DEMPO CHARITIES TRUST's

Dhempe College of Arts and Science, Panaji-Goa

Department of Biotechnology

Report on 2-day Hands-on Training on 'Computer Aided Drug Design & Discovery' 7th & 8th October 2024

A comprehensive 2-day hands-on training on 'Computer Aided Drug Design & Discovery' was organized by the Department of Biotechnology at DCT's Dhempe College of Arts and Science, in association with make-Intern and E-Cell, IIT Hyderabad, supported by the DBT Star College Scheme, Government of India from 7th – 8th October 2024. This training was designed particularly for students & researchers and aimed to enhance participants' understanding and skills in computational methods applied to drug discovery.

The **Objectives** of the training included:
1. Introduction to fundamental concepts in computer-aided drug design (CADD).
2. Hands-on experience with popular drug design software and databases.
3. Exposure to molecular modeling, docking studies, and virtual screening processes.
4. Building foundational skills to accelerate drug discovery workflows.

Day 1 summary: The workshop commenced with an inaugural ceremony amidst the presence of esteemed dignitaries Dr. Karunakar Tanneeru, the Resource Person, Prof. (Dr) Ramu Murthy, Principal, Dr. Swati Pawar (Vice Principal), Mrs. Mrunal Phadke (Department In-Charge). A total of 40 enthusiastic students along with faculty members of the biotechnology department were also present. The principal explained the significance of hands-on skill training for the students for better job and research prospects.
Sessions included an introduction to the role of CADD in modern drug discovery, discussing its advantages in speeding up the development of effective therapeutic agents. Topics covered included:
- Basics of molecular modeling and drug design
- Software installation and environment setup for CADD
- Exploration of chemical databases for drug discovery, including PubChem.
Participants were introduced to molecular docking principles and virtual screening techniques. Practical exercises included setting up molecular structures, visualizing ligand-protein interactions, and using AutoDock and PyMOL software.

Day 2 Summary: On the second day, the focus shifted to advanced CADD applications, including:
- Molecular dynamics simulations to predict the stability of drug-receptor complexes

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Event coordinator

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- Quantitative Structure-Activity Relationship (QSAR) modeling for predicting biological activity
- ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) predictions to assess drug safety and efficacy

The hands-on sessions provided participants with practical experience in running simulations and analyzing docking results, culminating in an interactive Q&A session where participants could discuss challenges and gain feedback.

A time-bound assessment of students was carried out via the circulation of a Google questionnaire as part of the Zonal Championship. Based on the scores and interaction throughout the training, the top 5 students were awarded special certificates and will now stand a chance to compete at the National level championship to be held at IIT later this year.

Outcomes: Participants gained practical skills in utilizing computational tools for drug discovery, from structure visualization to docking studies. The training gave attendees the knowledge and resources to implement CADD methodologies in their research projects.

Conclusion: The 2-day training was highly beneficial, equipping participants with essential CADD skills and fostering a deeper understanding of drug design and discovery processes. The hands-on experience ensured that participants could apply these tools in real-world drug research, positioning them to contribute effectively to advancements in pharmaceutical sciences. The two-day hands-on training concluded with a vibrant valedictory ceremony and distribution of certificates to the participants.

Total no: of beneficiaries: 40 (Males: 08; Females: 32)

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