AI-based Drug Design Schedule

March 17-22, 2025 (Hybrid mode)

Date	March 17, 2024	March 18, 2025	March 19, 2026	March 20, 2027	March 21, 2028	March 22, 2029
Day	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
09:00-09:30 AM		Title: Emerging opportunities in computational biology driven by AI **Dr. Ashutosh Shandilya, IIT Delhi**	Title: ML, DL and LLM-based models for designing protein based drugs **Prof. G.P.S. Raghava, IIIT Delhi**	Title: Machine learning and deep learning techniques **Dr. Manjari Gupta, IIT BHU**	Title: Decoding GPCRs and Hormonal Ligands in Crustaceans: Insights from the Machine Age **Prof. N.S. Gandhi, MIT, Karnataka**	Title: Unveiling Molecular Dynamics for Drug Discovery Training session **Dr. Suyash Pant, Schrodinger, Hyderabad**
09:30-10:00 AM	Inaugural session:					
10:00-10:30 AM	High Tea Break					
10:30-11:00 AM	Title: Illustrating machine learning-guided approaches in lead optimization **Prof. G.N. Sastry, IIT Hyderabad**					
11:00-11:15 AM		Tea break				
11:15-12:30 AM		Title: To be announced **Prof. Anshuman Dixit, ILS, Bhubaneswar**	Title: Density Functional Theory, Docking, and Molecular Dynamics-based Simulations for Drug Design **Dr. N.R. Jena, IIITDM Jabalpur**	Title: To be announced **Prof. S.K. Singh, Alagappa University, Tamilnadu**	Title: QSAR-based Drug Design **Prof. Mukesh Doble, IIT Madras**	Reserved for Activities
12:30-01:15 PM	**Lunch Break**					
01:15-02:30 PM		**Lunch Break**				
02:30-03:30 PM	Title: Molecular property prediction using machine learning and Artificial Intelligence **Dr. Rajnish Kumar, IIT BHU**	Title: To be announced Training session **Prof. Anshuman Dixit, ILS, Bhubaneswar**	Title: Development of AI-based models for proteins using Python Training session **Prof. G.P.S. Raghava, IIIT Delhi**	Title: Machine learning and deep learning techniques Training session **Dr. Manjari Gupta, IIT BHU**	Title: Integrating Molecular Docking, Virtual Screening, and Molecular Dynamics: A Comprehensive Approach to Computational Drug Discovery **Dr. Suyash Pant, Schrodinger, Hyderabad**	Title: Protein-ligand Docking with GOLD: Optimising Drug Discovery Through Structure-based Drug Design Training Session **Dr. Rupesh Chikhale, CCDC, UK**
03:30-4:30 PM						
04:30 - 4:45 PM	Tea break					Concluding Remarks
04:45-05:00 PM	Title: ML and AI-based drug design Training session **Dr. Rajnish Kumar, IIT BHU**	Title: Structure visualization by Pymol Training session **Mr. Ramprakash Yadav, IIITDM Jabalpur**	Title: Virtual Screening to Molecular Docking using our in-house tools (Sanjeevini) and MD Simulations by AMBER on our supercomputing resources Training session **Dr. Ashutosh Shandilya, IIT Delhi / Mr. Dheeraj Chaurasia**	Title: To be announced Training session **Prof. S.K. Singh, Alagappa University, Tamilnadu**	Title: QSAR-based drug design Training session **Prof. Mukesh Doble, IIT Madras**	
05:00-06:45 PM						