INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title: A computational study on the molecular recognition in water using endo-functionalized molecular tubes and uses of these receptors as drug delivery vehicles

Name of Thesis Supervisor(s) : Prof. Sandip Paul

Thesis Submitted to the Department/ Center : Chemistry

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Key words for description of Thesis Work : Computational biophysics, endo-functionalized molecular tube, molecular recognition, drug delivery.

SHORT ABSTRACT

My doctoral research focused on the molecular recognition in water using endo-functionalized molecular tube receptors and uses of these receptors as drug delivery vehicles. Host-guest coupling investigations indicate the driving factors behind complexation and offer insight into noncovalent interactions between the host and guest moiety. We have also analyzed the water thermodynamics using grid inhomogeneous solvation theory (GIST). This study also provides interaction between these receptors and different model lipid bilayers to find the possibility of using these receptors as drug delivery vehicles. The expertise accumulated leads to the design of therapeutic functional compounds, such as molecular reactors for catalysis, or the advancement of structure-based drug design and their delivery in medicinal chemistry.