MEDICINAL CHEMISTRY
M. S. (Pharm.)

Course no.	Course Name	Credits
Semester I		
CORE SUBJECTS (ALL COMPULSORY)		
MC-510	Basics of Drug Action	2
MC-520	Organic Synthesis-I	2
MC-530	Spectral Analysis	1
MC-540	Principle and Applications of NMR	1
NP-510	Separation and Chromatographic Techniques	1
GE-510	Biostatistics	2
GE-511	Seminar	0.5
LG-510	General Laboratory Experience	2.5
	Total	**12**
ELECTIVE SUBJECTS (4 CREDITS)		
EL-501	Biochemical Engineering Fundamentals	2
EL-502	Biotechnology in Pharmaceutical Sciences	1
EL-503	Microbiology	1
EL-504	Industrial safety and green chemistry	1
EL-505	Computer Application in Biomedical Engineering	1
EL-506	Biological System Analysis and Control	1
EL-507	Productivity in management and reengineering (Neha	1
EL-508	Biosynthesis of Natural Products	1
EL-509	Chemotherapy of Parasitic and Microbial Infections	1
	Choose any core courses of other department (BT/MD/NP/PA/PC/PE)	
	Total Credits	**16**
Semester II		
CORE SUBJECTS (ALL COMPULSORY)		
MC-610	Drug design and discovery	2
MC-620	Organic Synthesis-II	3
MC-630	Chemical biology	2
MC-640	Stereochemistry in drug action	1
MC-650	Industrial Process and Scale-up Techniques	1
GE-611	Seminar	0.5
LS-610	General Lab Experience in the Area of Specialization	2.5
	Total	**12**

ELECTIVE SUBJECTS (4 CREDITS)		
EL-601	Biomechanics	2
EL-602	Mathematical Methods in Biomedical Engineering	1
EL-603	Logistics & distribution	1
EL-604	Total quality control	1
EL-605	Lean system, 6 sigma	1
EL-606	Introduction to Ayurveda and Polyherbal Formulations	1
EL-607	Chemotherapy and Immunopharmacology	2
EL-608	Pharmacovigilance and Medical Writing	2
	Choose any core courses of other department (BT/MD/NP/PA/PC/PE)	
	Total Credits	**16**
	Semester III	
TH- 598	Synopsis, Presentation	9
	Semester IV	
TH-698	Thesis Writing and Thesis Defense	9
	TOTAL CREDITS (I TO IV SEMESTERS)	**50**

Medicinal Chemistry
NIPER-Ahmedabad

Semester I

MC-510 (Basics of Drug Action); Credit -2

1. **Receptorology and Enzymology:** Drug-receptor interactions, Receptor theories and drug action, Receptor Complexes and Allosteric Modulators, Enzyme kinetics in drug action, Mechanisms of enzyme catalysis, Coenzyme Catalysis, Drug action through enzyme inhibition, Theories of enzyme inhibition and inactivation, Enzyme activation of drugs and prodrugs **(10 hr)**

2.Druglikeness: Drug like molecules and theories associated with the recognition of drug like properties. Physical organic chemistry of drug metabolism, drug de-activation and elimination, Phase I and phase II transformations, Concept of hard and soft drugs, Chemistry of ADME and toxicity properties of drugs. Role of transporters, ion-channel, CYP in permeability (CaCo-2), drug resistance and ADMET properties (8 hr)

3. Drug-receptor interactions: Inter and intramolecular interactions. Weak interactions in drug molecules. Chirality and drug action, Covalent, ion-ion, ion-dipole, hydrogen bonding, C5H Bonding, C-H hydrogen bonding (with protein/peptides as example), dihydrogen bonding, van der Waals interactions and the associated energies **(4 hr)**

4. **Introduction to Peptides, peptidomimetics and Nucleic acids:** Introduction to peptoids/peptidomimetics, ODN, and their Therapeutic

implications, synthetic ODNs and their role in drug discovery, Nucleic acids (NA) as targets for drug action,NA-interactive agents, NA-alkylation, NA-strand breaking and their importance in drug action **(10 hr)**

