

Title of the project for student internship/student trainees

On

DFT Investigation on theoretical spectroscopic, ELF, MEP, Hirshfield surface and molecular docking studies of phenyl benzothiazole, mercaptobenzimidazole, dibenzothiophene, and 2-aminothiazole



**HANSRAJ COLLEGE
UNIVERSITY OF DELHI**

**INSTITUTION INNOVATION COUNCIL
Research and development cell**



Inviting applications for student internship/student trainees

on

“DFT Investigation on theoretical spectroscopic, ELF, MEP, Hirshfield surface and molecular docking studies of phenyl benzothiazole, mercaptobenzimidazole, dibenzothiophene, and 2-aminothiazole ’

Applications invited from 8th April 2022

Project Investigator
Dr. Manoj Kumar
Dr. Sonu Kumar

IIC, CONVENOR
DR. ARCHANA SINGH

PRINCIPAL, HANSRAJ COLLEGE
PROF. RAMA

Faculty Involved

Dr. Manoj Kumar

Dr. Sonu Kumar

Students Involved -3

Duration- 1 year

Learning outcome

- 1. Learning how to study protein ligand interaction by docking**
- 2. Learning how to validate interaction by simulation**
- 3. Identification of new potent bio active chemical**