BIC & NNP, JNU WORKSHOP(s)

ETT
Enabling Technology Training

January 20 - **March 02**, 2024
on **Saturday**(s)

Workshop Themes

- Medical data analysis with python
- Gene enrichment and biological pathway analysis
- Predicting drug resistance in tuberculosis from whole genome sequencing
- Molecular modeling and drug design
- How to calculate accurate binding free energy for drug design
- NGS data QC and transcriptome analysis
- NGS data analysis with DNA shape and dynamics

http://ccbb.jnu.ac.in/bic

Venue & organised by -

School of Computational & Integrative Sciences
Jawaharlal Nehru University
New Delhi.

Funded by -
Bioinformatics Center and **National Network Project, JNU**
Department of Biotechnology, Government of India

We proudly announce series of hands-on **"Enabling Technology Training (ETT) Weekend Workshops"** embedded with a Distinguished-lecture Series at School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi. In this series, we present a total of SEVEN workshops on wide range of topics in the areas of Bioinformatics expertise of our respective faculty members who will individually organize each one of them.

Highlights of the Workshops

- Each workshop will be held from 1400 to 1800 hours on a Saturday and participation will be through registration and selection.
- Each workshop will be independent and on a specific theme.
- Participants need to register for each of them separately on the ETT-workshop website.
- Registration for each will start 15 days before the workshop and close 07 days before it. Selected candidates will be informed 05 days before the workshop. (Only limited seats are available)
- There is no registration fees for the workshops.

Highlights of Distinguished Lectures:

- Each workshop will be preceded by a Distinguished Lecture by an eminent scientists related to the theme of the workshop.
- Each distinguished lecture will be held from 11:00-12:00 hours onwards on the day of the workshop.
- Participation in ETT Distinguished Lectures will be open to all and no registration will be required.

Register for the event:

- Visit: http://ccbb.jnu.ac.in/bic/index.php/registration-ett2024

- OR **Scan** QR Code

Distinguished Speakers

- **Dr. Bharti** (University of Delhi)
- **Dr. Dipika Bansal** (NIPER, Mohali)
- **Prof. Seyed Ehtesham Hasnain** (IITD & Sharda University)
- **Prof. P. Bharatam** (NIPER, Mohali)
- **Prof. Debnath Pal** (IISc, Bangalore)
- **Prof. Saurabh Raghuvanshi** (University of Delhi South Campus)
- **Dr. Dipak Dutta** (CDRI, Lukcnow)

Individual Workshop Organizers

- **Dr. Jyoti Singh Kirar**
- **Dr. Pallavi Somvanshi**
- **Prof. Shandar Ahmad**
- **Prof. Naidu Subbarao**
- **Prof. Pradipta Bandopadhyay**
- **Prof. Mukesh Jain**

Series Organizers

- **Prof. Shandar Ahmad** (Coordinator)
- **Prof. Mukesh Jain**
- **Prof. Naidu Subbarao**
- **Dr. A. Krishnamachari**

Technical Team

- **Mr. Sudhir Patwal**
- **Mr. Ravindra**

Workshop on

Organiser: **Prof. Shandar Ahmad** and **Manisha Kalsan**

ETT 7

NGS data analysis with DNA shape and dynamics

Saturday, March 02, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

Tool: DynaSeq; Readout

Workshop Summary

Transcription factors (TFs) are the key proteins that regulate gene expression. In a cellular environment a single TF regulates thousands of genes by recognizing their target DNA sequences. It has now become known that the target DNA sequence alone cannot explain how TFs select to bind in some and not the other sequences at different locations of a genome. Sequence-dependent DNA shape and conformational dynamics have been used to identify this second level of regulation. We have developed tools such as DynaSeq and ReadOut, which can provide deep insights into the role of DNA shape and dynamics into transcription factor binding specificities and affinities. This workshop will provide a hands-on approach to Biologists to use these tools to analyze their NGS data, particular those produced by ChIP-Seq, DNAse-Seq and related methods

