



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Comprehending the Aggregation Aptitude through Structural Variation within Small Molecular Framework: Comparative Analysis and Interaction Studies**

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SHORT ABSTRACT

This Thesis entailed investigating the outcome of structural alteration (Aromatic Core substitution and Fluorophore substitution) on the aggregation prospective of simple urea and Schiff base derivatives and furthermore probed their sensing potential by studying the effect of their aggregation behaviour due to their interaction with biological macromolecules and other environmentally relevant analytes.

A set of three already reported *meta*- nitro-phenyl functionalized bis-urea derivative has been purposefully synthesized by varying the aromatic core (*ortho*-, *meta*- and *para*- position) and the systematic survey has directed to the discovery of noteworthy isomeric effect in case of **2** in the formation and stabilization of aggregates compared with other two in the aqueous medium. Further we examined the outcome of external factors such as temperature, urea, salt (NaCl), pH on the aggregation characteristics to simplify molecular designing for a particular application. Then we continued with another series of neutral naphthyl bis-urea derivatives **4**, **5** and **6** to overcome the spectroscopic limitations and recognized the effect of core substitution on their aggregation ability with the change in the solvent nature. Moreover, we checked the interaction with the electron-deficient nitro-phenols for the aggregated form of the compound **4** and **5** in the aqueous medium and the systematic assessment encountered a significant effect in the case of PA (Picric Acid) among the nitro-phenols due to its strong electronic acceptor nature. Keeping in mind the bonus advantage of introduction of AIE core, next we attempted to realize the role of planar fluorophores with different sizes and π -electron clouds in the aggregation aptitude of the

small fluorescent molecules. Interestingly, simple di-substituted urea probe **7** is capable of displaying interesting AIE characteristics and a selective turn-on fluorescence response towards HSA over other proteins and bio-analytes in 100% aqueous medium with a very low detection limit. But **8** displayed negligible change in emission intensity with change in water fraction and remain silent when interacted with HSA/BSA. Proceeding on the same lines, this work was further challenged by replacing the anthracene moiety by more conjugated pyrene moiety along with crafting ICT prospect in two Schiff base derivatives **9** and **10**. It is worth mentioning that simply regulating the water content of the medium leads to in an exhibition of the already anticipated AIE properties of the two compounds without the presence of any external stimuli. In addition, **9** and **10** can selectively sense Hydrazine both in solution and vapour phase in their aggregated state over other amines with a very impressive detection limit. Thus, the overall findings in the thesis revise the design strategy for developing functional-assembly of small molecular system and successfully established the some of the various fundamental concepts of small molecule aggregation through sequential approach of spectroscopic and microscopic studies.
