**SS840** **BIOCHEMISTRY FOR COMPUTER SCIENTISTS**
**4-0-0-4**

## COURSE OBJECTIVE

This course starts with introduction to the basic concepts of organic chemistry and biochemistry to students from a non-life sciences background (eg. engineers). The objective is not to get them to be experts in biochemistry or organic chemistry, but to be able to understand enough to be able to model them using modeling techniques.
Specific learning objectives for this course are:

1. To provide a working knowledge of organic chemistry and biochemistry
2. Understand what makes small molecules behave as drugs
3. To develop an understanding about macromolecular structure
4. Get students to start modeling in complex molecular modeling environments and manipulate structures through computer applications
5. Understand basics of molecular dynamics

| Serial No. | TOPICS TO BE COVERED |
|---|---|
| **Unit 1** | **Small molecules and basics of drugs** |
| 1. | Physicochemical properties in relation to biological action: solubility, partition coefficient, dissociation constant, |
| 2. | Physicochemical properties in relation to biological action: hydrogen bonding, ionization, drug shape, protein binding, bioisosterism. |
| 3. | Stereo chemical aspects of drug action - stereo-isomerism, optical isomerism |
| **Unit 2** | **Macromolecular structure** |
| 4. | Protein Structure and Function: Introduction/ Amino acids, peptide bonds |
| 5. | Protein Structure and Function: polypeptide chains. Secondary structure. |
| 6. | Protein Structure and Function: Tertiary structure. Quarternary structure. |
| 7. | DNA: Flow of information. Nucleic acids. DNA replication. |
| 8. | Gene expression. Amino acid coding by 3 bases |
| 9. | Enzymes and hormones: nomenclature, classification and characteristics - enzyme mechanism of action, factors affecting enzyme action |
| 10. | Enzymes and hormones: cofactors and coenzymes, enzyme inhibition, enzymes in organic synthesis. Hormones and vitamins - representative cases. |
| **Unit 3** | **Basics of drugs** |
| 11. | Topics in biochemistry that affect drug design: Definition of drugs, Characteristics of different routes of Drug Administration, site of drug action, mode of drug action. |

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| 12. | Topics in biochemistry that affect drug design: Classification of drugs, mechanism of drug action. Drug-receptor complex, agonist, antagonist. Assessment of drug activity, receptor and drug action. |
| **Unit 4** | **<u>Computational Drug Design</u>** |
| 13. | Force fields |
| 14. | manipulation of structure using VMD **(X 5)** |
| 15. | VMD: scripting in Python or Tcl **(X 3)** |
| 16. | Molecular modeling and minimization |
| 17. | Docking **(X 5)** |
| 18. | Conformational searching **(X 5)** |
| 19. | QSAR basics |
| 20. | Assessment/prediction of drug activity using computational tools and molecular databases |
| 21. | Basics of cheminformatics |

**TEXT BOOKS / REFERENCES:**


1. "Principle of Organic Medicinal Chemistry" by Prof. Rama Rao Nadendla.
2. "Molecular Modeling and Simulation: An Interdisciplinary Guide", Tamar Schilk
3. "Molecular Modeling and Applications", Andrew Leach