DEPARTMENT OF BIOINFORMATICS
SCHOOL OF BIOENGINEERING
SRM UNIVERSITY
LECTURE PLAN

Subject code: BI0625 Credits: 3
Subject: Molecular Dynamics Semester: III
Staff: Dr. S.K.M. Habeeb.

Hour	Contents	Learning Outcome
1 2 3 4	**Unit 1:** Introduction to Molecular Dynamics, Statistical Mechanics for Molecular Dynamics Energy Minimization, First order derivative methods, second order derivative methods, Steepest descent, and Conjugate Gradient method.	• .Basics of molecular dynamics • Importance and methods of energy minimization.
5 6 7 8	**Unit II:** Equations of motions, Finite difference methods Predictor corrector method, Constant energy MD simulation. Constant temperature and pressure dynamics simulations.	• Integration of Newton's law of motion • Exposure to performing simulation at different ensembles.
9 10	**Unit III:** Brownian Dynamics MD simulations, Introduction to molecular dynamics packages. GROMACS, AMBER, CHARMM & DESMOND.	• Exposure to various molecular dynamics packages
11 12	**Unit IV:** Energy calculations for complex interactions potentials. Energy Minimization for complex interaction potentials.	• Thermodynamics properties from MDS. • Binding Energy.
13 14 15	**Unit V:** Molecular Dynamics simulation of macromolecules. Free energy calculations & Analyzing molecular dynamics trajectories.	• Macromolecular dynamics & trajectories.

REFERENCES

1. Andrew R. Leach, *Molecular Modeling- Principles and applications*, Prentice hall, IIedition, 1996.

2. Alan Hinchliffe, *Modelling Molecular Structures*, John Wiley, 2000.

3. Charles R. Cantor, Paul ReinhardSchimmel, *Biophysical Chemistry: The Behavior ofBiological Macromolecules PART III*, W. H. Freeman, 1980.

Signature of the Subject in charge **Signature of the HOD**