M. Sc. - II Organic Chemistry
Semester – III
CHO-5301: Designing of organic synthesis and Heterocyclic Chemistry
(48 L+ 12 T) (4 Credit)

1. Designing of organic synthesis **(24 L)**

Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide, enamines, Umpolung in organic synthesis, Retrosynthesis-FGI, divergent vs. convergent syntheses.Synthesis of some typical organic molecules- Abscisic acid, Longifolene
Ref. 1-9

2.Heterocyclic Chemistry **(24 L)**

a) Five and six membered heterocycles with one and two hetero atoms:
Synthesis, reactivity, aromatic character and importance of following heterocyclic rings:
Furan, Pyrrole, Thiophene, Pyrazole, Imidazole, Pyridine
b) Condensed five and six membered heterocycles:
Benzofuran, Indole, Quinoline
c) Condensed five membered heterocycles:
Benzoxazole, Benzthiazole, Benzimidazole
d) Synthesis of ranitidine, papavarine, amlodipine, bromouridine, tryptophan, thiamine, chloroquine Ref. 10-17

References:

1. Designing of organic synthesis – S. Warren (Wiley)
2. Some modern methods of organic synthesis – W. Carruthers (Cambridge)
3. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
4. Organic synthesis – Michael B. Smith
5. Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007)
6. Guidebook to organic synthesis-R K Meckie, D M Smith and R A Atken
7. Organic synthesis- Robert E Ireland
8. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako
9. Organic synthesis through disconnection approach- P. S. Kalsi
10. Heterocyclic Chemistry -T. Gilchrist
11. An introduction to the chemistry of heterocyclic compounds-R M Acheso
12. Heterocyclic Chemistry- J A Joule and K Mills
13. Principles of modern heterocyclic chemistry- A Paquette
14. The essence of Heterocyclic Chemistry- A. R. Parikh, Hansa Parikh, Ranjan Khunt
15. Handbook of Heterocyclic Chemistry- A R Katritzky, A F Pozharskii
16. Heterocyclic Chemistry-II- R. R. Gupta, M Kumar, V Gupta, Springer (India) pvt
17. 17.Heterocyclic Chemistry- R. K. Bansal

CHO-5302: Spectroscopic Methods in Structure Determination
(48 L+ 12 T) (4 Credit)

^{1}H NMR Spectroscopy (14 L)

Recapitulation of basic principle,Fourier Transform technique, Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei (alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant "*J*", classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2. Spin decoupling,

Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear over-hauser effect (NOE), and resonance of other nuclei like ^{31}P

^{13}C NMR spectroscopy (8 L)

FT NMR, Types of ^{13}C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT with 3 different angles, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, chemical shifts of solvents, Homo nuclear (^{13}C-^{13}C) and Hetero nuclear (^{13}C-^{1}H)coupling constants.

2D NMR Techniques (6 L)

General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)-Homo COSY (^{1}H-^{1}H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications. Illustrative example of COSY, HSQC in carbohydrate characterization.

Mass Spectrometry (10 L)

Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrapole mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation

Problems based on joint application of UV, IR, PMR, CMR, and Mass. **(10 L)**

(Including reaction sequences)

References:

1. Introduction to Spectroscopy - D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wileyand Sons.
3. Spectroscopic methods in organic chemistry - D. H. Williams and I. Flemming Mc Graw Hill
4. Absorption spectroscopy of organic molecules - V. M. Parikh
5. Nuclear Magnetic Resonance - Basic Principles- Atta-Ur-Rehman, Springer-Verlag (1986).