5. Introduction to Biosimilars and Vaccines: Basics concept of immunology in biosimilar and biologics, vaccines; Introduction to biosimilars and vaccines **(3 hr)**

6. Drug Discovery and Free energy methods in drug design, Introduction of thermodynamics in drug discovery, case studies, drug discovery in combating the threats of pandemic" **(5 hr)**

Note: All chapters should include at least one example as case study from current research articles

READING MATERIAL

1. The organic chemistry of drug design and drug action. Richard B. Silverman Academic Press.
2. The Pharmacological Basis of Drug Action Goodman and Gilman.
3. Advanced organic chemistry, Fourth Edition Jerry March Wiley-VCH
4. The Practice of Medicinal Chemistry by Camille Wermuth
5. Molecular Mechanism of Drug Action by C.J. Coulson , Taylor & Francis
6. A primer of Drug Action by R.M. Julien, Worth Publishers
7. Drug-Receptor Thermodynamics by R.B. Raffa, Wiley
8. Principles of Drug Action by W.B. Pratt, P. Taylor, Churchill Livingstone
9. H. D. Jakubke, N. Sewald, Peptides from A to Z, Wiley-VCH Verlag GmbH & Co. KgaA (2008)
10. From research articles and web information

LEARNING OUTCOME

Upon completion of this course students shall

- Demonstrate the assessment of drugs for therapeutic purpose
- Identify the key parameters of pharmacokinetic properties and toxicity for molecules.
- Demonstrate the importance of peptides and peptidomimetics in drug discovery.
- Derive the key interactions of drugs with receptors
- Derive basic knowledge about bio-similar and vaccines

MC-520 (Organic Synthesis-I); Credit -2

1. Introduction to Reaction Mechanism and Reaction intermediates: Basics of reaction mechanism, kinetic and non-kinetic methods of determining reaction mechanisms: reaction intermediates, crossover experiments and isotopic labeling, solvent, ionic strength and salt effect, Basics of acid-base catalysis, fundamental principles of organocatalysis, transition metal catalysis, Nucleophilic substitution reactions, Electrophilic substitution reactions, Addition and elimination reactions, Aromatic electrophilic substitution reactions, Aromatic nucleophilic substitutions reactions; Principles of Resonance, Inductive effects, mesomeric effect, neighbouring group participation etc. in organic synthesis. **(10 hr)**

2. Rearrangement, Oxidation and Reduction reactions: Fundamental principles of oxidation and reduction: A brief introduction to oxidation, reduction, rearrangement reactions with mechanism and examples. Metal based oxidizing reagents: A review and detailed discussion of chromium, manganese, ruthenium, silver and other metal based reagents. Non-metal based oxidizing reagents: DMSO, peroxide, peracid

and oxygen based oxidation. Miscellaneous oxidizing reagents like IBX, DMP, CAN, DDQ, periodate etc. Homogeneous and heterogeneous hydrogenations; Discussion on borane based racemic and chiral reagents, aluminum, tin, silicon based reducing agents. Dissolving metal reductions. Illustration of electron deficient and electron rich skeletal rearrangements with examples **(10 hr)**

3. Introduction to heterocyclic Chemistry: Classifications and Nomenclature of Heterocyclic compound (Fused, Spiro, Aromatic and Aliphatic) and methods of preparation with examples, Chemical Reactions and properties of 3/4/5/6-membered heterocyclic compounds with one/more hetero atoms **(10 hr)**

4. Photochemistry. Basic introduction of photochemistry, Singlet and triplet states, photosensitization, quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-1 and type-11 cleavages, Paterno-Buchi reaction, photo-reduction, photochemistry of enones and para-benzoquinones,, Pericyclic reactions including cycloaddition, electrocyclic and chemotropic reactions; Sigmatropic rearrangements **(5 hr)**

