



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title: **Synthesis and Structural Evaluation of Neutral Acyclic Receptors for Recognition of Ionic Analytes in Solid- and Solution-State**

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SHORT ABSTRACT

This thesis deals with ‘supramolecular host-guest recognition chemistry’ where the host mainly anions or the hydrated anions or anionic associations are formed by some simply synthesized monopodial or dipodal acyclic receptors (**L₁-L₆**) decorated by the positional or electronic effect of terminal aryl substituents or anionic dimension or molecular host architectures in solid-state. Interestingly the dipodal receptors **L₁-L₄** formed various halides/hydrated halide complexes whereas, among simple monopodial receptors **L₅** and **L₆**, only **L₅** could be able to form a dimeric association of $[\text{HCO}_3 \cdots \text{HCO}_3]^{2-}$ as well as of $[\text{HSO}_4 \cdots \text{HSO}_4]^{2-}$ which were supported by various non-covalent supramolecular interactions. Like dipodal receptors (**L₁-L₄**), monopodial receptors **L₅** and **L₆** also displayed the tendency to form various halide/hydrated halide complexes at room temperature. On the other hand, we are also interested in solution-state recognition of various ionic analytes in a physiological medium. To aim that, at first, we have designed two simple pyrene/anthracene-based chemodosimeters namely, **L₇** and **L₈** connected through a C=C bond-forming D- π -A-type structure to facilitate interactions with ionic species where we have verified and studied the reactivity of C=C double bonds towards colorimetric (LOD = 0.09 ppm for **L₇** and 0.76 ppm for **L₈**) and fluorometric (LOD = 0.55 ppm at 376 nm and 0.053 ppb at 455 nm for **L₇** whereas 0.85 ppm for **L₈**) sensing of HSO_3^- based on Michael-type addition reaction in a

mixed aqueous medium. To prove the feasibility of the probe in practical applications, we used **L**₇ for the quantitative detection of HSO₃⁻ in food, water samples, and dip-stick analysis.

Furthermore, probe **L**₉ was synthesized and the same displayed a selective “turn-on” emission response towards Al³⁺ (LOD = 1.97 μM) *via the* chelation-enhanced fluorescence (CHEF) process. It could also deliver a naked-eye colorimetric response toward Cu²⁺ in a mixed aqueous medium. The *in situ* prepared [**L**₉-Al³⁺] complex could selectively sense phosphate ions, particularly pyrophosphate (PP_i). The suggested detection pathway is the complexation-decomplexation pathway. As for biological applications, we have also investigated the DNA tracking ability of the ensemble mentioned above, and the present study established the utility of probe-coated dip-stick analysis with **L**₉ to detect Al³⁺ ions in the experimental medium. Finally, we have designed and synthesized a simple chromone derivative-based multi-selective chemical probe **L**₁₀ for selective “turn-on” detection of Al³⁺ (LOD = 5.5×10⁻⁷ M) in an aqueous medium followed by [**L**₁₀-Al³⁺] ensemble-based subsequent detection of PP_i (LOD = 1.02 × 10⁻⁷ M) among all other common anions under the same experimental condition at physiological pH. On the other hand, **L**₁₀ could also be able to detect F⁻ (LOD= 6.4×10⁻⁸ M) in an acetonitrile medium by deprotonation mechanism. The adduct (**L**₁₀-F) could also be used for the recognition of Zn²⁺ (LOD = 2.96 μM) under an identical experimental milieu.