6. One and Two dimensional NMR Spectroscopy - Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998)
8. Organic structural Spectroscopy- Joseph B.Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).
9. Organic structures from spectra -Field L.D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sonsLtd.
10. Spectroscopic identification of organic compound- R. M. Silverstein, G. C.Bassler and T. C.Morril, John Wiley
11. Introduction to NMR spectroscopy-R. J.Abrahm, J. Fisher and P. loftus Wiley
12. Organic spectroscopy-William kemp, E. L. B. with McMillan
13. Spectroscopy of organic molecule-P.S.Kalsi,Wiley, Esterna, New Delhi
14. Organic spectroscopy-R. T. Morrison and R. N. Boyd
15. Practical NMR spectroscopy-M. L. Martin, J. J. Delpench, and D. J. Martyin
16. Spectroscopic methods in organic chemistry-D. H. Willson, I. Fleming
17. Spectroscopy in organic chemistry- C. N. R. Rao and J. R. Ferraro
18. NMR –Basic principle and application-H. Guntur
19. Interpretation of NMR spectra-Roy H. Bible
20. Carbohydrate Characterization through Multidimensional NMR: An Undergraduate OrganicLaboratory Experiment. *J. Chem. Educ.* **2020**, 97(1), 195-199
21. Mass spectrometry organic chemical applications-J H Banyon

CHO-5303: Organic Stereochemistry-I and Organic Reaction Mechanism (48 L+ 12 T) (4 Credit)

Organic Stereochemistry-I

1. Stereochemistry of six membered rings. Ref. 1, 3, 4, 5 **(11 L)**
2. Stereochemistry of rings other than six membered Ref. 1, 3, 4, 5 **(7 L)**
3. Fused Bridged and caged rings Ref. 1, 2, 3, 4 **(6 L)**

Organic Reaction Mechanism

1. Carbanions: Formation, geometry, stability and related reactions- Aldol, α-halogenation, haloformreaction, Michael reaction, Robinson annulations, Mannich, Stobbe, Cannizaro's, Darzons, Dieckmann, Knoevegel, Benzoin, Perkin, Benzoin condensation, Grignard, Claisen condensation, Baylis-Hilman,Appel reaction,Corey-Fuchs reaction Ref. 6, 7, 8, 10 **[12 L]**
2. Enamines: formation and applications of enamine in organic synthesis. Ref. 9 **[4 L]**
3. NGP:Neighbouring group participation Ref. 6 **[4 L]**
4. Synthesis and reactions of carbenes and nitrenes Ref. 9 **[4 L]**

References:

1. Stereochemistry of carbon compounds - E. L. Eliel
2. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen
3. Stereochemistry of organic compounds –Nasipuri
4. Stereochemistry of organic compounds-Kalsi
5. Organic stereochemistry – Jagdamba Singh
6. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
7. Advanced organic chemistry by J. March, 6th Ed.
8. Advanced organic chemistry. F. A. Carey and R. J. Sundberg, Part A 5th Ed. Springer (2007)
9. Advanced organic chemistry. F. A. Carey and R. J. Sundberg, Part B 5th Ed. Springer(2007)
10. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers

CHO-5304: Photochemistry, Free radicals and Pericyclic Reactions and (48 L+ 12 T) (4 Credit)

1. Photochemistry (16 L)

General basic principles, photochemistry of carbonyl compounds, alkenes, dienes and aromatic compounds and their application in organic synthesis (Norrish type I and II reaction, isomerization, Patterno-Buchi reaction)photorearrangements (di-π-methane, oxa di-π and aza di-π-methane rearrangements), photoreduction, photosubstitution reaction-Barton reaction.
Photochemistry in nature- chemistry of vision, Application of photochemical reactions in synthesis– Isocomene
Ref. 1,2,3,4

2. Free radicals: [16 L]

Generation of radicals, Stability of Free Radical, types of free radicals, Nucleophilic and electrophilic radicals, methods for detection and formation of free radicals, radical initiators, Characteristics reactions, -Free radical substitution, addition to multiple bonds, free radical halogenation- chlorination and bromination- NBS, autoxidation,Thermal decomposition of hydroperoxides, Radicals in synthesis: Hunsdiecker reaction, Barton Nitrite Photolysis reaction, Barton Decarboxylation, Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol dionors, cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling. C-C bond formation in aromatics, SNAr reactions-Sandmeyer reaction
Ref. 1, 3, 6

