Abstract

Index No. 4/19/Chem./26

Title of Thesis: Synthesis and characterization of Schiff bases and their diverse applications.

The structures of Schiff bases consist of exocyclic imine/azomethine (C=N) functional unit who is considered as a versatile component for various applications. The imine unit can serve as coordinating group or chelating site in the coordination chemistry. Some of the properly functionalised Schiff bases have been used as a functional material for recognition of bio-relevant ions/molecules at a very low concentration (µM to nM) level. Cations, Anions and certain molecules regulate concentration dependent bioactivity in human body and can be beneficial or toxic than the requisite amount to trigger health issues. Therefore, for normal functioning of the living system, the determination of concentration of these active species must be monitored carefully. Considerable efforts have been invested for the development of efficient chemosensor based on imine framework (CH=N) for sensitive detection of analytes. In addition, the coordinating environment of such molecule with metal centre can form discrete complex and coordination polymers (CPs) which is considered as the natural extension of coordination compounds towards polymerization. In my research work, five Schiff bases bearing different fluorogenic entities such as triphenylamine, benzimidazolyl, pyrazolyl, coumarinyl, naphthyl have been formulated. The probes are synthesized by Schiff's condensation reaction followed by extensive characterization through different spectroscopic techniques (IR, Mass, NMR, elemental analysis) and structural confirmation of some of the molecules by Single Crystal X-Ray Diffraction measurements, Chapter II: Triphenylamine-naphthyl appended Schiff base, an emissive probe, (λ_{em} , 550 nm) selectively senses Cu^{2+} through fluorescence quenching (CHEQ) with a LOD value of 7.3 nM in 7:3 (v/v) CH_3CN/H_2O medium (HEPES buffer, pH 7.2) which exhibits reversibility in presence of Cysteine and restores the emission of the probe due to strong binding of Cysteine to Cu²⁺ and the LOD of sensing is 36 nM. The probe has been used in cytotoxicity analysis in normal WI-38 Cell line and intracellular imaging was performed with HepG2 Cell line. Chapter III: Benzimidazolyl-ethoxysalicyldehyde derivative recognizes Zn²⁺ in 9:1 (v/v) DMSO/H₂O (HEPES Buffer, pH=7.4) medium through chelation and fluorescence intensity (λ_{em} , 461 nm) is

enhanced and the LOD is 3.2 nM. The emissive [Zn(L¹)OAc] complex is further capable of disclosing a selective fluorescence 'turn-off' detection towards H₂PO₄⁻ (LOD: 0.238 μM) accomplishing the reversibility of Chemosensor. **Chapter IV**: Coumarin-Pyrazolyl appended probe detects Zn²⁺ (λ_{em}, 497 nm) and CN⁻ (λ_{em}, 447 nm) with two distinctive emissive responses in CH₃CN/H₂O (99:1, v/v) (HEPES Buffer, pH 7.5) medium and the LOD values are 34.76 nM (Zn²⁺) and 19.91 nM (CN⁻). On interaction of the probe with Zn²⁺ a hexanuclear metallocryptand [Zn₆L₆] is structurally verified by Single Crystal X-Ray Diffraction data. The probe is successfully applied for biological applications such as MTT Assay, cellular imaging and FACS in MD-MBA cells. **Chapter V**: Naphthyl-dimethoxy scaffold is AIE active probe and a strong solid-state emitter which enables a reversible acidochromic behaviour in presence of HTFA/TEA vapour. The LOD estimated for HTFA vapour is found to be 1.41 ppm. The probe further detects a chromogenic and fluorogenic receptor selectively towards CN⁻ (λ_{em}, 565 nm) in CH₃CN/H₂O (99:1, v/v) (HEPES Buffer, pH 7.3) and the LOD is 45.42 nM. MTT analysis and AIE phenomena along with CN⁻ detection of the probe is clearly depicted from the intracellular imaging. **Chapter VI:** Coumarinyl-pyridine molecule has been utilized for the fabrication of Zn(II) 2D coordination polymer (Zn(II)-CP) which has been explored as a semiconducting Schottky diode device and possess effective anticancer efficacy against HeLa cell line.

From my research work, I have published a total of six original research articles and more results will be published shortly.

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