



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student : Haobam Kisan Singh

Roll Number : 176122035

Programme of Study : Ph.D.

Thesis Title: **Computational Investigation of Noncovalent Interactions in Supramolecular Host-Guest and Amyloid- β (A β) Protein-Ligand Systems**

Name of Thesis Supervisor(s) : Dr. Manabendra Sarma

Thesis Submitted to the Department/ Center : Chemistry

Date of completion of Thesis Viva-Voce Exam : 29-04-2024

Key words for description of Thesis Work : Noncovalent interaction, host-guest, Amyloid- β protein

SHORT ABSTRACT

This thesis covers the computational investigation of noncovalent interaction in the supramolecular host-guest and protein-ligand systems. Different quantum chemical and classical molecular dynamics (MD) calculation methods were employed to understand the noncovalent interactions. Initially, we have investigated the noncovalent interactions (both intra and inter) present in the conformers of the host 1,6-bis(2,6-bis(benzothiazol-2-yl) pyridine-4-yloxy) hexane and their host-guest complex formation with resorcinol guest. Further, the electron transport through noncovalent interactions, such as π - π interaction present in the host-guest complex, was also studied in this thesis. In addition, the effect of the electron-withdrawing and donating groups on the π - π interaction and hydrogen bonding was also investigated. Our investigation also proceeds to the interaction of the amyloid- β (A β) protein with the amino acids functionalized perylene diimide (PDI) molecule.