Distinguished Lecture

Understanding therapeutic vulnerabilities of Triple Negative Breast Cancer (TNBC)

Speaker

Dr. Dipak Datta

CSIR-Central Drug Research Institute, Lucknow

https://cdri.res.in/1792.aspx?id=1792

ETT 1

Organiser: **Dr. Jyoti Singh Kirar**

Workshop on

Medical data analysis with python

Saturday, January 20, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

Workshop Summary

Medical data analysis is a crucial task since it demands accurate interpretation of the acquired and available data for the correct therapy of the patients. Voluminous data is being generated in medical domain on daily basis. Manual analysis of medical data is a monotonous and cumbersome task. Also, it is highly subjective to the expertise of the clinicians/practitioners. Further, the availability of limited number of experts elevates the need of the computer-aided medical data analysis for identification of hidden patterns, revealing the correlations among the various disease and their symptoms and more. Thus, there is a need to design and develop computer aided analysis systems that can support the faster and accurate analysis of the data.

Thus, the workshop aims to dive into medical data analysis using Python. Its objective is to inculcate medical data analysis skills in the participants by introducing them to: (a) different types of the medical data and their challenges; (b) various analysis tools to analyze the data; and (c) hands-on the developing decision/predictive models for classification/prediction of various diseases or its stage. With this workshop, they can form a base for in-depth understanding of the medical data analysis.

Distinguished Lecture

Data fusion in medical data analysis

Speaker

Dr. Bharti

Department of Computer Science,
University of Delhi.

http://people.du.ac.in/~bharti/

Workshop on

Organiser: **Dr. Pallavi Somvanshi**

ETT 2

Gene enrichment and biological pathway analysis

Saturday, January 27, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

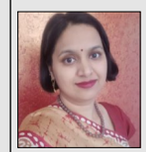
Workshop Summary

Gene set enrichment analysis (GSEA) and biological pathway analysis are crucial bioinformatics tools that help researchers interpret large-scale genomic data. GSEA identifies a gene set's statistically significant association with experimental data, suggesting it is coordinately regulated or functionally related. Biological pathway analysis maps enriched gene sets to known biological pathways, providing a comprehensive understanding of underlying biological mechanisms. These analyses help researchers understand the molecular basis of biological phenomena, including diseases, and identify potential therapeutic targets.

Session major topics:

- Biological insight into gene set enrichment analysis
- Estimate the role of statistically significant genes and visualization.
- Single gene and multiple gene expression analysis.
- Find out how a set of genes is connected by e.g. protein interactions and identify pathways, systems, and modules within this network (STRING).
- Insights into WebGeStalt, OmicsNET, NetworkAnalyst, DAVID etc.
- Gene Over-representation analysis (ORA).
- Network Topological Analysis and Visualization using Cytoscape.

Distinguished Lecture



Indirect Evidence synthesis using network analysis for efficacy and safety of drug therapy

Speaker

Dr. Dipika Bansal

Associate Professor,
Clinical Research Unit, NIPER, Mohali

https://niper.gov.in/faculty_newpage.htm

ETT 3

Organiser: **Prof. Shandar Ahmad** and **Anuja Jain**

Workshop on

Predicting drug resistance in tuberculosis from whole genome sequencing

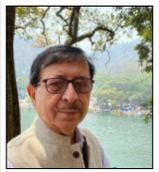
Saturday, February 03, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

Tool: MycoVarP

Workshop Summary

Tuberculosis has largely been regarded as a treatable disease for most patients. However, many patients have been diagnosed with drug resistance leading to unexpected failure of treatment. There is a growing interest in identifying patients with resistance to specific MTB drugs before the start of therapy. Whole genome sequencing (WGS) of the MTB strains can provide a powerful guide on which drugs to use to a patient suffering from a specific variant of the disease. In this workshop we will introduce MycoVarP a recently developed pipeline with our collaborators, which can make such predictions automatically from scratch starting from WGS data.