5. **Alkylation:** a) Enolates: Regio- and stereo-selective enolate generation, "O" versus "C"- alkylation, effects of solvent, counter cation and electrophiles, Symbiotic effect, Thermodynamically and kinetically controlled enolate formations, Various transition-state models to explain stereoselective enolate formation. (b) Enamines and metallo-enamines: Regioselectivity in generation, applications in controlling the selectivity of alkylation**. (5 hr)**

READING MATERIAL

1. The Logic of Chemical Synthesis E. J. Corey and Xue-Min Cheng
2. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag
3. Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
4. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure by Michael B. Smith, and Jerry March
5. Designing Organic Syntheses by Stuart Warren
6. Modern Synthetic Reactions by Herbert O. House
7. T. Eicher, S. Hauptmann, A. Speicher, *The Chemistry of Heterocycles*, 2nd Ed, Wiley-VCH Verlag GmbH & Co. KgaA (2003).
8. J. McMurry, *Organic Chemistry*, 5th Ed, Boroks/Cole (2006).
9. From research articles and web information

LEARNING OUTCOME

Upon completion of this course students shall

- Demonstrate the logics behind organic reactions and develop skill to analyze the reaction mechanism.
- Identify the reaction intermediates and various underlying mechanism involved in oxidation, reduction, rearrangements.
- Demonstrate the knowledge of applications of enolates and enamines in synthesis of drug molecules.
- Derive the fundamentals of heterocyclic chemistry.
- Derive basic knowledge about principle of photochemistry and its applications

MC-530 Spectral Analysis Credit 1

1. UV-Vis Spectroscopy Energy levels and selection rules: Definitions, molecular orbital approach for energy absorption, various modes of transitions. b) Correlation of structural variation with UV absorption:

Factors influencing the position and intensity of absorptions, Inductive and resonance effects, effect of ring size, influence of stereo chemical factors. c) Predicting UV absorption: Woodward-Fieser, Fieser-Kuhn and Nelson rules. d) Other factors: Non-conjugated interactions, Solvent effect, S-Cis band **(4hr)**

2. Infrared (IR) spectroscopy: Characteristic regions of the spectrum: Various modes of vibrations, Energy levelsCorrelation of structure with IR spectra: Influence of substituents, ring size, hydrogen bonding, vibrational coupling and field effect on frequency.Applications: Determination of stereochemistry, structural elucidations of biomolecules (conformation of secondary structure of peptides), Spectral interpretation with examples. **(4hr)**

3. Mass-Spectrometry: Molecular ion and metastable peak, fragmentation patterns, nitrogen and ring rules, McLafferty rearrangement, electron and chemical ionization modes, applications. Basics of Instrumentation (Ionization sources, Mass filters/analyzers and detectors), Tandem Mass analyzers, High Resolution and Accurate Mass, Applications in biomolecules (**9hr)**

4. Introduction to ORD, CD, Atomic absorption spectroscopy (AAS) and Inductively Coupled Plasma-Mass spectrometry (IPC-MS)

Basic principles with one examples from each (**3 hr**)

Note: All chapters should include at least one example as case study from current research articles

READING MATERIAL

1. Introduction to Spectroscopy: A Guide for Students of Organic Chemistry Donald L. Pavia, Gary M. Lamlman and George S. Kriz Thomson

2. R. S. Drago, Physical Methods for Chemists, W. B. Saunders,1992.
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell, McGraw-Hill, 1966
4. Instrumental Methods of Analysis, Seventh Edition Hobart H. Willard, Lynne L. Merrit, John A. Dean and Frank A. Settle CBS Publishers
5. Spectrometric Identification of Organic Compounds, Sixth Edition Robert M. Silverstein and Webster Fransis Wiley-VCH
6. Spectroscopy by Donald L Pavia, Gary M Lampman, George S Kriz, James A Vyvyan
7. Organic spectroscopy by William Kemp
8. Spectroscopic Methods in Organic Chemistry by Dudley H. Williams & Ian Fleming
9. Spectrometric Identification of Organic Compounds by Robert M. Silverstein, Francis X. Webster & David J. Kiemie
10. Applications of Absorption Spectroscopy of Organic Compounds by Dyer
11. Edmond de Hoffmann, Vincent Stroobant: *Mass Spectrometry, Principles and applications*, 3rd Edition, Wiley, 2007
12. E. de Hoffmann and V. Stroobant, *Mass Spectrometry: Principles and Applications*, 3rd edition, Wiley Interscience (2007).

