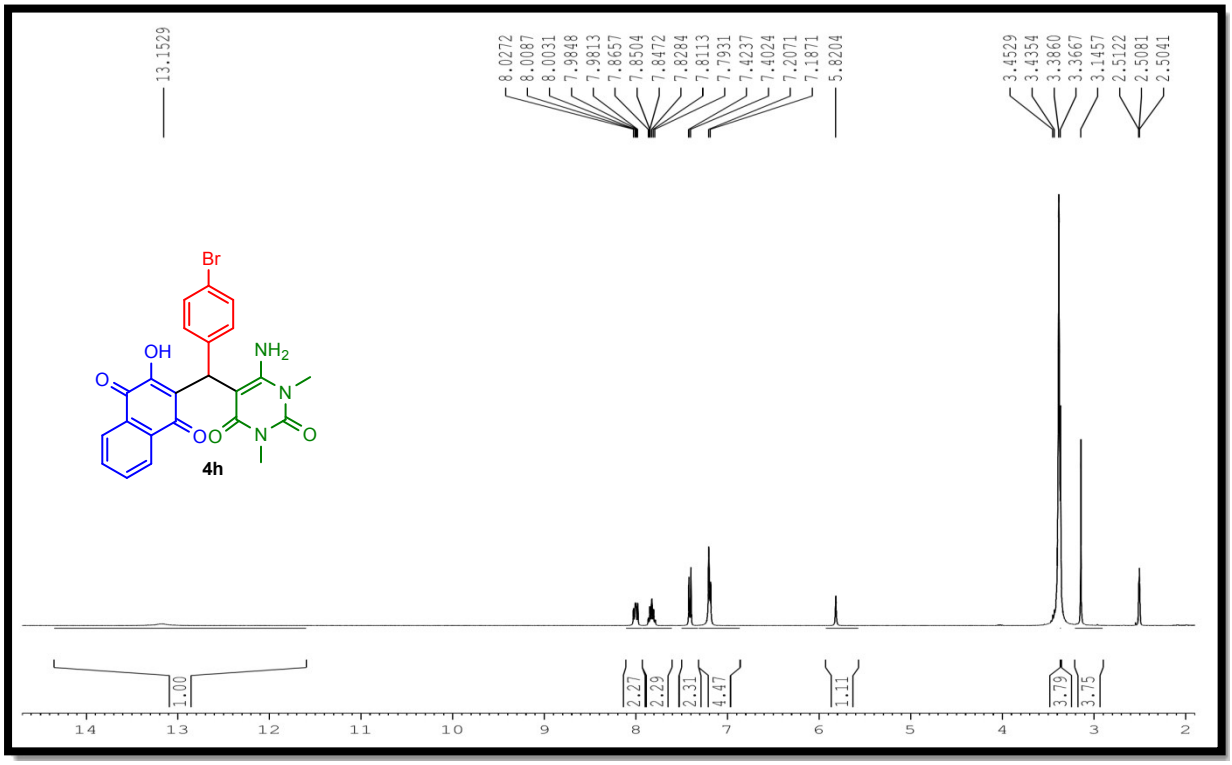

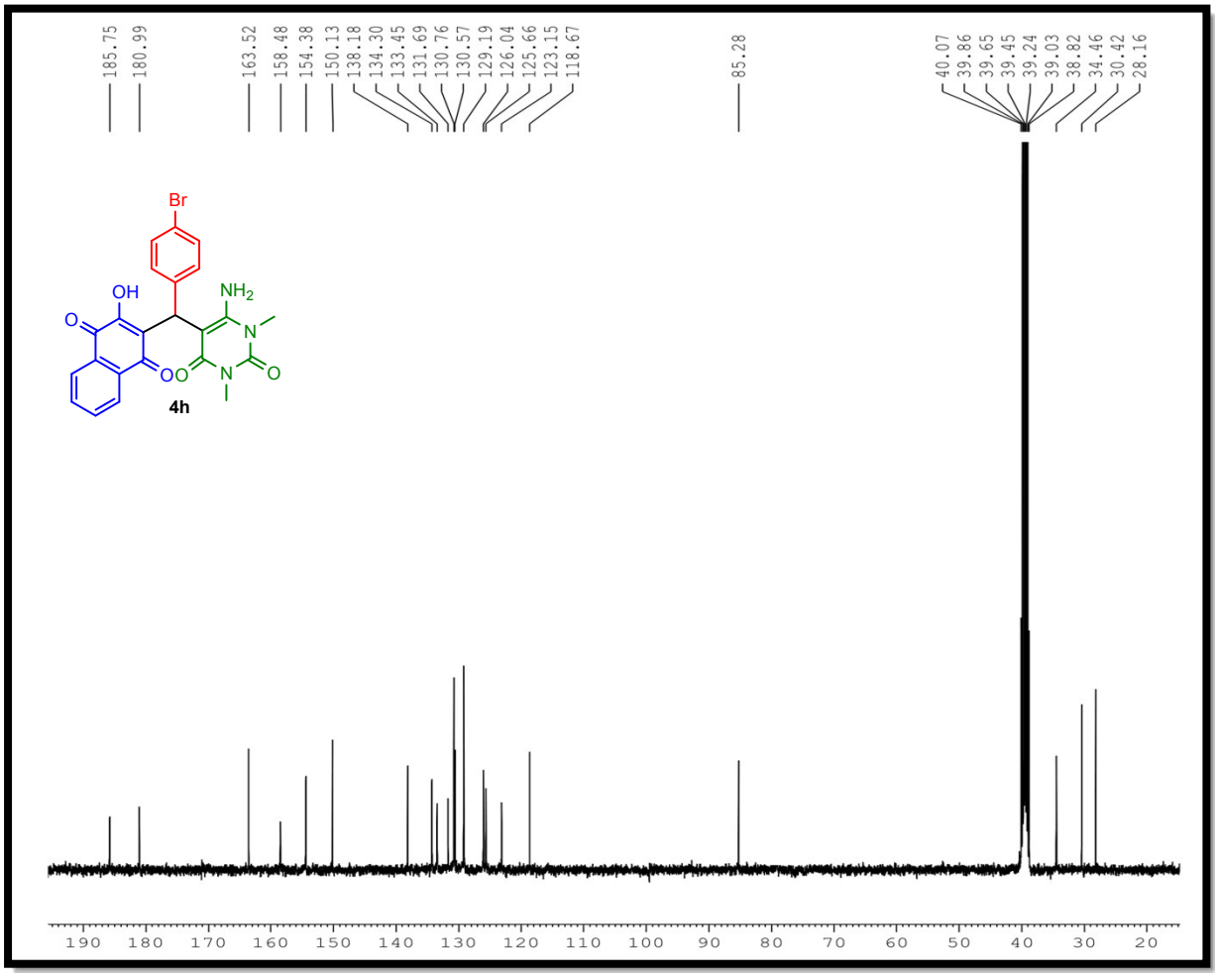

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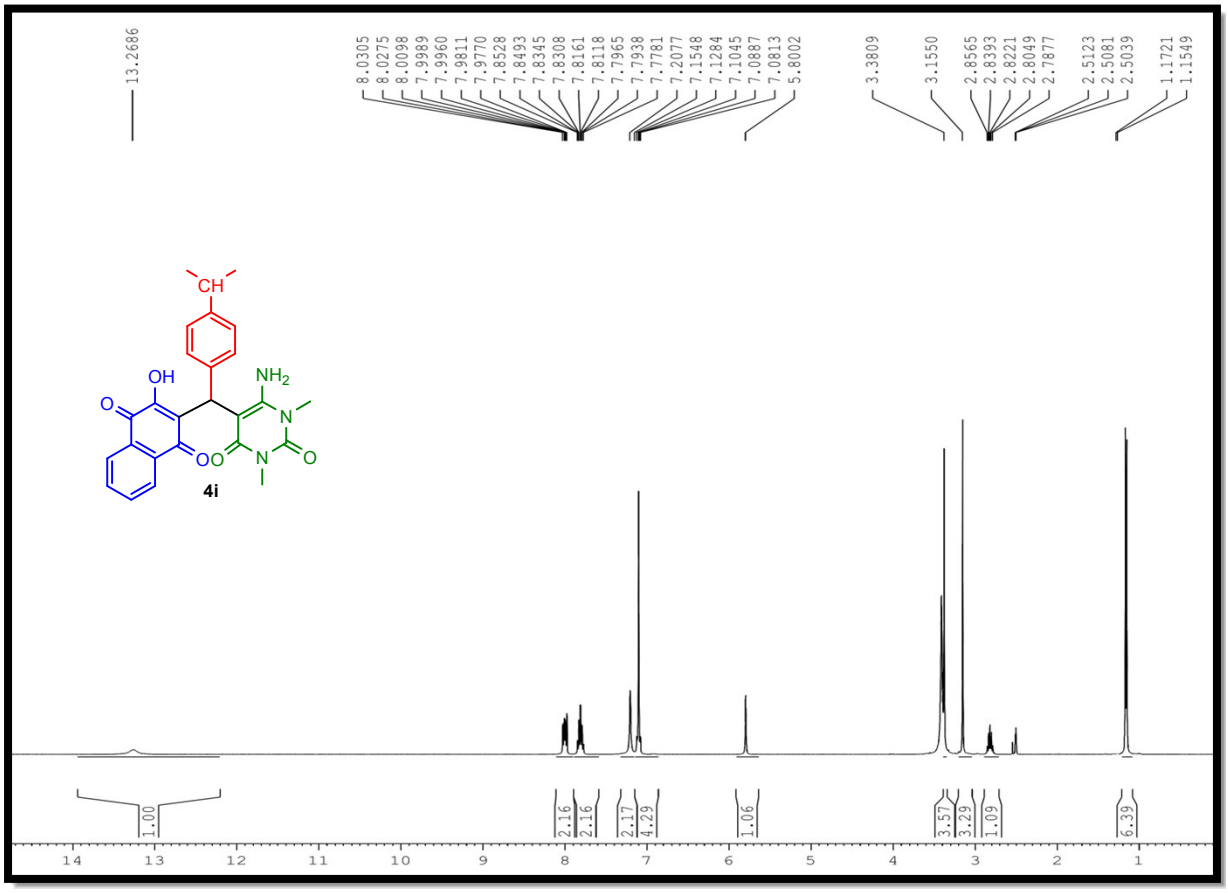

