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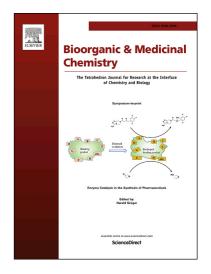
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## **ACCEPTED MANUSCRIPT**

A reusable magnetic nickel nanoparticle based catalyst for the aqueous synthesis of diverse heterocycles and their evaluation as potential antibacterial agent

Deboshikha Bhattacharjee, Sanjoy Kumar Sheet, Snehardinarayan Khatua, Koel Biswas, Sataram Joshi<sup>b</sup> and Bekington Myrboh<sup>a\*</sup>

<sup>a</sup>Centre for Advanced Studies in Chemistry, Department of Chemistry, North-Eastern Hill University, Mawlai Shillong -793022 India.

<sup>b</sup>Microbiology Laboratory, Department of Biotechnology and Bioinformatics, North-Eastern Hill University, Shillong – 793022, India

#### Abstract

A library of biologically important heterocycles, viz. pyrazolyl pyrimidine-triones, bis(heterocyclyl)methanes were successfully synthesised by the condensation of barbituric acid, pyrazolone with an aldehyde and dimedone/4-hydoxy coumarin with various substituted aldehydes in aqueous medium at room temperature catalysed by nickel nanoparticles which proved to be an efficient magnetically recyclable catalyst. The method is simple, eco-friendly and gave excellent yields of the products without taking recourse to column chromatographic separation procedures. Computational method was employed to elucidate the selective formation of uncyclised product in reaction course. The biological activity of the synthesized compounds were investigated and the results demonstrated profound antibacterial activity.

#### 1. Introduction

The discovery of multi-component reaction has led the synthesis of library of diverse heterocycles in a simple, efficient and concerted steps minimising the by-products and maximising the atom economy in a more environment friendly manner. Keeping in mind the green principles of chemistry, the use of harmful volatile organic solvents have been avoided and in lieu of hazardous solvents many alternative reaction media have been introduced. One such reaction medium is the 'universal solvent' i.e. water as it is the safest and most abundant substance on our planet. Besides as a solvent, water tends to enhance the reaction rate due to its polarity, hydrophobic packing and hydrogen bonding. The search for a catalyst which is nontoxic, affordable, easy to recycle and having high catalytic efficiency is an ongoing

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