REG. NO. 1074/2006-07

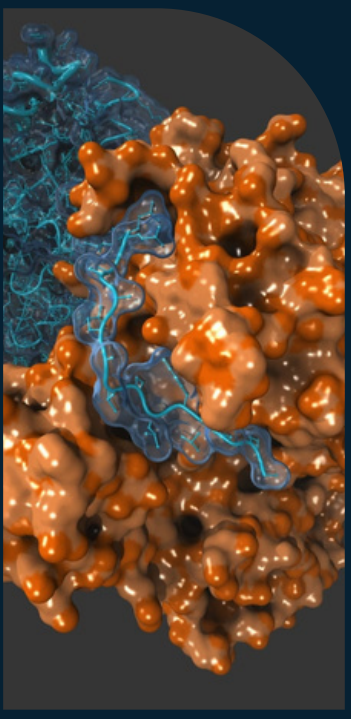
CENTRE OF BIOINFORMATICS TRAINING AND RESEARCH

Short Term Bioinformatics Training on

Computer-Aided Drug Design (CADD)

19-28 NOVEMBER 2022, 7:00 PM IST

ONLINE HANDS-ON TRAINING SESSION



Registration Fee

~~INR 6000/-~~

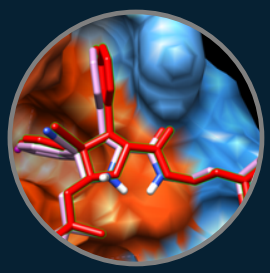
INR 1500/-only

(Only Selected Candidates will be contacted for fee submission)

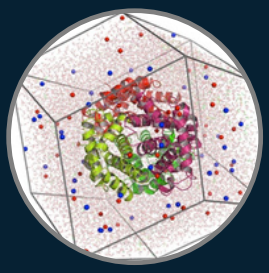
CLICK/SCAN FOR REGISTRATION

HTTPS://FORMS.GLE/NQANA3YMRCCDDNQG6

PHARMACOKINETICS ANALYSIS



MOLECULAR DOCKING



MOLECULAR DYNAMICS SIMULATIONS

- E-CERTIFICATE
- TRAINING REPORT
- VIDEO RECORDING

CONTACT US

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TOPICS TO BE COVERED....

Theory + Hands-on session

MODULE - I

Pharmacokinetic Analysis of compounds/Drugs (Ligand Based Drug Design)

- Introduction to Bioinformatics and Understanding of Databases (NCBI-Gene databases and Protein databases, PubMed, PubChem, DrugBank, RCSB-PDB
- Understanding file formats (sdf, mol, pdb)
- Lipinski's rule of five analysis (Drugability of Compounds)
- Pharmacokinetics analysis of compounds/drugs based on their Absorption-Distribution-Metabolism-Excretion (ADME)
- Toxicity screening (Carcinogenicity and Mutagenicity)

MODULE - II

Molecular Docking Analysis (Structure based Drug Design)

- Introduction to Structure based Drug Design and process layout of Docking
- Data mining, literature study and acquisition of target structure
- Installation of Discovery Studio, MGL Tool, AutoDock and other Software
- Protein structure validation
- Preparation of Protein and Ligand (Compound/Drug)
- Active site/ Pocket identification of target protein
- Molecular Docking analysis (Ligand-Target Docking)
- Docking analysis (based on binding energy, Hydrogen bond interactions, electrostatic interactions, hydrophobic interactions, etc.
- Visualization of protein-ligand interactions in Discovery studio
- Building protein-ligand complex and visualization (publication standard)

MODULE - III

Molecular Dynamics (MD) Simulation

- Introduction to Molecular Dynamics Simulations
- Basic Principles of Molecular Dynamics Simulations
- Installation of Ubuntu and software required for simulations (GROMACS)
- Molecular Dynamics Simulation using GROMACS
- Initialization (Ionization and Solvation)
- Energy minimization and Heating (300K)
- Equilibration (NVT& NPT) and Production
- Analysis (simulation trajectories)
- RMSD and RMSF Graph analysis and interpretation

Who is Eligible

Students of B.Sc./M.Sc./B.Tech/M.Tech/Ph.D and Postdoctoral Fellow/Faculty members from Life Sciences, Biological Science, Pharmacy, Agriculture, Microbiology, Biochemistry, Biotechnology, Molecular biology, Medicine, clinical research and other relevant areas can join