



Department of Pharmaceuticals  
Ministry of Chemicals and Fertilizers  
Government of India



SKILL VIGYAN INITIATIVE SCHEME OF THE DEPARTMENT OF  
BIOTECHNOLOGY, GOVT. OF INDIA, COORDINATED BY TSCOST

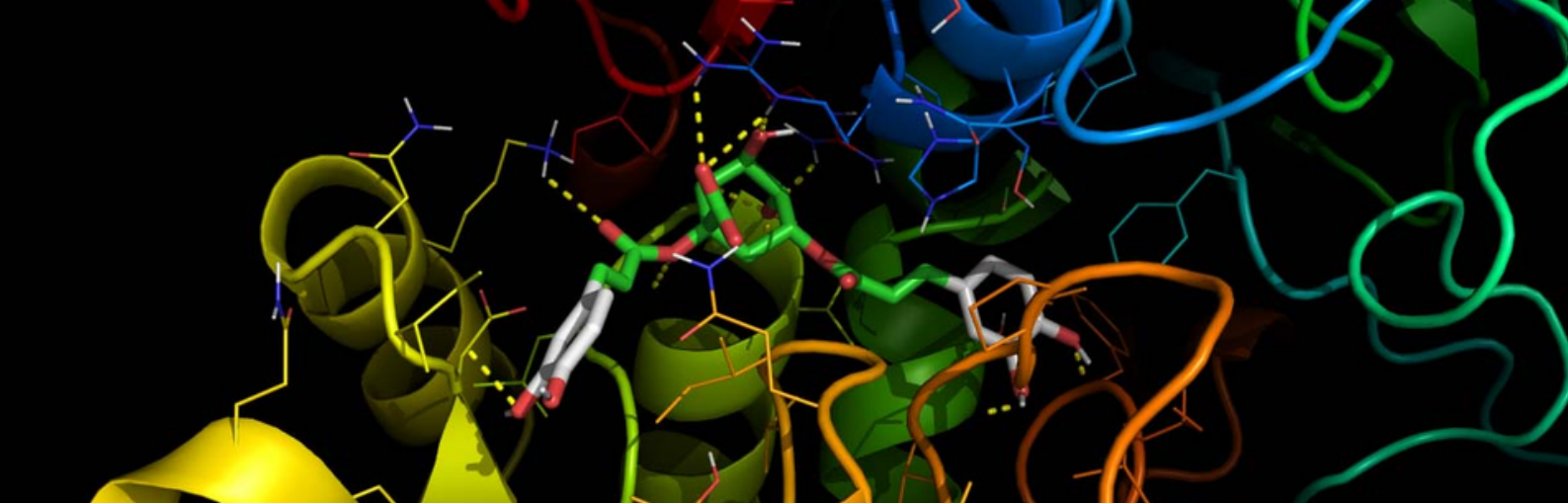
# FACULTY TRAINING PROGRAM 'WORKSHOP ON MOLECULAR DOCKING, VIRTUAL SCREENING AND COMPUTATIONAL BIOLOGY'

FROM 26TH FEB TO 8TH MARCH, 2024  
AT NIPER HYDERABAD



ORGANIZED BY

NATIONAL INSTITUTE OF PHARMACEUTICAL EDUCATION AND RESEARCH (NIPER)-  
HYDERABAD, BALANAGAR, HYDERABAD-500037, TELANGANA



### Workshop Topics:

The workshop has been designed to provide the theoretical background as well as a hands-on approach to Molecular Docking and Virtual screening. The workshop covers different Pharmacoinformatics and Cheminformatics methods and the use of software for lead identification and optimization.

Topics include:

- Introduction to biological databases
- Introduction to drug discovery
- Virtual screening of small molecules
- Molecular interaction analysis
- Phylogenetic analysis for biological sequences
- Biological sequence alignment techniques: pair-wise & multiple sequence alignment
- Methods and advances in computer aided drug design
- Protein database & structure modeling
- Identification and evaluation of binding pocket / active site
- Generating protein-ligand complexes by molecular docking
- Refinement of novel leads using ADME prediction
- QSAR modeling and lead optimization
- Introduction of molecular dynamics simulation

### Invited Speakers:

- NIPER- Hyderabad faculty
- External Speakers from Industry & Academia
- Schrodinger Scientific team

### Participants:

- **Faculty members from Telangana State Universities/ Institutes/ Colleges are eligible to apply (preference will be given to faculties from Pharmacy and Chemical Sciences background).**
- **Total number of participants is restricted to 20.**
- **There is no fee for the workshop.**
- The program is sponsored by Skill Vigyan Initiative Scheme of Department of Biotechnology, Govt. of India coordinated by the Telangana State Council of Science & Technology (TSCOST), EFS&T Department, Govt. of Telangana.

### Important Dates:

- **Scanned copy of completed registration form should reach on or before 9th Feb, 2024 to [ftp.niperhyd@gmail.com](mailto:ftp.niperhyd@gmail.com)**
- The selected candidates will be informed by e-mail.

# **FACULTY TRAINING PROGRAM 'WORKSHOP ON MOLECULAR DOCKING, VIRTUAL SCREENING AND COMPUTATIONAL BIOLOGY'**

## **REGISTRATION FORM**

**Name:**

**Department/ Specialization:**

**Institution/University/College:**

**Date of entry in to service:**

**Address:**

**Pin:**

**E-mail:**

**Phone:**

**Declaration:**

I.....agree to abide by the rules and regulations of the FTP programme. The information provided herewith is true to the best of my knowledge.

**Place:**

**Signature:**

**Forwarded and Recommended by:**

**Signature with seal**

**Head of institution**

**NOTE:**

- Participants are requested to bring their own laptops for hands-on and software installation.
- NIPER Hyderabad does not have the guest house facility therefore participants are advised to book their accommodation directly.



### **About NIPER Hyderabad**

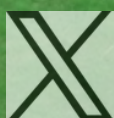
NIPER Hyderabad is an "Institute of National Importance" with proclaimed objectives of becoming Centre of Excellence for advanced research in pharmaceutical sciences. NIPER Hyderabad has excellent Lab facilities to update the knowledge and expose the students to various advanced techniques essential for Drug Discovery Research.

### **About the Programme**

The Skill Vigyan Initiative Scheme of Department of Biotechnology, Govt. of India and TSCOST Sponsored Faculty Training Programme (FTP) is designed to train the faculty who wish to upgrade the knowledge and skills in area of Drug Discovery. Hands on training will be provided to strengthen the practical knowledge with emphasis on Drug Design, Pharmacoinformatics, Pharmaceutical Sciences & Chemical Sciences.



[facebook.com/niperhyd/](https://facebook.com/niperhyd/)



[@NIPERHyd](mailto:ftp.niperhyd@gmail.com)



[@niperhyd](https://www.instagram.com/niperhyd)

## **PROGRAMME COORDINATORS**

**Dr. K. VENKATA RAO**  
**ASSISTANT PROFESSOR**  
**NIPER-HYDERABAD**

**Dr. VASUNDHRA BHANDARI**  
**ASSISTANT PROFESSOR**  
**NIPER-HYDERABAD**

**Dr. N. SHANKARAI AH**  
**ASSOCIATE PROFESSOR**  
**NIPER-HYDERABAD**

For any queries write to [ftp.niperhyd@gmail.com](mailto:ftp.niperhyd@gmail.com)