LEARNING OUTCOME

Upon completion of this course students shall

- Demonstrate the knowledge of various spectroscopic and other techniques.
- Identify the structures of API by using UV-vis, IR and Mass Spectrometry.
- Demonstrate the knowledge of advanced techniques like ORD, CD, AAS and IPC-MS.
- Derive the applications of the spectroscopic and spectrometric tools for identification of complex molecules.
- Demonstrate the analytical skill for various samples including impurity profiling.

MC-540: Principles and Applications of NMR-Spectroscopy Credit-1

1. Fundamentals of NMR spectroscopy: Physical basis, Magnetic nuclei, resonance, relaxation processes, signal sensitivity ^{1}H NMR: chemical environment and shielding, chemical shift and origin of its concept, reference compound, local diamagnetic shielding and magnetic anisotropy, relation with chemical shift, chemical and magnetic non-equivalence, spin-spin splitting and its origin, Pascal's triangle, coupling constant, mechanism of coupling, integral, NMR solvents and their residual peaks, protons on heteroatoms, quadrupole broadening and decoupling, effect of conformations and stereochemistry on the spectrum, Karplus relationship, diastereomeric protons, Heteronuclear coupling to 19F and 31P. 1^{3}C NMR: Chemical environment, shielding and carbon-13 chemical shift, calculation, proton-coupled 13C spectra, Proton-decoupled 13C spectra, Nuclear Overhauser Enhancement (NOE), Problem with integration, Heteronuclear coupling for carbon to deuterium, carbon to 19F, carbon to 31P, Introduction of qNMR with examples **(12 hr).**

2. NMR Instrumentation: Different component of NMR spectrometer, operation of NMR spectrometer, Fourier transform NMR instruments **(2 hr)**

3. Distortionless Enhancement by Polarisation Transfer (DEFT): Introduction of DEPT Spectroscopy, Types of DEPT NMR, Examples and applications **(2 hr)**

4. 2D NMR spectroscopy: Introduction of 2D NMR with examples and its applications in elucidation of complex natural products and biomolecules (**4hr**)

Note: All chapters should include at least one example as case study from current research articles

READING MATERIAL

1. R. S. Macomber, A Complete introduction to modern NMR techniques, 1st Ed, John Wiley & Sons, England (1998).
2. M. H. Levitt, Spin dynamics: Basics of Nuclear Magnetic Resonance, 2nd Ed, John Wiley & Sons, England (2008).
3. C. P. Slichter, Principles of Magnetic Resonance, 3rd Ed, Springer Verlag, Berlin (1996).

LEARNING OUTCOME

Upon completion of this course students shall

- Demonstrate the knowledge of various NMR techniques.
- Identify the structures of molecules by using NMR- techniques.
- Demonstrate the knowledge of advanced NMR-techniques like 2D-NMR and DEFT.
- Derive the knowledge of ^{13}C-NMR for structural elucidation

Semester II

MC-610 (Drug Design and Discovery); Credit -2

1. Introduction to drug discovery Historical prospective of drug discovery, Sources of drugs, including natural products as examples , Stages of drug discovery (from target identification to post market surveillance), Target identification and validation, Screening of drugs,

High throughput screening(HTS), Random and Systematic screening. Hit identification. Rational drug designing. **(7 hr)**

2. Structure activity relationship (SAR) and Quantitative Structure activity relationship (QSAR)

Approaches to Lead Optimization Bioisosteric replacement, Conformation restriction, Molecular dissection, Metabolic stabilization , Homologation of alkyl chain(s) or alteration of chain branching, design of aromatic ring position isomers, and alteration of ring size, Alteration of stereochemistry, or design of geometric isomers or stereo isomers, Design of fragments of the lead molecule that contain the pharmacophoric group, Alteration of interatomic distances within the pharmacophoric group or in other parts of the molecule. Introduction to QSAR, molecular descriptors, QSAR model developments and validation, Example of 2D QSAR and 3D QSAR. **(9 hr)**

