

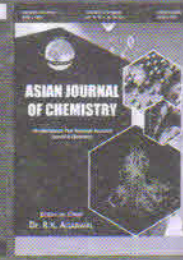


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Fe₃O₄@SiO₂@(CH₂)₃@4-(2-Aminoethyl)morpholine as a Reusable Magnetic Organocatalyst for Synthesis of Pyrano[3,2-*c*]chromene Derivatives Along with Docking Study

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Pyrano[3,2-*c*]chromene derivatives, as an important category of heterocyclic compounds, have received much attention due to their various biological activities. Different synthetic methods using various catalysts have been reported for the synthesis of these compounds. Here, a green, magnetically separable catalyst functionalized with nitrogen-containing groups was used for the synthesis of a series of pyrano[3,2-*c*]chromene derivatives. The target compounds were synthesized by employing the catalytic activity of the previously synthesized composite under environmentally friendly and mild conditions. The reaction proceeded efficiently in a water/ethanol mixture within a short time and resulted in high product yields. A multicomponent reaction was used to synthesize pyrano[3,2-*c*]chromene derivatives from malononitrile, 4-hydroxycoumarin and various aldehydes. The purity of the final compounds was checked by melting point determination and comparison with literature values. Since pyrano[3,2-*c*]chromene derivatives are proposed as potential inhibitors of DNA topoisomerases, especially TOPII, in the second part of this study, a computational study was performed targeting the DNA-TOPII complex. The results revealed that some of the synthesized compounds are known to inhibit topoisomerases, supporting their role as promising anticancer agents.

Keywords: Pyrano[3,2-*c*]chromene, Magnetically catalyst, Docking, Topoisomerase.