IQAC and IPR Cell Driven

International Workshop on Computational Tools and

Data-Driven Transformation in Drug Discovery

Date: 16-18 AUGUST 2023,

Location: Maliba Pharmacy College, Uka Tarsadia University, Surat, Gujarat, India

Report

The **inauguration ceremony** was a momentous occasion, attended by esteemed guests, speakers, and workshop participants and students of Maliba Pharmacy College. It set the stage for the three days of intensive learning and collaboration. The ceremony began with a warm welcome by Dr. Sandesh Lodha, the event organizer, who highlighted the importance of the workshop in advancing drug discovery through computational tools and data-driven methods. The key note address for inauguration was give by Dr. Vijay Masand. Dr. Shailesh Shah, Dr. Ashish Mishra, Dr. Debanjan Sen and Dr. Renu Chauhan graced the occasion. Dr. Gajanan Kalyankar gave the formal vote of thanks for inaugural ceremony.

Day 1: Molecular Docking and Hands-on Tools

The first day of the International Workshop on Computational Tools and Data-Driven Transformation in Drug Discovery was dedicated to the exploration of Molecular Docking and various hands-on tools that facilitate the drug discovery process.

Morning Session: Introduction to Molecular Docking

The morning session commenced with an introductory presentation on Molecular Docking by Dr. Vijay Masand, a renowned expert in the field. Attendees gained insights into the principles of Molecular Docking, its applications, and its significance in the drug discovery process. Key topics included:

Molecular Docking Algorithms: Discussion on various docking algorithms, such as AutoDock, AutoDock Vina, and GOLD.

Case Studies: Real-world examples showcasing the successful application of Molecular Docking in drug discovery.

Afternoon Session: Hands-on Tools for Drug Discovery

In the afternoon, participants had the opportunity to engage in a hands-on workshop where they explored a range of tools and software that facilitate drug discovery. These tools covered areas such as ligand preparation, receptor preparation, and result analysis.

Ligand and Receptor Preparation Tools: Participants learned how to prepare ligands and receptors for docking using tools like Open Babel and Avogadro.

Result Analysis: Attendees explored various tools for analyzing and visualizing docking results, such as PyMOL and Discovery Studio Visualizer.

Day 2: Pharmacophore Modeling and Molecular Dynamics Simulation

The second day of the workshop was centered on Pharmacophore Modeling and Molecular Dynamics Simulation, two crucial techniques in the drug discovery process.

Morning Session: Pharmacophore Modeling

The morning session was led by Dr. Debanjan Sen, an expert in the field of pharmacophore modeling. Key topics included:

Fundamentals of Pharmacophore Modeling: Introduction to the concept of pharmacophores and their role in drug discovery.

Software Tools: Overview of popular software tools for pharmacophore modeling

Afternoon Session: Molecular Dynamics Simulation

The afternoon session delved into Molecular Dynamics Simulation (MD), a technique that allows researchers to study the dynamic behavior of biological systems at an atomic level. Highlights of the session included:

Introduction to MD Simulation: A comprehensive overview of MD simulations and their applications.

Software and Resources: A review of software tools, such as GROMACS and AMBER, used for MD simulations.

Hands-on Session: Practical exercises in setting up and running MD simulations.

Day 3: Antibody and its role, Result Analysis of MD Simulation and Machine Learning

The third and final day of the workshop emphasized the critical aspects of result analysis in MD simulations and the integration of machine learning techniques in drug discovery.

Morning Session:

Mr. Manoj Sabnani from USA in online mode emphasized on importance of antibody designing and its significance in disease treatment with future perspectives

Result Analysis of MD Simulation

The morning session was dedicated to interpreting and analyzing MD simulation results. Topics covered included:

Trajectory Analysis: Techniques for analyzing trajectories, including RMSD, RMSF, and PCA.

Visualization Tools: Utilizing visualization software like VMD and PyTraj.

Case Studies: Real-world applications of MD simulation analysis.

Afternoon Session: Machine Learning in Drug Discovery

The workshop concluded with a focus on the integration of machine learning in drug discovery. The key elements included:

Introduction to Machine Learning: An overview of machine learning concepts and algorithms.

Drug Discovery Applications: How machine learning can be applied in various stages of drug discovery, including target identification and virtual screening.

Hands-on Exercises: Participants had the opportunity to explore machine learning tools and apply them to real drug discovery datasets.

Closing Remarks and Networking

The workshop concluded with a closing session, where attendees had the opportunity to share their experiences and insights gained during the three-day event. It was followed by a networking session, allowing participants to interact, share ideas, and build collaborations in the field of computational drug discovery.

The International Workshop on Computational Tools and Data-Driven Transformation in Drug Discovery was a resounding success, providing participants with valuable knowledge and practical skills in utilizing computational tools for drug discovery. The combination of expert presentations, hands-on sessions, and real-world case studies made it a highly informative and engaging event. Participants left with a deeper understanding of cutting-edge techniques and their applications in drug discovery.

The valedictory function was a moment of reflection, recognition, and celebration as the workshop came to a close. The chief Guest for Valedictory function was Honorable Dr. Dinesh Shah Sir, Provost, Uka Tarsadia University who emphasizing the importance of interdisciplinary research and the role of universities in fostering knowledge exchange and innovation. Their dynamic leadership and vision were evident in the impactful words shared with the audience. His presence and encouragement inspired the attendees. The function witnessed a momentous and exhilarating announcement by the Provost of Uka Tarsadia University. The Provost declared the establishment of a state-of-the-art Pharmacoinformatics Lab right on the university campus, much to the delight and applause of the participants. Dr. Shailesh Shah, Dr. Ashish Mishra, Dr. Debanjan Sen and Dr. Renu Chauhan graced the occasion.

Participants were invited to share their experiences and insights gained during the workshop. Their feedback was a testament to the positive impact of the event. Feedback from participants was overwhelmingly positive, reflecting their appreciation for the workshop's content, organization, and the valuable skills acquired. Certificates of participation were distributed to all attendees, and awards were presented to exceptional contributors and participants. Dr. Sandesh Lodha expressed his gratitude to the distinguished speakers, management, colleagues, volunteers, participants and all those who contributed to the success of the workshop in his vote of thanks.

The inauguration and valedictory function of the "International Workshop on Computational Tools and Data-Driven Transformation in Drug Discovery" was marked by enthusiasm, knowledge sharing, and an overwhelming sense of accomplishment. These two pivotal events encapsulated the essence of the workshop's journey, from its promising beginning to its successful conclusion.

This event will undoubtedly serve as a cornerstone for future endeavors in the field of drug discovery through computational tools and data-driven transformation for the participants.

Details of Participation

Total Participants – 52

Male participants – 26

Female Participants – 26

Outside UTU participants – 12

Faculty participants - 13

Speakers – 3