

**ANDHRA UNIVERSITY**  
**DEPARTMENT OF ORGANIC CHEMISTRY & FDW**  
**Revised Syllabus for M.Sc Chemistry (Organic chemistry specialization)**  
**(With effect from the Admitted batch of 2021-2022 Academic Year)**

**Programme objectives:**

1. To provide students in the scientific skills and chemical knowledge essential to develop and apply the knowledge in chemical sciences for preparing chemists of exceptional skills and abilities.
2. To provide knowledge, application, skills in required areas of chemical education
3. To equip students with effective scientific communication skills
4. To encourage the pursuit of lifelong education
5. To develop each student into a committed individual with ethical and social responsibility

**Programme Specific objectives:**

The students who complete the M.Sc. Organic Chemistry course shall:

1. Have strong foundation in the fundamentals and applications of chemical knowledge and understanding
2. Have the abilities to think critically, logically and analytically and solve problem in the area of chemical sciences, materials, environmental aspects, medicines and energy
3. Have the abilities to carry out chemical experiments, record and analyze the results and design advanced models
4. Have the abilities to use modern library and information retrieving tools to obtain information and assimilate to generate concepts and apply them in challenging situations
5. Have the abilities to effectively communicate their knowledge and skills to other chemists and non-chemists in oral or written formats
6. Secure suitable employment in the areas of chemical industries like pharmaceutical, steel and metals, polymers, fuels and nuclear, environmental and pollution control, nanotechnology and composite materials, teaching and research, etc.
7. Have the personal attributes and ethical sensibilities to enable them to function as effective scientists and citizens

M.Sc. Chemistry (Final Year)  
**Specialization: ORGANIC CHEMISTRY**  
 Syllabus (w.e.f.2021-22 admitted batch)

Scheme of Instruction and Examination for **III Semester**

S.No.	Course Title	Course Type	Instruction Periods per week	External Marks	Internal Marks	Total Marks	Duration of External Examination	Credits
1	Paper-I: Organic Reaction Mechanisms, Pericyclic Reactions and Photochemistry	Theory	4	80	20	100	3 hours	4
2	Paper-II: Organic Spectroscopy	Theory	4	80	20	100	3 hours	4
3	Paper-III: Organic Synthesis	Theory	4	80	20	100	3 hours	4
4	Paper-IV: Chemistry of Natural Products	Theory	4	80	20	100	3 hours	4
5	Practical - I: Multi Stage Organic Synthesis	Lab	3	80	20	100	6 hours	4
6	Practical - II: Chromatography & Viva-Voce	Lab	3	80	20	100	6 hours	4
7	MOOCs Course	-				-	-	2
		Total:				600		26

Scheme of Instruction and Examination for **IV Semester**

S.No.	Course Title	Course Type	Instruction Periods per week	External Marks	Internal Marks	Total Marks	Duration of External Examination	Credits
1	Paper-I: Modern Synthetic Methodology in Organic Chemistry	Theory	4	80	20	100	3 hours	4
2	Paper-II: Organic Spectroscopy and Structure determination of Natural Products	Theory	4	80	20	100	3 hours	4
3	Paper-III: Designing Organic Synthesis and Synthetic Applications of Organo-Boranes and silanes	Theory	4	80	20	100	3 hours	4
4	Paper-IV: Drug Design and Drug Chemistry	Theory	4	80	20	100	3 hours	4
5	Project Work	Lab	-	100	-	100	-	4
5	Practical - I: Organic Mixture Analysis	Lab	3	80	20	100	6 hours	4
6	Practical - II: Estimations and Isolation	Lab	3	80	20	100	6 hours	4
8	Viva-Voce	-	-	-		50	-	2
9	MOOCs Course	-				-	-	2
		Total:				750		32

M.Sc. Chemistry (First Year)  
SEMESTER I  
Paper III- Organic Chemistry  
(w.e.f. 2021-22 admitted batch)

Scheme of Instruction and Examination for **I Semester**

Course code	Course Title	Course type (Theory/ Practical)	Instruction periods per week	Internal Marks	External Marks	Total Marks	Duration of Examination	Credits
	General Chemistry-I	Theory	04	20	80	100	3 hrs	04
	Inorganic Chemistry-I	Theory	04	20	80	100	3 hrs	04
	Organic Chemistry-I	Theory	04	20	80	100	3 hrs	04
	Physical Chemistry-I	Theory	04	20	80	100	3 hrs	04
	Inorganic Chemistry Laboratory-1	Practical	06	15	60	75	3 hrs	03
	Physical Chemistry Laboratory-1	Practical	06	15	60	75	3 hrs	03
	Organic Chemistry Laboratory-1	Practical	06	15	60	75	3 hrs	03
		Total	34					25