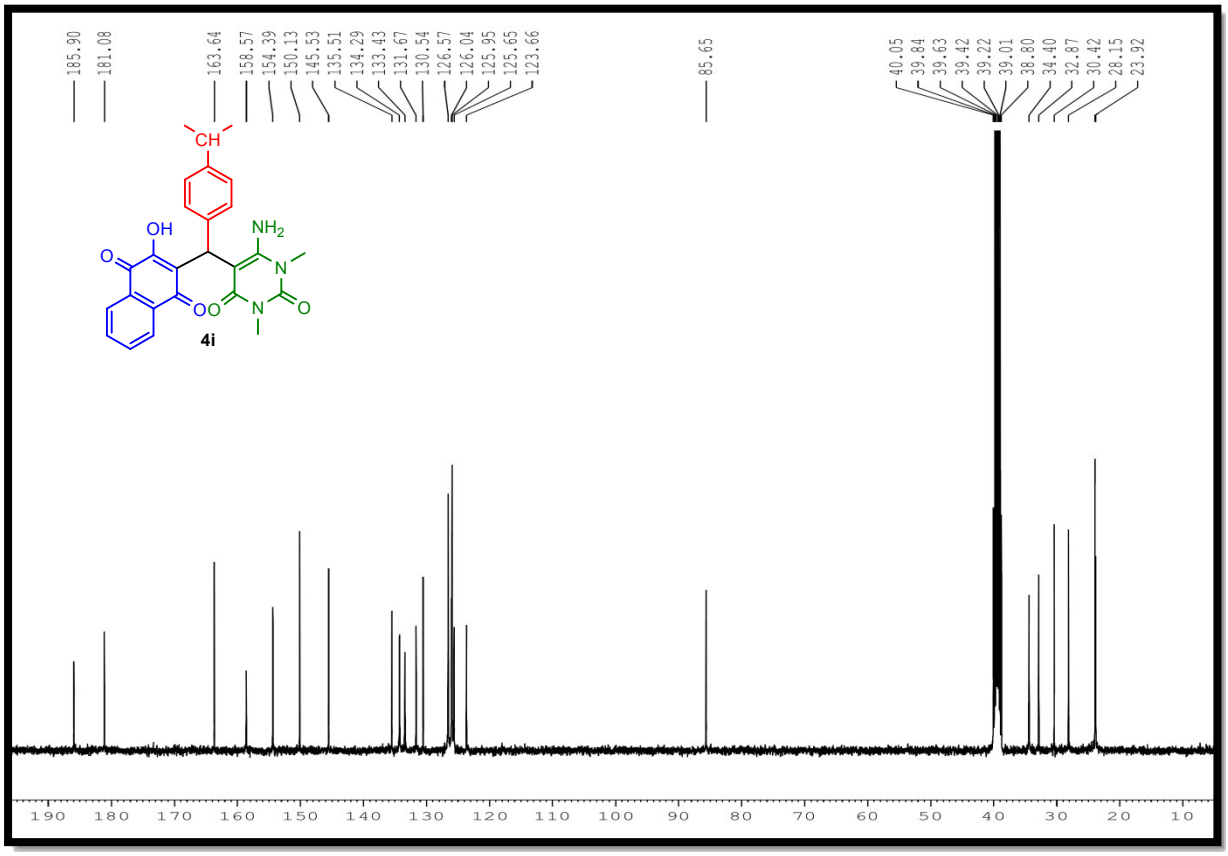

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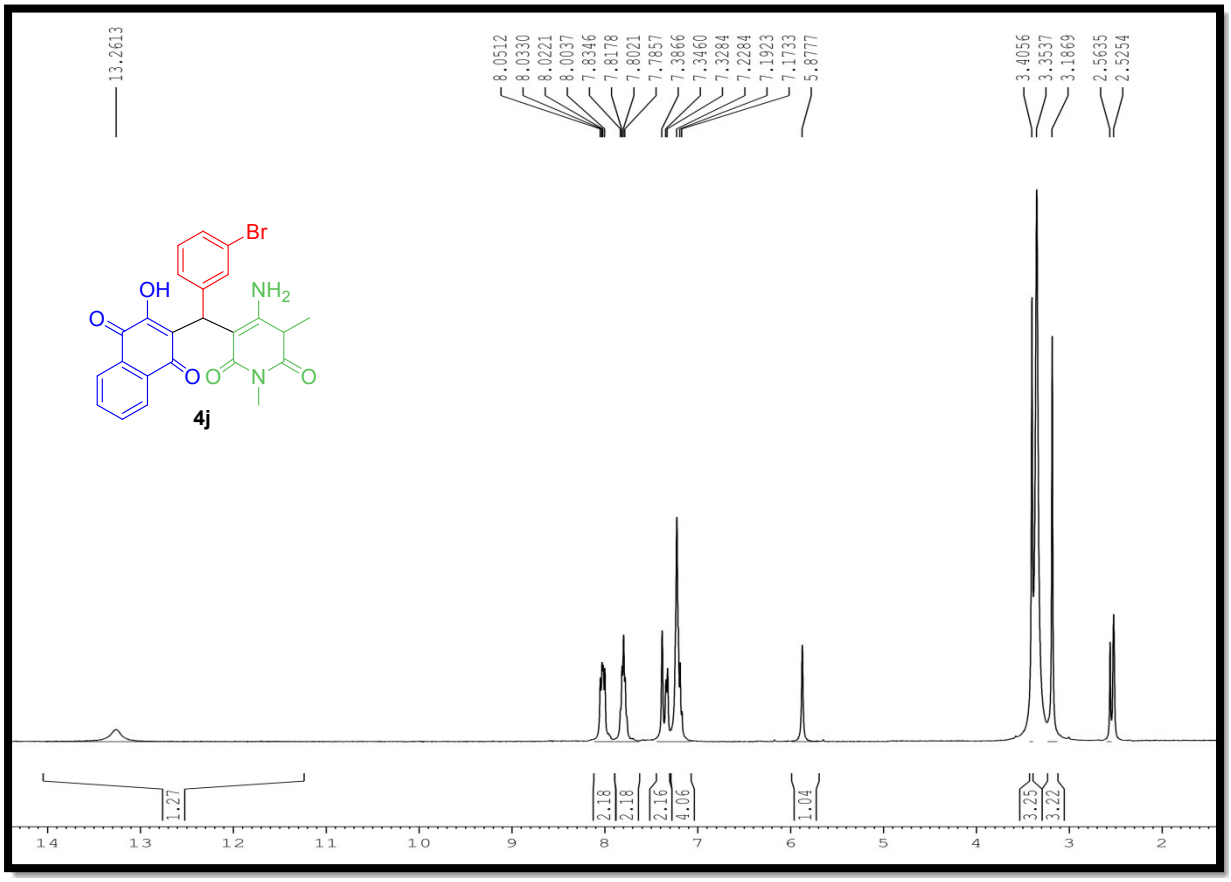

