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Thesis Title: Synthesis, Structural Characterization and Biological Studies of Metal Complexes of Dithiocarbamate Derivatives.

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FINDINGS

The thesis entitled "**Synthesis, Structural Characterization and Biological Studies of Metal Complexes of Dithiocarbamate Derivatives**" consists of six chapters. The thesis details out the development of various biologically active complexes containing dithiocarbamate ligands. The synthesized metal dithiocarbamate complexes were evaluated for their antimicrobial, anti-leishmanial and DNA binding agents.

A brief chapter-wise description of the findings is given below.

Chapter I deals with the general chemistry, synthetic approaches and different binding modes of metal dithiocarbamate complexes. It also describes the general chemistry, pharmacological activities of metal dithiocarbamate adducts. The chapter also deals with various mode of DNA binding of drug compounds.

A general description on the sources and solvents of all the instruments used during the research work is provided in the chapter II.

Chapter III deals with synthesis of new functionalized homo and heteroleptic zinc(II) and cadmium(II)dithiocarbamate complexes and then characterized by elemental analysis, IR, UV-Vis., ^{1}H and ^{13}C NMR spectroscopy. Anti-leishmanial activity evaluation revealed the promising anti-promastigote activity of complexes **1** and **2**with IC_{50} values4.6±0.41 and 3.37±0.28 μgmL^{-1}. All the complexes showed potential antioxidant activity.

Chapter IV describes four homo and heteroleptic complexes were prepared and characterized by IR, UV-Vis., NMR (^{1}H, ^{13}C) spectroscopic techniques. The anti-leishmanial activity evaluation of complexes **1** and **2** revealed promising anti-promastigote activity with IC_{50} values of 18.50±0.86 and 14.58±0.78 $\mu g\ mL^{-1}$, and anti-amastigote activity with IC_{50} values of 33.95 ± 1.75 and 28.63 ± 1.63 $\mu g\ mL^{-1}$, respectively.

Chapter V details out the synthesis of new homoleptic heteroleptic complexes and then characterized by an elemental analysis, IR, ^{1}H, ^{13}C NMR and UV-Vis. spectroscopy. All the complexes showed significant scavenging activity. The *in vitro* antifungal potential of complexes (**1-4**) against three *Candida* strains (*C. albicans, C. glabrata* and *C. tropicalis*) by taking fluconazole (FLC) as a reference drug, showed that **3** exhibit significant activity with MIC around 500 μgmL^{-1}against all strains.

In chapter VI, synthesis of four new complexes of dithiocarbamate ligand were described and well characterized by elemental analyses, IR, UV-Vis., ^{1}H and ^{13}C NMR spectroscopy. All the complexes exhibit significant DPPH scavenging activity. The *in vitro* antifungal potential of all the complexes (**1-4**) towards three *Candida* strains (*C. albicans, C. glabrata* and *C. tropicalis*) showed that complexes **3** and **4** exhibit moderate activity. The complexes **2** and **4** have bind effectively with calf thymus DNA (Ct-DNA) through intercalative mode of interaction, which was further supported by molecular docking study.