

**UNIT – I**

**A Revisit to 2-D QSAR:** Free- Wilson Model, Fugita- Ban Model, Hansch analysis, Electronic factors, steric factors, & hydrophobic factors. Comparison between Free-Wilson model and Hansch analysis. Molecular Connectivity Index (MCI).

**UNIT – II**

- Recent techniques and applications in **Pharmacophore Mapping**.
- **3-D QSAR Analysis:** Receptor independent 3-D QSAR Analysis, Receptor dependent **3-D QSAR Analysis**.
- Receptor pre-organization for activity and its role in identifying Ligand-binding sites on
- Docking molecules into protein binding sites
- *de-novo* Ligand design

**UNIT – III**

**Enzyme Inhibitors:** A detailed study of the following types of enzyme inhibitors, related drugs and their pharmaceutical significance;

- a) P.G.Synthetase (cyclooxygenase and lipoxygenase inhibitors)
- b) Phosphodiesterase (PDE) inhibitors.
- c) Carbonic anhydrase inhibitors.
- d) Angiotensin converting enzyme (ACE) Inhibitors
- e) Acetyl choline Esterase (AChE) inhibitors.

**UNIT – IV**

**Miscellaneous classes of drugs:** Recent advances in the following classes of drugs:

- a) Proton-pump Inhibitors as antiulcer agents.
- b) Immunosuppressive and immunostimulant agents.
- c) Antiviral agents
- d) Beta – Adrenergic blockers (Beta 1 and Beta 2 )

**REFERENCES:**

1. Medicinal Chemistry by Alfred Burger
2. Drug Design by Arie4ns.
3. Introduction to the principles of drug design by Smith & Williams.
4. Strategy of drug design by Purcell.
5. Textbook of medicinal and pharmaceutical chemistry by Wilson and Gisvold.
6. Principles of medicinal chemistry by William Foye
7. Organic synthesis by Michael. B .Smith    Mac Graw Hill