ABSTRACT

The dissertation entitled " Molecular Recognition : Design, Synthesis and Binding Studies of Model Receptors for Mono and Dicarboxylic Acids" embodies in detail the model studies on hydrogen bondings involved in molecular complexation of highly associated mono and dicarboxylic acids with the designed receptors. X-ray crystal structure of water assisted hydrogen bonding in the formation of supramolecular assembly of a simple heterocyclic molecule is also described. The content of the thesis has been divided into five chapters. Chapter I presents an introduction to molecular recognition including the definition and its interdisciplinary nature with various disciplines. This chapter also covers a brief discussion on the nature of noncovalent forces and their existence in nature. The necessary criteria for the design of host and guest and the different physico-chemical methods to study their molecular complexation are also discussed in this chapter. Chapter II describes a critical survey of various reports and reviews on the recognition of both mono and dicarboxylic acids. The binding of monocarboxylic acids that are present in dimeric or in highly associated forms, is very difficult with the designed receptors. Binding studies of a number of aliphatic and aromatic monocarboxylic acids into the binding core of the designed receptors based on three point hydrogen bonding along with the π- stacking interactions have been studied. The variation of the interacting groups in the designed receptors changes the receptor property toward the preferential recognition of either aliphatic or aromatic monocarboxylic acids. Variation in alkyl groups by aliphatic versus aromatic in the binding zone of three point hydrogen bonds to carboxyl group has been studied to see their influence in preferential recognition of aliphatic versus aromatic carboxylic acids. All these phenomena are included in chapter III. Role of C-H---O hydrogen bonding in water assisted supramolecular assembly of small organic molecule has been described on the basis of crystal structure analysis in chapter III. The selective binding of dicarboxylic acids of longer as well as shorter chain lengths by the designed receptors is another interesting aspect of carboxylic acid recognition study. Chapter IV deals with the synthesis and binding studies of dicarboxylic acids within a new molecular scaffold based on Troger's base spacer. Various new Troger's

base receptors for dicarboxylic acid recognition have been synthesised and binding studies with dicarboxylic acids have been undertaken. Fluorescence experiments have been performed with the Troger's base receptors for dicarboxylic acids and significant fluorescence enhancement has been noted for selective dicarboxylic acid complexation. Design of photoresponsive receptors for dicarboxylic acids and their hydrogen bonding induced configurational locking by dicarboxylic acids, based on chain lengths complementarity with the generated cavity of the receptors are also addressed here. Chapter V defines the problem of solubilization and analytical detection of insoluble tartaric acid into the common organic solvents by the hydrogen bonding receptors. Naphthyridine fluorescent receptors are developed for solubilisation by complexation of insoluble tartaric acid into chloroform as well as fluorescense studies have been made to show their possible analytical use for detection of tartaric acid into chloroform. The synthesis of a chiral Troger's base containing macrocycle on chiral tartaric acid template has also been discussed in this chapter. Binding of amino acids with designed new receptors have been discussed. In making these synthetic receptors, functionalised heterocycles are important synthons, the synthesis of which are not straight forward. The detailed study of bromination reaction on the various heterocycles under various conditions (especially in presence or absence of water) has been demonstrated in this chapter.