

## **ABSTRACT**

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Title: *“Development of new organic probes for optical detection of metal ions: Synthesis, characterization and sensing studies”*.

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In the present submitted thesis novel design and synthesis of several colorimetric and fluorescence chemosensor molecules has been demonstrated along with rigorous spectral studies and binding studies with respect to the particular ionic analytes. These newly fabricated molecules behave as chemosensors for certain environmentally and biologically important metal ions. Thorough spectral study viz. HRMS, IR-studies,  $^1\text{H}$  as well as  $^{13}\text{C}$  NMR, UV-Vis and fluorescence has been done to determine the structure of the receptor. By various analytical studies the binding of the receptors and the ions has also been confirmed. Biological application of these molecules as bio-markers in live-cell imaging studies has also been investigated.

### **Chapter 1**

This chapter serves as a brief introduction to the basic concepts of the present research work, the basic definition of a chemosensor along with its classification. It explains the basic concept of different non-covalent forces involved in host-guest binding. The necessary criteria for the designing of molecular probes are also incorporated in this chapter. A concise literature survey of various reported chemosensors has also been discussed elaborately.

### **Chapter 2**

This chapter is about the instruments and methods that were used during the course of the present research work. It serves as a brief description of instrumented procedures such as HRMS, IR,  $^1\text{H}$ ,  $^{13}\text{C}$  NMR, UV-Vis, fluorescence detection, lifetime decay measurement, crystallography etc. along with the basic theory behind some of the relevant analytical procedures.

### **Chapter 3**

This chapter briefly describes the synthesis and characterization of a fluorescence “turn-on” receptor (HL) for both  $\text{Al}^{3+}$  and  $\text{Hg}^{2+}$  ions based on Rhodamine and coumarin moieties. The absorption,

emission properties and cation sensing properties have been studied thoroughly. The structure has been optimized by computational methods and TDDFT and DFT calculations have also been done.

#### Chapter 4

This chapter demonstrates the design, synthesis and characterization of a thioether containing fluorescence “turn-on” probe ( $H_2L$ ) for the selective detection of  $Zn^{2+}$  in DMSO:water, 1:5 medium. An INHIBIT logic gate was constructed using  $Zn^{2+}$  and EDTA as the chemical inputs. The chapter also contains live-cell imaging studies using the ligand  $H_2L$ ,  $Zn^{2+}$  solution and MCF-7 cell line.

#### Chapter 5

This chapter presents a selective colorimetric chemosensor for  $Ni^{2+}$  ion, based on a pyridyl azo derivative and its synthesis, characterization, photo-physical properties and various cation sensing studies. DFT and TDDFT calculations also have been done.

#### Chapter 6

This chapter is about a new coumarin-based “turn-on” probe HMBH for  $Al^{3+}$  along with its synthesis, characterization and cation sensing studies. TDDFT computations have also been done to obtain the optimised structure of the ligand and the metal complex and their spectral properties.

#### Chapter 7

This chapter illustrates the synthesis, characterization, spectral studies, cation sensing studies of a novel fluorescence “Turn-on” probe (HBSA) for the selective detection of  $Zn^{2+}$  ion. Electronic structure and sensing mechanism have been interpreted by DFT and TDDFT calculations.

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