Scheme of Instruction and Examination for **II Semester**

Course code	Course Title	Course type (Theory/ Practical)	Instruction periods per week	Internal Marks	External Marks	Total Marks	Duration of Examination	Credits
	General Chemistry-II	Theory	04	20	80	100	3 hrs	04
	Inorganic Chemistry-II	Theory	04	20	80	100	3 hrs	04
	Organic Chemistry-II	Theory	04	20	80	100	3 hrs	04
	Physical Chemistry-II	Theory	04	20	80	100	3 hrs	04
	Inorganic Chemistry Laboratory-1I	Practical	06	15	60	75	3 hrs	03
	Physical Chemistry Laboratory-II	Practical	06	15	60	75	3 hrs	03
	Organic Chemistry Laboratory-1I	Practical	06	15	60	75	3 hrs	03
		Total Number of credits						25

**M.Sc., CHEMISTRY (Organic Chemistry Specialization)**  
**SEMESTER – I SYLLABUS**  
**(From the batch admitted during the academic year 2021-2022)**

**PAPER III - ORGANIC CHEMISTRY**

**Course Objectives: To make the students**

- CO 1: Acquire the knowledge of aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- CO 2: Understand aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- CO 3: Apply the knowledge and understanding of aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products to new situations
- CO 4: Develop interest in the areas of aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products

**Learning Outcomes:** At the end of the course, the learners should be able to:

- LO 1: Explain aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- LO 2: Interpret aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- LO 3: Compare aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- LO 4: Analyse aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- LO 5: Solve aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- LO 6: Identify aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products
- LO 7: Apply aliphatic nucleophilic, aliphatic electrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products

## UNIT - I

**Aliphatic Nucleophilic Substitutions:** The  $S_N2$ ,  $S_N1$ ,  $S_Ni$  and SET mechanisms. Substitution reactions of ambident nucleophiles, anchimeric assistance, the neighbouring group mechanism: neighbouring group participation by O, N, S, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acyclic and bicyclic systems (Non- classic carbocations). Nucleophilic Substitution at allylic, trigonal and Vinylic carbons. Effect of substrate, attacking nucleophile, leaving group and reaction medium.

## UNIT-II

**Aliphatic Electrophilic Substitutions:**  $SE1$   $SE2$  and  $SEi$  mechanisms. Reactivity-effects of substrate, leaving group and solvent. Reactions- hydrogen exchange, migration of doublebonds, halogenation of aldehydes, ketones, carboxylic acids, acyl halides, sulfoxides and sulphones.

## UNIT-III

**Stereochemistry and Conformational Analysis :** Optical Isomerism: optical activity, molecular dissymmetry and chirality - elements of symmetry. Fisher's projection D,L. and R,S. configurations - relative and absolute configurations optical isomerism due to asymmetric carbon atoms - optical isomerism in biphenyls, allenes and spirans- optical isomerism of nitrogenous compounds, racemisation and resolution. Geometrical isomerism: E, Z -configurations, properties of geometrical isomers. Conformational analysis: Conformations of acyclic molecules –alkanes and substituted alkanes- compounds having intramolecular hydrogen bonding. Conformations of cyclohexane, mono and disubstituted cyclohexanes and decalins, effect of conformations on reactivity.

## UNIT-IV

**Chemistry of Heterocyclic Compounds :** Structure, reactivity and synthesis of three membered Heterocycles: (a) Oxirane: Sharpless method, Shi epoxidation, Jacobsen epoxidation, etc, (b) Aziridine; four membered Heterocycles: (a) Oxetane (b) Azetidine; five membered Heterocycles: (a) Pyrrole: Paal Knorr, Hantzsch Methods, etc, (b) Thiophene: Paal Knorr, Hinsberg method, etc. (c) Furan: Paal Knorr, Fieser-Benary, Industrial Method, etc.; (d) Pyrazole, (e) Imidazole, (f) Oxazole, (g) Thiazole; Six membered Heterocycles: (a) Pyridine, (b)Pyridazine,(c) pyrimidine and (d) Pyrazine; Aromatic heterocyclics: a) Indole: Fischer indole synthesis, Bischler synthesis, and Madelung synthesis (b) Quinoline and Isoquinoline, (c) Coumarins and Chromones.

## UNIT-V

### **Chemistry of Natural Products:**

**A) Terpenoids:** - Occurrence, Isolation, isoprene rule, structure elucidation and synthesis of  $\alpha$ - Terpineol and  $\alpha$ - pinene

**B) Steroids:-** Nomenclature of steroids, structure elucidation, synthesis and stereochemistry of cholesterol and progesterone

**C) Lipids:-** Classification, properties and function-free fatty acids, triglycerides, phospholipids, glycolipids & waxes conjugated lipids-lipoproteins

### **Reference Books**

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March,  
Mc.Graw Hill and Kogakush.
2. Organic Chemistry Vol. I (Sixth Ed.) and Vol. II (Fifth Ed.) by I L Finar ELBS.
3. Organic Chemistry (fifth Ed., ) by Morrison and Boyd, PHI, India.
4. Organic Chemistry (fifth edition) by Francis A. Carey Tata Mc Graw Hill publishing  
Company Limited, New Delhi.
5. Stereochemistry of Organic compounds by Ernest L. Eliel, Samuel H. Wilen
6. Chemistry of natural products by S. V. Bhat, B. A. Nagasampangi and M. Sivakumar  
Narosa Publishing House, 6th reprint 2010

