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$CoFe_2O_4$-Al_2O_3-TiO_2 Nano catalyst: Magnetically retrievable platform for medicinal precursors

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ABSTRACT

The significance of the reaction of *α, β-unsaturated* products in pharmaceutics and industry makes the design of economically efficient heterogeneous catalysts for the Knoevenagel condensation reaction essential. To manufacture Knoevenagel condensation products, using benzaldehydes and ethyl cyanoacetate, an active methylene compound, we have developed and produced titania-coated magnetically retrievable cobalt ferrite nanoparticles with interlayer alumina $CoFe_2O_4$-Al_2O_3-TiO_2 nanocatalyst by sequential polyol, coprecipitation and sol-gel hydrolysis techniques. To precisely characterise the nanocatalyst, herein several advanced techniques have been utilised, such as powder X-ray diffraction (XRD), Fourier transform infrared (FT-IR), transmission electron microscopy (TEM), Brunauer-Emmet-Teller (BET), and vibration sample magnetometry (VSM). Based on these characteristics, we have successfully developed a new magnetic nanocatalyst, $CoFe_2O_4$@Al_2O_3@TiO_2 (CFAT), which has cubic phase $CoFe_2O_4$ (CF) for its superparamagnetic capabilities, anatase phase TiO_2 (T) for improved catalytic action, and γ-Al_2O_3 (A) for thermal stability and support. The current approach's advantageous characteristics include outstanding catalytic performance, easily available solvent conditions for EtOH:H_2O (1:1), ease of catalyst retrievability, an easy workup procedure, a large substrate tolerance, high turnover frequency (TOF) values (up to 1470.58 h^{-1}), green chemistry metrics like E-factor (0.09), reaction mass efficiency (RME) value (91.69 %), carbon efficiency (100 %), and atom economy (AE) value (93.08 %) that are near their ideal values, and recyclability for up to ten runs without substantially reducing activity. A molecular docking study finds some of the *α, β-unsaturated* products show higher binding energy (ΔG) of -5.7 to -6.1 kcal/mol compared to the reference drug chloroquine's binding energy of -5.6 kcal/mol and equal to hydroxychloroquine's binding energy of -6.1 kcal/mol.

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