

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

Vision

Faculty of Pharmacy aspires to create skilled and competent pharmacy professionals by imparting quality education in pharmaceutical sciences to meet the global health challenges for the betterment of mankind

Mission

Faculty aims to impart quality education to develop pharmacy professionals to lead the progress in global healthcare, to evolve into center of excellence in pharmaceutical research, to create entrepreneurs and problem solvers in multi-disciplinary arena and to inculcate professional ethics and passion for lifelong learning

2 Days Hands-On Workshop

Introduction and Structure Based Designing Tools

by  **Molsoft**



Resource Person

Dr. Shamshair Singh Sardar

Senior Application Scientist,
Advent Informatics, Pune

Learn • Explore • Apply

Build your skills in
structure-based drug design
with industry expert guidance



Who can attend?

Pharmacy, Life Sciences & Allied Health Sciences

- PG Students
- Research Scholars
- Faculty Members



Date

14-10-2026 &
15-10-2026



Venue

Council Hall,
FPH



Time

09:00 AM -
05:00 PM

Convener

Dr. Judy Jays
Professor and Head

Co-ordinators

Dr. Vijaybhanu P
Assistant Professor

Dr. Liklesha B M
Assistant Professor

Registration fee Rs. 600/- (including GST)

Limited Seats
Register Now



Registration Link

https://ruasportal.msruas.ac.in/asd_EventPublicUserMaster.htm?eventID=218



Scan for Registration



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About the Workshop

Introduction and Structure-Based Designing Tools by Molsoft is a two-day hands-on workshop designed to provide practical exposure to modern computer-aided drug design using the ICM platform. Participants will explore molecular visualization, small-molecule and virtual library screening, molecular dynamics simulations, covalent and induced-fit docking, peptide and protein-protein docking, along with ligand optimization using the ICM 3D Ligand Editor and ADMET assessment. The workshop also introduces PROTAC modelling, Rapid Isostere Discovery Engine (RIDE), and 2D/3D QSAR and structure-activity relationship analysis. Through guided demonstrations and hands-on sessions, participants will gain an integrated understanding of structure-based drug design, hit optimization, binding analysis, and computational lead development

Ramaiah University of Applied Sciences

Ramaiah University of Applied Sciences (RUAS) is a state private university, under the aegis of Gokula Education Foundation. The innovative university focuses on academics, research, consultancy, training and leadership development. RUAS offers outcome-based education in health and allied sciences, engineering, and humanities. RUAS is oriented towards student-centric education and services with applied research whilst maintaining the highest academic and ethical standards in a creative and innovative environment. RUAS inspires critical thinking, personal development, and a passion for lifelong learning. RUAS is accredited with A+ Grade by NAAC.

Faculty of Pharmacy

Faculty of Pharmacy (FPH), formerly M.S. Ramaiah College of Pharmacy, was established in 1992. Faculty of Pharmacy, ranked 56 in the AIR- NIRF 2025, is a leading Pharmacy college with a legacy of 33 years. It imparts outcome-based pharmaceutical education to meet the growing demands of well-trained healthcare professionals globally. The faculty offers B.Pharm (NBA-Accredited), Pharm.D, M.Pharm in Pharmaceutical Chemistry, Pharmaceutics, Pharmacology, Pharmacognosy, Pharmacy Practice, Regulatory Affairs, and Ph.D programme.

Department of Pharmaceutical Chemistry

Department of Pharmaceutical Chemistry was originally established as a part of M S Ramaiah College of Pharmacy. PG program in Pharmaceutical Chemistry was started in the year 2008. The department was integrated into Faculty of Pharmacy in 2014. The department provides outcome-based education and training skills on various aspects of drug design using bioinformatics and computational tools, synthesis by conventional and green chemistry approaches, spectral characterization, and pharmacological evaluation of small molecules. Moreover, students get practical training in handling various advanced instruments including Microwave synthesizer, ATR-IR, Flame photometer, HPLC, HPTLC and utilising GPU powered Computational Lab.

Workshop-Schedule

DAY 1 (14.10.2026)		DAY 2 (15.10.2026)	
Sessions	Time	Sessions	Time
Registration	9:00 AM - 9:30 AM	Learn about optimal docking areas and Protein-Protein docking with ICM	9:00 AM - 9:45 AM
Inauguration	9:30 AM - 10:00 AM	Learn how to optimise a Ligand in its binding site with ICM 3D ligand editor and ADMET	9:45 AM - 11:00 AM
Science Behind Molsoft Technologies, Briefing about various Modules, Molecular graphics, Movies, Knowing the interface and visuals	10:00 AM - 11:00 AM		
Tea Break			11:00 AM - 11:15 AM
Small molecule docking + some addons with ICM, Virtual library screening with ICM batch docking	11:15 AM - 12:15 PM	Introduction and demonstration of ICM Protac model builder	11:15 AM-12:15 PM
Molecular dynamic simulation using ICM (open mm), Analysis of MD simulation results along with additional stack calculations	12:15 PM - 1:00 PM	ADMET and Introduction and demo on Rapid IsoSter Discovery Engine (RIDE) by ICM	12:15 PM - 1:00 PM
Lunch Break			1:00 PM - 2:00 PM
Covalent Docking & Induced Fit Docking (IFD)	2:00 PM - 4:00 PM	Learn 2D and 3D Quantitative Structural Activity Relationship (QSAR) using ICM & Learn about different types of Structural activity relationships with ICM	2:00 PM - 4:00 PM
Tea Break			4:00 PM- 4:15 PM
Peptide Docking	4:15 PM - 5:00 PM	Q&A	4:15 PM - 4:30 PM
		Valedictory	4:30 PM - 5:00 PM