

# ONE WEEK SUMMER SCHOOL 2025

## From *In Silico* to *In Vitro* – Empowering Anticancer Drug Discovery with Computational and Experimental Synergy (Hands-on workshop)

1<sup>st</sup> to 5<sup>th</sup> July 2025

Organized by  
Department of Pharmaceutical Chemistry

### Techniques covered

#### Critical Concepts & Hands-on-Training:

- AI/ML Methods
- Molecular Docking
- Molecular Dynamic Simulations
- ADME Screening
- Network Pharmacology
- *In-Vitro* Cell line studies

### Objectives

#### One week intensive summer school is aimed at meeting the objectives of

- Making the attendees able to understand the concept of *in silico* drug design for cancer therapy
- Getting trained on handling the applications of various computational techniques
- Demonstrate cell line models and techniques for evaluation of NCEs/Phytochemicals/Formulations for anticancer properties.

### Eligibility

#### Any passionate learner is eligible to participate, preferably

- Faculty, Industry Personal
- Post-Doctoral Fellows
- Ph.D. Research Scholars
- M. Pharm. Students

### Committee

#### Convener

Dr. Jagannath Sahoo, Dean, SPPSPTM

#### Workshop Coordinators

Dr. RajaSekhar Reddy Alavala

Dr. Mahesh Palkar

Department of Pharmaceutical Chemistry,  
SPPSPTM



### Registration

#### Online Registration Process

- Registration Fee:  
Faculty students - Rs. 2000/-  
Students (NMIMS) - Rs. 1500/-
- Working lunch included on all the days
- Fill the below registration form  
<https://forms.gle/hyQ5ZccPh7UjN2ka9>  
Limited to 45 seats (On a first come, first serve basis)
- Last Date to Register: 20<sup>th</sup> June 2025

**Venue:** SPPSPTM, SVKM's NMIMS Deemed to be University, V.L. Mehta Road, Vile Parle (W), Mumbai-400056

For any queries, please contact: Workshop Coordinators  
alavala.rajasekharreddy@nmims.edu (or) mahesh.palkar@nmims.edu  
Contact: 98852 71223 (or) 94483 16466

## Day-1

Time	Topic
10:00 – 10:30	Inauguration & Welcome Address
10:30 – 11:30	Overview of Anticancer Drug Discovery: Challenges & Opportunities
11:30 – 11:45	Tea Break
11:45 – 01:00	Introduction to In Silico Drug Design: Concepts & Applications
01:00 – 02:00	Lunch Break
02:00 – 04:30	Hands-on: Molecular Docking & Visualization

## Day-2

Time	Topic
10:00 – 11:30	Molecular Dynamics Simulations in Cancer Drug Design
11:30 – 11:45	Tea Break
11:45 – 01:00	QSAR and 3D-QSAR Techniques
01:00 – 02:00	Lunch Break
02:00 – 04:30	Hands-on: QSAR Model Building

## Day-3

Time	Topic
10:00 – 11:30	Network Pharmacology in Cancer
11:30 – 11:45	Tea Break
11:45 – 01:00	Target Prediction Tools & Pathway Analysis
01:00 – 02:00	Lunch Break
02:00 – 04:30	Hands-on: Protein-Drug Network model building (String & Cytoscape)

## Day-4

Time	Topic
10:00 – 11:30	Cell Line Models in Anticancer Research
11:30 – 11:45	Tea Break
11:45 – 01:00	Cytotoxicity Assays and Apoptosis Studies
01:00 – 02:00	Lunch Break
02:00 – 04:30	Hands-on/Virtual Demo: In Vitro Assays and Data Analysis

## Day-5

Time	Topic
10:00 – 11:30	Role of AI/ML in Drug Discovery: Current Trends
11:30 – 11:45	Tea Break
11:45 – 01:00	Introduction to ML Algorithms for Drug Prediction (SVM, RF, ANN)
01:00 – 02:00	Lunch Break
02:00 – 03:30	Hands-on: AI Model Building using Python (scikit-learn, TensorFlow)
03:30 – 04:30	Valedictory Session, Certificate Distribution & Feedback

### Registration

Name of the A/C Holder:	SVKM'S NMIMS
Bank Name:	Kotak Mahindra Bank
	JUHU - Vile Parle West
NEFT IFSC Code:	KKBK0000661
Account No:	2311578254
Type of Account:	Current
MICR Code:	400485022
SWIFT Code:	KKBKINBB

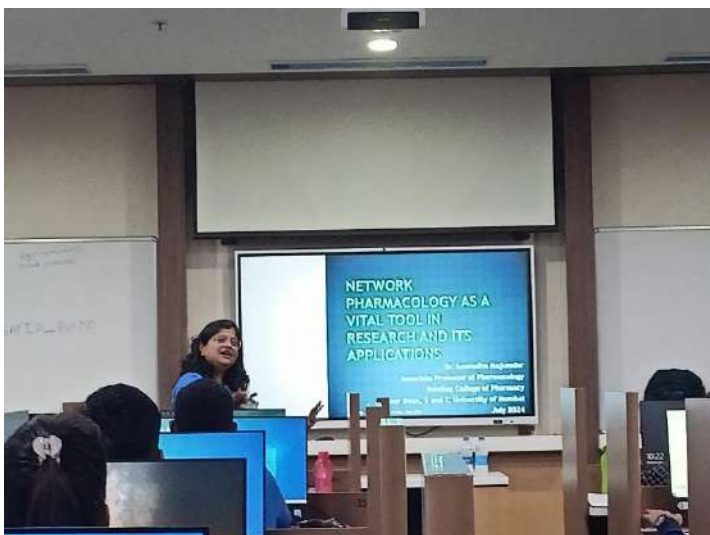
### Tools

#### Molecular Modelling:

- Docking – Autodock, PyRx, Biovia
- Pharmacophore – Biovia, Pharmmapper
- Network model – Cytoscape, STRING
- Visualizer – Biovia, Chimera
- FACS Data Analysis
- Python

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## Glimpses from Summer School 2024



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