Supporting information

Design, preparation and characterization of functionalized magnetic nanoparticles with chitosan/Schiff base and using as a reusable nanocatalyst for green synthesis of 1H-isochromenes under mild conditions

Mahshid Zarei, Hossein Naeimi*

General multicomponent procedure for the synthesis of 1H-isochromene

1H-isochromene was synthesized by the MCR. In this reaction, 1 mmol of cyclohexanone and 1 mmol of malononitrile were mixed in an ethanol solvent. After adding 10 mg of Fe3O4@CS-S.B-CaMgFe2O4, the mixture was stirred at 25 °C for 5-10 minutes. 1 mmol of benzaldehyde was added after the first step was completed, and the reaction was allowed to proceed at room temperature for 10–15 minutes. After the completion of the reaction, the nanocatalyst was separated from the reaction mixture by an external magnet, Then the reaction mixture was filtered using a porous glass filter with the help of a vacuum pump. In the end, to purify the product, the precipitate obtained was washed with normal hexane and distilled water and finally dried in an oven at a temperature of 80 °C for 24 hours. The product obtained was characterized by melting points, IR, and ¹H NMR spectra.

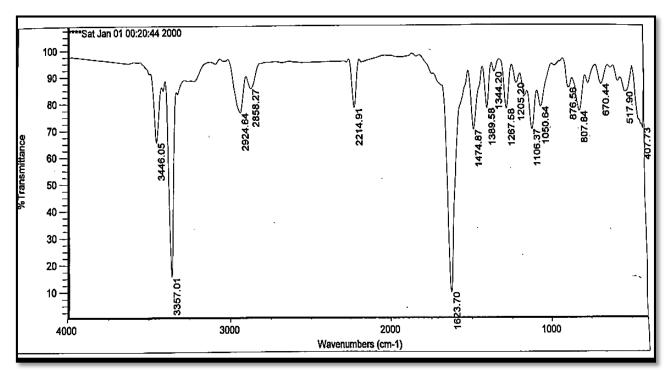


Fig. S1. FT-IR of 3-Amino-1-(2,4-dichlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4a**)

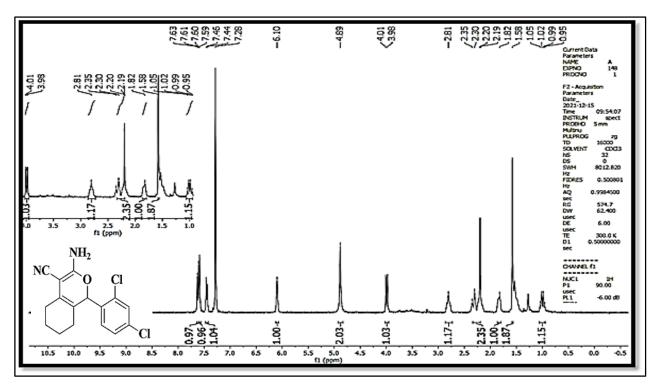


Fig. S2. ¹H NMR of 3-Amino-1-(2,4-dichlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4a**)

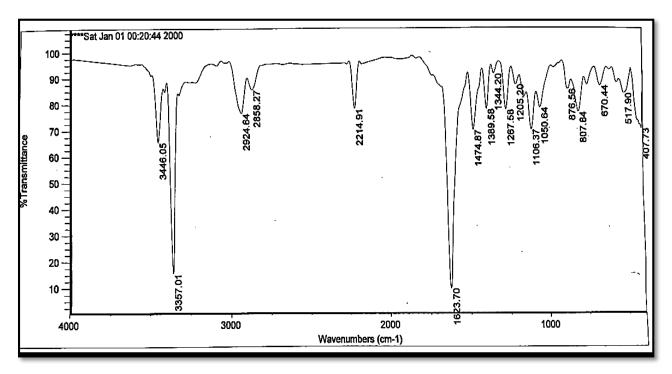


Fig. S3. FT-IR of 3-Amino-1-(4-chlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4b**)

