MANGALORE UNIVERSITY

Department of Industrial Chemistry

ICH 503: SYNTHETIC, HETEROCYCLIC AND MEDICINAL CHEMISTRY

Course Outcomes:

- Planning and execution of multistep synthesis with retro synthetic approach.
- Photochemical reaction with pericyclic reaction, cycloaddition, sigmatropic reactions.
- Heterocyclic and medicinal chemistry used for drug discovery process
- Classification, synthesis and mode of action, some of drugs which are in practice.

UNIT I: Planning and Execution of Multistep Synthesis **14 hrs**

Basic principles and technologies used in disconnection approach, synthons and synthetic equivalents, Interconversion of functional groups, one group C-X and two group C-X disconnections. Protecting groups-Principles of protection of hydroxyl, amino,carboxylic and carbonyl groups. Use of C-C one group and C-C two group disconnections in the synthesis of 1,2; 1,3; 1,4; 1,5 and 1,6-difunctionalised compounds. Retrosynthetic analysis of alcohols, carbonyl compounds, cyclic and acyclic alkanes, benzocaine, p-methoxyacetophenone, acetocyanohydrin, 2-methyl-6-methoxy-indole-3-acetic acid, 6-methylquinoline and. Illustrative synthesis of Juvabione, Longifolene, Prelog-Djerassi lactone, Solid phase synthesis of polypeptides.

UNIT- II: **14 Hours**

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. Woodward-Hoffmann correlation diagram and FMO approach.

Electrocyclic Reactions: Introduction, Con-rotatory and dis-rotatory Process, 4n and 4n+2 systems. Reactions of cations and anions, formation and cyclisation of Dipolar molecules.

Cycloaddition reaction: Suprafacial and Antrafacial addition, 2+2 and 4+2 systems, 1,3-dipolar cycloaddition reactions and their applications in the synthesis of five membered heterocycles, nitrile oxide and sydnones

Sigmatropic reactions: Suprafacial and Antrafacial shift of H, [1,3] and [3,3]-sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

UNIT III: Heterocyclic Compounds **14 hrs**

Hantzsch-Widman system for naming monocyclic, fused and bridged heterocycles. Chemistry of derivatives of pyrazole, imidazole, oxazole, thiazole, benzofuran, indole, benzothiophene, pyridine, quinoline. Inter conversion of coumarin to benzofuran, pyrrole to pyridine, Pyrimidine to pyrazole, indole/isatin to quinoline, furans to pyrrole. Uses of

furan,pyrrole,thiophene in the synthesis of non heterocycles.

UNIT IV: Medicinal chemistry **14 hrs**

Introduction, Drug discovery- Historical examples, Natural products. Classification and nomenclature of drugs, concept of lead compounds, analogues and prodrug, Factors governing drug design ADME, drug design through molecular disjunction and conjunction. Drug receptor interactions- Forces involved in drug receptor interactions Theories of drug action-occupancy, rate, induced fit theory. Structurally specific and non-specific drugs, Classification, synthesis and mode of action of following classes of drugs-Antipyretic analgesics (Cinchophen), General anaesthetics (Thiopental sodium), Local anaesthetics (benzocaine,), cardiovascular drugs (diazoxide), antimalarials (chloroquine phosphate), antineoplastic agents (methotrexate and fluorouracil), antiviral drugs (methisazone).

References

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4. Organic Synthesis- A Disconnection Approach, Stuart
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7. Organic Reaction Mechanisms, V.K.Ahluwalia & R.K.Parashar, Narosa, 2006
8. Heterocyclic Chemistry, J. Joule & G. Smith, Van-Nostrand, ELBS, 1978.
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10. Heterocyclic Chemistry, Raj K. Bansal, New Age International, 1999.
11. Stereochemistry- Conformation and Mechanism, P.S.Kalsi, Wiley Eastern, New Delhi, 1993.
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13. Pericyclic reactions, S. M. Mukherji (The McMillan Bangalore), 1979.
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