3. **Computer assisted drug design (CADD) :** Introduction to CADD, Structure and ligand based drug discovery, Applications of CADD in Drug design. Molecular docking and its subtype. Advantages and Its limitations, Overview of Docking tools Introduction to molecular dynamics, Force fields, Energy minimization and geometry optimization, drug-receptor complexes and conformational search Pharmacophore mapping, methods of conformational search used in pharmacophore mapping; Comparison between the popular pharmacophore methods De novo drug design techniques, Receptor/enzyme cavity size prediction. Predicting the functional components of cavities, designing drugs fitting into cavity. Brief introduction to bioinformatics, and its application to drug design **(16 hr)**

4. Modern analytical tools in drug discovery: Introduction to Proteomics, genomics and metabolomics.**(5 hr)**

5. Prodrugs: Basic concept and definition, Prodrug Design Considerations Prodrugs of functional group, Drug release and activation mechanisms, Application of prodrugs in drug discovery. **(3 hr)**

Note: All chapters should include at least one example as case study from current research articles

READING MATERIAL

1. An Introduction to Medicinal Chemistry, Fourth Edition Graham L. Patrick Oxford Press
2. 3D QSAR in Drug Design Hugo Kubinyi, Gerd Folkers, Yvonne C. Martin Spinger
3. .Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set (Burger's Medicinal Chemistry and Drug Discovery) Donald J. Abraham and David P. Rotella
4. Molecular Modelling, byA. R. Leach
5. Organic Chemistry of Drug Design and DrugAction, by R.B. Silverman
6 Practical Applications of computer aided drug design, by P.S. Charifson
7 Molecular modeling in Drug Design, by C. Cohen
8. Chemical Applications of Molecular modeling, by J. Goodman
9. Pharmacophore perception, by O.F. Guner

Learning outcome

Upon completion of this course students shall

- Demonstrate the knowledge of various stages of drug discovery process.
- Identify the key requirements for converting HIT molecules to Lead.
- Demonstrate the knowledge of Computer assisted drug discovery
- Derive the approach of Structure-activity-relationship of drugs
- Demonstrate the skill for applying advanced tools in drug discovery process

- Derive the fundamentals of prodrug concepts.

MC-630 (Chemical Biology) Credit -2

1. Introduction to chemical biology: Chemistry and Biology — Historical and Philosophical Aspects, Central dogma in molecular biology; chemical genetics in DD. Biomimetic synthesis **(3 hr)**

2. Bioorthogonal chemistry: Bioorthogonal chemical reactions and their importance. Bioconjugation strategies, protein and peptide labeling, Site specific modification of proteins and peptides. Staudinger ligation, Native chemical ligation. (**5 hr)**

3. Biomolecules: Structure and function of carbohydrates, lipids, polysaccharides and Nucleic acids and their pharmaceutical importance and applications, Structure of lipoproteins and glycoproteins in relation to their function. Protein structure building block to quaternary structure of proteins: Ramachandran plots. **(8 hr)**

4. Targets, mechanism of action of drugs in Cancer, Diabetes and CNS related disease Case studies in case of Cancer, Diabetes and CNS related disorder **(12 hr)**

5. Techniques for structural analysis of biomolecules : Basic principles of fluorescence spectroscopy, fluorescent group, sensitivity of fluorescence to environment, applications for structure determination of biomolecules, ORD/CD application to Nucleic acids and proteins, Various thermodynamics based instrumental methods for estimation of

structural features of biomolecules, Crystallographic method for structure of biomolecules, Various Mass spectrometric methods (MALDI-TOF, Soft ionization) for structural determination of biomolecules.**(12 hr)**

Note: All chapters should include at least one example as case study from current research articles

