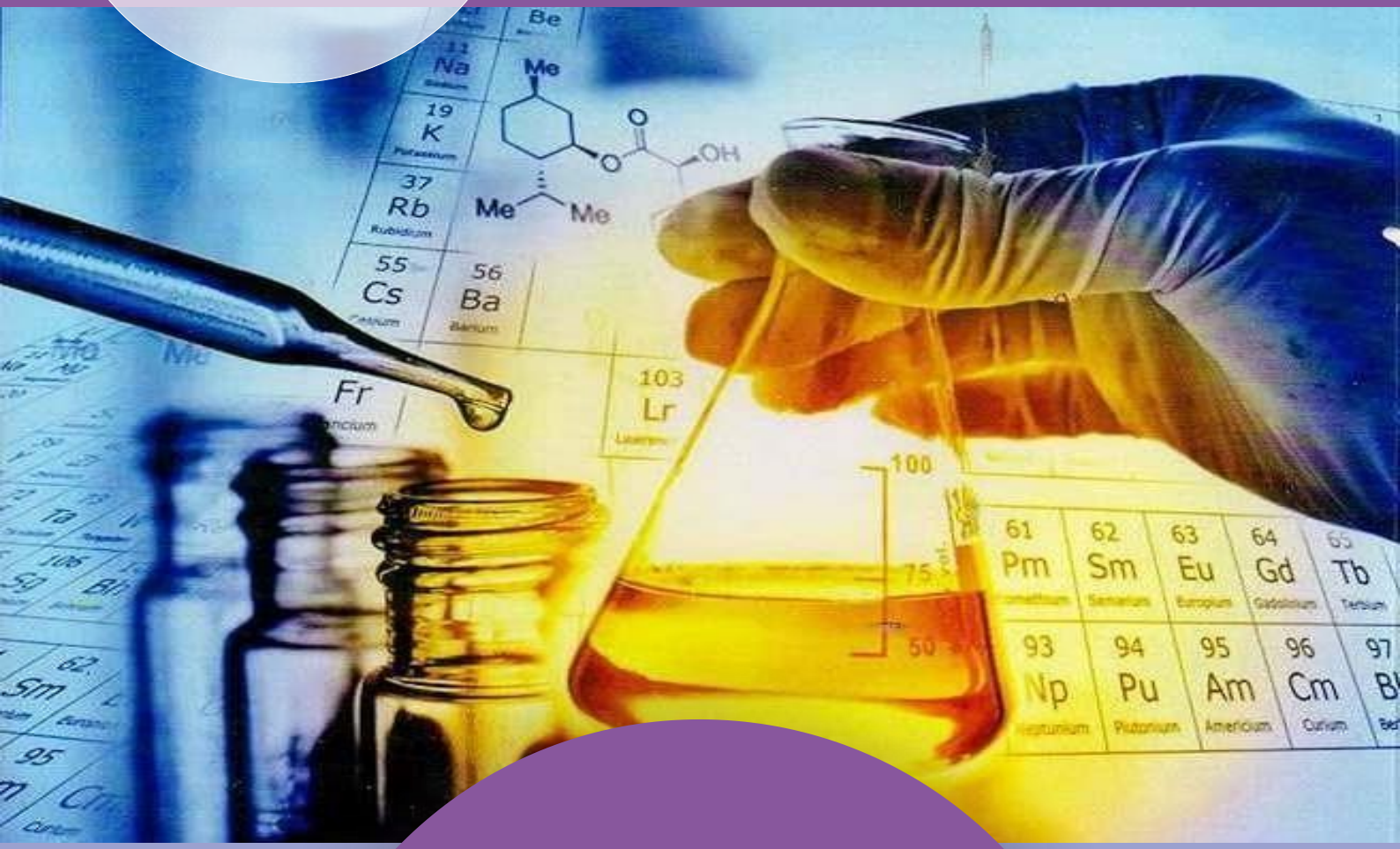
SHARDA UNIVERSITY
Beyond Boundaries

NAAC A+ ACCREDITED

# SHARDA SCHOOL OF ENGINEERING & SCIENCE

Department of Chemistry and Biochemistry




## COURSE

# Molecular Docking (NV33114)

## VALUE ADDED COURSE BROCHURE 2025-26

## SHARDA UNIVERSITY

Sharda University envisions to serve the society by being a global University of higher learning in pursuit of academic excellence, innovation and nurturing entrepreneurship. It has 13,000+ students from 95+ countries, 29 states, and Union Territories, providing cultural diversity and global exposure to students. It has 26000+ alumni who are today leaders in their realms. Sharda University is NAAC A+ University with Overall NIRF Rank of 87. Teaching Learning Center at Sharda University is to equip the faculty members with the expertise, skills and knowledge they need for capacity building of students. Teaching as a profession requires highly specialized skills and knowledge to impact significantly on student learning and therefore teachers must refine their conceptual and pedagogical skills.

