Indian Journal of Heterocyclic Chemistry
Vol. 36 - Number 01 (Jan-Mar 2026) 99-108
https://connectjournals.com/01951.2026.36.99
https://doi.org/10.59467/IJHC.2026.36.99

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Multifunctional Imidazole–pyrazole hybrids: Design, synthesis, and therapeutic potential

Vikram Punia[1], Pratibha Periwal[1], Swati Sehrawat[2], Ashwani Kumar[3], Vikas Verma[1]*, Meenakshi Bhatia[3], Vikramjeet Singh[3] and Sonia Rohilla[1]

[1]Department of Chemistry, Guru Jambheshwar University of Science and Technology, Hisar, Haryana, India
[2]Department of Physics, Deenbandhu Chotu Ram University of Science and Technology, Murthal, Haryana, India
[3]Department of Pharmaceutical Sciences, Guru Jambheshwar University of Science and Technology, Hisar, Haryana, India

ABSTRACT Imidazole–pyrazole hybrids represent a class of compounds that have gained significant attention due to their diverse pharmacological activities. In this study, a focused library of derivatives (**3a–3f** and **5a–5f**) was synthesized through the Debus–Radziszewski reaction and a multi-step hybridization approach, and thoroughly characterized using nuclear magnetic resonance, Fourier-transform infrared, and mass spectrometry techniques. The antimicrobial potential of all the synthesized compounds was evaluated by determining minimum inhibitory concentration (MIC) values against a panel of bacterial and fungal strains, revealing potent activity for several derivatives. Among them, compound **5d** emerged as the most effective candidate, with MIC values as low as 0.0104 µmol/mL against *Escherichia coli*, *Staphylococcus aureus*, *Candida albicans*, and *Aspergillus niger*. Similarly, compound **3d** showed strong dual antibacterial and antifungal activity. Structure–activity relationship analysis highlighted the importance of halogen substituents (–Br, –F) and thiophene rings in enhancing antimicrobial potency. Molecular docking studies further validated the experimental results, showing robust interactions of **5d** with bacterial DNA gyrase, consistent with its superior MIC values. Furthermore, predictions of drug-likeness and bioavailability-related parameters were also carried out. Insights into these molecular interactions provide a foundation for the rational design of next-generation pyrazole–imidazole hybrids with enhanced pharmacological profiles. This research underscores the potential of these hybrid compounds as promising antimicrobial agents.

KEY WORDS Antibacterial, Antifungal, Hybrids, Imidazole, Pyrazole.

How to cite this article: Punia, V., Periwal, P., Sehrawat, S., Kumar, A., Verma, V., Bhatia, M., Singh, V. and Rohilla, S. Multifunctional Imidazole–pyrazole hybrids: Design, synthesis, and therapeutic potential, *Indian J. Heterocycl. Chem.*, **2026**, *36*, 99–108. *https://doi.org/10.59467/IJHC.2026.36.99*