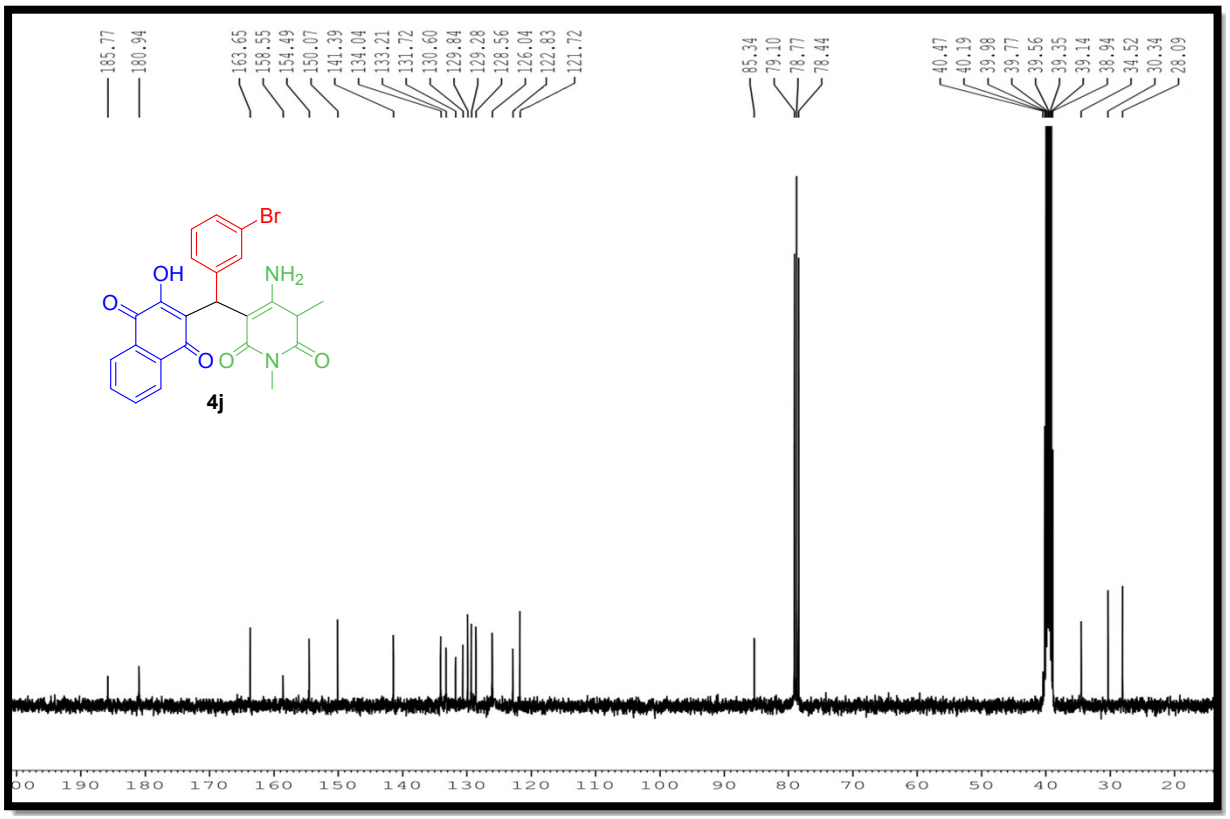

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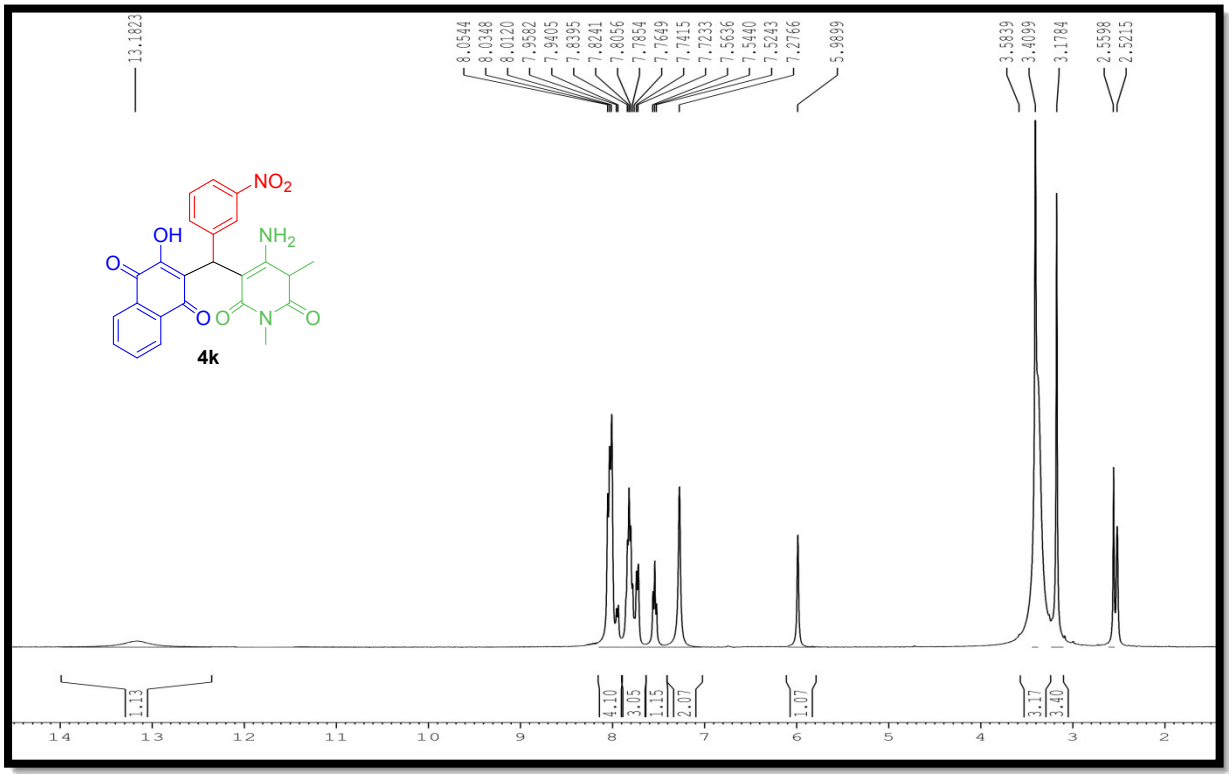

