

JANUARY 28, 2026

Programme

INAUGURAL SESSION; 10:00 AM - 11:15 AM (IST)

- Intro to AI Impact Pre-Summit: Dr. Gitanjali Yadav, BRIC-NIPGR
- CODATA TG Overview: Dr. Narinder Mehra, INSA
- AI In Structural Biology: Dr. Debasisa Mohanty, Director, BRIC-NII, Chairperson, India CODATA

SESSION 1 (11:15 AM - 12 PM IST)

- **How AI/ML and Rational Drug Design are Transforming Drug Discovery** – Dr. Raghu R. CEO- Molecular solutions software Pvt Ltd (An overview of cutting-edge AI and computational methods that are reducing timelines, enhancing accuracy, and reshaping the discovery-to-development pipeline.)

SESSION 2 (12PM - 1 PM IST)

- **Fundamentals of Generative AI and Ultra Large Chemical Space Docking Methods** (Presentation and Demo) by Dr. Faizan Syed, Applications Scientist (A clear explanation of Gen AI, Ultra large molecular docking, Scaffold hopping, R Group replacement, scoring functions, and the science behind predicting binding interactions between ligands and proteins.)

LUNCH BREAK (01:00 PM - 02:30 PM IST)

SESSION 3 (02:30 PM - 03:30 PM IST)

- **02:30 PM (IST):** How Do We Assess This Work? Beyond Publications and Impact Factors; Prof. Peter Murray-Rust, Cambridge University
- Audience Q & A
- **03:00 PM (IST):** Talk by Simon Hodson, CODATA Exec Secy

SESSION 4 (03:30 PM - 04:30 PM IST)

- **Accurate Binding Free Energy Predictions and Unbinding Kinetics** by Dr. Viswanadhan, VP- Molecular Solutions
- Demo on Case Studies & Success stories in Drug Discovery by Anbu (Quick Binding Affinity and Unbinding kinetics prediction prediction and 11 Case studies to showcase how precise free energy perturbation can guide prioritization of drug candidates on variety of drug targets. Reproducibility, Provenance, and Explainability in AI-driven Science)

SESSION 5 (04:30 PM - 05:30 PM IST)

- Reflections for Policy, Data Governance, and ORAT Development: Panel Discussion
- Moderated by Dr. Neetu Singh (IITD)
- Panelists: Dr. Adrianna Baravalle (Argentina), Dr. Bortoluya (Mongolia), Dr. Renata Avila (Mexico) & Dr. Gitanjali Yadav (BRIC-NIPGR)