पेटेंट कार्यालय
शासकीय जर्नल

OFFICIAL JOURNAL
OF
THE PATENT OFFICE

निर्गमन सं. 35/2025	शुक्रवार	दिनांक: 29/08/2025
ISSUE NO. 35/2025	**FRIDAY**	**DATE: 29/08/2025**

पेटेंट कार्यालय का एक प्रकाशन
PUBLICATION OF THE PATENT OFFICE

(12) PATENT APPLICATION PUBLICATION

(19) INDIA

(22) Date of filing of Application :17/08/2025

(21) Application No.202521078022 A

(43) Publication Date : 29/08/2025

(54) Title of the invention : Bio-Based Catalytic System for the Synthesis of Bioactive Heterocycles in Aqueous Medium

(51) International classification	:C07C0253300000, B01J0035300000, A61P0029000000, C07D0317540000, C07C0045300000
(86) International Application No Filing Date	:NA :NA
(87) International Publication No	: NA
(61) Patent of Addition to Application Number Filing Date	:NA :NA
(62) Divisional to Application Number Filing Date	:NA :NA

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(57) Abstract :

ABSTRACT OF THE INVENTION: The present invention introduces a bio-based catalytic system for the sustainable synthesis of bioactive heterocycles in an aqueous medium, addressing the need for eco-friendly alternatives in organic chemistry. The system employs heterogeneous catalysts derived from abundant bio-waste sources, including pomegranate peels, bael fruit rinds, freshwater mussel shells, and Agave americana leaves, which are converted into active ash materials through a simple thermal process. These catalysts, characterized by high surface area (100-200 m^2/g), basic sites (4-8 mmol/g), and porous structures, enable efficient multicomponent reactions (MCRs) at room temperature without the use of toxic solvents or expensive metals. Bioactive heterocycles, such as 4H-pyrans, 2-amino-4H-chromenes, pyranopyrazoles, benzochromenes, and biscoumarins, are synthesized via one-pot protocols involving aldehydes, malononitrile or ethyl cyanoacetate, and cyclic 1,3-dicarbonyls or pyrazolones. The aqueous environment not only serves as a green solvent but also enhances reaction kinetics through hydrogen bonding and solvation effects. Typical reactions achieve excellent yields (85-95%) in short times (30-120 min), with broad substrate tolerance for electron-withdrawing and electron-donating groups on aromatic aldehydes. The catalyst preparation is straightforward and scalable: bio-waste is dried, carbonized at 500°C, and pulverized, yielding a reusable material that maintains >90% efficiency over multiple cycles. Mechanistically, the catalyst's basic components activate the methylene group for Knoevenagel condensation, followed by Michael addition and intramolecular cyclization, leading to the heterocyclic products. Characterization data from XRD (amorphous carbon phases), SEM (porous morphology), FT-IR (presence of -OH, $-CO_3$ groups), and BET analysis support the catalyst's efficacy. Preliminary biological evaluations indicate that the synthesized heterocycles possess significant antimicrobial activity (MIC 10-50 µg/mL against Gram-positive and Gram-negative bacteria), anticancer potential (IC_{50} 20-100 µM against HeLa and MCF-7 cell lines), and anti-inflammatory properties (inhibition of COX-2 enzyme). This underscores their relevance in drug development for treating infections, cancers, and inflammatory disorders. Compared to conventional methods using acids/bases like H_2SO_4 or piperidine in organic solvents, this system reduces environmental impact by minimizing waste, energy consumption, and hazardous materials. It aligns with the 12 principles of green chemistry, particularly in using renewable feedstocks and safer solvents. Potential industrial applications include large-scale production of pharmaceutical intermediates, with extensions to other transformations like transesterification or C-C bond formations. Challenges such as catalyst deactivation in highly substituted substrates are mitigated by optimization of loading and reaction pH. Overall, this invention provides a versatile, low-cost platform for green synthesis, contributing to sustainable development in chemical sciences and offering economic benefits through waste valorization.

No. of Pages : 15 No. of Claims : 6