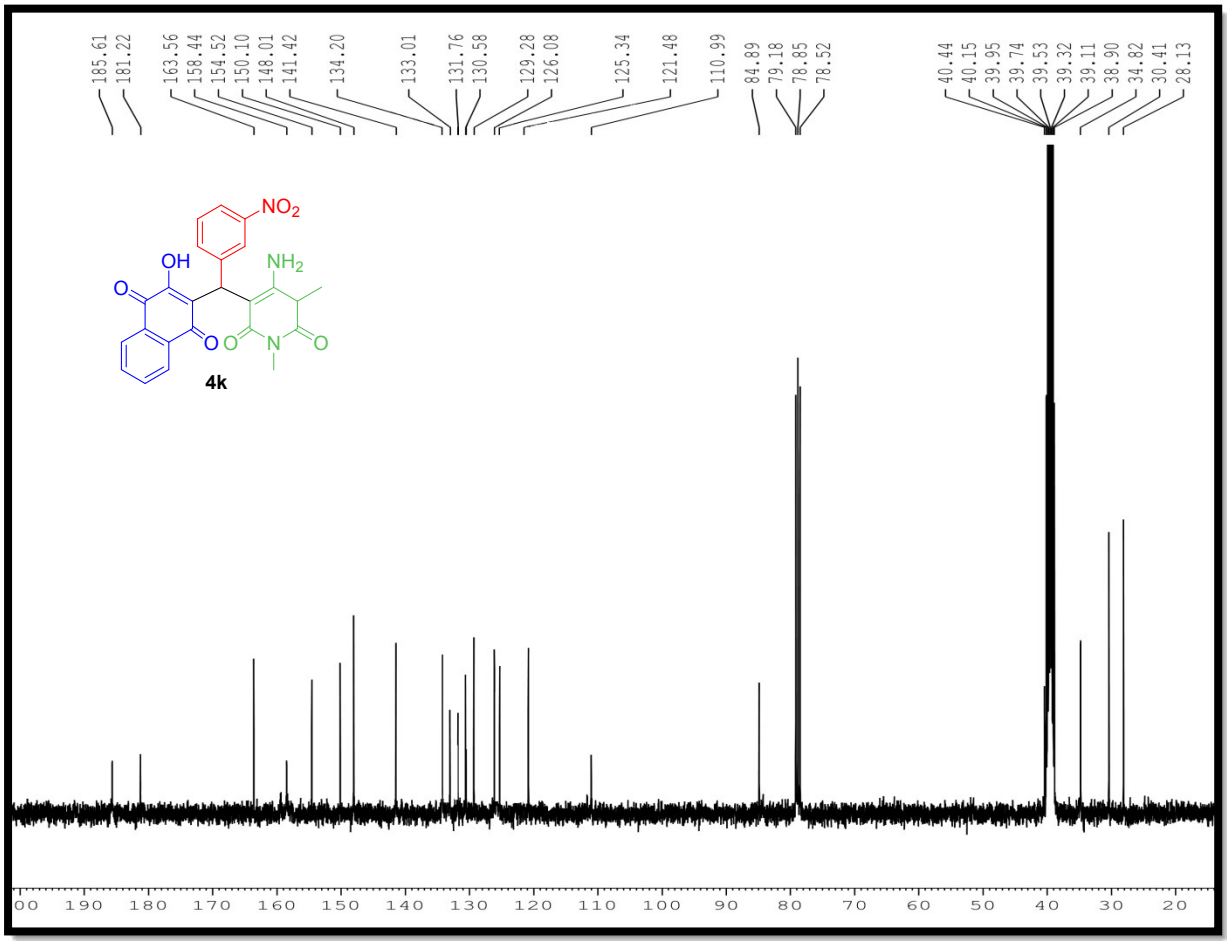

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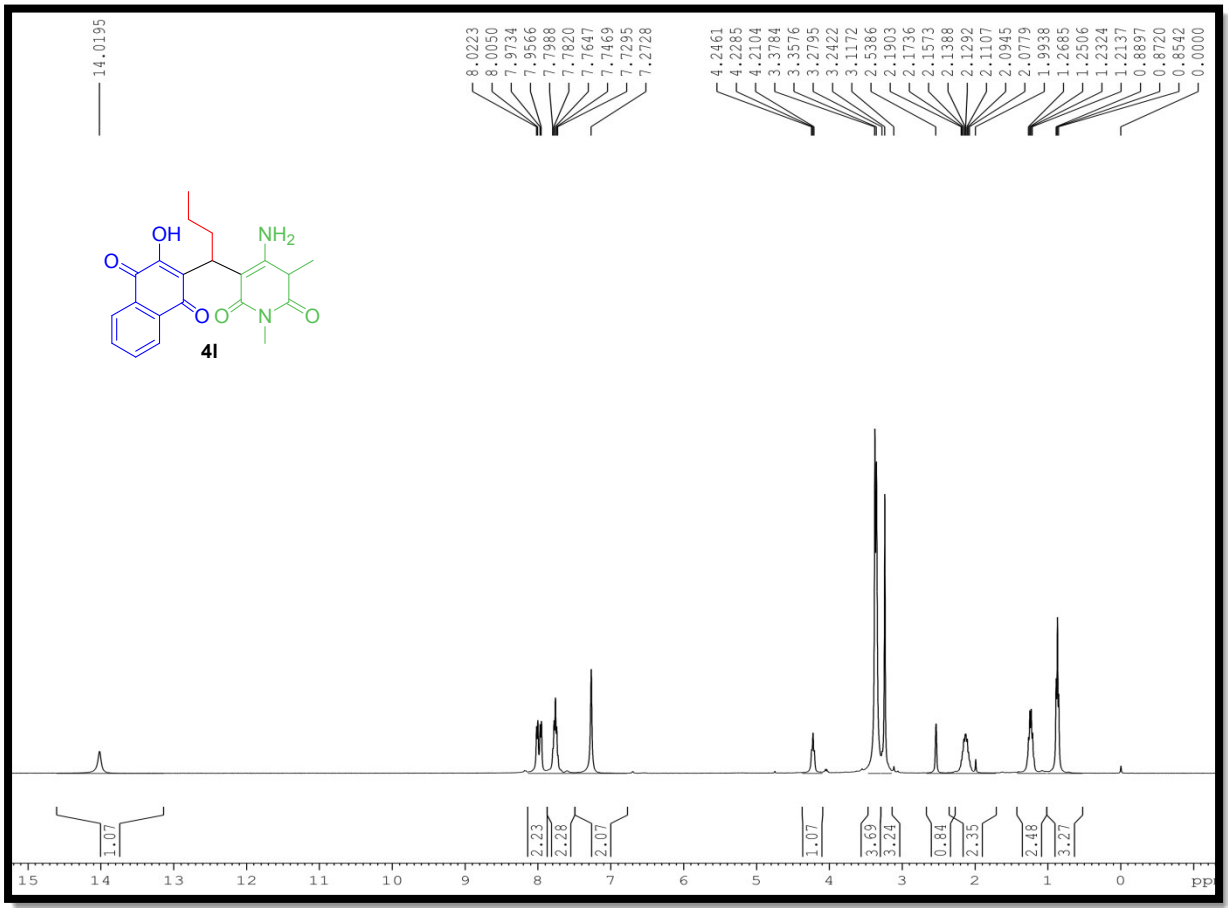