3. Pericyclic reactions

Recapitulation of Molecular Orbitals, their symmetry properties, Woodward –Hoffmann's Conservation oforbital symmetry property rule. **(4 L)**
Application of Woodward –Hoffmann's Conservation of orbital symmetry property rule to the ground state and excited state Electrocyclic reactions, Cycloaddition reactions, Chelotropic reactions, Sigmatropic reactions,and1,3-dipolar additions, Analysis by correlation diagrams, FMO approach, Mobius-Huckel theory and ATS concept. Application of pericyclic reactions: Ene reaction, Sommelet-Hauser rearrangement, Claisen and Cope rearrangements, fluxional molecules, synthesis of Endiandric acid. **( )**
Ref. 1, 3, 5, 7, 10-14

References:

1. Advanced Organic Chemistry, Part A – F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
2. Excited states in Organic Chemistry- J.A. Barltrop and J.D.Coyle, John Wiley & sons
3. Photochemistry and Pericyclic reactions-Jagdamba Singh, Jaya Singh 3rd Ed.
4. Organic photochemistry: A visual approach-Jan Kopecky, VCH publishers (1992).
5. Conservation of orbital symmetry – R. B. Woodward and R. Hoffmann; Verlag Chemie, Academic press (1971).
6. Radicals in Organic Synthesis B. Giese, Pergamon press (1986)
7. Orbital Symmetry : A problem solving approach- R. E. Lehr and A. P. Marchand;Academic (1972)
8. Classics in total synthesis- K. C. Nicolaou and E. J. Sorensen; VHC (1996)

9. P. A. Wender and J. J. Howbert *J. Am. Chem. Soc.* **1981**,*103*, 688-690.
10. Organic reactions and orbital symmetry, 2nd Ed. T. L. Gilchrist and R. C. Storr
11. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers
12. Pericyclic reactions: A text book –S. Sankararaman
13. Pericyclic reactions- Gill and Willis
14. Frontier orbitals and organic chemical reactions-Ian Fleming, John Wiley & sons 7

Practical course I

CHO-5305: Single stage preparations [4 Credits]

At least nine single stage and five isolation of Natural products and two quantitative analysis should carried out. The preparation should be carried out on micro scale.

A) Advance organic practical (any 9)

a) Preparation of dry solvents eg THF, DCM, DMF, DMSO, CH_3CN

b) Synthesis and purification and characterization

1) Ethyl cinnamate from benzaldehyde (Wittig reaction)
2) 2-phenyl indole by Fischer indole synthesis
3) Cyclohexanone to enamine
4) Triphenyl or diphenyl methyl carbinol(Grignard reaction)
5) 4-chlorotoulene from p-toluidine (Sandmeyer reaction)
6) Cyclohexanol from cyclohexanone ($NaBH_4$ reduction)
7) Glucose pentaacetate fromglucose
8) Stilbene from benzyl chloride (Wittig reaction)
9) Vilsemeir Haack formylation of 2-methoxy naphthalene
10) Diels Alder reaction of anthracene and maleic acid.
11) 4-Nitro Benzonitrile from 4-Nitrobenzaldehyde
12) Quinoline from Aniline (Skraup synthesis)
13) Synthesis of imidazo[1,2-a]pyridines
14) 1-phenyl,3-methyl pyrazole-5-one from phenyl hydrazine and ethyl acetoacetate

B) Isolation of Natural products (Any 5)

1) Caffeine from tea leaves (Soxhlet extraction)
2) Piperine from pepper (Soxhlet extraction)
3) Lycopene from tomatoes
4) Trimyristin from nutmeg
5) Eugenol from clove
6) Curcumin from turmeric powder
7) Casein and lactose from milk
8) β-Carotene from carrots

C) Organic quantitative analysis (any 2)

1) Estimate amount of sulphadiazine present in given tablet
2) Estimation of paracetamol and ibuprofen in given tablet
3) Estimation of glucose using Fehling's solution
4) Estimation of sucrose using Fehling's solution
5) Estimation of amino acid by formol titration

Practical course II

CHO-5306: Double and multiple stage preparations 4 credits]

At least five double stage and two multiple stage preparations should be carried out. The preparation should be carried out on micro scale.