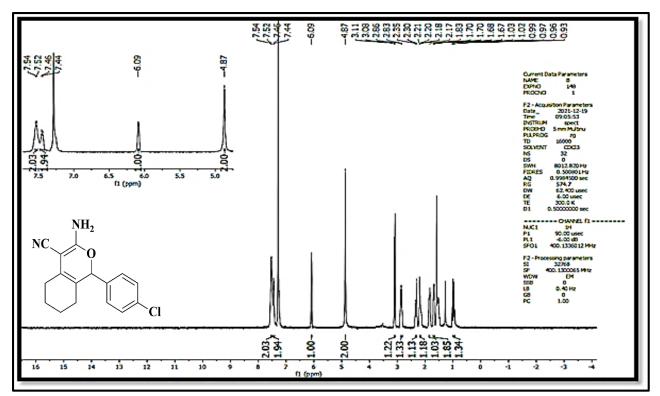


Fig. S4. ¹H NMR of 3-Amino-1-(4-chlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (4b)

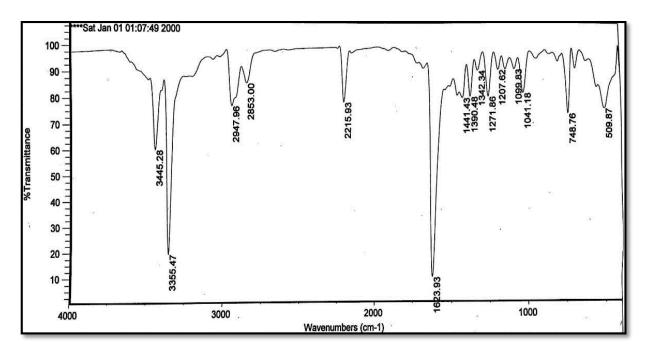


Fig. S5. FT-IR of 3-Amino-1-(2-chlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4-

carbonitrile (4c)

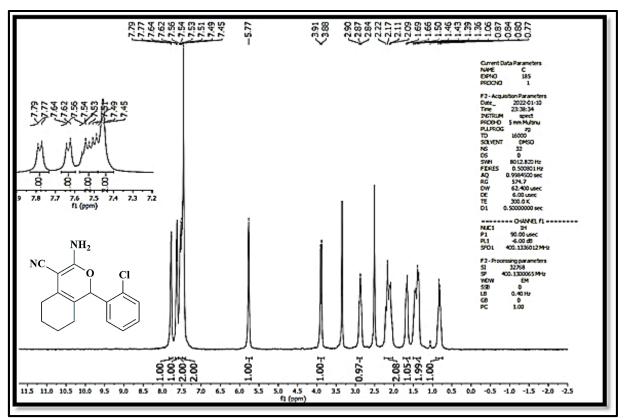


Fig. S6. ¹H NMR of 3-Amino-1-(2-chlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4c**)

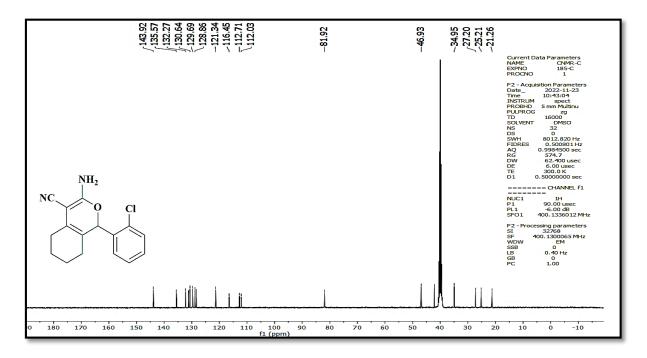


Fig. S7. ¹³C NMR of 3-Amino-1-(2-chlorophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4c**)

