



College of Arts,  
Science &  
Commerce (Autonomous)

RISE WITH EDUCATION

NAAC REACCREDITED - 'A' GRADE

**Department of Biochemistry and Food technology and Nutraceuticals**

**A. Title of Workshop/Activity:** 'In-silico Approach to Drug Discovery- Molecular Docking'

**B. Background:** The purpose of this workshop is to orient the participants to structure-based *in-silico* drug discovery process.

**C. Aims/Objective:** The workshop aimed to

- i. Introduce chemical databases (cheminformatics) and their applications
- ii. Give Hands on experience of *in-silico* tools employed for studying physiochemical and pharmacokinetics properties of small molecules.

**D. Location:** Mini Auditorium & Computer laboratory, SIES College.

**E. Target audience/participants with expected numbers:** 31 Post-Graduates Students + 08 Research Scholar + 06 Faculty

**F. Date of Activity:** 24<sup>th</sup> Nov.2023 to 26<sup>th</sup> Nov.2023

**G. Name of Resource Person:**

Day 1 Dr Deepali Kotheekar; Day 2 Dr Sanket Bapat (MIT Pune)

**H. Outcome/Feedback:** Two-day workshop was good interactive session for both students and faculty. They learnt introduction to drug discovery and application of databases like Swiss ADME, PubChem, Swiss Target prediction. Participants learnt how to use softwares of docking and apply it in their research work. The participants realised the significance of *in-silico* work in absence of wet lab data.

**I. Annexures:**

i) Photographs (Geotagged)

ii) List of Participants

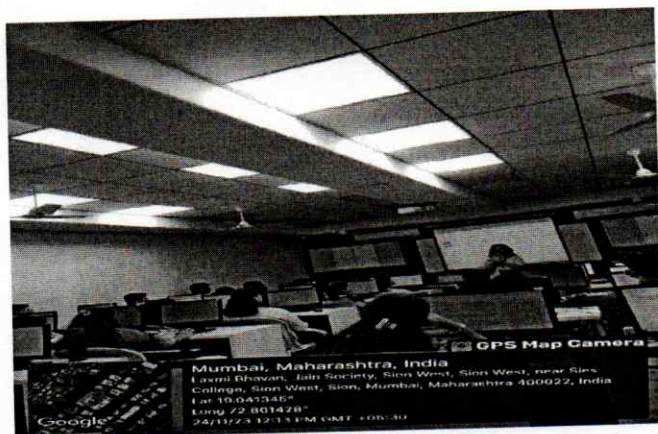
Report Prepared by: Rani A Shinde

  
Signature of HOD

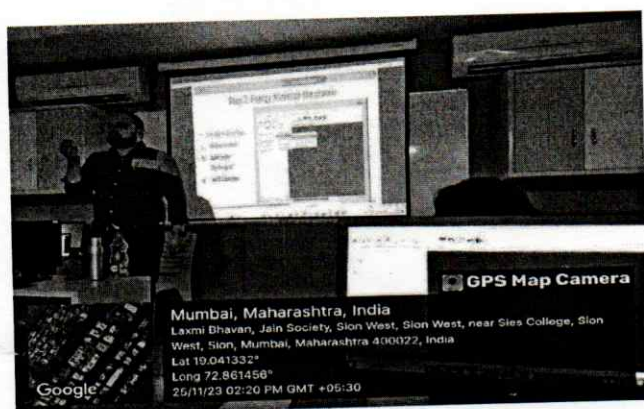
Department: Department of Biochemistry



## Photographs of Molecular Docking Workshop (Geotagged)



*In frame – Dr. Deepali Kothekar explaining about the PubChem.*



*In frame - Dr. Sanket Bapat explanation for hands on session on Introduction to Molecular Docking*



*In frame - Dr. Sanket Bapat & Dr. Deepali Kothekar with participants*

## List of Participants for Molecular Docking workshop

SIES College of Arts, Science & Commerce (Autonomous)  
Department of Biochemistry  
'In-silico approach to drug discovery- Molecular Docking Workshop'  
WORKSHOP ATTENDANCE

DAY 1: 24<sup>th</sup> November, 2023  
Module: Introduction to structure-based drug discovery  
Resource person: Dr Deepali Kothekar  
Session Timing: 9:00 am to 4:00 pm

### BATCH I

Sr. no	Name of the participant	Signature of the participant	
		Morning Session (9:00 am to 1:00 pm)	Afternoon Session (1:30 pm to 4:00 pm)
1	Swetha Sunder Kanagalla		
2	Thevar Bhavani Murugan		
3	Siddhi Sanjay Choudhari		
4	Mariya Antony		
5	Omkar Vijay Ghag		
6	Priji Rajkumar Yadav		
7	Rachana Ramesh Machha		
8	Sanjana Menon		
9	Alex Jose		
10	Faiak Afreen Badshah Mahmood Ansari		

11	Iqra Mansuri		
12	Yashashree Dattatray Bhisce		
13	Utkarsha Rakesh Mhatre		
14	Wagh Samruddhi Shamkant		
15	Chelsia D'souza		
16	Angel Yesurathnam Mhetre		
17	Jyotsna Boddu		
18	Vidhi Kiran Thakur		
19	Zehra Sudanwala		
20	Pratik Jadhav		
21	Lakshan Nadar		
22	Akshata Salvi		
23	Dr Wajed Khan		

24 Rani Shinde  
25 Niyati Nali

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### BATCH II

Sr. no	Name of the participant	Signature of the participant	
		Morning Session (9:00 am to 1:00 pm)	Afternoon Session (1:30 pm to 4:00 pm)
1	Sumaiya		
2	Niditha Harish Shetty		
3	Arthi Manohar		
4	Ritika Kantaram Kavar		
5	Ms. Mamta Vishwanath Bhusara		
6	Saili Suresh Chavan		
7	Vaishnavi Ghurahoo Ram		
8	Sana Sajjad Jalili		
9	Aditi Vijay Kud.		
10	Vrushali Anant Rane		

11	Bhunia Suraj Rajkumar		
12	Ridha Rehan Ghawte		
13	Romil C. Dagha		
14	Rohit Shashikant Patil		
15	Dwijalee Rajendra Deo		
16	Dr. Talib Yusuf Abbas Hussain		
17	Pallavi Uttam Rai		
18	Yash Krishnan		

19. Kavika Ganpurnam  
20. Suvreena Pellyay