**M.Sc., CHEMISTRY (Organic Chemistry Specialization)**  
**SEMESTER – II SYLLABUS**  
**(From the batch admitted during the academic year 2021-2022)**

**PAPER III - ORGANIC CHEMISTRY**

**Course Objectives: To make the students**

- CO 1: Acquire the knowledge of aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- CO 2: Understand aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- CO 3: Apply the knowledge and understanding of aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids to new situations
- CO 4: Develop interest in the areas of aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

**Learning Outcomes: At the end of the course, the learners should be able to:**

- LO 1: Explain aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- LO 2: Interpret aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- LO 3: Compare aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- LO 4: Analyse aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- LO 5: Solve aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- LO 6: Identify aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids
- LO 7: Apply aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

**UNIT-I: Aromaticity****[12 Hours]**

**A) Aromaticity:** Concept of Aromaticity, Aromaticity of five membered, six membered and fused systems - non-benzenoid aromatic compounds: cyclopropenylcation, cyclobutadienyldication, cyclopentadienyl anion – tropyliumcation and cyclooctatetraenyl di anion – metallocenes, ferrocenes, azulenes, fulvenes, annulenes, fullerenes. Homo aromaticity, Anti aromaticity and Pseudo aromaticity.

**B) Aromatic Nucleophilic Substitutions:** The S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne and S<sub>RN</sub>1 mechanisms. Reactivity: Effect of substrate, leaving group and attacking nucleophile. The Von-Richter, Sommelet-Hauser and Smiles rearrangements.

**UNIT-II: Reactive Intermediates and Name Reactions****[12 Hours]**

**A) Reactive Intermediates:** Generation, structure, stability and reactivity of Reactive intermediates: carbanion, carbocation, free radicals, carbenes and nitrenes.

**B) Name Reactions:** - Wittig reaction, Grignard reaction, Stork enamine reaction, Michael addition, Mannich Reaction, Diel's-Alder reaction and Ene- reaction,

**UNIT-III: Molecular Rearrangements****[12 Hours]****Molecular Rearrangements:**

Types of molecular rearrangements, migratory aptitude;

**Rearrangements to electron deficient carbon:** Pinacol-pinacolone, Wagner-Meerwein and Benzil-Benzilic acid,

**Rearrangements to electron deficient nitrogen:** Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements;

**Rearrangements to electron deficient oxygen:** Baeyer-villiger, Dakin rearrangements;

**Other rearrangements:** Neber rearrangement and Favorskii rearrangements

**UNIT - IV: Spectroscopy****[12 Hours]**

**A) UV Spectroscopy:** Various electronic transitions, selection rules, effect of solvent on electronic transitions, the absorption laws, chromophores, auxochromes, bathochromic and hypso chromic shifts, hyperchromic and hypochromic effects, Woodward-Fieser rules for conjugated dienes and carbonyl compounds.

**B) Infrared Spectroscopy:** Basic principles: types of molecular vibrations, fingerprint region and identification of functional groups.

**C) Nuclear Magnetic Resonance Spectroscopy (<sup>1</sup>H-NMR):** nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shifts, factors affecting the chemical shift, and assignment of chemical shifts.

**D) Mass Spectroscopy:** Basic principles, nitrogen rule and fragmentation pattern of carbonyl compounds and alcohols

**UNIT – V Alkaloids, Peptides, Proteins and Nucleic acids****[12 Hours]**

**A) ALKALOIDS:** Occurrence, Isolation, classification based on nitrogen heterocyclic ring and synthesis of quinine and nicotine

**B) Peptides and Proteins:** α-Amino acids, their general properties and synthesis, Synthesis of peptides by Merrifield solid phase synthesis. Primary, secondary and tertiary structures of proteins

**C) Nucleic acids:** Heterocyclic bases; Purines: Adenine and Guanine; Pyrimidines: Cytosine, Uracil and Thymine; nucleosides, nucleotides Basic concepts of the structures of RNA and DNA



**Text books:**

1. Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Edn.) by I.L. Finar ELBS.
2. Organic Chemistry (fifth Edn., ) by Morrison and Boyd, PHI, India.
3. Organic Chemistry (fifth edition) by Francis A. Carey Tata McGraw Hill publishing Company Limited, New Delhi.
4. Reaction Mechanism in Organic Chemistry by Mukherjee Sirigh, N Ternitarr, Indiar
5. A guide book to mechanism in Organic Chemistry by Peter Sykes, ELBS.
6. Advanced organic chemistry by Jerry March (4th Edition)Wiley Eastern. .
7. Stereochemistry of carbon compounds by E.Eliel, John Wiley & Sons, Inc.
8. Stereochemistry of Organic compounds by D. Nasipuri.  
Chemistry of Natural products by R.S. KalsiKalyani Publ

**M.Sc., CHEMISTRY (Organic Chemistry Specialization)**  
**SEMESTER – III SYLLABUS**  
**(From the batch admitted during the academic year 2020-2021)**