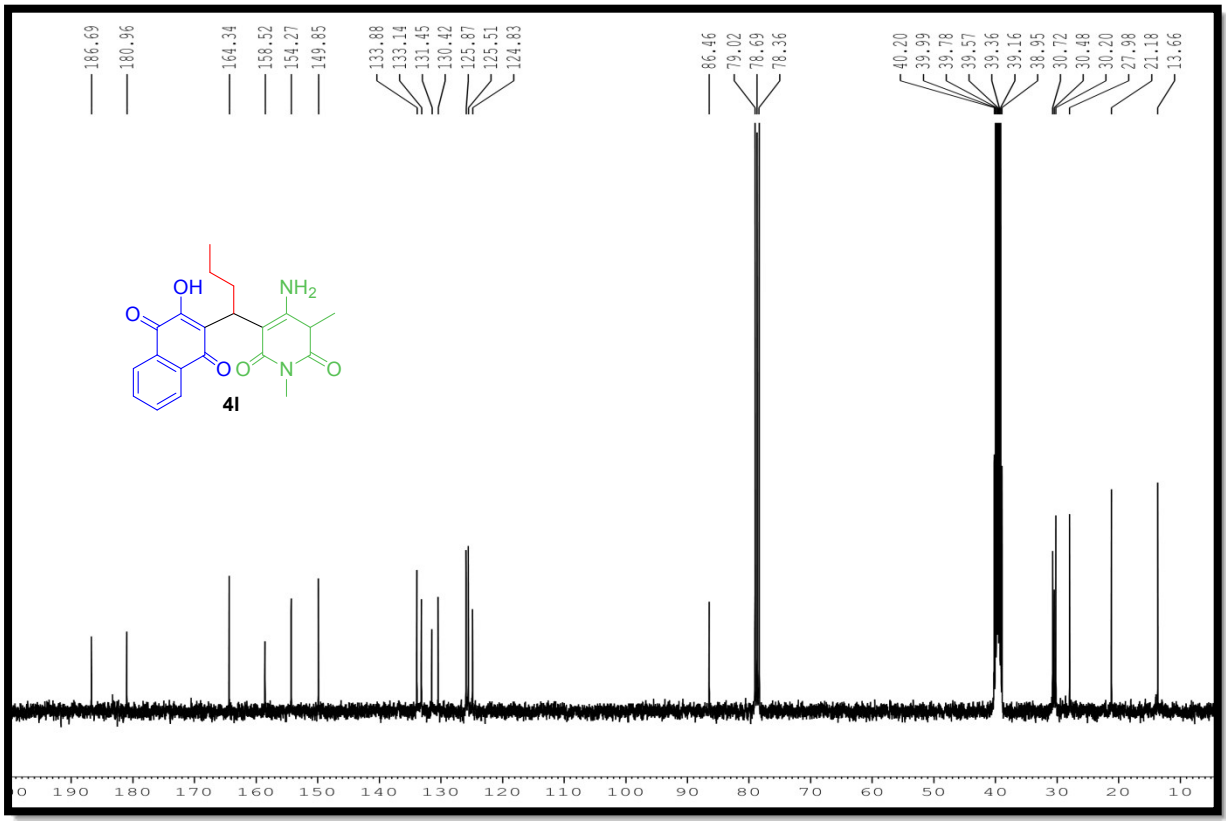

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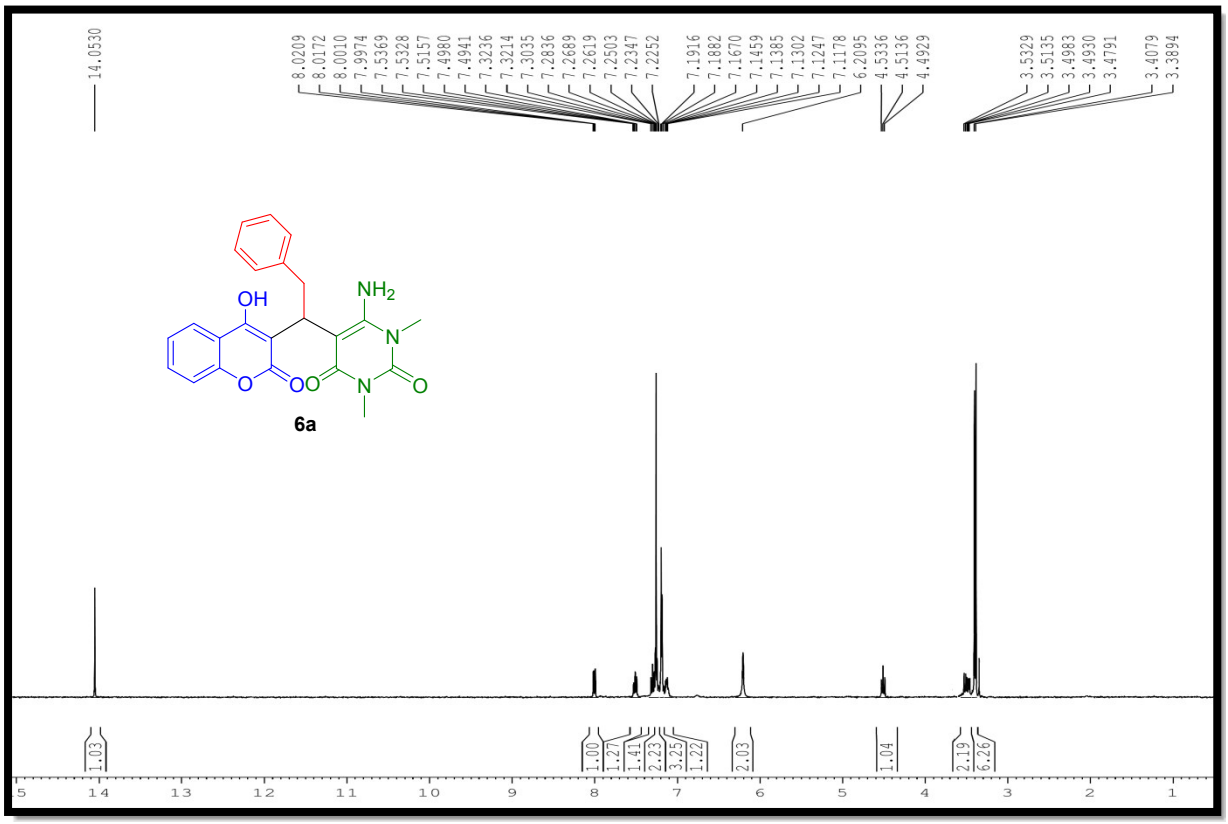

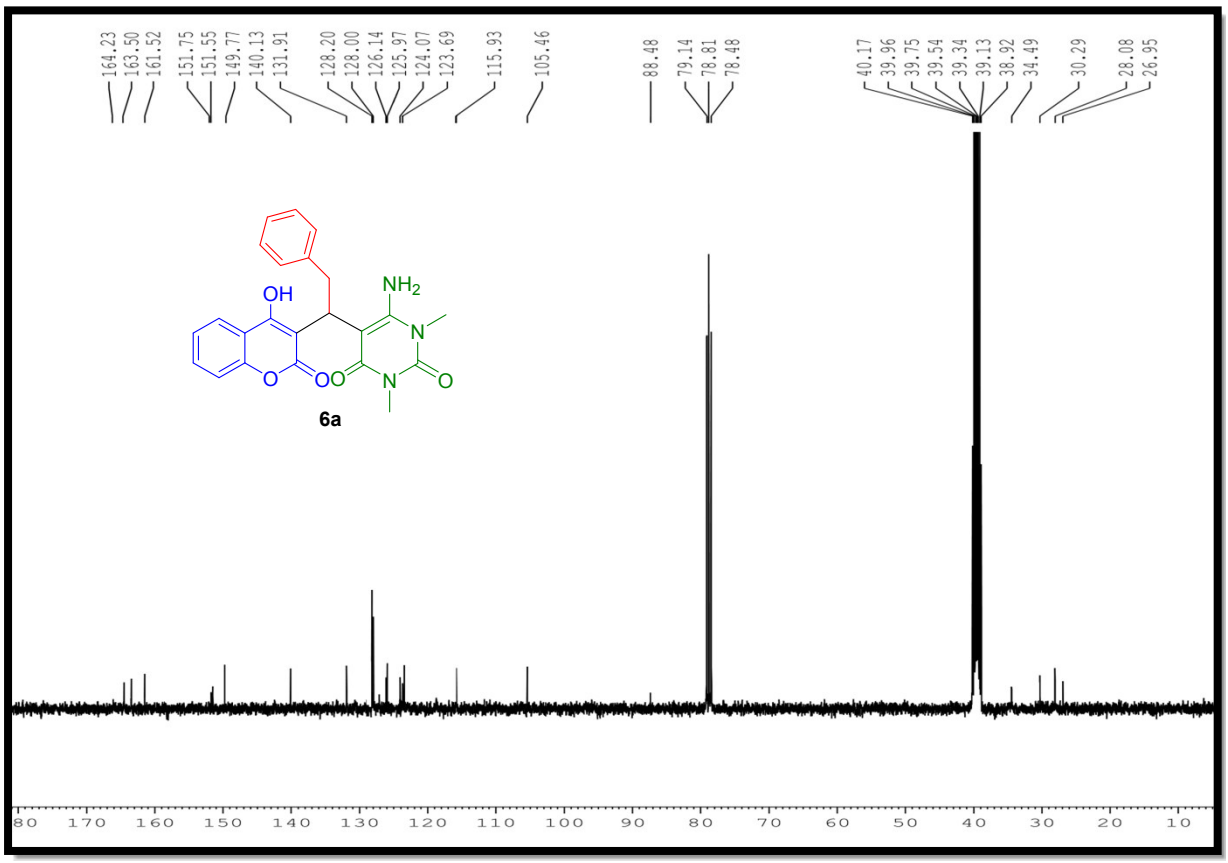

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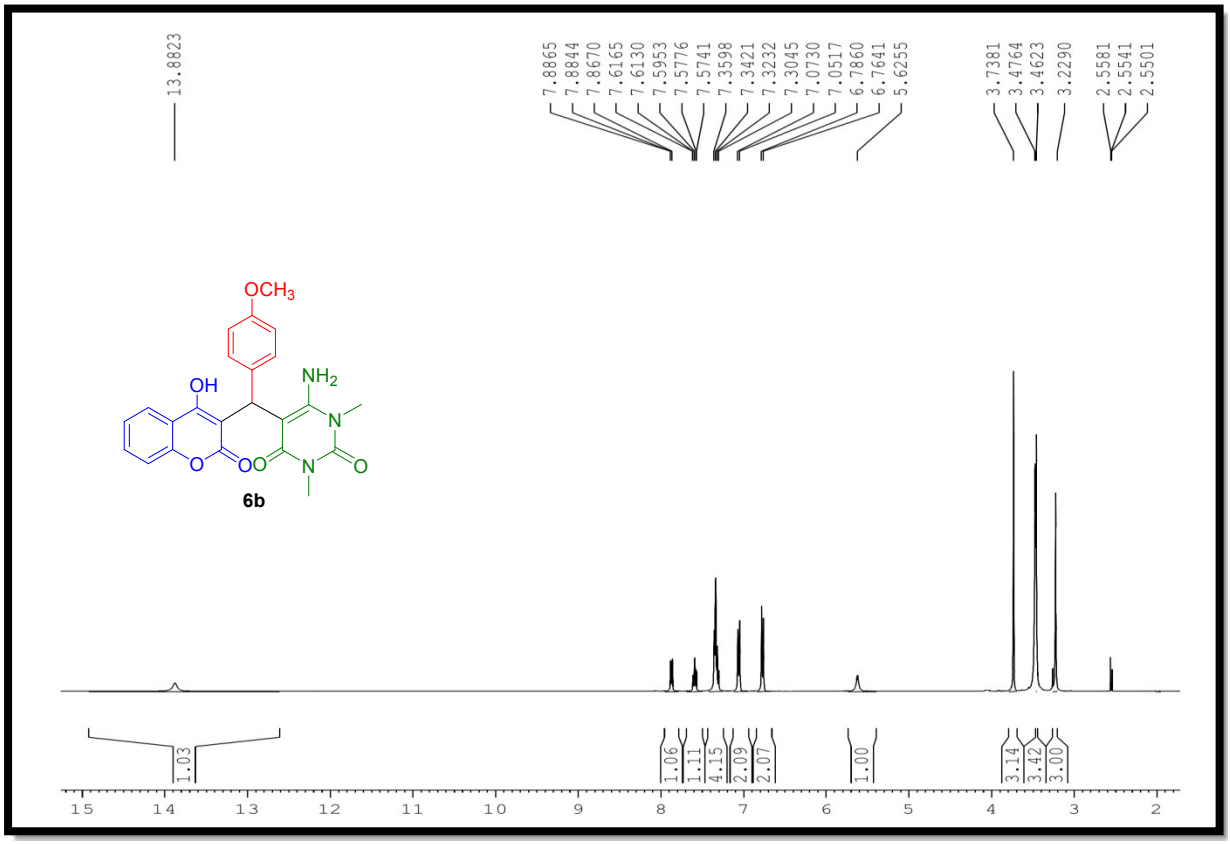

