



BITS Pilani
Pilani Campus

Workshop on Cheminformatics and Machine Learning in Drug Discovery

March 18-19, 2024

Organized by:

Department of Pharmacy, BITS Pilani, Pilani campus

About the Department

The Department of Pharmacy at BITS Pilani is a renowned institution in the field of pharmacy education and research. Founded in 1950 by the late Prof. M.L. Schroff, a pioneer in pharmacy education in India, the department has since established itself as one of the leading pharmacy schools in the country. In 2023, the department secured the 3rd rank in the prestigious NIRF (National Institutional Ranking Framework) in the Pharmacy category. Moreover, our department has been placed within the impressive 100-150 band in the QS world ranking for Pharmacy and Pharmacology. Its broad-based education system and strong university-industry linkages have been instrumental in its success. The department completed 70 years of its existence in 2021 as a premier institution in the field of pharmacy education and research in India and abroad, a testament to its continued excellence. The alumni of the department are well-placed in India as well as abroad, in various pharmaceutical companies and government organizations, including drug control, research laboratories, and several premier academic institutions. Three faculty members of the department recently started start-ups, demonstrating the department's commitment to fostering innovation and entrepreneurship among its faculty members and students.

Objectives of Workshop

The role of big data analytics is emerging in all research areas, including drug design and discovery. This two-day workshop intends to expose participants to the cheminformatics and machine learning (ML) approaches used in drug design and discovery. The workshop intends to cover basic theoretical and practical aspects of various techniques used in cheminformatics and ML. Experts in the field will deliver the lectures and hands-on tutorials. The workshop also intends to expose participants to various open-source and commercial tools and databases that can be employed for cheminformatics and machine learning applications. The participants will also get the opportunity to network with each other and well-known researchers in the field. The participants will be provided with a limited period license for Cresset and Schrodinger commercial software for hands-on training.

Topics covered

- Basic concepts in cheminformatics and ML.
- Performance evaluation and validation of models. Best practices followed for predictive modeling.
- Real-world applications of cheminformatics and ML in Drug Discovery
- Hands-on training with cheminformatics and ML software from Schrodinger (DeepAutoQSAR, Active Learning Glide) and Cresset group (FLARETM).

Who is eligible?

Due to the advanced nature of the topic, only Master's and PhD students, postdoctoral researchers, and early career professionals involved in teaching or research in chemical, pharmaceutical, and related sciences areas are eligible.

Registration fees & details

Please fill Google form via link: <http://tinyurl.com/4nnfa5sa>

Deadline 1st March 2024

₹500 (BITS participants); ₹950 (External participants). Includes 2 lunches, 1 dinner, refreshments, kit.

Accommodation

Participants are requested to arrange accommodation on their own. Limited accommodation is available at the on-campus BITS guest house on a first-come-first-serve basis. In addition, there are several hotels at the walking distance to the institute. See Google Form for more details.

Bank details

| | |
|------------------|---|
| Beneficiary Name | Birla Institute of Technology & Science, Pilani |
| IFSC CODE No. | UTIB0001188 |
| Account | CURRENT ACCOUNT |
| Bank Account No. | 918010089946355 |
| Bank | AXIS BANK LTD |
| Branch | PILANI |
| City | PILANI |
| MICR No. | 333211177 |



SPEAKERS



Prof. Narasimhan

Director-IQAC, Former Head and Dean at Maharshi Dayanand University, Rohtak



Prof. Manoj Kumar

Senior Principal Scientist and Head of the Virology Unit at Bioinformatics Centre, CSIR-Institute of Microbial Technology (IMTECH) Chandigarh



Prof. Kamlesh Tiwari

Associate Professor
Department of Computer Science & Information Systems, BITS Pilani, Pilani Campus



Dr. Boyli Ghosh

Application Scientist at Cresset Biomolecular Discovery Ltd., Bengaluru, Karnataka



Dr. Lahari Murali

Support Scientist at Cresset Biomolecular Discovery Ltd, Bengaluru, Karnataka



Mr. Vinod Devaraji

Senior Scientist I at Schrödinger Bengaluru, Karnataka



Dr. Abhijit Koyal

Senior Scientist II at Schrodinger Bengaluru, Karnataka

LEADERSHIP

Prof. V. Ramgopal Rao, Vice Chancellor, BITS Pilani

Prof. Sudhirkumar Barai, Director, BITS Pilani, Pilani campus

HEAD OF THE DEPARTMENT

Prof. Anil Gaikwad, Department of Pharmacy, BITS Pilani, Pilani campus

ORGANIZING COMMITTEE:

Prof. Sandeep Sundriyal; Prof. Hemant R. Jadhav;

Prof. S. Murugesan; Prof. Atish T. Paul

For any query, you may contact to:

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