**PAPER I - ORGANIC REACTION MECHANISMS, PERICYCLIC REACTIONS  
AND PHOTOCHEMISTRY**

**Course Objectives: To make the students**

- CO 1: Acquire the knowledge of reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- CO 2: Understand reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- CO 3: Apply the knowledge and understanding of new situations reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- CO 4: Develop interest in the areas of reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry

**Learning Outcomes:** At the end of the course, the learners should be able to:

- LO 1: Explain reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- LO 2: Interpret reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- LO 3: Compare reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- LO 4: Analyse reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- LO 5: Solve reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- LO 6: Identify reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry
- LO 7: apply reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry

**UNIT-I: Radical Substitution Reactions**

**[12 Hours]**

Reactivity for aliphatic substrates, reactivity at Bridgehead, Reactivity in aromatic substrates, neighbouring group assistance in free radical reactions, reactivity in the attacking radical, effect of solvent on reactivity, halogenation at an alkyl carbon and allylic carbon, hydroxylation at aromatic carbon by means of Fenton's reagent, formation of cyclic ethers with Pb (OAc)<sub>4</sub>, Hunsdiecker reaction, Kolbe reaction, Reed reaction and Sandmeyer reaction.

**UNIT-II: Elimination Reactions:**

**[12 Hours]**

Mechanisms of E<sub>2</sub>, E<sub>1</sub>, and E1CB, factors-effects of substrate, attacking base, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems. Saytzeff elimination, Hoffman elimination and pyrolytic elimination.

**UNIT-III: Addition Reactions:**

**[12 Hours]**

(a) **Addition to carbon-carbon multiple bonds-** Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms. Stereochemistry and reactivity. Hydrogenation of double and triple bonds, Birch reduction, Hydroboration, Michael reaction, Prins reaction. Addition of oxygen and N<sub>2</sub>O<sub>4</sub>.

(b) **Addition to carbon-hetero atom multiple bonds:** Mechanism and reactivity. Reductions of carbonyl compounds, carboxylic acids, esters, nitriles. Addition of Grignard reagents, Mannich reaction, Reformatsky reaction, Tollen's reaction, Wittig reaction,

**UNIT-IV: Pericyclic reactions:**

**[12 Hours]**

Molecular Orbital Symmetry, MO diagrams of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene and allyl system. Woodward- Hoffman correlation diagram method, Frontier molecular orbital approach (FMO) and Perturbation molecular orbital approach (PMO) for the explanation of pericyclic reactions under thermal and photochemical conditions.

Classification of pericyclic reactions: **Electrocyclic Reactions:** Conrotatory and Disrotatory motions.  $4n\pi$  and  $4n+2\pi$  electrons systems. **Cycloadditions:** Antarafacial and Suprafacial additions. 2+2, 4+2 cycloadditions and chelotropic reactions. **Sigmatropic rearrangements** - Suprafacial and Antarafacial shifts of H, Sigmatropic shift involving carbon moieties (1,3), (1,5), (3,3) and (5,5) sigmatropic rearrangements. Claisen, Cope, Oxy-cope and aza- Cope rearrangements. Ene reaction.

**UNIT-V: Organic Photochemistry:**

**[12 Hours]**

Photochemistry of carbonyl compounds-  $n\pi^*$  and  $\pi\pi^*$  transitions. Norrish type I and Norrish type II cleavages. Paterno-Buchi reactions, Photoreduction, Photo chemistry of  $\alpha,\beta$ -unsaturated ketones, photochemistry of enones and cyclohexadienones. Photochemistry of unsaturated systems (Olefins): cis-trans isomerisation, dimerization, and addition. Acetylenes- dimerisation. Photochemistry of 1,3 butadienes, di- $\pi$ -methane rearrangement. Photochemistry of aromatic compounds – 1,2, 1,3, and 1,4- additions. Photo-Fries rearrangement, Photo-Fries reactions of anilides.

**Text Books:**

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
2. Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
3. Pericyclic reactions by S.N. Mukharji, Mcmilan.
4. Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Richgardsen.
5. The modern structural theory in Organic Chemistry by L.N.Ferguson, Pretice Hall

## PAPER II- ORGANIC SPECTROSCOPY

### Course Objectives: To make the students

- CO 1: Acquire the knowledge of UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- CO 2: Understand UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- CO 3: Apply the knowledge and understanding of new situations UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- CO 4: Develop interest in the areas of UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained

### Learning Outcomes: At the end of the course, the learners should be able to:

- LO 1: Explain UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- LO 2: Interpret UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- LO 3: Compare UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- LO 4: Analyse UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- LO 5: Solve UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- LO 6: Identify UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained
- LO 7: Apply UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained

### UNIT-I: UV SPECTROSCOPY:

[12 Hours]

UV spectra of aromatic and heterocyclic compounds,  $\alpha$ -diketones,  $\beta$ -diketones, enediones and quinones. Applications of UV Spectroscopy-study of isomerism, determination of strength of hydrogen bonding and conformations of  $\alpha$ -substituted cyclohexanones. Steric effect in biphenyls.