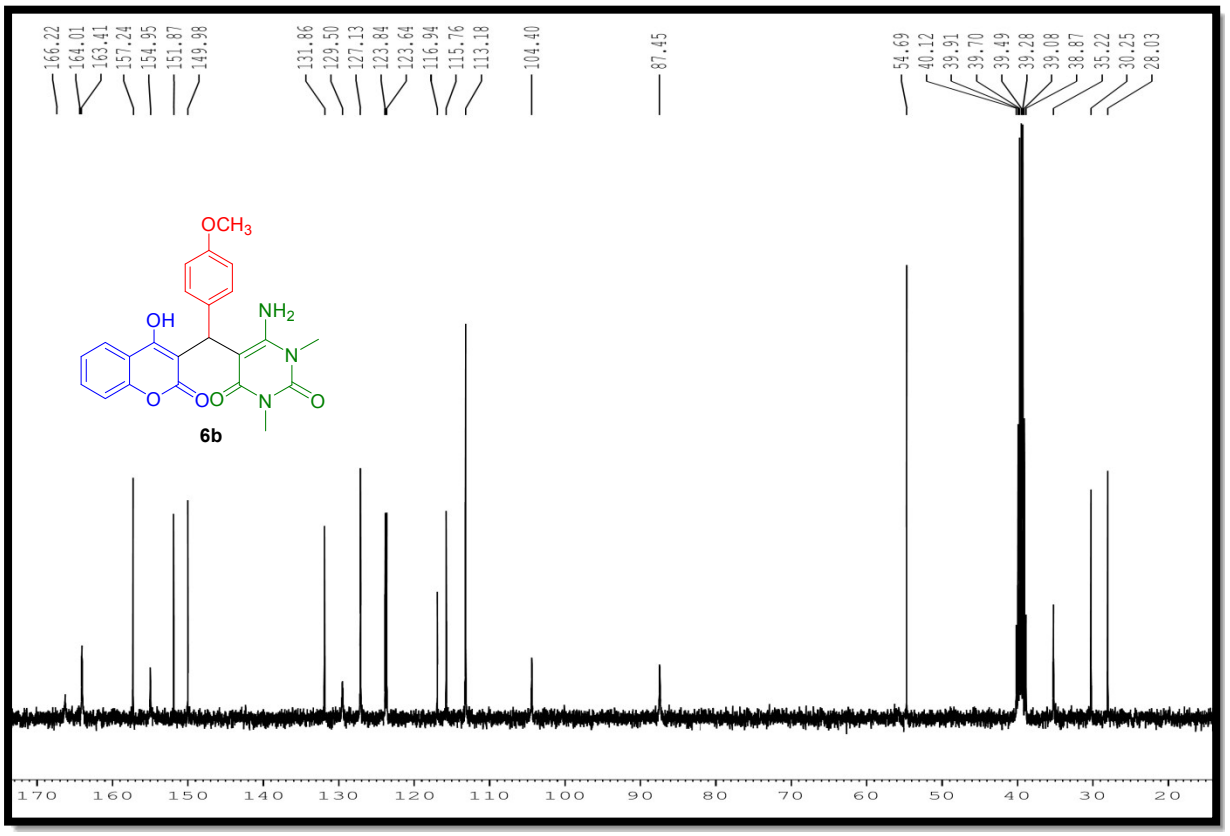

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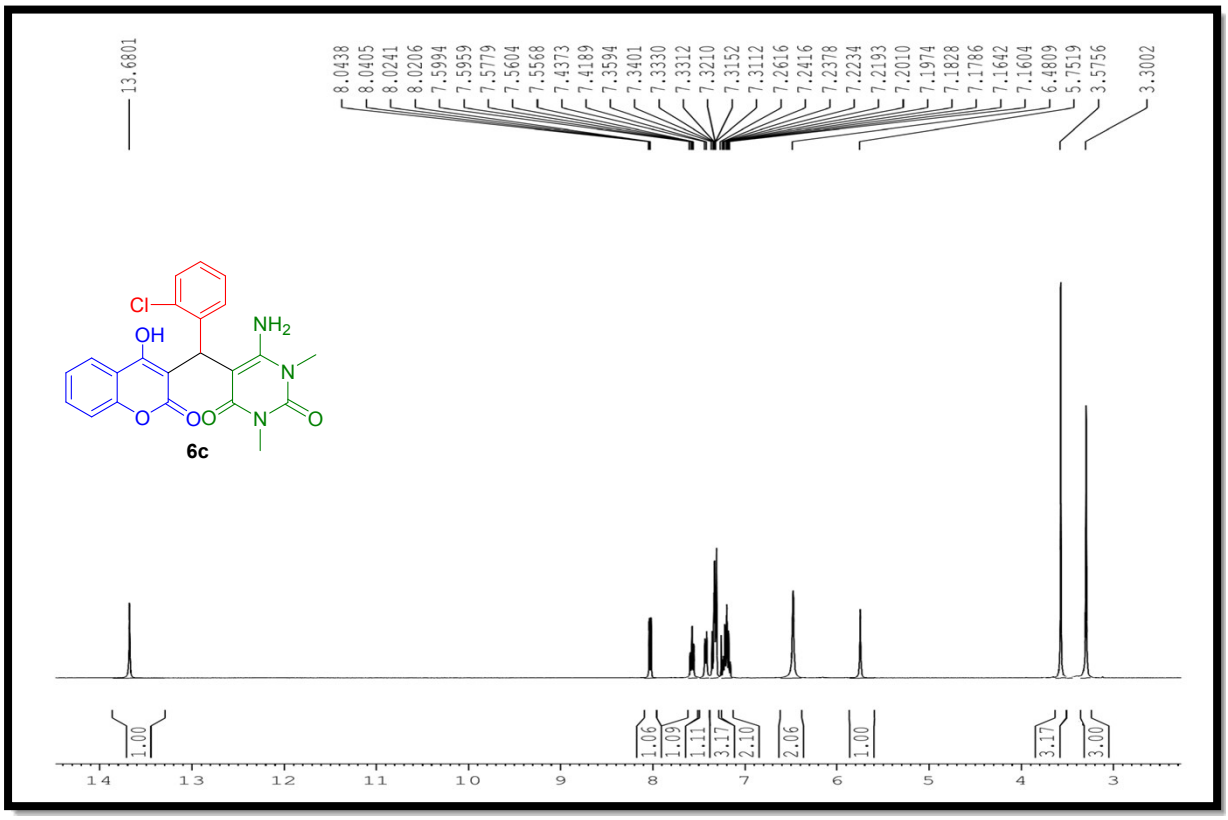

