Subject Code : P8BIE2A

MOLECULAR MODELLING AND DRUG DESIGN

UNIT - I

Basic concepts of molecular structure (bond length, bond angle, torsion angle and non-covalent interactions – Molecular structure and internal energy - Energy minimization of small molecules – Empirical representation of molecular energies – Use of force fields and the molecular mechanics method –Discussion of global energy minimum – Molecular representation in graphics.

UNIT - II

Basic principles of molecular dynamics and Monte Carlo Simulation for conformational analysis - ab initio – Density-Functional Theory and semiemperical methods**.**

UNIT - III

Macromolecular modeling – Identification and mapping of active sites - Design of ligands for known macromolocular target sites. Drug-receptor interactions. Classical SAR/QSAR studies and their Implications to the 3-D modeler. 2-D and 3-D database searching –pharmocophore identification and novel drug design.

UNIT – IV

Cancer and related diseases – mechanism and action of available anti-cancer drugs - New targets for anti-cancer drugs - Drugs that rescue mutant p53's and tubulin.

UNIT – V

Enzyme background – Theories of enzyme inhibition - Enzyme inhibition as a tool for drug development – Structured-based drug design – structural bioinformatics in drug discovery - Examples.

Reference Books

1. Andrew Leach, Molecular Modelling: Principles and Applications (2nd Edition), Addison Wesley Longman, Essex, England, 1996.
2. Alan Hinchliffe, Modelling Molecular Structures, 2nd Edition, John-Wiley, 2000.
3. Alan Hinchliffe, Molecular Modelling for Beginners, John-Wiley, 2003.
4. N. Cohen (Ed.), Guide Book on Molecular Modeling in Drug Design, Academic Press, San Diego, 1996.
5. D. Frenkel and B. Smith, Understanding Molecular Simulations. From Algorithms to Applications, Academic Press, San Diego, California, 1996.
6. C. Rauter and K. Horn, X-ray crystallography and drug design, Elsevier, 1984.
7. M. Kalos and P. A. Whitlock, Monte Carlo Methods**.** John Wiley & Sons, New York, 1986.
8. J.A. McCammon and S.C. Harvey. Dynamics of Proteins and Nucleic Acids. Cambridge University Press, Cambridge, 1987.
9. D.C. Rapaport. The Art of Molecular Dynamics Simulation.Cambridge University Press, Cambridge, England., 1995