A) Double stage preparation(any 5)

1) Benzaldehyde to benzalacetophenone to epoxide
2) Phthalimide to *N*-benzylphthalimide to benzylamine
3) Cyclohexanone to phenyl hydrazone to 1,2,3,4-tetrahydrocarbazole
4) Hydroquinone to hydroquinone diacetate to 2,5-dihydroxy acetopheneone
5) Resorcinol to 4-methyl-7-hydroxy coumarin to 4-methyl-7-acetoxy coumarin
6) Phthalic acid to phthalimide to anthranilic acid
7) Hydroquinone to hydroquinone diacetate to 1,2,4-triacetoxy benzene
8) Synthesis of indigo and its vat dyeing of cotton
9) Acetanilide to 4-nitro acetanilide to 4-nitroaniline

B) Multiple stage preparations(any 2)

1) Glycine to Hippuric acid to Azalactone to 4-Benzylidene 2-phenyl oxazol-5-one
2) Aldehyde to benzoin to benzil to benzilic acid
3) Acetanilide to *p*-acetamidobenzene sulphonyl chloride to *p*-acetamidobenzene sulphonamide to sulphanilamide.
4) D-glucose to 1,2,5,6-Di-*O*-isopropylidene-α-D-glucofuranose to S-methyl dithiocarbonate derivative to 3-deoxy-1,2,5,6-Di-*O*-isopropylidene-α-D-glucofuranose.

M. Sc. - II Organic Chemistry
Semester – IV
CHO–5401 Chemistry of Natural Products-I
(48 L+ 12 T) (4 Credit)

1. Isolation of Natural Products (5 L)

1.1 General methods of isolation and purification:

i) Extraction and fractionation- Maceration, enfleurage, Soxhlet extraction, supercritical fluid extraction, extraction with solvents, hydrodistillation, steam distillation

ii) General methods of separation/purification:

Separation by chromatographic techniques: column chromatography, ion exchange and charcoal chromatography, Size exclusion chromatography, HPLC,

Ref. 1-8

2. Methods of structure determination of Natural Products (5 L)

Chemical methods: Based on functional group- Bicarbonate extraction, sodium bisulphite adduct formation, derivatization of functional group; degradation of alkaloids- Emde's degradation, etc.

Physical/Spectral methods: UV, IR, NMR spectroscopy, MS spectrometry, optical polarimetry, XRD.

Ref. 1-8

3. Synthesis and Structure elucidation involving stereochemistry, spectral and chemical methods (14 L)

3.1 Terpenoids: Menthol (Takasago) and Caryophyllene (E J Corey)

3.2 Alkaloids: Reserpine (R B Woodward)and morphine (Marshall Gates)

3.3 Prostaglandins: Prostaglandins E_2(E. J. Corey)

3.4 Antibiotics: Cephalosporin (R B Woodward)

Ref. 1-8

4. Biogenesis of natural products (20 L)

4.1. Terpenoids and Steroids – Mono, Sesqui, Di, Triterpenoids

Steroids: biosynthesis of cholesterol- mevalonic acid pathway

4.2. Alkaloids

a) Derived from ornithine- hygrine, cocaine, tropine, cuscohygrine, hyoscymine, retronecine,
b) Derived from Lysine-anaferin, lobeline, piperine, pelletierine, lupinine,
c) Derived from Tyrosine- mescaline, anhalonine, reticuline, thebaine, codeine, morphine, emetine, cephaeline,
d) Derived from nicotinic acid- biosynthesis of nicotinic acid, biogenesis of nicotine, nornicotine
e) Derived from tryptophan- psilocin, Harman, harmine, ajmalicine, yohimbine, cinchonine, quinidine, camptothecin, lysergic acid.

Ref. 9, 10,11

5. Mechanisms in biological chemistry (4 L)

Mechanisms involving NAD/NADP to NADH/NADPHreductive amination in nature, nature's acyl anion equivalent, shikimic acid pathway, oxidation with FAD.

