International Journal of Advanced Research in Science, Engineering and Technology
ISSN: 2350-0328
Vol. 12, Special Issue, December 2025
National Conference on Earth, Elements and Energy: Interdisciplinary Perspectives (NC3EIP–2025)
IMPACT FACTOR 7.150

Synthesis and Biological Study of noval pyrazole derivatives

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ABSTRACT: We report an efficient and eco-friendly protocol for the synthesis of a new library of pyrazole derivatives. The synthesis was carried out via a green synthesis methods, affording the target compounds in high yields and high purity. The structures were elucidated using elemental analysis and spectral data. Subsequent biological screening for antimicrobial and antifungal properties was conducted. The results demonstrated that the introduction of lipophilic electron-withdrawing substituents enhanced the bioactivity of the pyrazole core. All derivative exhibited the good potency against Ecoli, s. aureus and C. albicans. This study highlights a robust synthetic route to access biologically active pyrazoles that warrant further investigation as therapeutic agents.

KEY WORDS: Pyrazole derivatives, Biological evaluation, antimicrobial properties, antifungal properties.

I. INTRODUCTION

Heterocyclic compounds play an important role in medicinal chemistry due to their wide range of biological activities. Among them, pyrazole and its derivatives have attracted significant attention because of their unique structural features and strong pharmacological potential. Pyrazole is a five-membered nitrogen-containing heterocycle consisting of two adjacent nitrogen atoms, which allows it to interact effectively with various biological targets.

Pyrazole derivatives are well known for exhibiting diverse biological properties such as antimicrobial, antifungal, anti-inflammatory, analgesic, anticancer, antidiabetic, and antioxidant activities. The presence of nitrogen atoms in the pyrazole ring enhances hydrogen bonding and improves binding affinity with enzymes and receptors, making these compounds valuable scaffolds in drug design [1,2].

Several studies have reported the synthesis of substituted pyrazole derivatives using different synthetic strategies, including cyclocondensation reactions, multicomponent reactions, and green chemistry approaches. Modifications at different positions of the pyrazole ring significantly influence their biological activity. For example, electron-donating or electron-withdrawing substituents on aromatic rings attached to pyrazole have been shown to enhance antimicrobial and anticancer properties [3,4].

In recent years, pyrazole derivatives have shown promising antimicrobial activity against both Gram-positive and Gram-negative bacteria, as well as antifungal strains such as *Candida albicans*. The increasing resistance of microorganisms to existing drugs has created an urgent need for the development of new antimicrobial agents. Pyrazole-based compounds have emerged as potential candidates to overcome this challenge due to their broad-spectrum activity and structural versatility [5,6].

Furthermore, biological screening studies have demonstrated that pyrazole derivatives can inhibit key enzymes and cellular pathways involved in disease progression. Structure–activity relationship (SAR) studies indicate that slight structural modifications in pyrazole molecules can lead to significant changes in biological performance, highlighting the importance of designing novel derivatives with improved efficacy and reduced toxicity [7].

Based on the above findings, the synthesis of novel pyrazole derivatives and their biological evaluation remains an active and important area of research. The present work focuses on the design and synthesis of new pyrazole derivatives followed by their biological screening to explore their potential as antimicrobial and antifungal agents.

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II. MATERIAL AND METHOD

All melting points were measured in an open capillary tube using a silicon oil bath and are uncorrected. IR spectra were recorded on a Nicolet-Impact 400 FT-IR spectrometer. The ^{1}H NMR spectra were taken on a Bruker AC300 (300 MHz) instrument, using TMS as the internal standard. Nitrogen content was determined by the Kjeldahl method. The purity of the compounds was checked by thin-layer chromatography (TLC) on silica gel-G plates.

Diones were heated under reflux with semicarbazide, thiosemicarbazide, or isonicotinic acid hydrazide in ethanol for about two hours. After the reaction, the mixture was cooled and then poured into water. The solid product that formed was filtered, washed with water, and recrystallized from ethanol to obtain titled compounds (1a–c). Their physical data are listed in the table.

