PROGRAMME SCHEDULE

Structural Bioinformatics & Computer Aided Drug Designing (CADD)

DAY – 1 (15 / 11 / 2024): Introduction to Structural Bioinformatics	
08:30 – 9:00 am	**REGISTRATION**
09:00 –10:00 am	*Session-I: Protein Modeling and Structure Prediction* ✓ Sequence Structure Gap ✓ Protein Modeling: Homology Modeling and Threading ✓ Secondary structure prediction
10:00 – 10:30 am	**INAUGURATION**
10:30 – 11:00 am	**HIGH TEA**
11:00 – 12:15 pm	*Session-II: Protein Modeling and Structure Prediction* ✓ Extended modelling approach using Python* ✓ Tertiary structure prediction through Ramachandran plot ✓ Visualisation of 3D protein structure*
12:15 – 12:30 pm	Doubt Clearing Sessions
12:30 – 01:45 pm	**LUNCH**
01:45 – 03:00 pm	*Session-III: Mutational Analysis and Thermodynamics* ✓ Generation of mutants & Thermodynamics* ✓ Energy minimisation of protein structures* ✓ Relative RMSD calculation*
03:00 – 03:30 pm	**HIGH TEA**
03:00 – 03:30 pm	Doubt Clearing Sessions
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DAY – 2 (16 / 11 / 2024): Computer Aided Drug Designing	
09:00 – 10:30 am	*Session-I: Introduction to small compound databases* ✓ Data retrieval from PubChem and DrugBank ✓ Drug Designing using Avogadro/GaussView* ✓ Pharmacokinetics (ADMET) Analysis
10:30 – 11:00 am	**HIGH TEA**
11:00 – 12:15 pm	*Session-II: Molecular Docking and Analysis* ✓ Introduction to Molecular Docking ✓ Molecular Docking using AutoDock* ✓ Intermolecular Interaction Analysis of Docked Poses
12:15 – 12:30 pm	Doubt Clearing Sessions
12:30 – 01:15 pm	**LUNCH**
01:15 – 03:00 pm	*Session-III: Molecular Dynamics Simulation* ✓ Introduction to Linux OS ✓ Molecular Dynamics Simulation of Protein in GROMACS ✓ MD Visualization in VMD
03:00 – 03:15 pm	**HIGH TEA**
03:00 – 03:15 pm	Doubt Clearing Sessions
03:15 – 03:30 pm	Valedictory Session and Vote of Thanks
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*Standalone softwares will be provided

Two Days Workshop & Hands-on-Training

Structural Bioinformatics & Computer Aided Drug Designing (CADD)

HIGHLIGHTS

- Introduction to Linux OS
- Computational Analysis using Python & ML
- Molecular Dynamics Simulation in GROMACS

Prerequisites

Personal Laptop (Windows / Linux OS)

Hurry !! Limited Seats

Registration Fees:

₹1500 (Ph.D. Scholars / Faculty)

₹1000 (Undergraduate / Postgraduate)

RESOURCE PERSON

Dr. Aniket Naha (M.Sc., Ph.D.)

Scientist & Student Coordinator

Medical Biotechnology & Computational Drug Designing Laboratory

Pushpagiri Research Centre, PIMS&RC, Tiruvalla

PAYMENT QR

Account Number: 024804176659190008
IFSC Code: CSBK0000248
MICR code: 689047003

Registration Link: https://forms.gle/8sHfkn7STUzWqLUJ9

15-16 November 2024 | **09:00 AM - 03:00 PM** | **Conference Hall, PRC**

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