5th Semester	RBT5D001	Molecular Modelling and Drug Designing	L-T-P 3-0-0	3 Credits

MODULE I   (**6 HOURS**)

Introduction to Molecular Modelling and its applications Biomolecular modeling problems:, protein folding, protein misfolding, nucleic acid/ protein interactions, and RNA folding, Basic concepts of quantum mechanics, ab initio, semi-empirical and density functional theory, calculations, molecular size versus accuracy.

MODULE II   (**8 HOURS**)

Molecular orbital theories. Molecular, mechanisms, energy calculations, Bond stretch, Angle bending, torsional terms, Electrostatic interaction- Van der waals interactions. Miscellaneous interactions,

MODULE III   (**10 HOURS**)

Introductionto molecular dynamics and simulations; Molecular Dynamics using simple models; Dynamics with continuous potentials, Constant temperature and constant dynamics; Conformation searching and systematic search; Monte-carlo simulation of biomolecules and bio-polymers.

MODULE IV   (**6 HOURS**)

Comparative modeling of protein: by homology- the alignment, construction of frame work, selecting variable regions, side chain placement and refinement, validation of protein models –Ramchandran plot, threading and ab initio modeling.

MODULE V   (**10 HOURS**)

Analog based drug designing : Introduction to QSAR. lead module, linear and nonlinear modeled equations, biological activities, physicochemical parameter and molecular descriptors, molecular modelling in drug discovery. Structure based drug designing: 3D pharmacophores, molecular docking, De novo Ligand, design, Free energies and solvation, electrostatic and non-electrostatic contribution to free energies. 3D data base searching and virtual screening, Sources of data, molecular similarity, and disimilarity searching, combinatorial libraries – generation and utility.

Books:

[1]   Molecular modelling and drug designing: Solomon K. Anand

Digital Learning Resources:

Course Name:	**Molecular Modelling and Drug Designing**
Course Link:	https://nptel.ac.in/courses/102/106/102106070/
Course Instructor:	PROF. MUKESH DOBLE Department of Biotechnology & Bioengineering IIT Madras