Poster Presentation

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Molecular recognition to self-assembly mediated by supramolecular interactons

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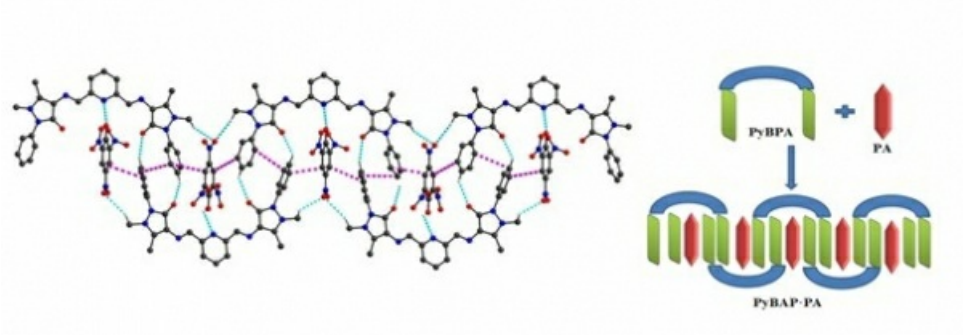
We report, synthesis and characterization of two classes of molecular receptors, one of which cationic organic synthetic receptor [C28H24N4]2+ and neutral receptor 2,6-Pyridine-bis(iminoantipyrine) (PyBAP). The cationic receptor, [C28H24N4]2+ shows conformational change from anti to syn upon molecular recognition of Zn(dmit)2]2− coordination complex anion. We show that conformational change of cationic receptor through electrostatic interactions to formation of supramolecular zipper. The PyBAP, a crab claws shaped open neutral molecular receptor showed selective molecular recognition of picric acid and stabilized in the pocket through supramolecular interactions including H-bonding, - and C-H… interactions to formation of extended supramolecular chain structure with turn-on fluorescence as well as intermolecular charge transfer induced colorimetric change was observed. Besides, the extended supramolecular interactions in the crystal lattice of PyBAP-PA rigidify the molecular structure of PyBAP and prevent the isomerisation of imine that lead aggregation induced emission at 620 nm. The selective host-guest formation of PyBAP-picric acid has been analysed using with FT-IR, 1H-NMR and computational studies. Two classes of receptors undergo supramolecular assembly through molecular recognition, that observations are described and the possible roles of the substrates are discussed. Detailed structural studies of host-guest complexes were carried out with the aid of single crystal X-ray structures analysis.

[1] Madhu, V. et al. (2015). CrystEngComm, 17, 3219–3223.



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