ICH 503: SYNTHETIC, HETEROCYCLIC AND MEDICINAL CHEMISTRY

Course Objectives:

- To study the retrosynthetic analysis for planning a synthesis, especially of complex organic molecules.
- To give a knowledge about pericyclic reactions.
- To learn synthesis. reactivity and industrial applications of heterocyclic compounds.
- To know about drugs, its synthesis and mode of action,

UNIT I: Planning and Execution of MultistepSynthesis 14 Hr

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: Pericyclic chemistry 14 Hr

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.

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.

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 Hr

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 Hr

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. Concept of fragment based drug discovery. 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).

Course Outcomes:

The students will be learning the following

- Planning and execution of multistep synthesis with retro synthetic approach.
- Different types of pericyclic reactions and its advantages.
- Reactivity, preparations and applications of heterocyclic compounds.
- Classification, synthesis and mode of actions of some drugs.

References

1. Organic Synthesis-Special Techniques, V.K.Ahluwalia and R. Aggarwal, Narosa, New Delhi, 2001.
2. Organic Synthesis, R.E.Ireland, Prentice Hall India,1969.
3. Advanced Organic Chemistry, IV Edn., Part A &B, F.J.Carrey&R.J.Sundberg, Kluwer, 2001.
4. Organic Synthesis- A Disconnection Approach,Stuart
5. Art in Organic Synthesis, Anand, Bindra&Ranganath, Wiley, New Delhi,1970.
6. Modern Methods of Organic Synthesis, N. Carruthers, Cambridge University,1996.
7. Organic Reaction Mechanisms, V.K.Ahluwalia&R.K.Parashar, Narosa,2006
8. Heterocyclic Chemistry, J. Joule & G. Smith, Van-Nostrand, ELBS,1978.
9. Comprehensive Heterocyclic Chemistry, Vol.I-VI Edn., Katritzky& Rees, Pergamon,1984.
10. Heterocyclic Chemistry, Raj K. Bansal, New Age International,1999.
11. Medicinal Chemistry, Ashuthosh Kar, Fourth edition, New Age International PvtLtd.
12. Pericyclic reactions, S. M. Mukherji (The McMillan Bangalore),1979.
13. V.K. Ahluwalia and Mahu Chopra, Medicinalchemistry.
14. Graham L Patrick, An introduction to medicinal chemistry,Oxford.
15. Ashutosh Kar, Medicinal chemistry.
16. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition,2006.
17. Johann Gasteiger (Editor), Thomas Engel (Editor), Chemoinformatics: A Textbook, Wiley Publisher ISBN: 978-3-527-30681-7, 2003.
18. Rajarshi Guha (Editor), Andreas Bender (Editor), Computational Approaches in Cheminformatics and Bioinformatics Wiley-Blackwell, 2012.
19. Fan Li, Developing Chemical Information Systems: An Object-Oriented Approach Using enterprise JAVA, John Wiley & Sons, 2006,ISBN,0470068787, 978047006878

ICS 504: Polymers and Soft materials

Course Objectives

- To learn polymer chemistry and properties and synthetic methods.
- To know the versatility of polymer materials in their applications
- To provide the knowledge of basic concepts of liquid crystals and its applications.
- To learn the aspects of soft materials and organic solids with structural details.

UNIT I **10 hr**

Polymers

Basic concepts and techniques in polymer chemistry. General structures & classifications of polymers. Techniques of polymerization and molecular weight determination. Uses of some commercial and engineering polymers. Thermoplastics, thermosets and elestomers. Polymer processing techniques, additives for improvement of polymer properties, spinning of industrial polymers, wet, dry melt spinning and elctrospinning.