



I-DAPT Hub Foundation IIT (BHU) sponsored Short-Term-Course (STC) on

Transforming Healthcare with AI-Driven Drug Discovery

18-22 December 2023, Indian Institute of Technology (BHU), Varanasi, India



About the Workshop

This STC aims to educate participants on the current and potential impact of AI in the field of drug discovery. It focuses on showcasing AI innovations and practical applications, fostering collaboration, and encouraging multidisciplinary discussions.

Hands-on sessions in the workshop will cover data preprocessing, machine learning model development, cheminformatics and bioinformatics tools, feature engineering, model evaluation, deep learning techniques, virtual screening, AI tools, and platforms. The sessions will also include real-world case studies, practical challenges, interactive workshops, and resource sharing to provide participants with practical skills and experience in applying AI to drug discovery.

Advisory Board

Prof. Pramod Kumar Jain, Director, IIT(BHU)
Prof. Vikash Kumar Dubey, Dean (Research & Development) IIT (BHU)
Prof. Rajeev Kumar Singh, Coordinator, I-DAPT Hub, Foundation IIT (BHU)
Prof. (Mrs.) Siva Hemalatha, Head, Dept. of Pharm. Eng. Tech., IIT (BHU), Varanasi

About the Institute

Established in 1919, the Indian Institute of Technology (Banaras Hindu University) owes its existence to the farsighted vision of its founder Bharat Ratna Mahamana Pandit Madan Mohan Malaviya. Initially, three engineering and technological institutions were established. Later, merged to form Institute of Technology (IT-BHU) in 1968. In 2012, IT-BHU was converted into IIT (BHU), Varanasi.

Apart from implementing rigorous academic programmes, the institute has been consistently promoting research on thrust areas of various engineering and science disciplines.

Organising Team

Organizing Secretary:

Dr. Rajnish Kumar, Assistant Professor
Dept. of Pharm. Eng. Tech., IIT (BHU), Varanasi

Co-organizing Secretaries:

Dr. Senthil Raja A., Associate Professor
Dept. of Pharm. Eng. Tech., IIT (BHU), Varanasi
Dr. S. K. Mishra, Assistant Professor
Dept. of Pharm. Eng. Tech., IIT (BHU), Varanasi
Dr. Gyan Prakash Modi, Associate Professor
Dept. of Pharm. Eng. Tech., IIT (BHU), Varanasi

About the I-DAPT Hub Foundation

I-DAPT Hub Foundation is established with the following objectives.

- To produce highly motivated and confident graduates for serving the nation.
- Continuous engagement of Industry, Professionals, R&D establishments, Alumni and the Society.
- Collaboration and interaction with Institutions of higher learning at Global and National Levels for enriching the academic and R&D processes, activities and functionalities.
- Working for National and Regional needs as may be identified by Government of India, and concerned State Governments.

Tentative Speakers

- Prof. G. Narahari Sastry, CSIR-NEITS, Assam
- Prof. GPS Raghava, IIIT, Delhi
- Prof. Prabha Garg, NIPER SAS Nagar, Punjab
- Prof. S. K. Singh, CSE, IIT(BHU), Varanasi
- Prof. Sanjeev K. Singh, Alagappa University
- Prof. Neha S. Gandhi, MAHE, Manipal
- Dr. Anshuman Dixit, ILS, Bhuvaneshwar
- Dr. Reiko Watanabe, Osaka University, Japan
- Dr. Vijayan Ramaswamy, University of Texas, MD Anderson Cancer Center, USA
- Dr. Manjari Gupta, DST-CIMS, BHU

Key Objectives

- To give an in-depth knowledge of the drug discovery paradigm and artificial intelligence.
- To provide hands-on training on QSAR, hit identification using deep learning, pharmacokinetic property prediction including toxicity, de novo ligand design using deep learning, and biomolecular simulations.
- To brief the participants on the use of high performance computers/super-computers (Param-Shivay) to ramp up the speed of computational modeling for drug discovery.
- To provide a networking opportunity to the participants to enhance broaden their research network.

Participants: Eligibility Criteria

This workshop is specifically designed for UG/PG/PhD students, researchers, faculties, and technical staffs with a background in pharmaceutical sciences or related areas and who are interested in the applications of Artificial Intelligence in Drug Discovery. The major focus of this workshop is on hands-on training.



Registration Information

- As the number of participants in the workshop is limited to fifty (50), applicants will be selected on the basis of their area of research, motivation to attend the workshop, and possible use and dissipation of knowledge gained from the workshop.
- Register at <https://forms.gle/XXY11hCJPW2iE9vM6>
- Registration Fees including 18% GST:
 - For faculties, scientists, and post-doctoral researchers: Rs. 3540/-
 - Industry personnel: Rs. 5900/-
 - For UG, PG and PhD students: Rs. 1180 (Rs. 590 for BIDDS member (<https://www.bidds.org/>))
- The method of payment will be communicated to only selected participants.
- The decision on final selection will be made by the organizing team.
- The registration fee only covers workshop cost and meals for the STC duration.
- Participants need to take care of the transport and accommodation themselves. Hostel accommodation and Guest house accommodation for the interested participants can be arranged at 100 and 1200 rs per night, respectively.
- Certificates will be provided after the successful completion of the workshop to the participants.

Register online before 30/11/2023

Link to registration:

<https://forms.gle/XXY11hCJPW2iE9vM6>

(Only 50 Participants will be selected)

Mode of workshop: Offline

Duration: Five Days



**I-DAPT Hub Foundation IIT(BHU), Varanasi
&
Department of Pharmaceutical Engineering & Technology
Indian Institute of Technology (IIT) BHU, Varanasi**