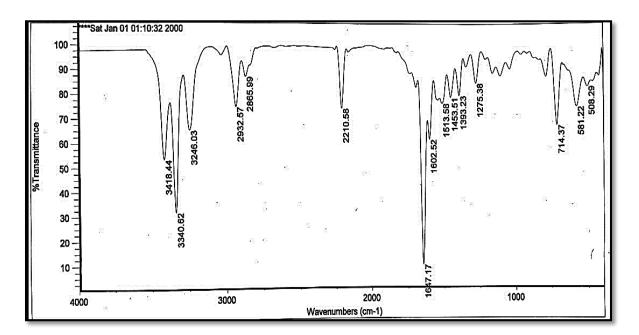


Fig. S8. FT-IR of 3-Amino-1-phenyl- 5,6,7,8-tetrahydro- 1H-isochromene-4-carbonitrile (4d)

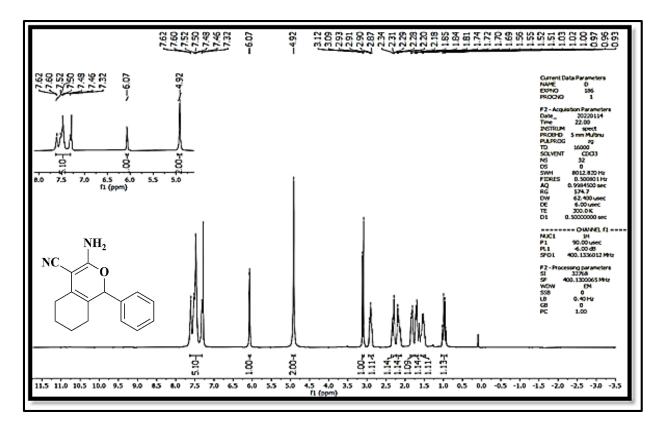


Fig. S9. ¹H NMR of 3-Amino-1-phenyl- 5,6,7,8-tetrahydro- 1H-isochromene-4-carbonitrile (4d)

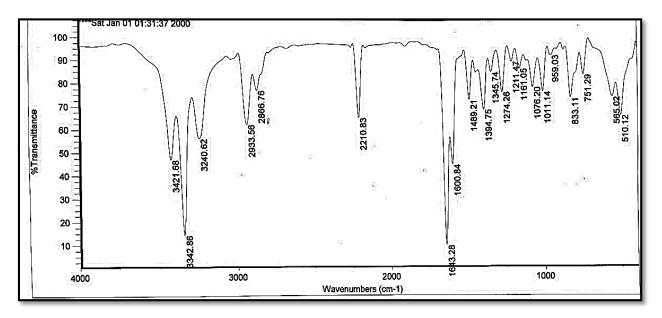


Fig. S10. FT-IR of 3-Amino-1-(4-bromophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (4e)

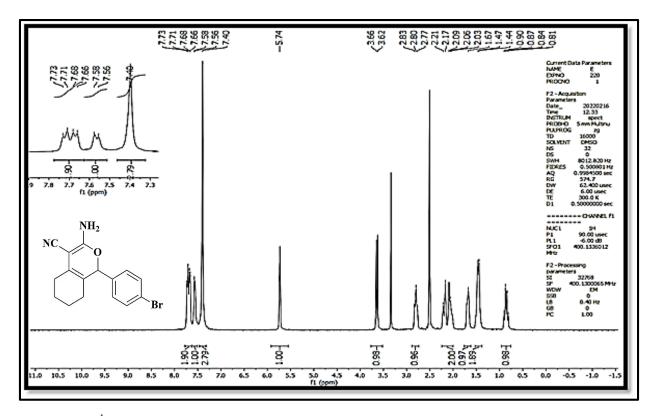


Fig. S11. ¹H NMR of 3-Amino-1-(4-bromophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4e**)

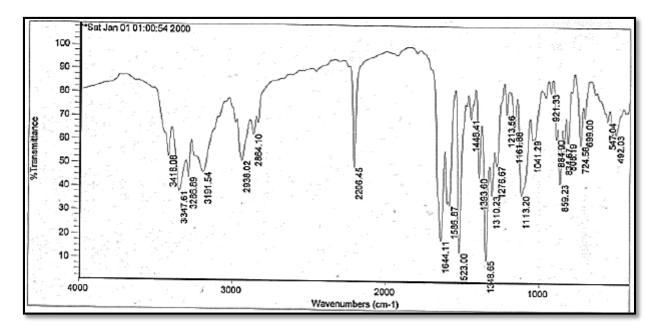


Fig. S12. FT-IR of 3-amino-1-(4-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4-carbonitrile

