

SUMMER SCHOOL 2026

Digital Chemistry in Action: Computational Tools for Organic, Medicinal, and Analytical Research

6th July to 10th July 2026

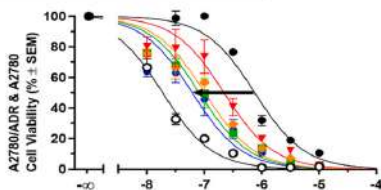
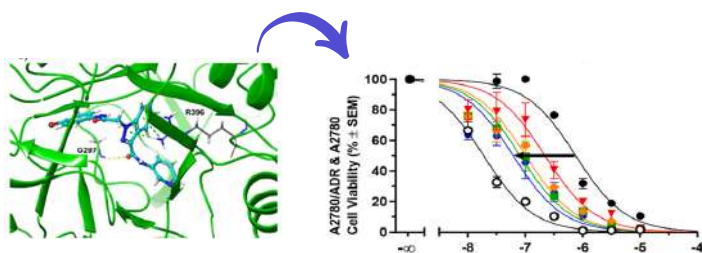
Organised by

Department of Pharmaceutical Chemistry

Topics covered

Critical Concepts & Hands-on-Training:

- Tools for drawing and property calculations
- Molecular Docking
- Molecular Dynamic Simulations
- ADME Screening
- Tools for NMR and Mass analysis
- Tools for PK/PD and QBD analysis



Organizers

Convener Dr. Jagannath Sahoo, Dean, SPPSPTM

Faculty Coordinator Dr. Kapil Juvale, Dr. Mahesh Palkar

Student co-ordinators

Amit Shimpi (9607774424)

Utkarsh Bhamare (9673206007)

Outcomes

Practical skills development in computational tools to:

- Perform molecular docking and MD simulations
- Analyze and interpret NMR and Mass spectral data
- Apply QBD approach for designing experiments
- Analyze the biological data
- Predict PK/PD parameters

Key learnings

- Molecular Structure drawing and property calculations: Biovia draw, ACD labs ChemSketch, DataWarrior
- Molecular Docking – Molegro, Biovia discovery studio, Autodock, Chimera
- Molecular Dynamics – Gromacs
- NMR and Spectra analysis – Mestrenova, SpinWorks
- QbD– Stat-Ease Design-Expert
- Biological data analysis – GraphPadPrism
- PK/PD – GastroPlus, PKSolver

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

For any queries, please contact:

kapil.juvale@nmims.edu, mahesh.palkar@nmims.edu

Day
01

• **Inauguration**

Introduction to basic tools- from drawing to property calculations

- Medicinal chemistry driven biological data analysis using Graphpad Prism
- Introduction to structure drawing tools – Drawing structures, biologics, reactions, naming, and properties calculations, edit stereochemistry, generate SDF files
- Sketching chemical structures and mechanisms using tools and templates available in software
- DataWarrior- scaffold analysis, library management

Day
02

Applications of computational tools in Medicinal Chemistry

- Introduction to molecular docking and molecular dynamics
- Protein and ligand preparation and binding site identification for molecular docking
- Hands-on training: Molecular docking and result analysis (Different tools paid vs free)

Day
03

Applications of computational tools in Medicinal Chemistry

- Molecular dynamics using Gromacs- system setup
- Molecular dynamics- trajectory analysis, RMSD, RMSF, SASA and H-bond analysis

Day
04

Applications of computational tools in Analytical Chemistry

- Fundamental of NMR and interpretation of NMR spectra
- Hands-on training: NMR spectra processing software (Paid and Free tools)
- Fundamentals of Mass spectra and analysis of mass spectrum

Day
05

Applications of computational tools for biological data analysis and PK/PD studies

- GastroPlus/PK-Solver Overview
- Design-Expert QbD overview and applications
- Applications of QbD in Chemistry
- Valedictory

Eligibility

- B.Pharm, M.Pharm Students
- PhD Research Scholars
- Faculty, Industry Professionals

Registration

Registration Fee:

Faculty / Students -Rs. 2000/-
Students (NMIMS) -Rs. 1500/-

Link for Registration:

<https://forms.gle/TPC6QkuKiPCo9oYM8>

Limited 30 seats (On a first come, first serve basis)

Last Date to Register: 20th June 2026



Scan for registration and
payment

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