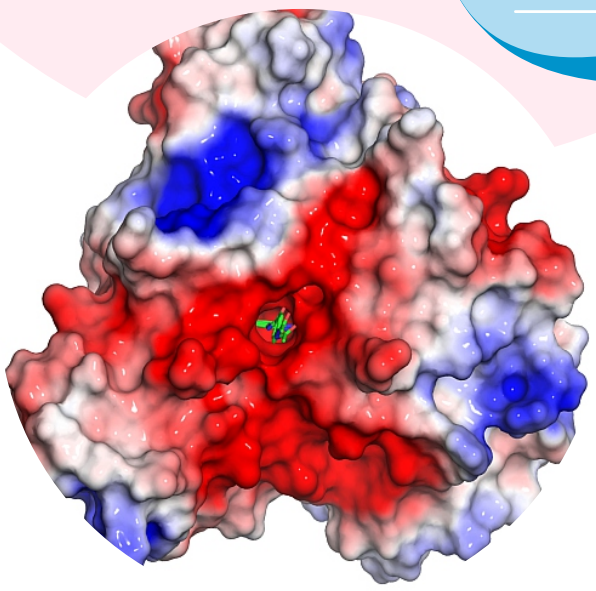
Two Days **Hands on** Workshop on

Machine Learning and High-Performance Computing in Computational Drug Design

virtual engineering

04-05th April 2024

Hotel IV Sanctum,
Gandhinagar
Bangalore



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Workshop Experts

Prof. Jayant K. Singh
Professor
Dept. of Chemical Engineering
IIT Kanpur

Dr. Prosun Haldar
Application Scientist
Prescience Insilico Pvt Ltd

Dr. Sudip Roy
Founder and Managing Director
PRESCIENCE INSILICO, Bangalore

Dr. Mohd. Aamir Khan
Tech Manager and Developer
Prescience Insilico Pvt Ltd

Dr. Aiswarya Pawar
Senior Application Scientist
Prescience Insilico Pvt Ltd

Ms. Mahima Kori
Application Scientist
Prescience Insilico Pvt Ltd

Workshop Schedule [Day 1]

virtual engineering

Workshop Starts at 10.00 am

Welcome and About the workshop

Mr. Santhosh N L
Director & CEO
DHIO Research and Engineering Pvt Ltd.,

Keynote Talk

Prof. Jayant K. Singh
Professor, Dept. of Chemical Engineering, IIT Kanpur

Dr. Sudip Roy
Founder and Managing Director, PRESCIENCE INSILICO, Bangalore

Session 1 : Introduction to *in silico* Drug Design

> Introduction to computer aided drug designing: motivation
> How to define and design a problem and solution:
> What are the available tools and computational methods that are applicable for drug designing:

Dr. Aiswarya Pawar and Ms. Mahima Kori
PRESCIENCE INSILICO, Bangalore

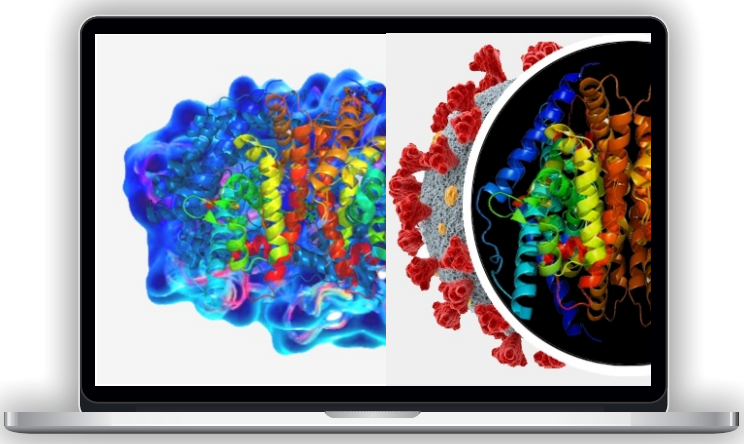
Session 2 : Methodologies – Structure-based and Ligand-based Screening

> Introduction to structure-based screening.
> Therapy/disease pathways and identification related targets, structure of targets. PDB structures, open databases, visualization of targets and available software.
> Molecular Docking, screening using docking, rigid and flexible docking.
> Computational/Theoretical methods used for docking, Monte Carlo Methods
> Introduction to chem-informatics.
> Database screening for identification of potential drug candidates.
> Pharmacophore modelling, chemical structure and property relationships.
> Quantitative Structure Property Relationship,linear regression theory.
> Lead optimization and identification

Ms. Adhithya & Ms. Mahima Kori
PRESCIENCE INSILICO, Bangalore

Session 3 : Hand-on: Compound Dataset design and Protein Design

> Integrated Databases for searching chemicals based on targets
> Sequence similarity search
> Chemical space expansion using AI
> Create input ligand structure
> Integrated RSCB database for searching targets
> Clean target structures by deleting unwanted protein chains, ligands, ions, water
> Model missing residues and loops
> Model numeric and alpha-numeric residue ID
> Homology modelling for unknown structures
> Adding various mutant to proteins
> Clean/rectify target biomolecules for input for MD
> SyMOG (Genetarive AI tool) for synthetic molecule generation
> Prepration of data set for HTVS



Workshop Schedule [Day 2]

Dr. Prosun Halder
PRESCIENCE INSILICO, Bangalore

Session 4 : Machine learning Aided Drug Screening

> Introduction to machine learning methods used in drug designing.
> Generative model, Knowledge graphs and reinforcement learning.
> Molecule optimization, molecular graph generation, multimodal graph -to-graph translation.
> Virtual drug screening, knowledge graph embedding methods for drug repurposing.

Dr. Sudip Roy
PRESCIENCE INSILICO, Bangalore

Session 5 : Basics of Molecular Simulations and its Application in Drug Screening

> Thermodynamics and Statistical Mechanics – connection to molecular simulation.
> Molecular simulations to calculate macroscopic properties. Methodology: Molecular Dynamics
> Introduction to Molecular Dynamics and its application in drug designing.
> Newton's equation of motion – algorithms to solve the equation of motion.
> Estimation of properties (RMSD, binding, interactions) and understanding mechanisms.
> Simulating biological systems – examples

Dr. Mohd Aamir Khan & Ms. Mahima Kori
PRESCIENCE INSILICO, Bangalore

Session 6 : Hands on training

> Docking
> Molecular Dynamics of Protein-ligand system and free energy calculation with MMPBSA

Registration Details

Registration Fee
Industry : INR 5000.00 + Tax
Faculty & Research Scholars : INR 3000.00 + Tax
Students : INR 2000.00 + Tax

Link for Expression of Interest

https://forms.office.com/r/fuxcM2BFM3

Link to pay registration fee and register

https://rzp.io/l/ComputationalDrugDesign

Contact for More Information

Mrs. Shilpashree
Product Manager
DHIO Research and Engineering Private Limited
shilpashree@dhioresearch.com +91 9900138009

Registration Form

virtual engineering

Students ☐	Industry ☐	Academic ☐

Name	
Designation	
Company / College	
Phone	
Fax	
Mobile	
Email	
Address	
Topic of Interest	
Signature and Seal	

Registration Details

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