Distinguished Lecture



A Multi-prong approach is the only way to intervene against the Tuberculosis bacterium

Speaker

Prof. Seyed Ehtesham Hasnain
National Science Chair, Indian Institute of Technology, Delhi
Distinguished Professor, Sharda University, Greater Noida.
http://seyedhasnain.org

ETT 5

Organiser: **Prof. Pradipta Bandyopadhyay** and **Dr. Hari O.S.Yadav**

Workshop on

How to calculate accurate binding free energy for drug design

Saturday, February 17, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

Workshop Summary

The important role of computation methods in structure-based drug design is well-known. However, the correct ranking of inhibitors based on their binding to drug targets is still a difficult problem to solve. Binding free energy calculations have been found extremely valuable to solve such problems. These data turn out to be complementary to cellular data, thus helping in decision-making and compound prioritization in the early stage of drug discovery. However, the evaluation of binding free energy, especially with good accuracy is a highly challenging problem because of complex networks of protein and water interactions. The challenge further arises from the complexities of length and time scales, which make the free energy calculation process computationally very expensive. But there are some enhanced sampling methods, through which these challenges can be overcome. To flourish drug-discovery field, it is essential to know and use various free energy calculation techniques for the problem at hand. In this workshop, several advanced free energy calculation techniques will be explained. Hands-on sessions will be performed from the basics.

Distinguished Lecture

Coarse-grained dynamics and protein molecular function

Speaker

Prof. Debnath Pal
Department of Computational and Data Sciences
Indian Institute of Science, Bangalore
http://cds.iisc.ac.in/faculty/dpal/

ETT 4

Organiser: **Prof. Naidu Subbarao**

Workshop on

Molecular modeling and drug design

Saturday, February 10, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

Workshop Summary

Molecular modeling has become a valuable and essential tool to medicinal chemists in the drug design process. Molecular modeling describes the generation, manipulation or representation of three-dimensional structures of molecules and associated physico-chemical properties. It involves a range of computational methods based on theoretical chemistry methods and experimental data to predict molecular and biological properties. These methods involve modifying the structure of the ligand to improve its binding affinity and selectivity. The proposed workshop will cover topics structure predication methods and database such as alphaFold, molecular docking methods(Search methods/Scoring functions) and Molecular docking programs Autodock/Autodockvina, Glide and Gold. Workshop will also present different Drug Target Databases, Chemical Databases (Pubchem/ZINC/Private databases) / Bioassay databases (Pubchem/ChEMBL). The Lectures will cover drug designing of antibacterial, antiviral, antimalarial and anticancer agents using Structure based drug designing, ligand based drug designing(QSAR and Pharmacophore modeling), Machine learning methods, MD Simulation using GROMACS and Free Energy of Binding calculations using MM_PBSA program. Recent technologies using genomics and transcriptomics to drug discovery will be discussed.

Distinguished Lecture

The importance of 3D thinking in Drug Design Strategies

Speaker

Prof. Prasad V. Bharatam
Department of Medicinal Chemistry
National Institute of Pharmaceutical Education and Research,
NIPER, Mohali
www.niper.gov.in/pvbharatam.pdf

ETT 6

Organiser: **Prof. Mukesh Jain** and **Dr. Khushboo Gupta**

Workshop on

NGS data QC and transcriptome analysis

Saturday, February 24, 2024 | Lecture-11.00-12.00 hrs, Workshop-14:00 to 18:00 hrs.

NGS QC Toolkit; FastQC

Workshop Summary

This workshop is aimed at providing a deeper understanding of the current next generation sequencing (NGS) technologies and their potential applications. The participants will be provided training on understanding the NGS data, finding potential issues in the data and performing basic transcriptome data analysis. The workshop is adapted to the needs of the beginners in the field of NGS data analysis and provides them a first hands-on experience.

Distinguished Lecture

'Big data' revolution in life sciences: Trends and Challenges

Speaker

Prof. Saurabh Raghuvanshi
Department of Plant Molecular Biology,
University of Delhi South Campus. New Delhi
https://www.dpmb.ac.in/index.php?page=SR