

UNIT – I

1. **Physico-chemical properties in relation to Biological action:**

Complex events between drug administration and drug action, route of administration, absorption, site of loss (storage site, protein binding, neutral fat), metabolism and excretion, biological activities of Homologous series, drug receptor interactions, isosterism, steric features of drugs, concept of drug receptor, forces involved theories on interaction, selected physico-chemical properties influencing biological action like ionization, hydrogen bonding chelation, oxidation-reduction potential, surface activity, solubility and partition coefficient.

Receptors, their types, location, isolation, Transduction mechanism

UNIT – II

2. **Metabolism of drugs:**

Role of cytochrome P-450 monooxygenase in oxidative biotransformation, oxidation of aromatic moieties, olefins, benzylic carbon all cyclic carbon, carbon nitrogen systems, carbon oxygen systems, carbon sulphur systems with examples of drugs, reductive reactions involving aldehydes, ketones, nitro and azo compounds, hydrolytic reactions with examples conjugation pathway with glucuronic acid, glycine, glutamine with specific example, acetylation and methylation of drugs.

Stereo chemical aspects of drug metabolism, production of pharmacologically active metabolites. Relationship of drug metabolism and drug design.

UNIT – III

3. **Combinatorial chemistry:**. High through put organic synthesis : Solid phase organic synthesis : Solution phase synthesis ;

Library construction strategy: Parallel synthesis, pooled synthesis,

Compound design within combinatorial library: Library diversity, controlling Molecular properties.

Looking for leads, Discovery Library : Synthesis of oligomers, efficient constructions, branching strategy, leveraging knowledge, targeted libraries.

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The fundamentals of Pharmacophore underlying in combinatorial chemistry.

UNIT – IV

4. **Strategies for synthesis of Candidate Drug:**

- Target selection
- Retro- synthesis (The disconnection approach, Consecutive versus convergent synthesis)
- Various strategic approaches including **LHASA**
- Strategic bond approach
- Strategic bond in ring approach
- Degradation techniques as a tool for Retro-synthesis.

REFERENCES:

1. Medicinal Chemistry by Alfred Burger
2. Drug Design by Ariens
3. Introduction to the principles of drug design by Smith and 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. Combinatorial library design & Evaluation by Arup. K. Ghosh & Vellarkad. N. Vishwanathan by Marcel Dekker. NYC