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Name of Department: **Chemistry**
Topic of Research: Design, Synthesis and Properties of Heterocyclic Systems Including Calix[4]pyrrole based supramolecular receptors.

Findings

The thesis entitled “Design, Synthesis and Properties of Heterocyclic Systems Including Calix[4]pyrrole based supramolecular receptors” consists of five chapters which deals with the synthesis of various heterocyclic systems under environmentally benigning conditions thereby utilizing deep eutectic solvents as catalysts as well as solvent medium. Besides this, the primary work which deals with the design, synthesis and diverse applications (anion binding and sensing studies) of functionalized dipyrromethanes, and calix[4]pyrroles (C4Ps). Chapter I deals introductory portion about with deep eutectic solvents, and calix[4]pyrroles, which briefly explores the importance, utilization, and diverse deep eutectic solvents mostly used in green chemistry. On the other this chapter also explores the historical background, about synthesis; applications (*anion and ion-pair binding studies, drug delivery, sensing mechanism, extraction of ions, and ion transport properties*) induced by C4Ps as well as include the objective of thesis. Chapter II, Part A also deals with the green synthesis of 2-substituted benzothiazoles and benzimidazoles in good to excellent yields by utilizing a deep eutectic solvent of *N,N'*-dimethyl urea (DMU) and L-(+)-tartaric acid (TA) in the ratio of 7:3 at 70 °C . Chapter II Part A, also deals with the generation of various derivatives ketazines & pyrazolines in good to better yields at 70 °C and 100 °C respectively, by utilizing a deep eutectic solvent of *N,N'*-dimethyl urea (DMU) and L-(+)-tartaric acid (TA) in 7:3 molar ratios. Chapter III Part A deals with synthesis of novel fluorescein based dipyrromethane receptors **DPM1** and **DPM2** from a simple and easily accessible fluorescein dye. Which have display colorimetric sensing (appearance of specific colour change in solution) towards fluoride, acetate and phosphate with limit of detection and quantification in the range of 1.28-13.54mg/L and 3.89-41.05mg/L respectively. Chapter III Part B deals with facial synthesis and anion binding studies of novel fluorescein/benzo-12-crown-4 ether based bis-dipyrromethane (**DPM3/DPM4**) receptor which reveals that binding constant (K_a) values of **DPM3/DPM4** with various tested anions in the range of 516.07 M^{-1} to 63789.81 M^{-1} . Chapter IV deals with facial synthesis, necked eye anion sensing and anion binding studies of novel fluorescein substituted one walled calix[4]pyrroles

(**C4P7**). The results revealed that the **C4P7** display selective and sensitive naked eye sensing towards fluoride, phosphate and acetate with limit of detection 4.27mg/L, 6.4mg/L, and 5.94mg/L respectively in acetonitrile solution. In addition to sensing behavior, the **C4P7** receptor system reveals that the formation of stable 1:1 complex with various tested anions (Br^- , Cl^- , I^- , NO_3^- , HSO_4^- , and SCN^-) in satisfied $K_{1:1}$ values within <10% error thereby capturing anions *via*. NH-anion, OH-anion as well as anion- π interactions. Chapter IV deals with the synthesis and anion binding studies of novel fluorescein based strapped calix[4]pyrroles (**C4P22**). The results reveals that the **C4P22** forms 1:1 complexes with the tested anions which were confirmed by the Job's plots. The **C4P22** receptor captures anions within binding constant in the range of 135.57 M^{-1} to 69059.16 M^{-1} through NH-anion bonding, and anion- π interactions which were confirmed by $^1\text{H-NMR}$ analysis.