



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
PhD-17 SHORT ABSTRACT OF THESIS

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Thesis Title : **Investigation on Molecular Self-Organisation in Peptide Systems: from Functional Assembly to Autonomous Replication.**

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SHORT ABSTRACT

The work presented in this thesis focuses deeply on supramolecular self-assembly of peptides, with particular emphasis on self-replication of cyclic peptides. We have unveiled a noteworthy and atypical characteristic of Thioflavin T (ThT), a benzothiazole dye. We observed that ThT has an affinity for and interacts with well-organized spherical aggregates formed by our designed self-assembled dipeptides. Additionally, we established a direct morphological transformation of the designed tripeptides with time from nano-spheres to rod-like structures through self-assembly. These self-assembled tripeptides have N_2 gas adsorption properties and can also encapsulate a powerful hydrophobic drug, curcumin. Furthermore, it also displays KCl-mediated salt-triggered disruption and release of encapsulated drug molecules. Moreover, we have successfully designed and synthesized the first-ever cyclic peptide-based model self-replicators. The designed self-replicating systems operate through templated autocatalysis while adopting random-coil conformations rather than conventional β -sheet or helical motifs. We have also successfully implemented a new ligating strategy by using benzyl-ester mediated amide bond formation, offering an alternative to the widely used Kent's ligation method.