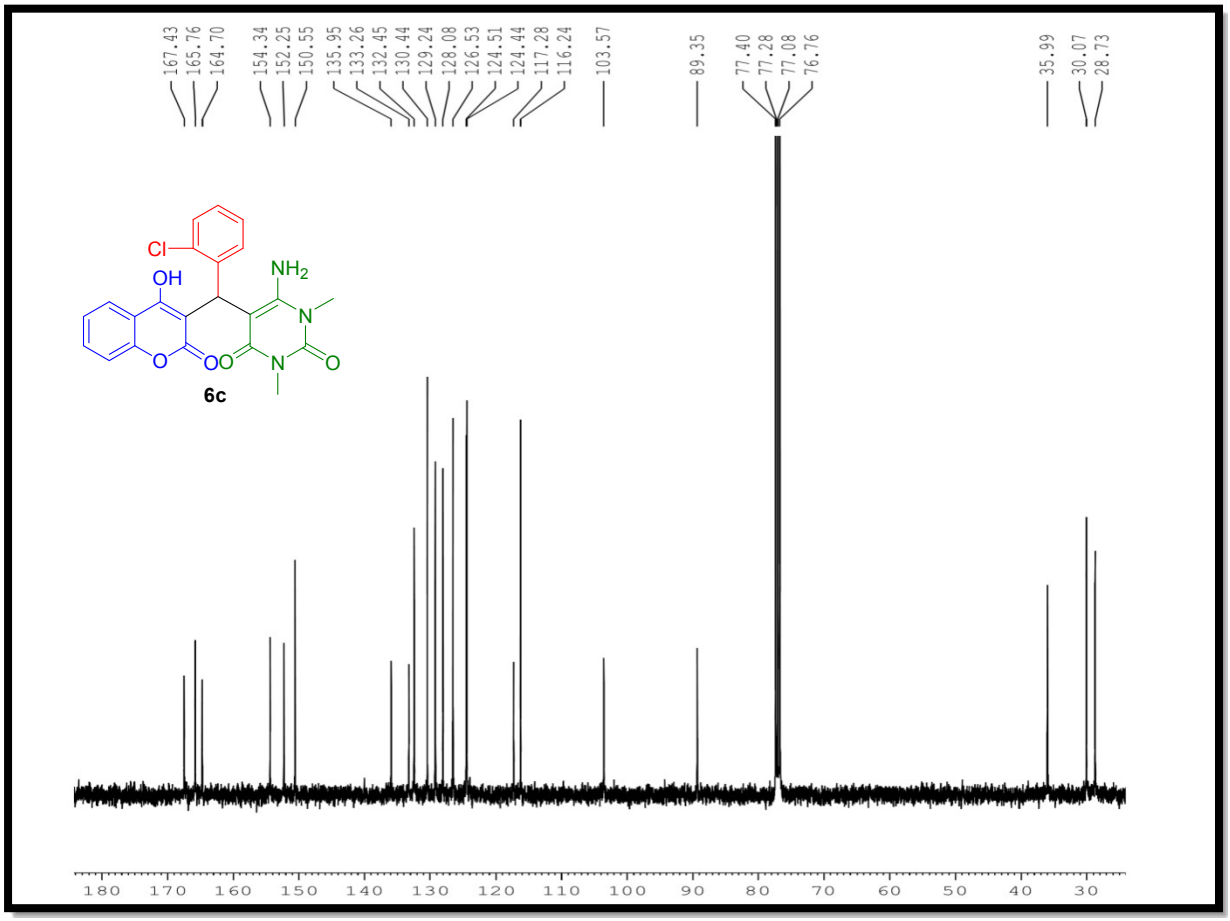

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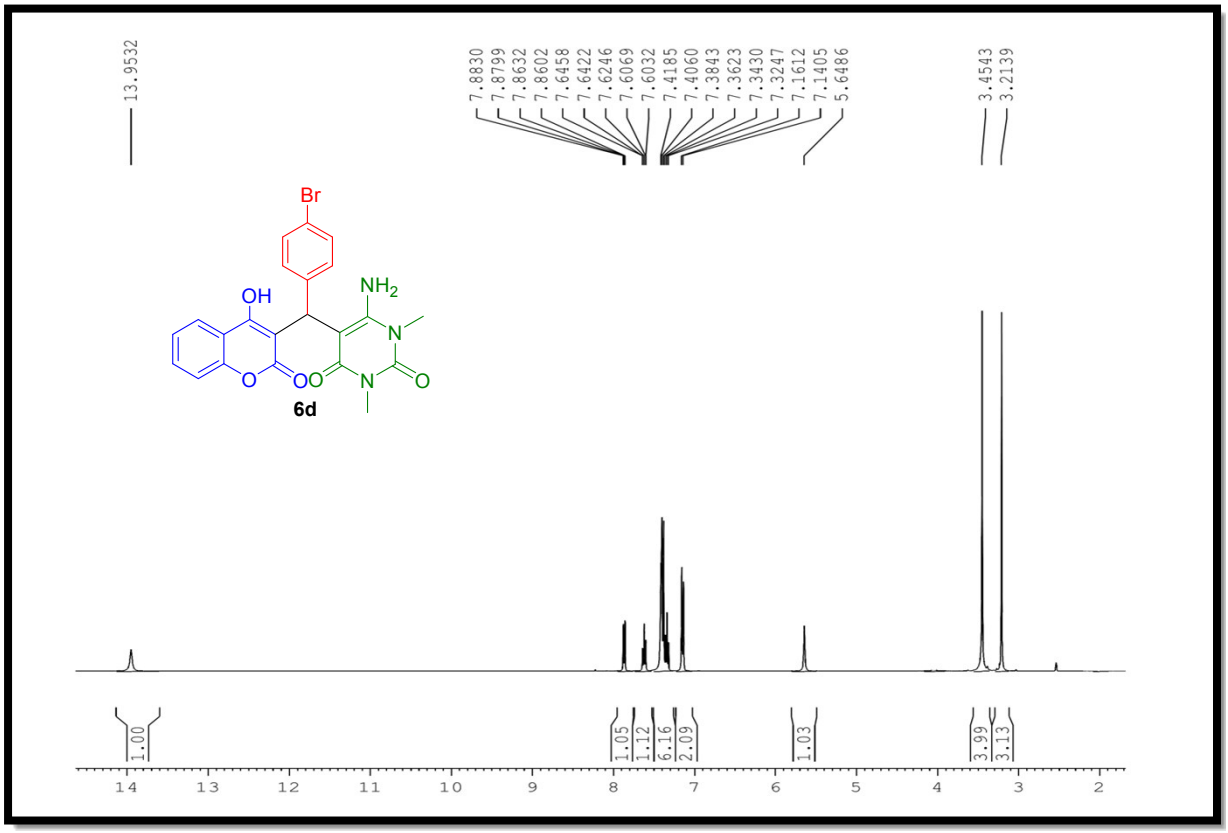