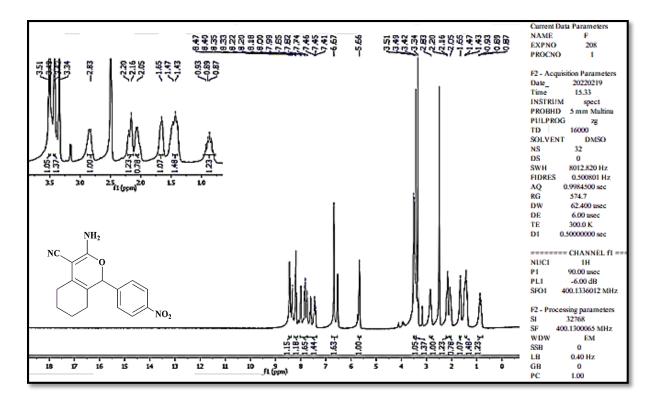


Fig. S13. ¹H NMR of 3-amino-1-(4-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4f**)

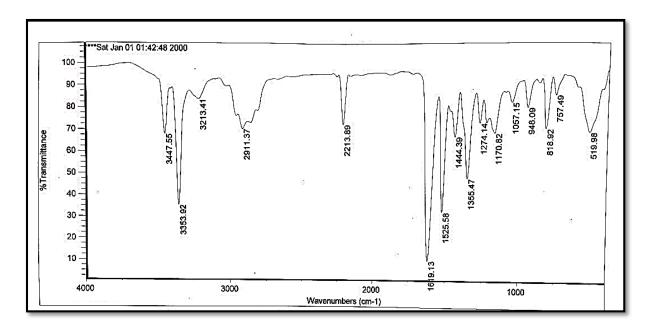


Fig. S14. FT-IR of 3-amino-1-(4-(dimethylamino)phenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4g**)

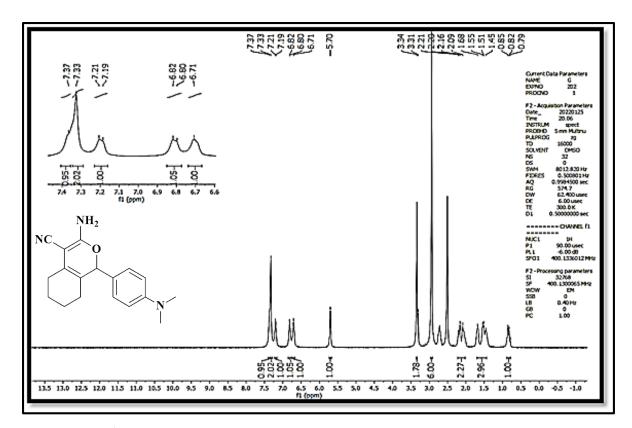


Fig. S15. ¹H NMR of 3-amino-1-(4-(dimethylamino)phenyl)-5,6,7,8-tetrahydro-1Hisochromene-4-carbonitrile (**4g**)

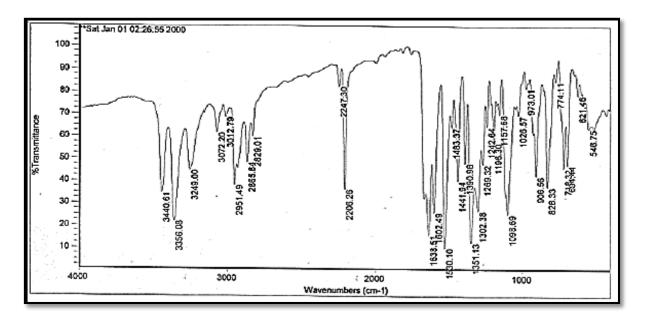


Fig. S16. FT-IR of 3-amino-1-(3-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4-carbonitrile

