

ABSTRACT

Index no.: 225/18/Chem./26.

Title: *“Synthesis, structure elucidation, and exploration of potential anti-cancer activity of newly designed palladium(II) Schiff base complexes”*

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In this thesis, synthesis of new Palladium(II) complexes using different type of NSO and NNO donor Schiff base ligands and their spectral and redox properties has been explored. The single crystal X-ray diffraction method confirms the complexes' structures. In addition, anticancer activity of the complexes has been studied and theoretical studies have also been undertaken to prove the electronic structures of the complexes. In addition, a selective and sensitive analytical method for the detection of palladium in the environment has been designed and developed.

Chapter-I

In this chapter, a review of the ligands containing ONS and ONN donor site and different complex of Palladium(II) has been described including their cancer activities and also their interaction with DNA and BSA along with the purpose of present investigations.

Chapter-II

In this chapter, a new palladium(II) complex, [Pd(LS^{Et})Cl] with benzothiazole based ONS donor pincer ligand (HLS^{Et}) was synthesized. The ability of the complexes to bind with CT DNA has been investigated by UV-Vis method and fluorescence method. Similarly, the interaction of the complex with BSA protein was investigated by UV-Vis and fluorescence methods. In vitro cytotoxicity of the complex towards human gastric cancer cell lines (AGS) was assessed by MTT assay method.

Chapter-III

In this chapter, synthesis of two new palladium(II) complexes, [Pd(L)Cl] and [Pd(L)PPh₃](ClO₄), with ONS donor thioether ligand (HL) is reported. All the complexes were thoroughly characterized by using numerous spectroscopic techniques like FT-IR, NMR and UV-visible spectroscopy and so forth. Moreover, DFT and TDDFT calculations were performed to interpret the electronic structure, redox and spectral properties of the complexes. Cytotoxicity of the complexes was evaluated in vitro using MTT assay on human gastric cancer cell lines (AGS).

Chapter-IV

In this chapter, two new ONN donor pincer ligands along with their palladium complexes are synthesized and thoroughly characterized by several spectroscopic techniques. The ability of the Pd(II) complexes to bind with CT DNA are investigated by UV-Vis method. Moreover, the interactions of Pd(II) complexes with bovine serum albumin (BSA) are also studied. The antiproliferative activity of the complexes are investigated with AGS, MDA-MB 231 and HepG2 cancer cell line. Electronic structure of the complexes is interpreted by DFT/ TDDFT computations.

Chapter-V

In this chapter, two new ONN donor pincer ligands and their palladium complexes are synthesized and thoroughly characterized by several spectroscopic techniques. The ability of the Pd(II) complexes to bind with CT DNA are investigated by UV-Vis method and Competitive binding study with ethidium bromide (EB) by fluorescence method suggests that the Pd(II) complexes efficiently displace EB from EB-DNA complex. Moreover, the interactions of Pd(II) complexes with bovine serum albumin (BSA) are also studied. The antiproliferative activity of the complexes are investigated with different cancer cell line.

Chapter-VI

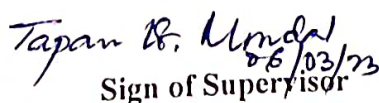
In this chapter, a new coumarin-morpholine O,N,N donor pincer ligand appended palladium(II) complex was synthesized and thoroughly characterized. Electronic structure and solution spectrum of the complexes are interpreted by DFT/TDDFT studies. The in vitro cytotoxic activity of the palladium complexes was carried out against human gastric cancer (AGS) cell lines and breast cancer cell lines (MDA MB 231 and MCF-7) by MTT assay. Intercalation of the complex with DNA was evaluated by performing agarose gel electrophoresis of various concentrations of the complex. The interaction of the complex with CT DNA and BSA protein was investigated by UV-Vis and fluorescence methods.

Chapter-VII

In this chapter, new coumarin based ONS donor ligand containing palladium(II) complexes were synthesized and thoroughly characterized by several spectroscopic techniques. Electronic structure and solution spectrum of the complexes are interpreted by DFT/TDDFT studies. The in vitro cytotoxic activity of the palladium complexes was carried out against breast cancer (MCF 7 and MDA MB 231) cell lines by MTT assay. The understanding of the complexes to bind with CT DNA and BSA investigated carefully through UV-Vis method and fluorescence method.

Chapter-VIII

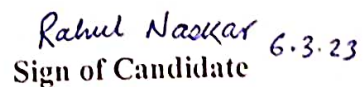
In the last chapter, a novel chromone based fluorescent probe (HMPM) is produced to selectively detect Pd²⁺ in the presence of other metal ions in the nM range. Interaction of HMPM with Pd²⁺ is determined by a variety of spectroscopic approaches. Density Functional Theory (DFT) is used to examine the electronic structures of HMPM and HMPM-Pd²⁺. Importantly, the probe can effectively detect Pd²⁺ using the dip-stick method.


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