## ABOUT THE SCHOOL

Sharda School of Engineering and Science (SSES) boasts of providing an interdisciplinary approach, exposure to different disciplines in science including Chemistry, Bio-Chemistry, Physics, Mathematics, and Environmental Sciences. The Sharda School of Engineering and Science is unique from other institutions of higher learning as it is committed to imparting knowledge in pure and applied sciences, which not only forms the foundation for further academic pursuits in science and technology but also acts as the foundation for students to pursue a career in multi facet directions. The academic programs are designed to meet the requirement of the latest technological developments and envisages to become a state-of-the-art department that cater the students at Graduate, Post- Graduate and Research level along with providing high-quality education and cutting-edge interdisciplinary research in sciences. SSES has well-equipped laboratories for Physics, MATLAB, Biochemistry, Physical, Organic and Inorganic chemistry for Graduate and Post-Graduate Programs. In addition, there are Central Instrumentation Facility (CIF) and other advance research labs to promote research culture.

## DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

The Department of Chemistry & Biochemistry endeavors to be nationally recognized model for nurturing students who can contribute to the ever changing technology of 21st century. The Department is committed to provide an excellent teaching & learning atmosphere for Undergraduate as well as post graduate students.

## RESOURCE PERSON

**Dr. Preeti Jain**

Dr.Preeti Jain has obtained her Ph.D in Coordination Chemistry from Gautam Buddha University and M.Tech in Chemical Analysis from IIT Delhi. She has also qualified CSIR-UGC JRF and GATE examinations. Her research interest involves the “Development of novel Chemotherapeutics and their theoretical and experimental investigations” and she is involved in publishing the research paper in the journal of international repute.

# MODULE

| | |
|---|---|
| **School: SSES** | **Batch : 2025-29** |
| **Program: M.Sc. (PG)** | **Current Academic Year: 2025-26** |
| **Branch: Chemistry/Biochemistry** | **Term : Even (2502), Semester : II** |

| | | |
|---|---|---|
| 1. Course Code | **NV33114** | |
| 2. Course Title | **Molecular Docking** | |
| 3. Credits | | |
| 4. LTPC | **(30 Hours)** | |
| Course Type | **Value added course** | |
| 5. Course Objective | Students will gain knowledge and skills on the various important software tools used in chemistry. They will learn how to plot a graph in Microsoft Excel, origin, draw, and visualize the chemical structure in ChemDraw, origin, CCDC, etc. Students will also develop presentation skills in this course.<br>Students will know of:<br>• Drawing the structures<br>• Performing molecular docking<br>• Students will also develop result visualization skills in this course. | |
| 6. Course Outcomes | CO1: The student will be able to understand the basis of molecular docking<br>CO2: The student will be able to Install useful software<br>CO3: The student will be able to Draw structures in chem sketch<br>CO4: The student will be able to do Ligand and Protein preparation<br>CO5: The student will be able to do docking and Visualization<br>CO6: The student will be able to gain knowledge of the important software used in chemistry | |
| 7. Course Description | This course introduces the most frequent and important software and tools in chemistry for making and analyzing the structure and basics of molecular docking | |
| 8. Outline syllabus | | CO Mapping |
| **Unit 1** | **Overview of drug discovery & molecular docking** | |
| A | Literature study and acquisition of disease target structure | CO1/CO6 |
| B,C | Lead molecule identification and optimization. | CO1/CO6 |
| **Unit 2** | **Installation of software** | |
| A | Understanding of Molecular docking tools and software | CO2/CO6 |
| B | Installation of Software Discovery Studio MGL Tool-AutoDock, Cygwin & PYMOL, PyRx | CO2/CO6 |
| C | Useful web servers for molecular docking | CO2/CO6 |
| **Unit 3** | **Drawing structures** | |
| A | Introduction of ChemDraw, chemical name to structure conversion, chemical structure to name conversion | CO3/CO6 |
| B | Introduction to ChemSketch, creating and modifying images of chemical structures, | CO3/CO6 |
| C | writing and performing chemical equations and diagrams. | CO3/CO6 |
| **Unit 4** | **Ligand and Protein preparation** | |
| A | Protein (disease target) structure validation and Preparation using SPDVB | CO4/CO6 |
| B | Active site Prediction | CO4/CO6 |
| C | Ligand optimization and docking parameters Preparation of PDBQT, DPF and GPF files | CO4/CO6 |
| **Unit 5** | **Docking and Visualization** | |
| A | Running docking commands, Building protein-ligand complex | CO5/CO6 |
| B | Visualization of protein-ligand interactions | CO5/CO6 |
| C | Pose Selection (publication standard),Result analysis and interpretation | CO5/CO6 |
| **Mode of examination** | Assignments, Quizzes & Viva | |