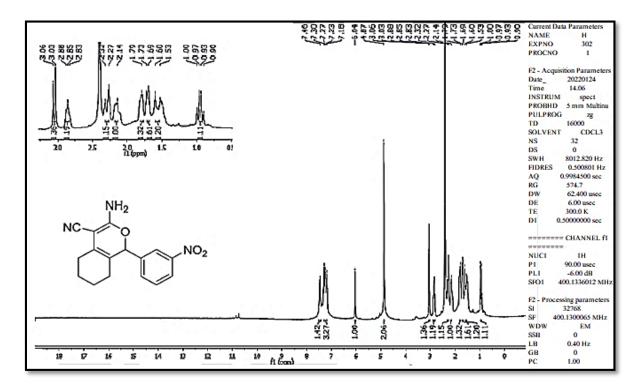


Fig. S17. ¹H NMR of 3-amino-1-(3-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4h**)

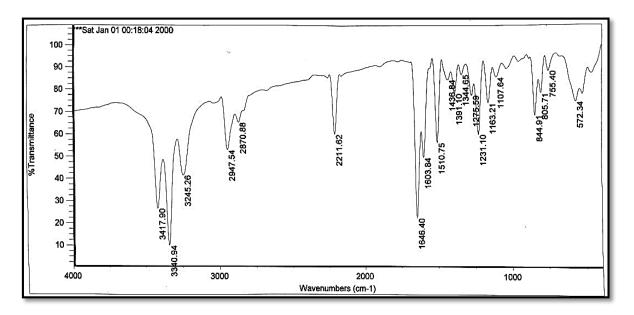


Fig. S18. FT-IR of 3-amino-1-(4-fluorophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4i**)

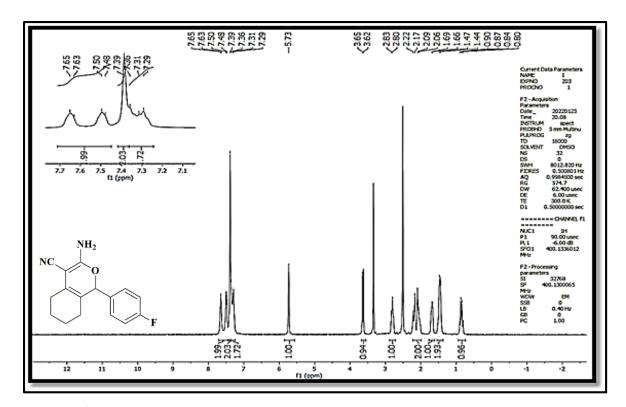


Fig. S19. ¹H NMR of of 3-amino-1-(4-fluorophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4i**)

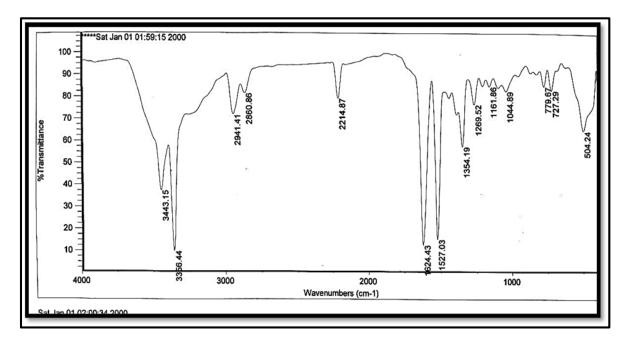


Fig. S20. FT-IR of 3-amino-1-(2-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4-carbonitrile

