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**Title of Thesis** - Development of Macromolecular Ligands for Multimetal Capturing Tendemcy: Physicochemical and Biological studies.

# ABSTRACT

The research work deals with the synthesis of the macromolecular ligands and its complexes and their characterizations. The scope and objective of the proposed work was discussed along with the experimental methods and chemicals used. The applications of dendrimers and their metal complexes has become very important research area in constant growth. Various aspects of the work have been explained. To illustrate the work being carried out in this field, an upto date literature survey has been presented. All the chapters deal with the synthesis of dendrimeric ligand and its metal complexes. The prepared ligand was complexed with metal ions. Both the ligand and its complexes were characterized by elemental analysis and spectroscopic studies (FT-IR, UV–vis, 1H NMR, and ESI-MS). In first two chapters and last chapter, the ligand and its complexes were screened on Candida albicans ATCC 90028 by determining MICs (minimal inhibitory concentrations) and inhibition in solid media (disk diffusion assay). In last two chapters, detection of DNA damage at the level of the individual eukaryotic cell was observed by commet assay. Molecular docking technique was used to understand the ligand–DNA interactions. In first chapter, response to an increasing demand for effective anticandidal agents, a new water-soluble dendrimeric ligand (L) was synthesized by Michael addition of ethylenediamine to methyl methacrylate. Square-planar and square-pyramidal geometries were proposed for Cu(II) and Co(II) on the basis of UV–vis spectroscopic data and molar conductance measurements. The synthesis of PAMAM dendrimer as ligand and its metal complexes is described in the next chapter. The development of drug resistant strains of the pathogenic fungi despite the availability of large number of drugs demands the development of new and more

potential drug molecules. Dendrimer based drug molecules are comparatively less researched upon and a recent advancement in this field. New water soluble dendritic ligand and its copper (II), nickel (II) and cobalt (II) complexes were synthesized. Tetragonal geometry was proposed for Cu(II) complex and square planar geometry was proposed for Co(II) and Ni(II) complexes on the basis of UV-Vis spectroscopic data. The compounds were fungicidal in comparison to fluconazole which is fungistatic only; however they are less active than fluconazole. A hemolysis assay of one of the reported compound was non toxic in comparison to the fluconazole. In the chapter, the synthesis of macromolecule with defined structure and properties and their metal complexes for their biomedical applications is described. In this chapter we report ligand with the porphyrin core. Porphyrin core dendrimeric ligand (L) was synthesized by Rothemund synthetic route in which p-hydroxy benzaldehyde and pyrrole were fused together. The prepared ligand was complexed with Ni(II), Cu(II) and Co(II) ions, separately. Square planar geometries were proposed for Cu(II), Ni(II) and Co(II) ions in cobalt, Nickel and copper complexes, respectively on the basis of UV-Vis spectroscopic data. The ligand and its complex were screened on Candida albicans (ATCC 10231), Aspergillus fumigatus (ATCC 1022), Trichophyton mentagrophytes (ATCC 9533) and Pencillium marneffei by determining MICs and inhibition zones. The activity of the ligand and its complexes was found to be in the order: CuL>CoL≈NiL>L. From docking experiment, we conclude that copper complex interacts more strongly than rest two. Next chapter deals with the development of macromolecular ligand and its complex as effective antifungal agents. Macromolecular ligand was prepared using ethylenediamine and methylmethacrylate as starting material via well known Michael addition reaction. The synthesized dendritic units were used as ligands to obtain metal-ligand complexes.