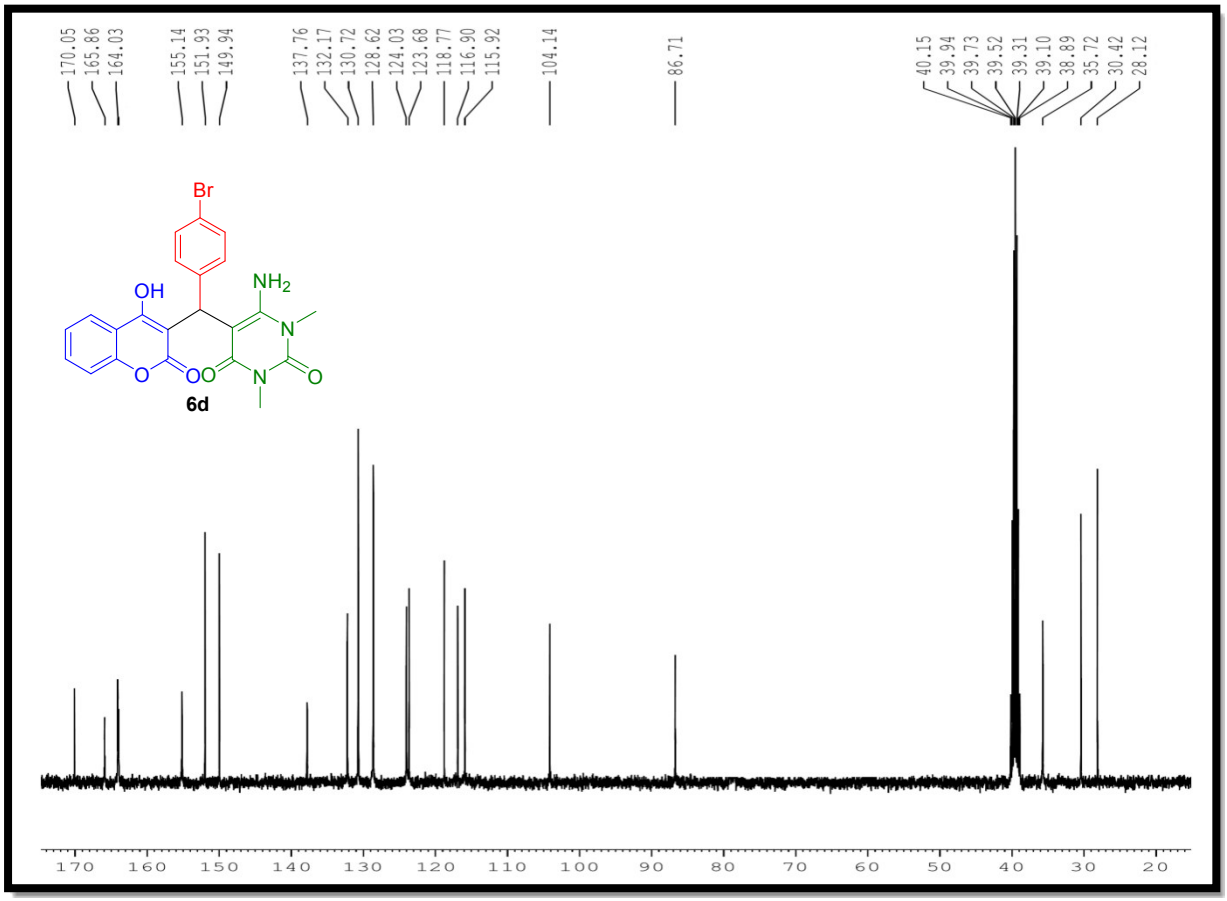

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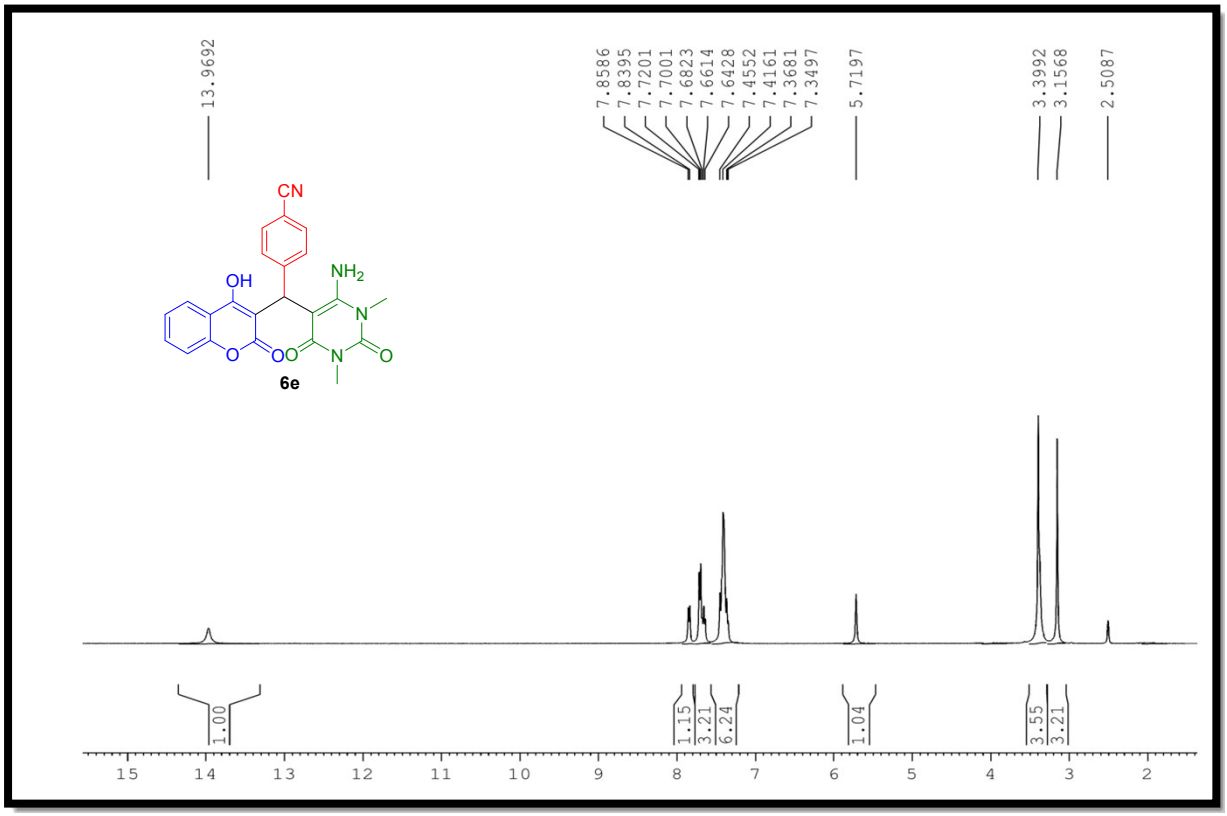

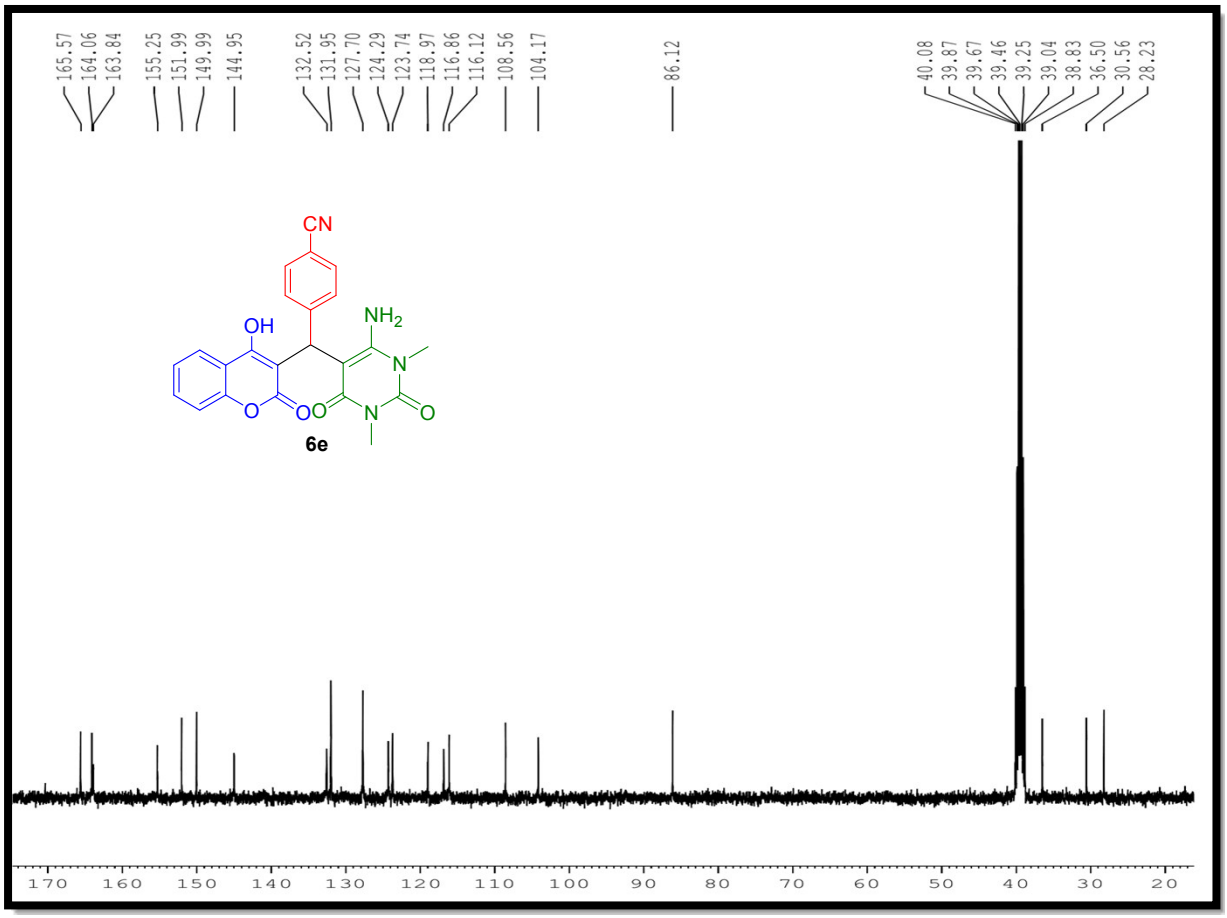

^{1}H & ^{13}C NMR Spectra of 6f