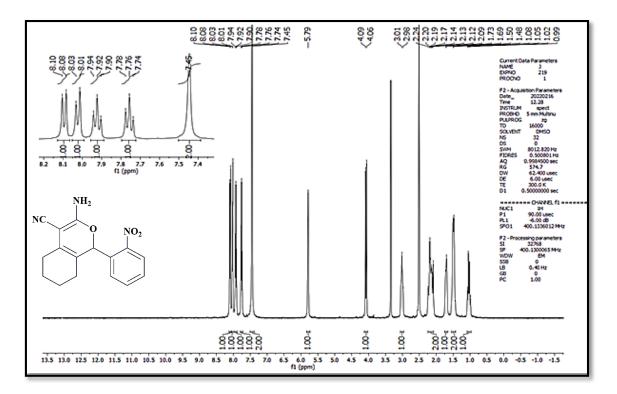


Fig. S21. ¹H NMR of 3-amino-1-(2-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4j**)

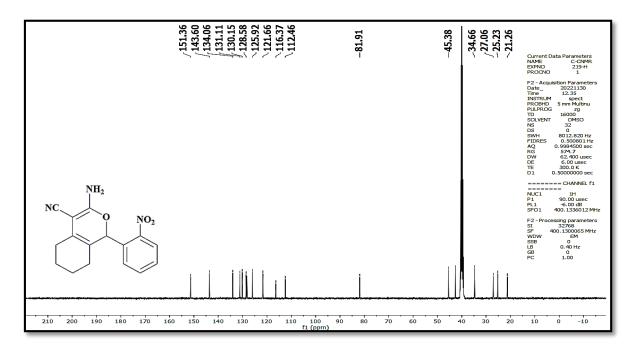


Fig. S22. ¹³C NMR of 3-amino-1-(2-nitrophenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4j**)

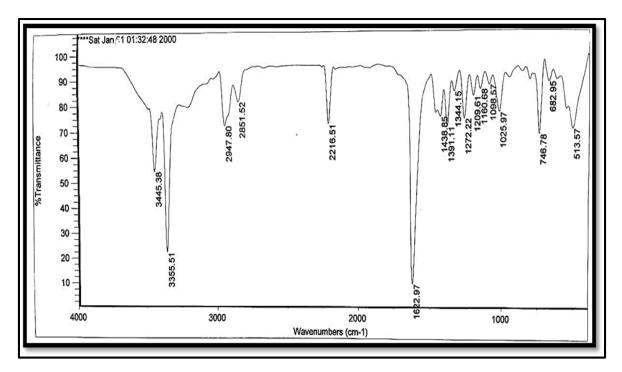


Fig. S23. FT-IR of 3-Amino-1-(2-bromophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (4k)

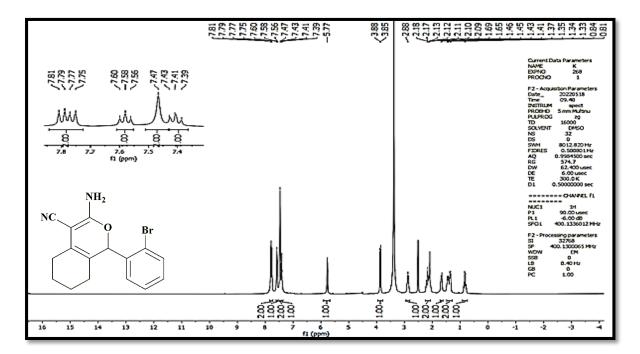


Fig. S24. ¹H NMR of 3-Amino-1-(2-bromophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4**k)

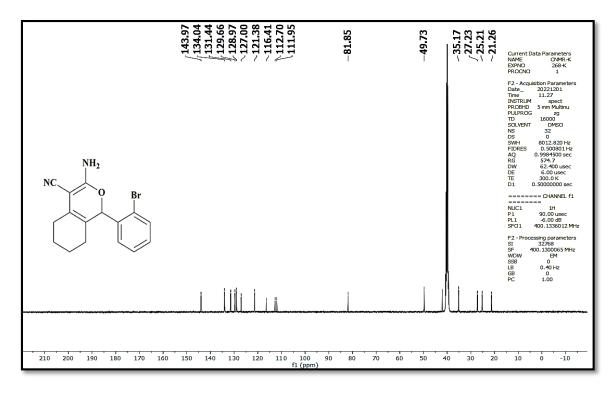


Fig. S25. ¹³C NMR of 3-Amino-1-(2-bromophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile (**4**k)

