Seven days

Online Skill Development Program

on

"In-Silico Drug Designing and Molecular Dynamics Simulations"

14 - 20 September 2022

(6:00 pm – 8:30 pm)

@

Google Meet Platform

CYTOGENE RESEARCH & DEVELOPMENT

CSC (B) – 301, 2ND FLOOR OLD COMPLEX, SAHARA STATES, JANKIPURAM, LUCKNOW -226021

www.cytogene.in

The concept behind:

This workshop designed to give participants a combination of lectures and Dry laboratory experience using various techniques. Delegate will gain experience to various tools used these day to reduce the working time and cost too. The live demo of software will add clear concept in mind about working of the tools and steps involved in it, Prediction of target protein, Drug Likeliness and screening, Homology Modelling and Docking. The Bioinformatic analysis of data on tools gives more accuracy than the traditional method. Experimental exposure will help to understand the direct interaction between the molecules.

Objectives of the Workshop:

The workshop aims at exposure of candidate to basics of techniques, its working & application. It will provide a platform to learn Techniques / software commonly used in Drug designing to get a better insight into computational biology through analysis of Protein – Ligand binding. It will also deal with homology modelling, docking of molecules & simulations.

Title: Molecular Dynamics Simulations and In-Silico Drug Designing

List of Major Experiments to be performed:

- o Introductory lecture on Molecular Dynamics Simulations and In-Silico Drug Designing.
- o Protein retrieval and Active site prediction (RCSB - PDB, Discovery studio, CASTp)
- o Selection of ligand and Dataset preparation (PubChem, ChemSpider, Open Babel)
- o Drug likeliness of compound and Screening of ligands on basis of Lipinski rule of 5
- o Ligand property prediction and screening (DriLiTo, ADMET-SAR, Swiss-ADME)
- o Homology modelling for structure of unknown proteins
- o Protein and Ligand Preparation on ADT
- o Docking in Autodock Vina
- o Docking in PyRx
- o ProteInteraction of Protein-ligand residues in the active site using LigPlot
- o Poses analysis using PyMol
- o Molecular Dynamics Simulation using GROMACS
- o Analysis of the plots of simulation
- o Final discussion/Conclusion, Certificate distribution & Feedback

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About the Hosting Institution:

CytoGene Research & Development, Lucknow is an autonomous Registered organization by Ministry of corporate affairs, Government of India under section 12(1) of LLP Act 2008 & Certified by ISO 9001:2015, ISO 14001:2015 & ISO 45001:20018.

Who Should Participate?

Teachers, Faculty member, PhD scholars, Students of M.Sc/M.Tech or B.Sc,/B.Tech from any division of Life sciences

Registration Fee:

Rs. 1,200/- (Only soft copy Certificate will be provided by email on last working day of Workshop)
Rs. 1,350/- (Hard copy Certificate by post/Courier and Soft copy certificate will be provided by email on last working day of workshop)

Compulsory requirement:

Laptop: All the participants must have laptop to perform the experiment to their own end on daily basis. Configuration of computer can be basic.

How to register:

Online:
Visit to www.cytogene.in and go to registration page select Workshop registration form. Fill the form completely followed by submit. The next window of Mode of payment will open by which the payment of registration fee can be done.

www.cytogene.in

Offline:

Download MS Word format of Registration form from our website www.cytogene.in and fill the form or ask us for form by email.

Send the duly filled registration form and payment screenshot by:

Email to workshop.cytogene@gmail.com

Whatsapp to 77-0309-5555

Mode of payment:

1) By online transfer / Cash deposit

Name : CytoGene Research & Development LLP

Type of account : Current

Bank name : Union Bank of India

A/C no. : 522601010036489

IFSC Code : UBIN0552267

Branch : Indira Nagar, Lucknow

2) By Phonepe

Name: SUJEET KUMAR SINGH

Mobile no: 8756658021

UPI ID: 8756658021@ybl

QR Code:

3) By Google pay

Name: SUJEET KUMAR SINGH

Mobile no: 8756658021

UPI: singh.sujeet121@oksbi

QR Code:

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Important Dates:

Date of Notification: **02 September 2021**

Start of registration: **02 September 2021**

Last date of Registration: **13 September 2021**

Date of Commencement of the workshop: **14 September 2021 (6:00pm – 8:30pm)**

Maximum No of Seat: 30 (Registration will be closed as soon as the seats will be filled)

Selection Process: First come first serve

Contact person:

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