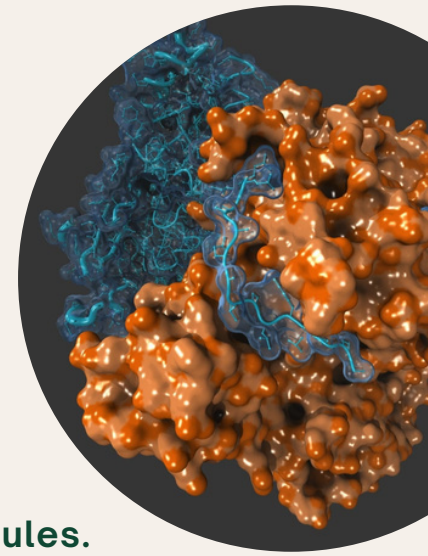
INTERNATIONAL ONLINE WORKSHOP

C·A·T·R
CENTRE FOR ADVANCED TRAINING AND RESEARCH
CERTIFIED & GOVT. APPROVED

COMPUTER-AIDED DRUG DESIGN

Pharmacokinetic Analysis-Molecular Docking-Molecular Dynamics Simulation



Gain expertise in Molecular Dynamics Simulation (MDS) and Molecular Docking, a highly effective computational method employed for investigating the dynamics and interplay of atoms and molecules. This technique holds immense significance in the field of drug discovery as it enables researchers to replicate the behavior of biological systems at the molecular scale. By mastering MDS, participants can:

- **Uncover the dynamic characteristics of biological molecules.**
- **Understand drug-protein interactions.**
- **Predict the stability and properties of drug candidates.**
- **Accelerate drug discovery processes.**

PROGRAMME SCHEDULE

01-10 JULY 2024

India/Sri Lanka	**7:00 PM**
Nepal	7:15 PM
Saudi Arabia/Qatar	4:30 PM
UAE /Oman	5:30 PM
Netherlands	3:30 PM
United Kingdom	2:30 PM
USA	6:30 AM
Italy/ Nigeria	2:30 PM

REGISTRATION

Scan/Click

https://forms.gle/GKHPCfJ5JycBc2719

WORKSHOP FEE & FEATURES

For Indian Participants:

2500 INR

For International Participants:

70 USD

Online mode
Certificate
Live Recording of Lectures
Software and Protocols
Complete practical based training
Hands-on-session

JOIN US NOW!

www.catredu.com

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Benefits of Attending This Workshop

Comprehensive Curriculum: Our 10-days program covers everything from drug discovery fundamentals to advanced Molecular Dynamics Simulation techniques.

Skill Enhancement: Acquire essential skills in Molecular Dynamics Simulation (MDS) crucial for success in drug discovery and computational biology.

Expert Guidance: Learn from experienced instructors, gaining practical knowledge & Hands-on session under their mentorship.

Hands-on Learning: Engage in interactive sessions and practical exercises, ensuring proficiency in MDS techniques.

Certification: Receive a recognized certificate upon completion, validating your expertise in MDS.

Career Boost: Enhance your career prospects in academia and industry, unlocking new opportunities in drug discovery and bioinformatics.

Who can join

This workshop is suitable for students and professionals in the following fields:

- B.Sc., M.Sc., MS B.Tech., M.Tech. in Biology, Biotechnology, Chemistry, Life science, Biochemistry, Bioinformatics, Pharmacy, and related disciplines.
- B. Pharm, M. Pharm, and Pharm. D. students.
- Ph.D. and Postdoc researchers in Life Sciences and Pharma and related field

Curriculum Overview

Module 1: Introduction to Drug Discovery with Drug-Like Property Analysis

- Overview of drug discovery and computational methods.
- Lead molecule identification and optimization.
- Drug like property analysis (Lipinski's rule of Five)
- Pharmacokinetic screening ADME
- Toxicity screening of molecules/Drug candidates

Module 2: Molecular Docking Studies

- Introduction to Structure based Drug Design
- literature study and acquisition of target structure
- Installation of Discovery Studio, MGL Tool, Docking tools, Cygwin and other Software
- Protein (Target) structure validation and Preparation
- Active site Prediction
- Ligand optimization and docking parameters.
- Running docking commands
- Building protein-ligand complex and Visualization of protein-ligand interactions
- Pose Selection (publication standard)
- Result analysis

Module 3: Molecular Dynamics Simulation Studies

- Introduction to Molecular Dynamics Simulation and software tools.
- Installation of Ubuntu and software required for simulations (GROMACS)
- Cleaning and preparation of protein and ligand files.
- Solvent selection and solvation box definition.
- Energy minimization and Heating (300K)
- Equilibration (NVT& NPT)