IV Year B.Tech. Biotechnology   VIII - Semester

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(BT434) MOLECULAR MODELLING & DRUG DESIGN

Objectives of the Course :
The main goal of this course is to gain some knowledge on modern approaches used in molecular modeling. powerful computer-based technology used to identify and design molecules for new medications greatly shortening the discovery phase of drug development by powerful computer-based technology.

UNIT - I : Quantum mechanics & concepts in molecular modeling :
Introduction – coordinate systems – potential energy surfaces   – introduction to quantum mechanics – postulates – Schrodinger wave equation – hydrogen molecule – Born-Oppenheimer approximation, introduction to computer hardware and software.

Unit II: Molecular mechanics and energy minimization:
Empirical force field models – Bond stretching – angle bending – torsional term – nonbonding interactions – thermodynamics properties using a forcefield – derived and non derived energy minimization method – simplex – sequential univariate method – steepest descent method – conjugate gradient method- Newton-Rapson method.

Unit III: Molecular Dynamics and Monte Carlo simulation :)
Introduction – Using single Model – time steps – Multiple steps – Setting up MD – energy conservation in MD Simulation Examples – Monte Carlo – Random number generation – Difference in MD & MC.

Unit IV: Homology modeling:
Comparative modeling of proteins – comparison of 3D structure – Homology – steps in homology modeling – tools – databases – side chain modeling – loop modeling.

Unit-V: Drug design:
General approach to discovery of new drugs - lead discovery – lead modification – physiochemical principles of drug action – drug stereo chemistry –drug action - 3D database search – computer aided drug design – docking - molecular modeling in drug design – structure based drug design – pharmacophores - QSAR.

TEXT BOOKS:

1.   A. R.Leach - Molecular Modeling Principles and Application, 2nd edition, Longman Publications, 1996.
2.   D. Baxivanis and Foulette - Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, Wiely Indian Edition, 2001.

REFERENCE BOOK:

1.   T K Attwood, D J parry-Smith, Introduction to Bioinformatics, Pearson Education, 1st Edition, 11th Reprint 2005.