INTEGRAL UNIVERSITY

LUCKNOW - INDIA

COLLEGE OF PHARMACY & DEPARTMENT OF PHARMACY

jointly offer

Under the Aegis of
FACULTY OF PHARMACY

Value Added Course on

COMPUTER-AIDED DRUG DESIGN AND APPLIED MEDICINAL CHEMISTRY:

FROM LEAD TO DRUG CANDIDATE

(PHV-O10, Online mode)

03 August 2026 – 18 September 2026

ABOUT THE COURSE

This course introduces the fundamentals of Computer-Aided Drug Design (CADD) and its application in modern drug discovery. Students will learn chemical structure drawing, data retrieval from online databases, and molecular docking to analyze drug-target interactions using tools such as ChemDraw, Avogadro, Chem3D, ChimeraX, SwissADME, AutoDock Vina, Discovery Studio, PyMOL and SwissDock.

The course also covers key medicinal chemistry concepts, including Structure-Activity Relationship (SAR), drug-likeness, and lead optimization. By the end of the course, participants will be able to apply computational tools alongside medicinal chemistry principles to design and optimize potential drug candidates.

COURSE MODULES (30 HOURS)

MODULE 1	Chemical Drawing & Molecular Modeling	6 HOURS
MODULE 2	Chemical & Protein Databases	6 HOURS
MODULE 3	Molecular Docking	6 HOURS
MODULE 4	ADME & Drug-Likeness Prediction	6 HOURS
MODULE 5	Applied Medicinal Chemistry (Lead Optimization)	6 HOURS

★ Total Duration: 30 Hours (5 Modules x 6 Hours Each)

COURSE HIGHLIGHTS

- Complete Drug Discovery Pipeline from Lead to Optimized Candidate
- Hands-on Training with Industry-Relevant CADD Tools
- Integrates Computational Methods with Medicinal Chemistry (SAR & ADME)
- Uses Free Tools Enabling Cost-Effective, Publishable Research
- Builds Industry-Ready Skills in Docking & Drug-Likeness Prediction
- Enhances Research Capability for High-Impact Publications
- Blended Learning Approach for Practical & Flexible Skill Development

COURSE DETAILS

Course Platform: Integral Learning Initiative – Learning Management System (LMS)

Delivery Mode: Online (Google Meet)

Course Duration: 30 Hours (6 Hours per week)

Lecture Timings: 6:00 PM – 8:00 PM (Monday, Wednesday & Friday)

Who Can Attend: Faculty Members, Technical Staff, Research Scholars and Students from domains like Pharmacy, Chemistry, Biosciences, Bioengineering, Medical Sciences, etc.

Course Completion: E-certificates to be provided to participants after successful completion of the course.

Course Fees: NA

REGISTER NOW!

Last Date for Registration

02 August 2026

SCAN TO REGISTER

Registration Link:
https://docs.google.com/forms/d/e/1FAIpQLSde3NSqf7Ut1fwyi0rut0g1DQ_LrB1-oJA80e-8EYvoNaKHQ/viewform

ASSESSMENT & CERTIFICATION

- Module Quizzes
- Practical Assignment
- Scientific Report
- Presentation

E-Certificate will be awarded to participants who meet the attendance and evaluation requirements.

COURSE OBJECTIVES

- Provide a fundamental understanding of CADD in modern drug discovery.
- Develop practical skills in molecular modeling, chemical data retrieval, and computational analysis.
- Enable students to apply molecular docking techniques for studying drug-target interactions.
- Understand key medicinal chemistry concepts such as Structure-Activity Relationship (SAR), drug-likeness, and ADME properties.
- Focus on lead identification and optimization using integrated computational and medicinal chemistry approaches.
- Prepare students for research and industry-oriented applications.

LEARNING OUTCOMES

- Understand the role of CADD in modern drug discovery.
- Perform chemical structure drawing and molecular modelling.
- Retrieve and manage data from chemical and protein databases.
- Conduct molecular docking and analyze drug-target interactions.
- Evaluate drug-likeness and ADME properties.
- Apply SAR principles for lead optimization.
- Develop practical skills for research and industry applications.
- Covers complete drug design pipeline from lead to optimized candidate.

SOFTWARE & TOOLS COVERED

ChemDraw	Chem3D	Avogadro	ChimeraX
OpenBabel	PubChem	RCSB PDB	ZINC Database
ChEMBL	SwissDock	AutoDock Vina	Discovery Studio
PyMOL	SwissADME	pkCSM	

COURSE COORDINATOR

Dr. Samar Mujeeb
Associate Professor
College of Pharmacy
Integral University, Lucknow
smujeeb@iul.ac.in
+91 8958351653

"Design Drugs. Explore Biology. Build Your Research Career.