### UNIT-II: Infrared Spectroscopy:

[12 Hours]

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, carbonyl compounds, esters, amides, carboxylic acids, anhydrides, lactones, lactams, nitriles and conjugated carbonyl compounds. Effect of hydrogen bonding and solvent on vibrational frequencies.

### UNIT-III: Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$ NMR):

[12 Hours]

Nuclear spin, resonance, saturation, shielding of magnetic nuclei, chemical shifts and its measurements, factors affecting chemical shift, chemical and magnetic equivalence of spins, spin-spin coupling, integration, the coupling constant, types of spin-spin couplings, factors influencing coupling constants, first-order and non-first order spectra, spin system notations (ABX, AMX, ABC,  $A_2B_2$  etc.). Simplification of non-first order spectra- use of higher magnetic fields, nuclear magnetic double resonance and contact shift reagents. Deuterium exchange, Nuclear Overhauser Effect difference spectra, Study of dynamic processes by Variable temperature (VT) NMR, restricted rotation DMF, cyclohexane ring inversion.

**UNIT-IV: Mass spectroscopy:****[12 Hours]**

Basic Principles, instrumentation, isotope abundance, the molecular ion, metastable ions, base peak, fragment ions, even-electron rule and nitrogen rule. McLafferty rearrangement, ortho effect. *retro*-Diels- Alder reaction, Fragmentation processes- fragmentation associated with various functional groups (alkanes, cycloalkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amides, amines, alkyl chlorides and alkyl bromides).

**UNIT-V: Application of UV, IR, NMR and MASS****[12 Hours]**

Structural elucidation of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral data.

**Text Books:**

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman

### PAPER III – ORGANIC SYNTHESIS

#### Course Objectives: To make the students

- CO 1: Acquire the knowledge of formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- CO 2: Understand formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- CO 3: Apply the knowledge and understanding of formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis to new situations
- CO 4: Develop interest in the areas of formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis

#### Learning Outcomes: At the end of the course, the learners should be able to:

- LO 1: Explain formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- LO 2: Interpret formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- LO 3: Compare formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- LO 4: Analyse formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- LO 5: Solve formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- LO 6: Identify formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis
- LO 7: apply formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis

#### UNIT-I: Formation of Carbon-Carbon (C-C) single bonds: [12 Hours]

Alkylations via enolate anions-1,3-dicarbonyl and related compounds, direct alkylation of simple enolates, imine and hydrozone anions, enamines. The aldol reaction, umpolung (dipole inversion). Via Organometallic reagents - organ palladium, organo nickel and organo copper reagents

#### UNIT-II: Formation of carbon-carbon double bonds: [12 Hours]

$\beta$ - Elimination reactions, Pyrolytic *syn* eliminations, alkenes form hydrazones, 1,2-diols, sulfones, sulfoxide-sulphonate rearrangement, the Wittig and related reactions

#### UNIT-III: Organic Polymers [12 Hours]

Introduction to organic polymers, general properties and classification of polymers. Methods of polymerization: (a) Addition polymerization-Definition, synthesis and applications, vulcanization. (b) Condensation polymerization- Definition, synthesis and applications. Radical polymerization. (With at least two examples in each category)

#### UNIT-IV: Reactions of unactivated carbon-hydrogen bonds [12 Hours]

Unactivated carbon-hydrogen bonds: Definition, mechanism and synthetic applications- The Hoffmann-Loeffler-Freytag reaction(HLF reaction)-cyclisation reactions of Nitrenes-the Barton reaction-Photolysis of organic hypohalites, hypochlorites, hypobromites and hypoiodites,

**UNIT-V: Asymmetric Synthesis****[12 Hours]**

Topocity – Prochirality – Substrate selectivity – Diastereoselectivity and enantioselectivity – Substrate controlled methods – use of chiral substrates – examples Auxiliary controlled methods – Use of chiral auxiliaries – Chiral enolates – alkylation of chiral imines-Reagent controlled methods – Use of chiral reagents – Asymmetric oxidation – Sharpless epoxidation – Asymmetric reduction – borate reagents.

**Text Books:**

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benjamin Inc. Menlo Park, California, 1972.
3. Principles of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
4. Advanced organic chemistry part A & B; Fourth edition; Francis A Cary and Richard J. Sundberg; Kluwer Academic/Plenum Publisher New York, 2000.
5. Organic chemistry Jonathan Clayden, Nick Greeves, Stuart Warren, 2nd Edition, 2012, Oxford University Press.
6. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri.
7. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen.
8. Stereochemistry: Conformation & Mechanism by P S Kalsi.
9. The third dimension in organic chemistry, by Alan Bassendale.
10. Stereo selectivity in organic synthesis by R S Ward.
11. Asymmetric synthesis by Noyori.
12. Asymmetric organic reactions by J D Morrison and H S Mosher.
13. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBÉ.

