

Center for AI in Medicine, Imaging & Forensics (CAIMIF)

is organising

Certified hands-on training on

# BIOINFORMATICS COMPUTATIONAL TOOLS FOR MOLECULAR DOCKING & VISUALIZATION

 27<sup>th</sup> & 28<sup>th</sup> Feb 2024

 1:30 PM - 04:30PM

 Center for AI in Medicine,  
Imaging & Forensics Block 2,  
1<sup>st</sup> Floor Room no- 103 B

Registration

Fee

UG Students- ₹ 500/-INR

PG/Ph.D Scholars- ₹ 800/-INR

Professionals- ₹ 1200/- INR

## Objectives of Event

- 1- Understanding Molecular Docking:** To comprehend the concept of molecular docking, its significance in drug discovery, and the various types of docking such as rigid and flexible.
- 2- Familiarity with Tools:** To become familiar with computational tools like PyRx and AutoDockVina that are used for molecular docking and visualization.
- 3- Hands-on Experience:** To gain practical experience by installing and using PyRx and AutoDockVina, thereby understanding their applications in real-world scenarios.
- 4- Problem-Solving Skills:** To develop the ability to troubleshoot common issues that may arise during the installation and usage of these computational tools.

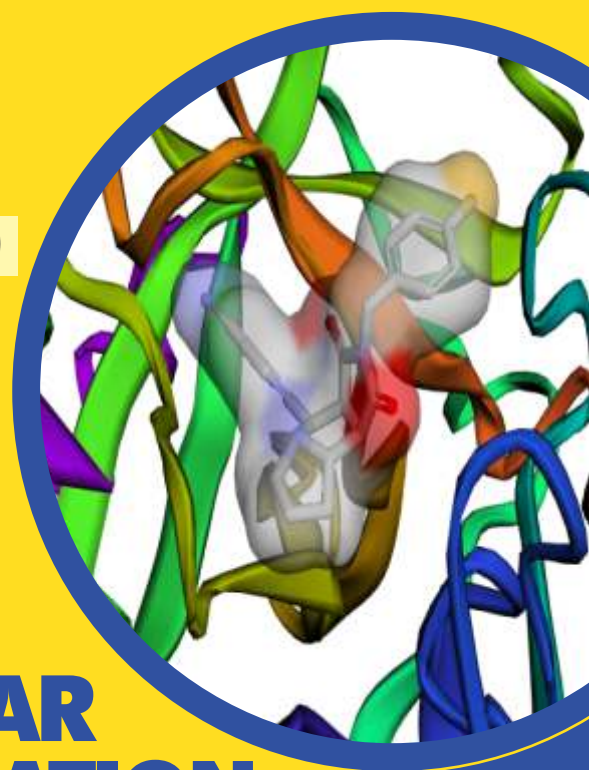
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Registration Link : <http://surl.li/qmcmg>

Whats app group link: <http://surl.li/qmcnv>



# Training Schedule

## Day 1 (27<sup>th</sup> Feb 2024)

### Session 1: Introduction to Molecular Docking and Types

- An overview of molecular docking, its importance in drug discovery, and the different types of docking (rigid, flexible, etc.).
- This session will also cover the principles behind these methods and their applications.

### Session 2: Hands-on Exercise - Installation of PyRx and AutoDock Vina

- A practical session where participants will install PyRx, a computational chemistry tool used for virtual screening, and AutoDock Vina.
- Hands-on session for installation process and troubleshooting common issues.

## Day 2 (28<sup>th</sup> Feb 2024)

### Session 3: Visualization Tools - Introduction to Chimera

- An introduction to Chimera, a visualization tool for molecular structures and related data.
- This session will cover the basic features of Chimera and how to use it for visualizing molecular docking results.

### Session 4: Hands-on Exercise - Chimera and PyMOL

- A hands-on session where participants will use Chimera and PyMOL for visualizing and analyzing molecular docking results.
- This session will provide practical experience in using these tools and interpreting the results.

Each lecture session is designed to last for approximately 1.5 hour, and the practical exercise for 4 hrs.

### Speaker

**Dr. Sunita Sharma**

Assistant Professor,  
Dept. of Biotechnology SSET

### Resource Person

**Ms. Shivani Singh**

**Harsh Pratap Singh**

### Patron

**Prof. (Dr.) Sibaram Khara**

Vice Chancellor,  
Sharda University

### Convener

**Prof. Ashok Kumar**

Head, CAIMIF & Professor  
Dept. of Physics, SSBSR

### Co-Convener

**Dr. Sunita Sharma**

Assistant Professor,  
Dept. of Biotechnology SSET

### Coordinator

**Ms. Bushra Khan**

Member CAIMIF &  
Asst. Professor Radiology, SSAHS

### Organizing Committee Members

**Prof. Ruqaiya Khanam | Ms. Shivani Singh**  
**Harsh Pratap Singh | Mr. Chanambam Mokaju Meitei**  
**Ms. Navita, Ms. Sanju | Mr. Rajat Mittal | Mr. Abhinav Singh**

**Sharda University**- Plot No. 32, 34 - Knowledge Park 3, Greater Noida-201310, Delhi- NCR, India.

