DBT-Sponsored

Short Term Training Program On

"Computer Aided Drug Designing and Molecular Dynamics Simulations"

(CAMDS -2022)

13th – 19th June 2022

Sponsored By

सत्यमेव जयते

Department of Biotechnology, Government of India.

Organised By

Department of Biotechnology & Medical Engineering, National Institute of Technology Rourkela.

About BIC at NIT Rourkela

The Centre for Bioinformatics and Computational Biology: Animal Bioinformatics (BIC) was established in the Department of Biotechnology and Medical Engineering at NIT Rourkela with funding from the DBT, Govt. of India. The BIC has been providing computational facilities and services to users in terms of hardware and software. Major activities includes human resource development, training and workshops, database creation and bioinformatics tool development. Research in the area of Big Data analysis, network analysis, database creation, computer-aided drug designing, protein modelling and comparative genomics are carried out at this facility.

About the Training Program

The training program aims to cover the fundamentals of molecular docking methods, scoring functions, and the conformational searching technique in this molecular docking training course. Furthermore, a full explanation of numerous protein-ligand interactions will be presented, which are required to determine binding energies. Protein-ligand complexes are used to explain docking sessions. Molecular Dynamics simulations (MD simulations) estimate time dependent behaviour of a macro molecular system. At present molecular docking and Molecular dynamics simulations methods are widely used to explore in drug discovery and to understand thermodynamics of biological macromolecules. Participants who complete this course will be familiar with molecular docking theory and molecular

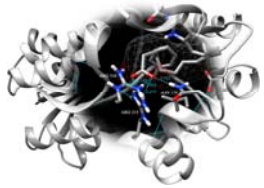
Target Participants

People working in the fields of bioinformatics, d discovery, biopharmaceuticals and Pharmaceuti industry or those who wish to have new venture biotechnology led entrepreneurship can particip Students, research scholars and young entreprene from start-ups are also allowed.

Brief Outline of Course Contents

- Introduction to Drug Discovery
- Protein database & Structure Modelling
- Molecular Docking
- Molecular Interaction Analysis
- Introduction of Molecular Dynamics simulation
- Molecular Dynamics Simulation
- Basics of Python and Python Data Types
- Basics of Linux Commands

The course will be delivered through few lectu demonstrations with examples, few hands-on trainings selected modules of the course such as Structure modelli molecular docking and molecular dynamics simulations.



How to Apply?

For registration please follow the Google link given here: https://forms.gle/ju36x2kK4idNr2Gw5

Or

Scan the QR code to register in CAMDS-2022.

A copy of the application form may be send through E-mail to **camdsnitrkl2022@gmail.com** for early confirmation. Please send the filled-in form to the coordinator on or before 13th June 2022 (09.00 AM).

The details of the training program and the form can also be downloaded from our website http://www.nitrkl.ac.in.

Registration and Course Fees

Dates and Venue

Date

13th – 19th June 2022.

Venue

Program will be conducted online through MS Team. Code will be shared with the registered participants only. Centre for Bioinformatics and Computational Biology, Department of Biotechnology & Medical Engineering, National Institute of Technology Rourkela, Odisha 769008.

Queries?

For any queries, please contact:

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Resource Persons

Dr. Mukesh K. Gupta
Dr. Pradeep Natarajan

Address of Correspondence

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E-mail: guptam@nitrkl.ac.in

Certification

Participants successfully completing the training program will be provided with E-certificate. A test will be conducted at the end of the program.

Prerequisites

The entire training will be online and shall have following prerequisites:

- Participants must have access to the laptop/desktop with stable internet connection.
- Participants must possess a Google account (xxxx@gmail.com).
- Pre-Installed MS team and make a login account, which is free.

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13th – 19th June 2022

REGISTRATION FORM

1	Name	:	
2	Designation	:	o Student o Research Scholar o Young entrepreneur o Others
3	Organization	:	
4	Address	:	
5	E-mail	:	
6	Telephone	:	
7	Mobile	:	

Date: Signature:

Note: ***Registration is mandatory*** (Participating link will sent ONLY to the registered candidates). Copies of th form can be used, if necessary. Please send the filled- form to the coordinator on or before 13th June 2022 (09.(AM). The details of the training program and the form c also be downloaded from our websi