## PAPER IV – CHEMISTRY OF NATURAL PRODUCTS

### Course Objectives: To make the students

- CO 1: Acquire the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- CO 2: Understand isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- CO 3: Apply the knowledge and understanding of new situations isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- CO 4: Develop interest in the areas of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments

### Learning Outcomes: At the end of the course, the learners should be able to:

- LO 1: Explain isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- LO 2: Interpret isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- LO 3: Compare isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- LO 4: Analyse isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- LO 5: Solve isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- LO 6: Identify isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments
- LO 7: Apply isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, terpenes, alkaloids, flavonoids and natural pigments

### UNIT-I: Antibiotics

[12 Hours]

Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Penicillin G, Cephalosporin-C, Streptomycin, Chloramphenicol and Tetracycline

### UNIT-II: Terpenes

[12 Hours]

Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Terpenes: Forskolin, Taxol and  $\beta$ -amyrin

### UNIT-III: Alkaloids

[12 Hours]

Isolation, structure elucidation, stereochemistry, synthesis, and biological properties of Alkaloids: Morphine, Reserpine and Vincristine



**UNIT-IV: Flavonoids****[12 Hours]**

Natural Flavonoids: Apigenin, Flavanones - Hesperetin, Isoflavones - Genistein, Flavonol quercetin, xanthone - Euxanthone.

**UNIT-V: Natural Pigments:****[12 Hours]**

Natural Pigments: Introduction structure elucidation and synthesis of quinones-Polyporic acid. Chlorophyll and haemin.

**Text Books:**

1. Organic Chemistry, Volume 2, Stereochemistry and chemistry of natural products, I.L. Finar, 5th Edition. ELBS.
2. Chemical Aspects of Biosynthesis, John Mann, Oxford University Press, Oxford, 1996
3. Chemistry of Natural Products. A Unified Approach, N.R. Krishnaswamy, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
4. Chemistry of Natural Products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010.

**M.Sc., CHEMISTRY (Organic Chemistry Specialization)**  
**SEMESTER – IV SYLLABUS**  
**(From the batch admitted during the academic year 2020-2021)**  
**PAPER – 1: MODERN SYNTHETIC METHODOLOGY IN ORGANIC CHEMISTRY**

**Course Objectives: To make the students**

- CO 1: Acquire the knowledge of various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- CO 2: Understand various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- CO 3: Apply the knowledge and understanding of new situations various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- CO 4: Develop interest in the areas of various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions

**Learning Outcomes:** At the end of the course, the learners should be able to:

- LO 1: Explain various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- LO 2: Interpret various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- LO 3: Compare various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- LO 4: Analyse various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- LO 5: Solve various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- LO 6: Identify various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions
- LO 7: Apply various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions

**UNIT – I: Modern Synthetic Methods** **[12 Hours]**

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reaction.

**UNIT-II: Multi component Reactions:** **[12 Hours]**

Passerini reaction, Biginelli reaction, Hantzsch reaction and Mannich reaction. Metathesis: Grubb's 1st generation and 2nd generation catalyst, Olefin Cross coupling Metathesis (OCM), Ring Closing Metathesis (RCM), Ring Opening Metathesis (ROM) and applications.

**UNIT-III: Oxidation** **[12 Hours]**

Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents). (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. (d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) (g) ketones to ester/lactones (Baeyer-Villiger)

**UNIT-IV: Reduction****[12 Hours]**

Reduction: (a) Catalytic hydrogenation (Heterogeneous: Palladium/ Platinum/ Rhodium/ Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) (c) Hydride transfer reagents-NaBH<sub>4</sub> triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; LiAlH<sub>4</sub>, DIBAL-H, and Red-Al.

**UNIT-V: NEWER METHODS IN ORGANIC SYNTHESIS:****[12 Hours]**

**Green Chemistry:** Introduction, principles, atom economy and scope (illustrate with two examples) **Microwave induced reactions:** Principle conditions, advantages over conventional heating methods-applications **Ionic liquids:** Introduction and applications in organic synthesis (illustrate with two examples). **Nanomaterials:** Introduction, methods of preparation, applications in organic synthesis **Phase-transfer catalysis:** solid-solid, solid-liquid systems-mechanism of catalytic action, type of catalysts, application in few important reactions

**Text Books:**

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
4. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.
5. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley-VCH, New York, 2000.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
7. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
8. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis Elsevier Academic Press, 2005.
9. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner.
10. New trends in green chemistry By V.K. Ahluwalia and M. Kidwai.
11. Organic Synthesis: Special techniques. V.K. Ahluwalia and Renu Agarwal

## PAPER II - ORGANIC SPECTROSCOPY AND STRUCTURE DETERMINATION OF NATURAL PRODUCTS

### Course Objectives: To make the students

- CO 1: Acquire the knowledge of  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- CO 2: Understand  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- CO 3: Apply the knowledge and understanding of new situations  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- CO 4: Develop interest in the areas of  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy

### Learning Outcomes: At the end of the course, the learners should be able to:

- LO 1: Explain  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 2: Interpret  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 3: Compare  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 4: Analyse  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 5: Solve  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 6: Identify  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 7: Apply  $^{13}\text{C}$  and Heteronuclear, 2D NMR and Instrumentation, ESR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy

### UNIT-I: $^{13}\text{C}$ NMR spectroscopy [12 Hours]

Introduction,  $^{13}\text{C}$ -chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of  $^{13}\text{C}$  NMR spectra: Proton-coupled, proton-decoupled and OFF-resonance decoupled (ORD) spectra, DEPT.  $^{13}\text{C}$ -NMR solvents:

### UNIT-II: Heteronuclear NMR spectroscopy & Electron Spin Resonance Spectroscopy (ESR): Heteronuclear couplings: $^{13}\text{C}$ - $^1\text{H}$ , $^{13}\text{C}$ -D, $^{13}\text{C}$ - $^{19}\text{F}$ , $^{13}\text{C}$ - $^{31}\text{P}$ . $^1\text{H}$ -D, $^1\text{H}$ - $^{19}\text{F}$ , $^1\text{H}$ - $^{31}\text{P}$ , $^1\text{H}$ - $^{15}\text{N}$ ESR Spectroscopy: Principles, hyperfine splitting

### UNIT-III: NMR Instrumentation, 2D-NMR techniques [12 Hours]

**NMR Instrumentation:** Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation

**2D-NMR techniques:** Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY ( $^1\text{H}$ - $^1\text{H}$  COSY), Hetero COSY ( $^1\text{H}$ ,  $^{13}\text{C}$  COSY, HMQC), long range  $^1\text{H}$ ,  $^{13}\text{C}$  COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

**UNIT-IV: Optical Rotatory Dispersion (ORD) and CD Spectroscopy: [12 Hours]**

Optical rotation, circular birefringence, and circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Application of the rules to the study of absolute configuration and conformations of organic molecules.

**UNIT-V: Structure Determination of Natural Products by Spectral Methods [12 Hours]**

Structure elucidation - Spectroscopic techniques IR, UV,  $^1\text{H}$ -NMR,  $^{13}\text{C}$ -NMR, COSY, HETEROCOSY, and MS- natural products - Examples, flavones - Apigenin, flavanones- Hesperetin, isoflavones - Genistein, coumarins-7-hydroxycoumarin, alkaloids - morphine, quinine, terpenoids - (-)-Menthol, Steroids - stigmasterol, Glycosides - salicin (Alcoholic  $\beta$ -glucoside)

**Text books:**

1. Spectroscopy, fourth edition, D. L Pavia, G. M Lampman CENGAGE Learning, 2012
2. Spectroscopic Methods in Organic Chemistry. Forth Edition D. M. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990. For all spectral methods except ORD and CD and ESR.
3. Organic Spectroscopy, Second Edition, W. Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6<sup>th</sup> reprint 2010 (For IV<sup>th</sup> unit)
5. Applications of absorption spectroscopy of Organic Compounds J.R. Dyer, Prentice Hall of India, New Delhi, 1984.
6. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein: G.C.Vassillir and T.C. Merrill, John Wiley, Singapore, 1981.
7. For ORD and CD "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds)
8. K.W. Bentley and G.W.Kirby John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).

### **PAPER – III: DESIGNING ORGANIC SYNTHESIS AND SYNTHETIC APPLICATIONS OF ORGANO- BORANES AND SILANES**

#### **Course Objectives: To make the students**

- CO 1: Acquire the knowledge of the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- CO 2: Understand the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- CO 3: Apply the knowledge and understanding of new situations the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- CO 4: Develop interest in the areas of the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes

#### **Learning Outcomes:** At the end of the course, the learners should be able to:

- LO 1: Explain the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- LO 2: Interpret the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- LO 3: Compare the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- LO 4: Analyse the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- LO 5: Solve the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- LO 6: Identify the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes
- LO 7: Apply the principles of disconnection approach, synthetic strategies for one group and two group disconnection, organoboranes and organosilanes

#### **UNIT-I: Disconnection Approach – Principles [12 Hours]**

Introduction, Terminology: Retrosynthesis, Target Molecule (TM), synthon, synthetic equivalent, functional group interconversion (FGI). Linear and convergent synthesis. Criteria for selection of target. Order of events in retrosynthesis with reference to Salbutamol, Proparacaine and Dopamine. Chemoselectivity, Regioselectivity, reversal of polarity and cyclizations. Protecting groups- Principles of protection of alcohols, amine, carbonyl and carboxyl groups

#### **UNIT-II: Synthetic Strategies - One group Disconnections [12 Hours]**

Introduction to one group disconnections: C-C disconnection-alcohols and carbonyl compounds; C-X disconnections- alcohols and carbonyl compounds and sulphides two group C-C and C-X Disconnections.

#### **UNIT-III: Synthetic Strategies - Two group Disconnections [12 Hours]**

Introduction to Two group C-C disconnections; Diels-Alder reaction, 1,5- difunctionalised compounds, Michael addition and Robinson annulation. Two group C-X disconnections; 1, 1-difunctionalised, 1, 2-difunctionalised and 1, 3-difunctionalised compounds. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.