READING MATERIAL

1. Foye's Principles of Medicinal Chemistry (Lemke, Foye's Principles of Medicinal Chemistry) Lippincott Williams & Wilkins
2. Principles of Biochemistry: Lehninger, Nelson and Cox; W.H. Freeman; 5th edition; 2008.
3. G. M. Blackburn, M. J. Gait, D. Loakes, D. M. Williams, *Nucleic Acids in Chemistry and Biology*, 3rd Edition, RSC Publishing, London, **2006**
4. S. Doonan, *Peptides and Proteins*, 1st Edition, RSC Publishing House, London, **2002**
5. Herbert Waldmann, *Chemical Biology: Learning Through Case Studies*; Wiley-VCH, Weinheim 2009.
6. Dobson, Gerrard & Pratt, *Foundations of Chemical Biology*; Oxford Univ. Press; 2002.
7. Miller & Tanner, *Essentials Of Chemical Biology: Structure and Dynamics of Biological Macromolecules*; Wiley; 2002.
8. Waldman & Janning, *Chemical Biology: A Practical Course*; Wiley-VCH; 2004.
9. Greg T. Hermanson, *Bioconjugate Techniques*; Academic Press, 2008.
10. Joseph R. Lackowicz, *Principles of Fluorescence Spectroscopy*; Springer; 2006.
11. Journal Articles/Web references

Learning outcome

Upon completion of this course students shall

- Demonstrate importance of biomolecules in life origin.
- Derive theory of various conjugation and labelling tools and methodologies.

- Demonstrate clear and concise importance of various therapeutic targets related to CNS, Cancer and Diabetes.
- Derive the mechanism of action of drugs.
- Demonstrate the skill for identifying and assigning the secondary and higher order structures of complex biomolecule by using various tools and techniques.

MC-650 (Industrial Process Scaleup technique); Credit -1

1. Introduction to generics: Status of Indian bulk drugs in international market, Generics vs Novel drugs. Current market scenario, scopes and challenges for API. Introduction to Pharmacopiae. **(3 hr)**

2. Process scale-up techniques: Introduction to scale-up techniques, route scouting, selection of starting materials. Introduction to impurities and control of impurities, Monitoring of reactions, in-process control (IPC), Purifications, recovery, Effluents and treatments, **Environmental concern**, and Green chemistry , Biocatalysis in process scale-up, Safety. Specifications, Introduction to technology transfer, Documentations of process. Process flow diagram, material balance, Material of constructs and equipments for scale-up.Case study (**12 hr)**

3. Regulatory requirements for API manufacturing: Introduction to regulatory affairs, ICH guidelines for API manufacturing, Introduction to, Regulatory markets, DMF, CEP and Written confirmation., Data integrity (ALCOA). **(5 hr)**

Note: All chapters should include at least one example as case study from current research articles

READING MATERIAL

1. **Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set (Burger's Medicinal Chemistry and Drug Discovery) Donald J. Abraham and David P. Rotella**
2. ICH guidelines (Quality and Inter-disciplinary)
3. Process Chemistry in the Pharmaceutical Industry by Kumar Gadamasetti, Marcel Dekker Inc.
2. Practical Process Research & Development by Neil G. Anderson, Academic Press
3. Principles of Process Research and Chemical Development in the Pharmaceutical Industry by O. Repic, John Wiley & Sons, Inc
4. Pharmaceutical Process Chemistry for Synthesis by Peter J. Harrington

Learning outcome

Upon completion of this course students shall

- Demonstrate the importance of process development in drug discovery.
- Identify the synthetic methods based upon green chemistry principles.
- Derive the key requirements for regulatory submission of API
- Distinguish the generics vs novel drugs.

