16BI350 MOLECULAR MODELING

UNIT - I

INTRODUCTION TO MOLECULAR MODELLING: Introduction Useful Concepts in Molecular Modelling,Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. computer; Hardware and Software.

UNIT- II

FORCE FIELDS: Force Fields. Bond Stretching. Angle Bending. Introduction to Nonbonded Interactions. Electrostatic Interactions. Van der Waals Interactions. Hydrogen Bonding i_n Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

UNIT - III

ENERGY MINIMISATION AND COMPUTER SIMULATION : Energy Minimization and Related Methods for Exploring the Energy Surface. Non Derivative method, 1st and 2nd order minimization methods. Computer Simulation Methods. Simple Thermodynamic Properties and Phase Space. Boundaries. Analyzing the Results of a Simulation and Estimating Errors. GROMACS.

UNIT - IV

Molecular Dynamics & Monte Carlo Simulation : Molecular Dynamics Simulation Methods.

Molecular Dynamics Using Simple Models. Molecular Dynamics with Continuous Potentials.

Molecular Dynamics at Constant Temperature and Pressure. Metropolis Method. Monte Carlo Simulation of Molecules.

UNIT- V

STRUCTURE PREDICTION AND DRUG DESIGN: Protein Structure Prediction Introduction to Comparative Modeling. Constructing and Evaluating a Comparative Model. Molecular Docking (AUTODOCK). Drug design: Structure based, De NOVO ligand design