

## 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

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**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 - 11:15 noon**

Tea break

**11:15 - 12:50 PM**

*Topic: to be announced.*

**Dr. Bhupesh Taneja, CSIR-IGIB**

**12:50 - 1:25 PM**

*Algorithms/LLMs underlying recent protein structural biology applications*

**Mr. Ashish Makani, Ashoka University**

**1:25 - 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 Mr. 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**

*Topic: to be announced.*

**Dr Debasisa Mohanty, NII Delhi**

**11:20 – 11:45 AM**

*TEA break*

**11:45 – 12:20 PM**

*Topic: to be announced.*

**Dr Kausik Chakraborty, CSIR IGIB Delhi**

**12:20 – 12:55 PM**

*Topic: to be announced.*

**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*