Ref. 1

References:

1. Pharmaceutical, medicinal and natural product Chemistry-P.S. Kalsi and Sangeeta Jagtap
2. Chemistry of natural products, a laboratory handbook- N. R. Krishnaswamy
3. Chemistry of natural products- S. V. Bhat, B. A. Nagasampagi, M. Sivakumar
4. Principles of organic synthesis by R. O. C. Norman and J.M.Coxon; Chapman and Hall
5. Classics in organic synthesis – K. C. Nicolaou & E. J. Sorensen
6. Natural products chemistry, sources, separations and structures- Raymond Cooper, George Nicola
7. Chemistry of plant natural products,stereochemistry, conformation, synthesis, biology and medicine- Sunil Kumar Talapatra and Bani Talapatra
8. Organic chemistry vol 2- Stereochemistry and chemistry of natural products- I. L. Finar
9. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley)
10. Secondary metabolism - J. Mann, 2nd edition.
11. Chemical aspects of Biosynthesis – J. Mann (1994).
12. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)

CHO-5402: Advanced Synthetic Organic Chemistry
(48 L+ 12 T) (4 Credit)

Transition metal complexes in organic synthesis: only Pd, Ni, Co, Fe (Metal mediated C-Cand C-X bond formation reactions): Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada,Hiyama, Negishi, Buchwald-Hartwig, Reppe Ref. 1-6

(14 L)

1. **C=C bond formation reactions:** Wittig, Horner-Wordworth-Emmons,McMurryShapiro, Bamford-Stevens,Julia-Lythgoe and Peterson olefination reactions,Titanium-carbene mediated olefination: Tebbe, Petasis. Ref. 2, 3, 4, 5, 7 **(8 L)**

2. **Click chemistry other important reactions:** criterion for click reaction, Sharpless azides cycloadditions and other ring formation reactions: Pausan-Khand, Bergman. Corey-Chaykovsky Reaction, Mitsunobu reaction. Ref. 8, 10 **(4 L)**

3. **Metathesis:** Grubbs 1st and 2st generation catalyst, Olefin cross coupling (OCM), ring closing(RCM) and ring opening (ROM) metathesis, Shrock catalysts, Buchwald catalysts, Knowels catalyst of Ruthenium and Rhodium – synthesis and uses its use in hydrogenation reactions-deallylation, C-C, C-O, C-N bond cleavages. Ref. 4, 5, 8 **(10 L)**

4. **Organoboranes:** reactions of organoborane reagents e.g. RBH_2,R_2BH,R_3B,9-BBN,catechol borane. Thexyl borane, cyclohexyl borane, $ICPBH_2$, IPC_2BH,Hydrboration-mechanism, stereo and regeoselectivity, uses in synthesis of primary,secondary tertiary alcohols, aldehydes, ketones, alkenes. Synthesis of EE, EZ, ZZ dienes andalkyenes. Mechanism of addition of IPCBH. Allyl boranes- synthesis, mechanism and uses.
   Use of Silicon in organic synthesis reaction Ref. 2, 4, 9 **(8 L)**

5. **Green Chemistry:**Introduction, Twelve principles of green chemistry, atom ecomony, Organic synthesis using crown ethers, PTC, ionic liquids, fluorous phase technique, nanoparticles in organic chemistry-synthesis of arylidenebarbituric acid, Prins condensation reaction of β-pinene and paraformaldehyde. Ref. 11-15 **(4 L)**

References:

1. Organic synthesis using transition metals-Roderick Bates (Wiley)
2. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
3. Designing of organic synthesis – S. Warren (Wiley)
4. Some modern methods of organic synthesis – W. Carruthers (Cambridge)
5. Organic synthesis – Michael B. Smith
6. Organometallics in organic synthesis – J. M. Swan and D. C. Black (Chapman and Hall)
7. Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007)
8. Guidebook to organic synthesis-R. K.Meckie, D. M. Smith and R. A. Atken
9. Organic synthesis- Robert E Ireland
10. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako
11. New Trends in Green Chemistry- V.K. Ahluwalia, M. Kidwai

12. Green Chemistry: Environmentally Benign Reaction- V. K. Ahluwalia
13. Green Solvents for Organic Synthesis- V. K. Ahluwalia, Ranbir S. Varma
14. Organic Synthesis: Special Techniques- V. K. Ahluwalia, Renu Aggarwal
15. Mini-review: Ferrite nanoparticles in the catalysis. *Arabian Journal of Chemistry*, **2019**, *12*, 1234-1246

CHO-5403: Biomolecules, Org chemistry of drug design and chiral drugs (48 L+ 12 T) (4 Credit)

1. Advanced carbohydrates (8 L)

Monosaccharides: Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of Glucose, conformation and anomeric effects in hexoses, mutarotation,glycoside formation, acetonide formation, reduction, synthesis of D-glyceraldehyde, Killani-Fischer Synthesis, glucal formation and reactions,Hanesian Reaction, Ferrier rearrangement.