Sr. No.	Compound	R1	R_2	R_3	Melting Point ^{0}C	% Yield	% Nitrogen		R.F. Value
							Found	Calculated	
1	1a	H	OH	$CSNH_2$	317	55	10.21	10.21	0.54
2	1b	OCH_3	OH	$CSNH_2$	311	65	9.52	9.52	0.62
3	1c	H	OH	C_5H_4NCO	217	45	9.19	9.19	0.65
4	1d	OCH_3	OH	C_5H_4NCO	319	64	8.62	8.62	0.55
5	1e	H	OH	$CONH_2$	290	72	10.63	10.63	0.59
6	1f	OCH_3	OH	$CONH_2$	228	49	9.88	9.88	0.52

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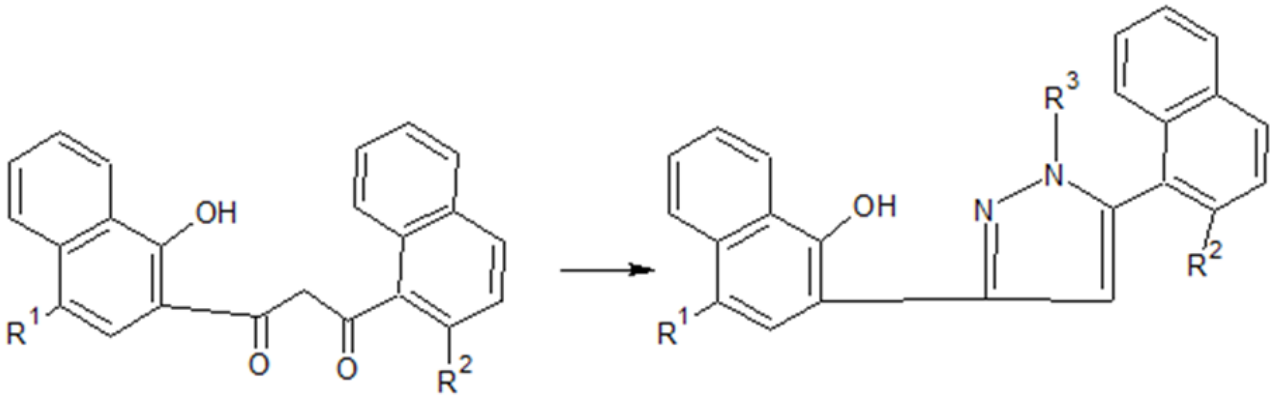
III. SCHEME



R1 = OCH3 , R2 = OH, R3 = $CSNH_2$, C_5H_4NCO

IV. SPECTRAL INTERPRETATION OF (1e)

IR (n_{max}) (cm^{-1}) : 3312 (OH, str), 3253 (NH_2, str), 1547 (C=N, str) 1710 (CO , str)

NMR (d ppm): 6.55 (s, 1H, =CH of pyrazole), 6.85-8.38 (m, 9H, Ar-H) , 6.06 (s, 2H, -NH_2), 09.73 (s, 1H, OH), 09.51 (s, 1H, OH)

V. BIOLOGICAL STUDY

The synthesized novel pyrazole derivative demonstrated promising antimicrobial potential against both bacterial and fungal pathogens. In antibacterial assays, the compound showed noticeable inhibitory activity against *Escherichia coli* and *Staphylococcus aureus*, indicating effectiveness against both Gram-negative and Gram-positive organisms. The zone of inhibition values suggested that the derivative disrupts microbial growth in a dose-dependent manner. In antifungal testing, the compound also exhibited significant activity against *Candida albicans*, reflecting its ability to interfere with fungal cell proliferation. Overall, the results indicate that this pyrazole derivative possesses broad-spectrum antimicrobial properties and could serve as a potential lead molecule for future drug development.

VI. ACKNOWLEDGEMENT

The authors are thankful to Dr.R D Deshmukh, Principal, RDIK and NKD college Badnera for providing necessary facilities .

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