**UNIT –IV: Organoboranes****[12 Hours]**

Hydroboration- Preparation of Organoboranes. Reagents – dicyclohexyl borane, disiamyl borane, thexyl borane, 9-BBN and mono-, di-isopinocampheyl borane. Functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organo boranes- carbonylation, cyanoboration.

**UNIT –V: Organosilanes****[12 Hours]**

Preparation and synthetic applications of trimethylsilyl chloride, dimethyl-t-butylsilyl chloride, trimethylsilylcyanide, trimethylsilyliodide and trimethylsilyltriflate. Protection of functional groups - Trimethylsilylethers, Silylenolethers. Synthetic applications of  $\alpha$ -silyl carbanions,  $\beta$ -silyl carbonium ions. Peterson's olefination.

**Text Books:**

1. Organic syntheses via boranes / Herbert C. Brown; with techniques by Gary W. Kramer,
2. Alan B. Levy, M. Mark Midland. New York : Wiley, 1975
3. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
4. Organic Synthesis: The disconnection approach, S. Warratt John Wiley & sons, New York, 1984.
5. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benjamin Inc. Menlo Park, California, 1972.
6. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
7. Organic Synthesis: Special techniques. V.K.Ahluwalia and Renu Aggarwal.
8. Organic Synthesis by C Willis and M Willis
9. Problems on organic synthesis by Stuart Warren

## PAPER IV-DRUG DESIGN AND DRUG CHEMISTRY

### Course Objectives: To make the students

- CO 1: Acquire the knowledge of drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs, antineoplastic drugs, cardiovascular drugs, oral hypoglycaemic drugs, local anti-infective and antiviral drugs
- CO 2: Understand drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs, antineoplastic drugs, cardiovascular drugs, oral hypoglycaemic drugs, local anti-infective and antiviral drugs
- CO 3: Apply the knowledge and understanding of new situations drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs, antineoplastic drugs, cardiovascular drugs, oral hypoglycaemic drugs, local anti-infective and antiviral drugs
- CO 4: Develop interest in the areas of drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs, antineoplastic drugs, cardiovascular drugs, oral hypoglycaemic drugs, local anti-infective and antiviral drugs

### Learning Outcomes: At the end of the course, the learners should be able to:

- LO 1: Explain drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs
- LO 2: Interpret drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs
- LO 3: Compare drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs
- LO 4: Analyse drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs
- LO 5: Solve drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs
- LO 6: Identify drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs
- LO 7: Apply drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs

### UNIT I: Introduction to Drugs

[12 Hours]

General Classification, nomenclature, drug metabolism. Development of drugs: Procedure followed in drug design, concepts of lead compound lead modification, concept of prodrugs, Structure Activity Relationship (SAR)-factors affecting bio-activity-resonance, inductive effect, isosterism, bio-isosterism, spatial considerations, Quantitative Structure Activity Relationships (QSAR)-Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials.

### UNIT II: Antineoplastic Agents:

[12 Hours]

Introduction, classification-alkylating agents- mechanism and mode of action, nitrogen mustards-synthesis, properties, uses and dosage - Chlorambucil, cyclophosphamide and melphalan. Antimetabolites- synthesis, properties, uses and dosage-pyrimidine analogues-5-fluorouracil, purine analogues-6-mercaptopurine, folic acid analogues-Methotrexate. Antibiotics-structure, properties and dosage-Doxorubicin, Mitomycin.

### UNIT III: Cardiovascular Drugs:

[12 Hours]



Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

#### **UNIT IV: Oral Hypoglycaemic Drugs:**

**[12 Hours]**

Introduction, Classification, Sulphonylureas- synthesis, mode of action, properties, uses and dosage- tolbutamide, glipizide. Biguanides- synthesis, mode of action, properties, uses and dosage- Metformin.  $\alpha$ -glucosidase inhibitors- synthesis, mode of action, properties, uses and dosage- Miglitol. Dipeptidyl Peptidase-4 (DPP-4) inhibitors- synthesis, mode of action, properties, uses and dosage-saxagliptin and sitagliptin

#### **UNIT V: Local Anti-infective & Antiviral drugs**

**[12 Hours]**

Local Anti-infective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, fluconazole, econazole and chloroquin.

Antiviral Drugs: Introduction, classification based on mechanism of action, Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NRTIs)-Synthesis, metabolism, properties and uses and dosage-Acyclovir, Zidovudine (Anti-HIV agent). Non-Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NNRTIs)-Synthesis, metabolism, properties and uses and dosage-Nevirapine, Efavirenz. Protease Inhibitors (PIs)- Synthesis, metabolism, properties and uses and dosage-Indinavir. CCR5-Inhibitors- Synthesis, metabolism, properties and uses and dosage-Maraviroc

#### **Text Books:**

1. Text book of medicinal chemistry, Volume 1 & II, Third edition by V Alagarsamy, CBS-publishers
2. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH.
3. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
4. An Introduction to Drug Design, S. S. Pandeya and J. R. Dimmock, New Age International.
5. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter.-9 and Ch-14), Ed. M. E. Wolff, John Wiley.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
7. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
8. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

