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Biogenic Synthesis of Pyrazole-Based Pharmacophores Using Onion Extract: A Sustainable Strategy for Antibacterial Drug Development

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ABSTRACT

Purpose: *The aim of the present study was to develop an eco-friendly and sustainable approach for the synthesis of substituted pyrazole derivatives using Allium cepa (onion) juice as a natural, green catalyst. The synthesized compounds were evaluated for their antimicrobial activity against selected Gram-positive and Gram-negative bacterial strains.*

Methods: *Fresh onion juice was extracted and used as a biocatalyst in the synthesis of various substituted pyrazole derivatives via condensation reactions. The structures of the synthesized compounds were confirmed by IR, NMR and mass spectrometry. Antibacterial screening was performed using the agar well diffusion method against Staphylococcus aureus, Bacillus subtilis (Gram-positive) and Escherichia coli, Pseudomonas aeruginosa (Gram-negative) bacteria. In silico studies, including molecular docking and ADME predictions, were also carried out to evaluate potential biological interactions and drug-likeness.*

Results: *All synthesized compounds were obtained in good yields with high purity. Antibacterial studies revealed that certain pyrazole derivatives exhibited significant activity, particularly against Gram- positive strains. Structure–Activity Relationship (SAR) analysis suggested that electron-donating substituents enhanced antibacterial potency. Molecular docking confirmed good binding affinities with target bacterial enzymes, while ADME predictions indicated acceptable pharmacokinetic profiles.*

Conclusion: *The study demonstrates that Allium cepa juice is an effective green catalyst for the synthesis of biologically active pyrazole derivatives. These compounds show promising antibacterial activity and favourable in silico drug-likeness, suggesting their potential as lead molecules for further pharmaceutical development.*

Keywords: Flavonoids; Flavone; Acacetin; Anticonvulsant; Pentylenetetrazole (PTZ) induced seizure; 4COF

INTRODUCTION

Pyrazoles, five-membered heterocyclic compounds containing two adjacent nitrogen atoms, are widely recognized for their broad spectrum of pharmacological activities and serves as a valuable template for both combinatorial and medicinal chemistry. The pyrazole ring system is a common scaffold in numerous biologically active compounds due to its structural versatility, ease of functionalization and favorable pharmacokinetic properties. Pyrazole derivatives have shown diverse biological activities, including antibacterial, antifungal, anticancer, antitubercular, anti-inflammatory antiviral and antiandrogenic properties. Additionally, some pyrazole derivatives have exhibited analgesic, antidiabetic, antioxidant, anthelmintic and analgesic activities. Beyond their biological significance, many pyrazoles are also known for their luminescent and fluorescent properties, this wide range of therapeutic applications has led to increased interest in the development of novel pyrazole-based molecules.

Traditionally, the synthesis of pyrazole derivatives often involves the use of harsh chemicals, toxic solvents and energy-intensive conditions, raising environmental and safety concerns. In response to the growing emphasis on sustainable chemistry, green synthetic methodologies have emerged as efficient and eco-friendly alternatives. These approaches focus on minimizing hazardous reagents, reducing energy consumption and employing renewable or natural resources [1].