Notification No: 549/2023

Date of Award: 31-10-2023

Name of the Scholar**:** **Rabiya Mehandi**

Name of the Supervisor**:** **Prof. Nahid Nishat**

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Name of the department**:** **Chemistry**

Topic of the Research**:** **Metal Catalyzed Synthesis, Characterization and Biological Applications of Some Heterocyclic Derivatives**

Findings

The thesis entitled "**Metal Catalyzed Synthesis, Characterization and Biological Applications of Some Heterocyclic Derivatives"** consists of six chapters. In this thesis we have mainly focused on Metal catalyzed synthesis and characterization of heterocyclic derivatives and their biological evaluation. The primary objectives of the thesis are to synthesize potentially active oxadiazole, pyrazole, and pyrazoline moieties as antifungal and antioxidant agents. All the synthesized derivatives were characterized by FT-IR, ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry. After synthesis and characterization, the *in-vitro* hemolysis assay of all derivatives was done against different fungi strains such as *Candida albicans*, *Candida tropicalis*, and *Candida glabrata*. Fluconazole was used as the standard drug. Based on the antifungal activity, the most active compounds were considered to investigation for the interaction property with calf thymus DNA and pBR322 plasmid DNA. The Antioxidant activity of all the compounds was also screened and percentage inhibition was calculated. DFT calculations of lead compounds was done to find out HOMO/LUMO energy levels and optimized geometry. MD studies of *C. albicans* CYP51 with compounds was carried out. The results were further validated by *In-silico* molecular docking (PDB ID: 1BNA) and the pharmacokinetic properties.