



Workshop on AI-Driven Drug Discovery: Advanced Tools, Techniques & Applications

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A three-day intensive workshop on “AI-Driven Drug Discovery: Advanced Tools, Techniques & Applications” was successfully organized at the CSIR-Human Resource Development Centre (CSIR-HRDC), Ghaziabad, from April 7 to 9, 2026. The programme was exclusively designed for CSIR Scientists and Technical Officers, with the objective of equipping them with advanced knowledge and practical exposure to cutting-edge Artificial Intelligence (AI) tools transforming modern drug discovery.

The workshop was inaugurated in the presence of eminent dignitaries including Prof. G. N. Sastry, Department of Biotechnology, IIT Hyderabad; Dr. T. S. Rana, Head, CSIR-HRDC; Dr. Vinay Kumar, Scientist G & Programme Convener; and Mrs. Preeti Chaudhary, Programme Coordinator. In his inaugural address, Prof. Sastry highlighted the transformative role of AI in revolutionizing the drug discovery process and emphasized the growing importance of interdisciplinary approaches in pharmaceutical research. Dr. Vinay Kumar also presented a comprehensive overview of the workshop, outlining its vision, objectives, and the rationale behind conceptualizing this programme to address emerging needs in AI-driven drug discovery..

Over the course of three days, the workshop featured a series of insightful lectures and interactive sessions delivered by distinguished experts from premier institutions. Notable contributors included Prof. Prabha Garg (NIPER, SAS Nagar), Prof. D. Sunder (Director, IBAB), Dr. Arijit Roy (TCS, Hyderabad), and Dr. S. Nagamani (CSIR-NEIST), who shared their expertise, real-world applications, and emerging perspectives in AI-enabled drug discovery.

The technical sessions on AI in Target Identification and Biomarker identification, AI-Assisted Molecular Docking & Scoring and AI in Bimolecular Simulation were particularly well-received. Experts such as Dr. Rajnish Kumar, Associate Professor (IIT BHU, Varanasi), Dr. Firoz Khan (CSIR-CIMAP), and Dr. Tarak Karmakar (IIT Delhi) provided in-depth knowledge and hands-on insights, significantly enhancing participants’ understanding of advanced computational approaches in drug discovery.

The workshop concluded on April 9, 2026, with the distribution of participation certificates by Dr. T. S. Rana and Dr. Vinay Kumar, recognizing the active engagement of participants throughout the programme.

The valedictory session concluded with a vote of thanks delivered by Mrs. Preeti Chaudhary, who expressed sincere gratitude to all distinguished speakers, dignitaries, and participants for their valuable contributions in making the programme a grand success.

The workshop received highly positive and encouraging feedback from participants, which will serve as a guiding framework for organizing future programmes. The programme successfully provided a dynamic platform for knowledge exchange, skill enhancement, and fostering innovation in the rapidly evolving domain of AI-driven drug discovery.

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