MC-620 (Organic Synthesis-II) 3 credit

1. Reaction of electron-deficient intermediates: Carbene, nitrene and free radical-their stability and modes of generation; Addition and insertion reactions of carbenoids and nitrenoids- regio- and stereo-selectivity, role of the metal catalysts in the transition metal-catalyzed

reactions, other types of reaction of carbenoids, e.g., ylide generation, 1,3-dipolar addition, rearrangement etc.; Intra-molecular radical trapping process leading to ring annulation - Baldwin's rule. **(10 hr)**

2. **Ylides and borons in organic synthesis(** a) Phosphorous ylides: Structure and reactivity, stabilized and non- stabilized ylides, effects of ligands on reactivity, Wittig reaction, Schlosser modification, Wittig-Horner and Horner Wadsworth-Emmons olefination reactions (b) Chemo-, regio- and stereo-selective hydroboration reaction, Alkylboranes as organometallic reagents e.g., 9-BBN, thexylboranes, siamylborane, chiral boranes- lpc2BH lpcBI-12 **(8 hr)**

3. Organometallic (a)Applications of Organometallics as reagents and catalysts for the synthesis and functionalizations of organic molecules. C-C bond forming reactions, examples as Sonogashira, Suzuki, Stile, Himaya etc., C-H activation, C-N bond forming reaction with examples including Buchwald-Hartwig. (**10hr)**

4. Peptide chemistry; Coupling reactions in peptide synthesis, Principles of solid phase peptide synthesis, site-specific chemical modifications of peptides, Segment and sequential strategies for solution phase peptide synthesis Side reactions in peptide synthesis. **(6hr)**

5. Introduction to Organocatalysis: Principles and reaction mechanism with examples. Ionic liquid catalysis, and Photo-redox catalysis (**3 hr**)

6. Modern synthetic tools: Microwave- and Ultrasound-assisted organic synthesis, Flow chemistry, Electroorganic synthesis. **(3hr)**

7. Asymmetric synthesis: Principles of asymmetric synthesis, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions. Synthesis of α-amino acids, synthesis of L-DOPA Sharpless enantioselective epoxidation, reduction of prochiral carbonyl compounds and olefins, Use of chiral auxiliaries in diastereoselective reductions. Use of chiral reagents in asymmetric transformations. Racemisation and resolution: Mechanism of racemisation, methods of resolution, Determination of enantiomer and diastereomer composition: Isotope dilution method, enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR). **(10hr)**

8. Retro-synthetic strategies Retrosynthetic Analysis and Synthetic Planning, Linear and convergent Synthesis, disconnections, Functional group interconversion, Strategies in Synthetic Planning, Examples **(10 hr)**

Note: All chapters should include at least one example as case study from current research articles. Applications of the synthesis in terms of complex drug synthesis need to be included wherever applicable.

READING MATERIAL

1. The Logic of Chemical Synthesis E. J. Corey and Xue-Min Cheng;
2. Organic Synthesis: The Disconnection Approach, Stuart Warren; Organic Chemistry ,Jonathan Clayden, Nick Greeves,Stuart Warren and Peter Wothers Oxford University Press

3. G. O. Spessard, G. L. Miessler, Organometallic Chemistry, Prentice Hall, 1997.
4. H. D. Jakubke, N. Sewald, Peptides from A to Z, Wiley-VCH Verlag GmbH & Co. KgaA (2008).
5. Organic Chemistry, 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
6. Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.
7. Wyatt, P., Warren, S. *Organic Synthesis: Strategy and Control*, Wiley, **2007**.
8. Warren, S. *Organic Synthesis: The Disconnection Approach*, Wiley, **1983**.
9. Nicolaou, K. C., Sorensen, E. *Classics in Total Synthesis*, Wiley-VCH, **2008**.
10. Nicolaou, K. C., Snyder, S. A. *Classics in Total Synthesis-II*, Wiley-VCH, **2003**.
11. Corey, E. J., Cheng, X-M. *The Logic of Chemical Synthesis*, Wiley, **1995**.
12. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals,* 3rd Ed.; Wiley-Interscience: New York, **2001**.
13. Hartwig, J. F. *Organotransition Metal Chemistry From Bonding to Catalysis,* 1st Ed.; University Science Books: Sausalito, CA, **2010**.