Disaccharides: Maltose, lactose, sucrose and their hydrolysis

Polysaccharides: Starch, end group analysis of amylose. Ref. 1, 2, 6

2. Chiron approach (8 L)

a) Introduction

b) The concept of chiral templates and chirons wherein the carbon skeleton is the chiral precursor.

c) Utilisation of the basic concepts for retrosynthetic strategy and synthesis ofthe following: (S) Propanediol, (R) and (S)-Epichlorohydrin, L (+)-Alanine, (-) Multistratin, (-) Pentenomycin, (-) Shikimic acid, Carbonolide BRef. 1,2,3

3. Amino acids, proteins, enzymes, and lipids (8 L)

Introduction to α-amino acids: acidic, basic, neutral, Streckersynthesis,modifiedGabriel synthesis, Erlenmeyer synthesis, reaction of amino acid with ninhydrin.

Introduction to proteins, calculation of weight of polypeptide, N-terminal amino acid determination, Carboxy-terminal amino acid determination, Edman degradation of peptides,sequence determination, synthesis of peptide: Merrifield solid-phase synthesis

Enzyme classification with their role in organic synthesis, Factors enhancing rate of enzyme catalyzed reactions, working of citrate synthase enzyme. Ref. 4, 5

4. Organic Chemistry of Drug Design

Organic chemistry of drug design and drug action-quantitative structure activity relationship Hammet equation, Taft equation Hansch analysis-derivations and application in drug design, illustration with examples **(4 L)**

Lypophilicity effect measurement of lipophilicities identification of active part molecular graphics and lead modifications **(2 L)**

SAR by mass and NMR **(2 L)**

Combinatorial chemistry- general aspects, split synthesis, peptide and non-peptide libraries **(2 L)**

Drug receptor interactions enzyme inhibitor and drug target **(4 L)**

Ref. 7-14

5. Chiral Drugs (10 L)

a) Introduction of chiral drugs, Eutomer, Distomer and eudesmic ratio

b) Distomers -i) with no side effects ii) with undesirable side effects

c) Synthesis of some drugs: Propanolol, Diazepam, Adrenaline, Omeprazole, S-Ibuprofen, S-Metaprolol, Captopril. Ref. 15,16

References:

1. Organic Chemistry – R. P. Morrison and R. N. Boyd
2. Organic Chemistry – I. L. Finar, volume II
3. Chiron Approach in organic synthesis – S. Hanessianh
4. Chemistry of Natural Products: Amino Acids, Peptides, Proteins, and Enzymes- V. K. Ahluwalia, Lalita S. Kumar, Sanjiv Kumar
5. Organic Chemistry- John McMurry
6. Organic Chemistry- Morrison and Boyd
7. Medicinal Chemistry an Introduction-Gareth Thomas 2nd Ed. Wiley
8. An introduction to medicinal chemistry-Graham L. Patrick 5nd Ed. Oxford
9. Introduction to Medicinal Chemistry-Alex Gringauz (Wiley)
10. Foye's Medicinal Chemistry
11. Medicinal Chemistry-A. Burger
12. Medicinal Chemistry-Ashutosh Karr
13. Pharmaceutical, medicinal and natural product Chemistry-P.S. Kalsi and Sangeeta Jagtap
14. Chemistry of natural products- S. V. Bhat, B. A. Nagasampagi, M. Sivakumar
15. Pharmaceutical Chemistry and drug synthesis –Rot and Kleeman
16. Drug Design –E.J. Arienes

CHO-5404: Organic stereochemistry II and Asymmetric Synthesis (48 L+ 12 T) (4 Credit)

1. Organic Stereochemistry-II

a) Resolution of racemic modification. Ref. 1, 4 **(7 L)**
b) Geometrical Isomerism and Stereochemistry of olefins. Ref.1, 2 **(12 L)**
c) Determination of stereochemistry organic compounds using NMR. **(5 L)**
Ref. 3 Chapters 32 (1st Edition)

