

Applications of AI and Data-Driven Approaches in Structural Biology

October 21-23, 2024

CSIR – Institute of Genomics and Integrative Biology, Mathura Road, New Delhi, 110025

Day 1: October 21, 2024

Venue: IGIB (Workshop 1)

Theme: TECHNICAL WORKSHOP DAY 1 – Hands on session

AI and Computational Methods in Structural Biology

09:30 – 9:45 AM

Welcome address by RWTH Aachen University and Forschungszentrum Jülich representatives

9:45 - 10:20 AM

Machine learning augmented enhanced sampling simulations of biomolecular recognition

Dr Tarak Karmakar, IIT Delhi

10:20 – 10:55 AM

Key post-processing analysis of MD simulations drive decisions for drug discovery

Dr Shailendra Asthana, THSTI Faridabad

10:55 - 11:30 AM

Tea break

11:30 - 12:05 PM

An integrated Structural and Computational approach to probe protein structural variants

Dr. Bhupesh Taneja, CSIR-IGIB

12:05 - 12:40 PM

Agentic Systems for Lifesciences : Cancer biomarker discovery

Mainak Chakraborty, AWS

12:45 - 2:30 PM

Lunch Break

2:30 - 4:30 PM

Application of machine learning algorithms to predict protein structures and estimate the pathogenicity of missense single nucleotide variants.

Hands-on session by Martin Danner, PhD student at RWTH Aachen University

Day 2: October 22, 2024

Venue: IGIB (Workshop 1)

Theme: TECHNICAL WORKSHOP DAY 2

Cryo-EM Methods and Practical Applications

10:00 – 10:45 AM

Integrated structural biology approach for developing next-generation antivirals.

Dr Dilip Kumar, Ashoka University

10:45 – 11:30 AM

Multi-scale structural model of autophagy receptor p62/SQSTM1.

Dr Alexandros Katranidis, Forschungszentrum Jülich, Germany

11:30 – 12:15 PM

Tea break

12:15 – 1:00 PM

In situ correlative light and electron microscopy: a case study of the cellular organization of autophagy receptor p62/SQSTM1.

Dr Sabrina Berkamp, Forschungszentrum Jülich, Germany

1:00 – 2:00 PM

Lunch Break

2:00 – 4:00 PM

Visit to DST-SATHI Cryo-EM Facility at IIT Delhi (For German delegation)

2:00 – 3:00 PM

Practical considerations for single particle cryo-EM sample preparation and data collection.

Ms Kirti Suhag, PhD Student, IIT Delhi

3:00 – 4:00 PM

Cryo-EM single particle reconstruction workflow by using Relion software.

Mr Niraj Kumar, PhD Student, RCB Faridabad

Day 3: October 23, 2024

Venue: IGIB (Auditorium)

Theme: Scientific Lectures on Applications of AI and Data-Driven Approaches in Structural Biology

10:00 AM – 10:40 AM

Capturing protein structures and their cellular context by cryo-EM

Dr Carsten Sachse, Forschungszentrum Jülich

10:40 – 11:20 AM

AI/ML based methods for prediction of novel folds, oligomeric complexes of proteins and binding affinity of protein-ligand complexes

Dr Debasisa Mohanty, NII Delhi

11:20 – 11:45 AM

TEA break

11:45 – 12:20 PM

Deep mutational scanning as a tool to study protein sequence

Dr Kausik Chakraborty, CSIR IGIB Delhi

12:20 – 12:55 PM

DNA intrinsic shape alphabet in genome recognition by Transcription factors

Dr Shandar Ahamad, JNU

12:55 PM– 1:30 PM

Bespoke protein recognition properties on membrane

Dr Lipi Thukral, CSIR-IGIB Delhi

1:30 PM– 1:35 PM

Concluding remarks by Dr. Carsten Sachse

1:35 PM onwards

Lunch