Notification No: 580/2025

Date of Award: 21/05/2025

Name of Scholar: Zohaib Saifi

Name of Supervisor: Professor Imran Ali

Name of Department: Chemistry

Topic of Research: "Design, Synthesis and Biological Studies of some New Heterocyclic Hybrid Molecules"

FINDINGS

This research presents the successful design, synthesis, and antibacterial evaluation of several novel heterocyclic hybrid molecules aimed at combating multidrug-resistant (MDR) bacteria.

Objectives:

- To design and synthesize heterocyclic hybrid molecules.
- To confirm the synthesized molecules by spectroscopic techniques such as ^{1}H-NMR,^{13}C-NMR, LC-MS, FT-IR, and HRMS.
- To perform in silico modeling (molecular docking, molecular dynamics) to predict receptor interactions and guide structural optimization.
- To evaluate biological activity through vitro assays.

A key focus was placed on the development of 1,2,4-oxadiazole-sulfonamide, quinoline-sulfonamide, and quinoline-indole chalcone hybrids. These compounds were synthesized through

efficient protocols and purified by column chromatography yielding high-purity products, confirmed by spectroscopic techniques such as ^{1}H-NMR,^{13}C-NMR, LC-MS, FT-IR, and HRMS.

Biological evaluation demonstrated significant antibacterial activity across multiple strains. Notably, compound 8f and QS3 showed potent activity with low MIC/MBC values and synergistic effects with standard drugs. In-silico study also support the result.

These findings provide a solid platform for further pharmacological optimization and preclinical development.