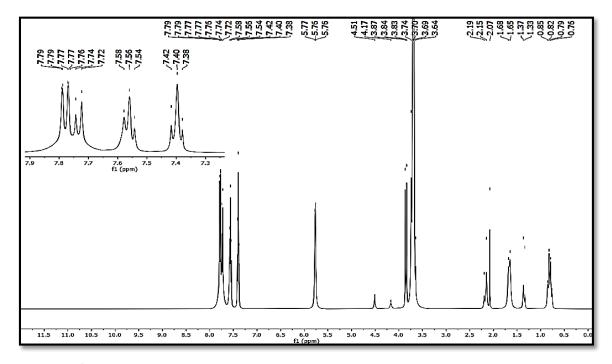


Fig. S26. ¹H NMR of 3-Amino-1-(2-bromophenyl)- 5,6,7,8-tetrahydro- 1H-isochromene-4carbonitrile in D₂O (**4**k)

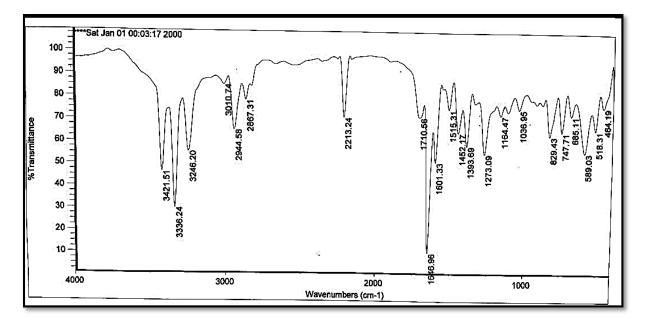


Fig. S27. FT-IR of 3-amino-1-(4-methylphenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4**I)

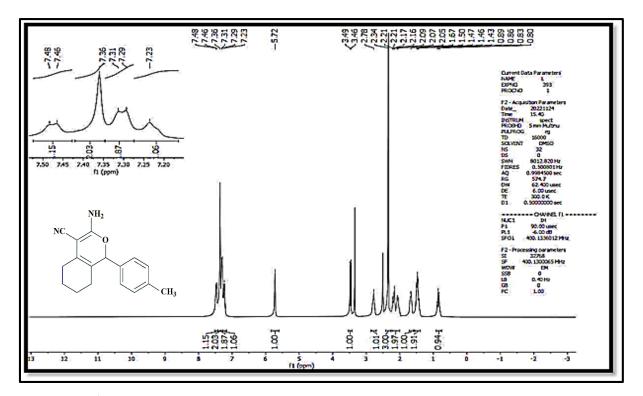


Fig. S28. ¹H NMR of 3-amino-1-(4-methylphenyl)-5,6,7,8-tetrahydro-1H-isochromene-4carbonitrile (**4**I)

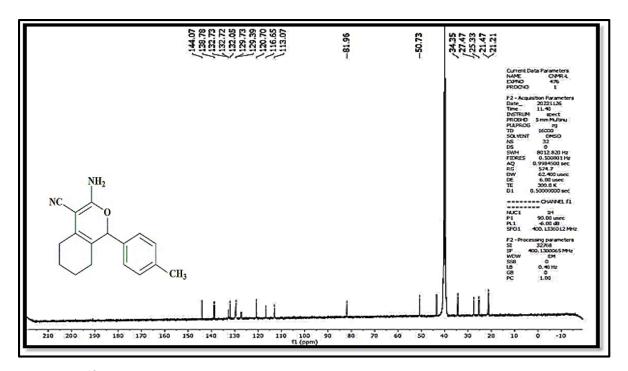


Fig. S29. ¹³C NMR of 3-amino-1-(4-methylphenyl)-5,6,7,8-tetrahydro-1H-isochromene-4-carbonitrile (**4**I)