Learning outcome

Upon completion of this course students shall

- Demonstrate the importance catalytic reactions in organic synthesis.
- Identify principle and mechanism of organometallic reactions involving electron deficient reaction intermediate.
- Derive the fundamentals of peptide synthesis
- Demonstrate the skill to analyze the complex molecules and propose route of synthesis.
- Derive the applications of boron-based reagents and ylides in organic synthesis.
- Demonstrate the knowledge of various modern tools in organic synthesis.

MC-640 Stereochemistry in Drug Action

1. Introduction to stereochemistry: Chirality and Prochirality, Nomenclature and representations; Various projectional formulae, molecule with chiral centre, axis and plane, symmetry elements and operation and conformational analysis of carbocyclic and heterocyclic system.

2. Conformational analysis Definitions: Internal co-ordinates, distinction between conformation and configuration, Conformational analysis of cyclic compounds: carbocycles and heterocycles, bi- and tri-cyclic compounds.

3. Group theoretical interpretation of chirality group: Laws of group theory, symmetry elements and operations, classification of symmetry operation into groups, chiral and achiral point groups, determination of molecular structures into symmetry point groups, platonic solids, disymmetrisation., Definitions: Internal co-ordinates, distinction between conformation and configuration. Conformational analysis of cyclic compounds: carbocycles and heterocycles, bi- and tri- cyclic compounds.

4. Chirality in drug discovery: Chiral switching, Eutomer and Distomer with example in drug discovery. Realization that stereoselectivity is a pre-requisite for evolution; Role of chirality in selective and specific therapeutic agents; Case studies; Enantio-selectivity in drug absorption, metabolism, distribution and elimination.

Note: All chapters should include at least one example as case study from current research articles.

READING MATERIAL

1. StereoChemistry of Organic Compounds by Ernest L. Eliel, Samuek H. Wilen, Lewis N. Mander
2. Stereo Chemistry of Carbon Compounds by Ernest L. Eliel
3. Chemical Application of Group Theory by F. Albert Cotton

Learning outcome

Upon completion of this course students shall

- Demonstrate the importance of chirality in drug action.
- Identify various rules and principles guiding assignment of stereocenters in drug molecules.
- Demonstrate the knowledge of various conformational analysis

EL-504: Introduction to Industrial safety and green chemistry (1Credit)

1.Introduction to laboratory safety: Laboratory and work ethics, Properties of hazardous and toxic chemicals and safe handling procedures: Classification of hazards, Safety symbols and safety measures case study Materials safety data sheets (MSDs), material handling, Handling and Chemical Storages **(8hr)**

2. Introduction to biological safety: Biological hazards, classifications and safety measures at laboratory-case study 2 example (**1hr**)

3. Cause and prevention of accidents, first aids, Fire safety, Spill measures (**3 hr**)

4. Safety & Health Guidelines for the Chemical Industry: OSHA and others (**3 hr**)

5. Green Chemistry and Industrial process: Environmental concern in bulk drug manufacturing, Catalysis in green chemistry, Case study Alternate reaction media (5 hr)

Note: All chapters should include at least one example as case study from current research articles.

READING MATERIAL :

1. **M. Ali, Bassam Ali, "Handbook of Industrial Chemistry: Organic Chemicals"**
2. **OSHA guidelines**
3. **Green chemistry by Paul Anastas**
4. **Green Chemistry and Catalysis by Isabel Arends, Roger A. Sheldon, and Ulf Hanefeld**
5. **C. A. Heaton, *Introduction to Industrial Chemistry*, 3rd Ed, Springer, New York (2009).**
6. **K. Weissermel, Hans-Jrgen Arpe, *Industrial Organic Chemistry*, 3rd Ed, Wiley-VCH, New York (2003).**
7. **Examples from Web information**

Learning outcome

Upon completion of this course students shall

- Demonstrate the skill to work in laboratory in safe manner
- Identify and distinguish various hazards associated with experiments.
- Derive the importance of safety.
- Demonstrate the skill to handle and store various chemicals under appropriate conditions
- Demonstrate the knowledge of various guidelines followed by industries as per safety norms.