



## *I-DAPT Hub Foundation IIT(BHU) sponsored Workshop On*



# **Applications of Artificial Intelligence In Drug Discovery (A2ID2)** **9-13 March 2023, Indian Institute of Technology (BHU), Varanasi, India**

### **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.

### **Tentative Key Speakers**

- Prof. Kenji Mizuguchi, Osaka University, Japan
- Prof. Andreas Bender, University of Cambridge, UK
- Dr. Ho-Leung Ng, Kansas State University, USA
- Dr. Vijayan Ramaswamy, University of Texas, MD Anderson Cancer Centre, USA
- Prof. B. Mishra, Indian Institute of Technology (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.

### **About the Workshop**

AI has become an integral part of Drug Discovery leading to an increase in the rate of success at a reduced cost and time. The aim of this workshop is to offer highly supervised and industry relevant training on the applications of Machine Learning and AI in early phase drug discovery by introducing the students to basic workflow of drug discovery, hands-on supervised training of various software packages supported by theory lectures for a compendious learning.

### **Organising Team**

#### **Organizing Secretary**

**Dr. Rajnish Kumar**

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#### **Co-organizing Secretary**

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#### **Organizing Committee**

Prof. Vikash Kumar Dubey

Project Director, I-DAPT Hub Foundation and Dean (R&D), Indian Institute of Technology (BHU), Varanasi

Dr. Rajeev Kumar Singh

Coordinator, I-DAPT Hub Foundation, Indian Institute of Technology (BHU), Varanasi

Prof. (Mrs) Siva Hemalatha

Head, Department of Pharmaceutical Engineering and Technology, Indian Institute of Technology (BHU), Varanasi



## 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.

**Register online before 25/2/2023**

**Link to registration: [shorturl.at/jkyG5](https://shorturl.at/jkyG5)**

**(Only 35 Participants will be selected)**

**Mode of workshop: Offline**

**Duration: Five Days**

## Participants: Eligibility Criteria

This workshop is specifically designed for UG/PG/PhD students, researchers, faculties, and industry professionals 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 35, 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.
- Participants have to register at the link provided ([shorturl.at/jkyG5](https://shorturl.at/jkyG5)) and after the deadline, selected candidates have to pay the registration fee for confirmation of their participation.
- The account details for payment of registration fee will be communicated to the selected participants only.
- The participants will be provided shared accommodation in the hostel and food for the whole duration of the workshop.
- Certificate will be provided after the successful completion of the workshop to the participants.

**Non-refundable Registration Fees including 18% GST (to be paid by selected candidates only):**

- For faculties, scientists and post-doctoral Fellow: Rs. 2360/-
- For participants from industry: 4720/-
- For UG/PG/PhD students: Rs. 590/-



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