2. Principles and applications of asymmetric synthesis: (24 L)

Asymmetric Synthesis: Brief introduction, the chiral pool-nature's "readymade" chiral centerstereoselective aldol reactions, predicting relative stereochemistry through T.S. model Zimmer-Traxler, Specific reactions: Evan's aldol, Mukaiyama, Masamune, Cram's rule, Felkin Anh rule, Cram's chelate model, Conforth model, Cieplak model Asymmetric synthesis, use of chiral auxiliaries: oxazolidinone and norephedrine-derived, chiral reagents and catalysts: preparation and use of CBS asymmetric reducing agent, Baker's yeast reduction, asymmetric hydrogenation, Sharpless asymmetric epoxidation/dihydroxylation.
Synthesis of propranolol/chloroamphenicol.Enantioselective carbonyl reductions: BINAP based Noyori type, CBS reaction, Brown reaction, Knowle's catalyst of Ruthenium and Rhodium- synthesis and uses its using hydrogenation reactions-deallylation, C-C, C-O, C-N bond cleavages .
Ref. 3 chapters 33, 34, 35

References:

1. Stereochemistry of carbon compounds - E. L. Eliel
2. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen
3. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers 1st. Ed.
4. Stereochemistry of organic compounds –Nasipuri

Practical course III

CHO-5405: Innovative experiments in organic chemistry [4 credits]

At least sixteen experiments should be carried out on micro scale.

1) Phase transfer catalyst-
    a) Oxidation of benzyl alcohol with hypochlorite solution
    b) Flavone from o-hydroxyacetophenone and benzoylchloride.
2) Microwave
    a) *o*-Phenylene diamine to Benzimidazole
    b) $KMnO_4$ oxidation of toluene
3) Photochemical
    a) Benzophenone to benzopinacol
    b) Dimerization of cinnamic acid to truxillic acid.
4) Enzyme catalysed reactions
    a) Sucrose to ethyl alcohol (Baker's yeast)
    b) Asymmetric reduction of EAA by using Baker's yeast
    c) Hydrolysis of cane sugar using invertase enzyme
5) Solid state reactions
    a) Preparation of 1, 1-bis-2-naphthol under grinding at room temperature.
    b) Solvent free aldol condensation between 3,4-dimethoxybenzaldehyde and 1-indanone
    c) Solvent free quantitative solid phase synthesis of azomethines from substituted anilines and substituted benzaldehydes
    d) Benzil Benzilic acid rearrangement under solvent free condition
6) Water mediated reaction
    a) [4+2] cycloaddition reaction in aqueous medium at room temperature
    b) Glucose to glucosazone
7) Ionic liquid mediated reaction
    a) Preparation of5-arylidene barbiturate using [Bmim]OH
    (Knovengel condensation)
8) Reactions using nanoparticles
    a) Preparation of ZnOnanoparticle
    b) Claisen Schmidt condensation using ZnOnanoparticle
9) To understand the atom economy
    a) Preparation of chalcone using conventional method
    b) Preparation of chalcone using green method
    c) Calculation of atom economy
10) Use of green catalysts
    a) Benzoin condensation using thiamine hydrochloride
    b) Clay catalyzed solid state synthesis of 7-hydroxy-4-methylcoumarin
    c) Bromination of *trans*-stilbene using sodium bromide and sodium bromated.
    d) Ecofriendly nitration of phenols and its derivatives using Calcium nitrate .

11) **Report on industrial visit or study tour.**

Reference:

1. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia and Renu Aggarwal
2. A text book of practical organic chemistry by A. I. Vogel, ELBS and Longman group.
3. Laboratory manual of organic chemistry by R. K. Bansal
4. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry Task Force Committee, DST
5. Practical organic chemistry by Mann and Saunders, ELBS and Longman group

Practical course IV

CHO- 5406: Project work [4 credits]

This is mandatory for every student to undertake the project work on selected area of study under the guidance of project coordinator. Student must carry out entire experimental work within the stipulated time and present it briefly in the form of the dissertation at the time evaluations.