Abstract

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Title: ***"Promising bio-active transition metal complexes with azo/imine functional O N S donor ligands: Synthesis, characterization and in vitro anticancer activity"***

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Chapter I represents a brief introduction on the a review of the azo/imine ligands containing O N S donor site and different transition metal complexes of Palladium(II), Platinum(II), Ruthenium(II), Rhenium(I). The anti-cancer activities of the metal complexes and their interactions with DNA and BSA have been described.

Chapter II deals with the synthesis and characterization of 5-fluorosalicylaldehyde-4(N)-substituted thiosemicarbazones ligands and their Pd(II) complexes. Structure of the complexes are confirmed by single crystal X-ray diffraction method. Electronic structure of the complexes is interpreted by DFT/ TDDFT computations. The ability of the complexes to bind with CT-DNA and bovine serum albumin (BSA) are investigated by UV-Vis method and fluorescence method.

Chapter III introduces the synthesis and thoroughly characterization of new Pd(II) and Pt(II) complexes with ONS donor azo-thioether pincer ligand. Electronic structure, solution spectrum and redox properties of the complexes are interpreted by DFT/TDDFT studies. The binding properties of the complexes toward calf thymus DNA (CT-DNA) and bovine serum albumin (BSA) are investigated with the help of absorption and fluorescence spectroscopy. *In vitro* antitumor activity of the synthesized complexes was tested on human liver (HepG2), colorectal (HCT116) and human lung (A549) cancer cell lines using MTT assay.

Chapter IV deals with the synthesis and characterization of two novel morpholine-based Pd(II) and Pt(II) complexes with N,N′ donor ligand. Electronic structure and solution spectrum of the complexes are interpreted by DFT/TDDFT studies. The investigation of the biological characteristics of the complexes have been carried out focusing on the binding properties with calf-thymus DNA (CT-DNA) and the affinity toward bovine serum albumin (BSA) investigated using UV-Vis and fluorescence spectroscopy. Finally, MTT assay has been used to evaluate the cytotoxic activity of the complexes against triple negative breast cancer cell line (MDA-MB-231) and normal kidney cell line (HEK-293).

Chapter V describes the synthesis and characterization of two new cyclometallated ruthenium(II) carbonyl complexes via C(aryl)-S bond activation. The compounds' electronic structure and UV-Vis spectra have been clarified by DFT and TD-DFT computations. The binding ability of

complexes with calf thymus DNA (CT-DNA) and Bovine Serum Albumin (BSA) have been explored by absorption and emission titration methods. In addition, the *in vitro* cytotoxicity of the ligands and complexes against human breast cancer cell line (MCF-7), human lung cancer cell line (A549), triple negative breast cancer cell line (MDA-MB-231) and gastric adenocarcinoma cell line (AGS) were investigated by using the MTT assay.

Chapter VI deals with the synthesis and characterization of two new Rhenium(I) tricarbonyl complexes with ONS donor azo-thioether ligands. Electronic structures and spectral properties of the complexes were interpreted by DFT and TDDFT calculations. The binding properties of the complexes toward calf thymus DNA (CT-DNA) and bovine serum albumin (BSA) are investigated with the help of absorption and fluorescence spectroscopy. *In vitro* cytotoxicity of the fabricated complexes was tested on human breast epithelial adenocarcinoma cell line (MCF-7) and human breast epithelial cell line (MCF-10A) using MTT assay.

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(Full signature of the candidate)

Date: 14/03/24

Signature with Seal of the Supervisor

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