Notification No.: 566/2024
Date of Award: 12-08-2024

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Topic of the research: Synthesis, Characterization, Biological and Catalytic Activity of Transition Metal Complexes of Some Heterocyclic Ligands

Keywords: Heterocyclic Derivatives, Transition Metal Complexes, Antifungal Activity, DNA Binding Study, Catechol Activity

Findings

This Ph.D. entitled "**Synthesis, Characterization, Biological and Catalytic Activity of Transition Metal Complexes of Some Heterocyclic Ligands**," was submitted by **Nouman**. A Ph.D. thesis consists of five chapters. The focus of the thesis is the design, synthesis, and characterization of heterocyclic derivatives and their transition metal complexes.

The **first chapter** deals with an introduction and brief literature survey of heterocyclic derivatives and their transition metal complexes.

Chapter 2 deals with design, synthesis, and heterocyclic derivatives (3a-3e) and their transition metal complexes (1-7). All the heterocyclic derivatives and their transition metal complexes have been thoroughly characterized with various spectroscopic techniques. The *in vitro* antifungal activity of heterocyclic compound and metal complex were performed by using different fungal strains. In addition, Ct-DNA binding studies were performed using various measurements with lead compounds. The catalytic activity of the lead compound was analysed for the oxidation of catechol to o-quinone. Furthermore, it was also concluded that potent heterocyclic analogues and complexes exhibited significant antioxidant activity against DPPH free radicals and hydrogen peroxide. Also, pharmacokinetics studies revealed that none of the heterocyclic compounds and metal complexes violate the Lipinski rule, and all the properties are in a considerable range for good oral bioavailability.

Chapter 3 deals with the design, synthesized and characterized the heterocyclic compounds **(4a-4f)** and metal complexes **(1–7)** using various spectroscopic techniques. Besides, the lead

heterocyclic compound and metal complex performed *in vitro* antifungal and antioxidant activities. The Ct-DNA studies were investigated using various measurements of lead derivatives and metal complexes. The catalytic activity of the potent complex was analyzed for the oxidation of catechol to o-quinone. A molecular docking study with (PDB ID: 1BNA) of all heterocyclic derivatives was also carried out. Also, pharmacokinetics studies revealed that none of the heterocyclic compounds or metal complexes violated the Lipinski rule.

Chapter 4 discusses the synthesis of heterocyclic derivatives **(2a-2n)** and **Ni(II)**, **Zn(II)**, and **Pd(II)** complexes of analog **2a** which were characterized by various spectroscopic techniques. All the heterocyclic derivatives and metal complexes had *in vitro* antifungal activity against fungal strains. The binding strength of all lead analogs with Ct-DNA was determined using various measurements. The antioxidant and catechol activities of potent compounds were measured. A molecular docking study with (PDB ID: 1BNA) of all heterocyclic derivatives and Pd(II) was also carried out. Also, pharmacokinetics studies revealed that none of the heterocyclic compounds or complexes violated the Lipinski rule.

In **chapter 5** the candidate reports two heterocyclic analogs **(5a** and **5b)** and transition metal complexes **(1-10)** with **5a** and (**11-20)** with analog **5b**. The reported compounds are adequately characterized based on different data techniques. . In addition, all the compounds had *in vitro* antifungal activity against *fungal strains*. The intercalative binding mode of lead analogs with Ct-DNA has been confirmed using various analytical measurements, which were further validated through molecular docking udies. The catalytic activity of the potent complexes was analysed for the oxidation of catechol to *o*-quinone with first-order kinetics that follow Michaelis-Menten enzymatic kinetics. Furthermore, it was also concluded that heterocyclic ligands and metal complexes exhibited significant antioxidant activity against DPPH free radicals and hydrogen peroxide. Pharmacokinetics studies revealed that none of the compounds or their metal complexes violate the Lipinski rule.