MAHARASHTRA EDUCATION SOCIETY

ABASAHEB GARWARE COLLEGE

(Autonomous)

(Affiliated to Savitribai Phule Pune University)

Two Year M.Sc. Degree Program in Chemistry
(Faculty of Science and Technology)

Syllabi under Autonomy
M.Sc. II (Organic Chemistry)

Choice Based Credit System Syllabus
To be implemented from Academic Year 2023-2024

Title of the Course: M. Sc. -II (Organic Chemistry)

Preamble:

The syllabus of Organic Chemistry for Second year has been redesigned for Autonomous Choice based Credit System (CBCS) to be implemented from 2023-2024.

In CBCS pattern semester system has been adopted for M. Sc.-II (Organic and Analytical Chemistry) which includes Compulsory and Elective Theory as well as Practical Paper at M.Sc. level. Additional Credit Courses have been introduced at M.Sc. level.

Syllabus for Organic Chemistry which includes seven Theory and three Practical subjects for two semesters of M. Sc. -II is to be implemented from the year 2023-24. Syllabus for M. Sc.-II Organic Chemistry will be implemented from the year 2023-24 as per structure approved.

Program Outcome

1. To impart knowledge of Organic Chemistry covering all the aspects viz. , advanced organic Chemistry, spectroscopy, stereochemistry, heterocyclic, medicinal, organometallic, synthetic and natural product chemistry

2. To provide laboratory experience to the students by performing experiments based on topics taught in theory

3. Create awareness and sense of responsibilities towards environment and apply knowledge to solve the issues related to Environmental pollution.

4. Apply knowledge to build up small scale industry for developing endogenous product

5. Apply various aspects of practical chemistry in natural products isolations, green chemistry, convergent, divergent synthesis and research projects and also to develop interdisciplinary approach of the subject

Eligibility:

Students should have completed 50% credits in M.Sc.-I Chemistry

Structure of the Course: M.Sc. -II (Organic Chemistry)

Basic structure/pattern (Framework) of the proposed postgraduate syllabus for the two year integrated course leading to M.Sc. (Chemistry) in the MES Abasaheb Garware College.

M. Sc.-II: Organic Chemistry

Year	Semester	Course Type	Course Code	Course Title	Remark	Credit	No. of Lectures /Practical to be conducted
2	III	Compulsory	PSCHO-231	Organic Reaction Mechanism	Theory	04	60
		Compulsory	PSCHO-232	Structure Determination of Organic Compounds by Spectroscopic Methods	Theory	04	60
		Compulsory	PSCHO-233	Stereochemistry and Asymmetric Synthesis of Organic Compounds.	Theory	04	60
		Elective	PSCHOELE-234	**A)** Protection - De-protection, Chiron approach and Carbohydrate Chemistry **B)** Designing Organic Syntheses and Heterocyclic Chemistry	Theory (Select any one)	04	60
		Compulsory	PSCHOP-235	Solvent Free Organic Synthesis and Ternary Mixture Separation	Practical -I	04	12 P + 12 P
	IV	Compulsory	PSCHO-241	Chemistry of Natural Products and Biogenesis	Theory	04	60
		Compulsory	PSCHO-242	Organometallic Reagents in Organic Synthesis	Theory	04	60
		Elective	PSCHOELE-243	**A)** Medicinal Chemistry	Theory	04	60

				B) Applied Organic Chemistry	(Select any one)		
		Compulsory	PSCHOP-244	Project	Practical -II	04	120
		Elective	PSCHOPELE-245	A) Convergent and divergent Organic Syntheses. **OR** B) Isolation of Natural Products	Practical -III (Select any one)	04	A) 24 P OR B) 12 P

The detailed course wise syllabus of M. Sc-II Organic Chemistry is as follows:

Semester-III

PSCHO-231: Organic Reaction Mechanism (4 Credits, 60 Hours)

Learning Outcome

1. Understand various methods for determining reaction mechanism.
2. Use of free radical reactions and mechanism.
3. Understand Linear Free Energy Relationships and Hammett equation.
4. Applications of carbanions, enamines, carbenes and nitrenes

Section I: (2 Credits, 30 Hours)

1. Methods for determining Reaction Mechanisms
(Kinetic and non-kinetic methods), Ref -1, **[4 L]**

2. Free Radicals: Generation, stability, reactivity, Free radical substitution, addition to multiple bonds, radicals in synthesis, Inter- and intra-molecular bond formation via mercury hydride, tin hydride, thiol donors, cleavage of C-X , C-Sn, C-S, O-O bonds, Oxidative coupling, C-C bond formation in aromatics, SNAr reactions, Free Radicals in Organic Synthesis. *(**Ref-**2, 3, 6, 7)*. **[10 L]**

3. Linear Free Energy Relationships, *Ref. 3, 4*. **[8 L]**

4. Hammett plots, Hammett equation, substituent constants, reaction constants, use of Hammet plots, calculation of k and K, Deviations from straight line plots, Taft equation, solvent effects. *Ref. 3, 4, 5* **[8L]**

References:

1. Mechanism and structure in Organic Chemistry E. S. Gould (Holt, Rinehart and Winston)
2. Advanced Organic Chemistry –J. March, 4th edition
3. Advanced Organic Chemistry- Part A: Structure and Mechanism- F. A. Carey and R. J. Sundberg,
5th Edition, Springer 2007)
4. A guidebook to mechanism in Organic Chemistry- Peter Sykes
5. The Hammett Equation by C. D. Johnson
6. Organic Chemistry-J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press
7. Radical in Organic Synthesis- B. Giese, Pergamon Press (1986)

Section-II: (2 Credits, 30 Hours)

1. Carbanions-Formation, stability and related name reactions **[16L]** Ref. 1, 2, 3 Vol. A
2. Enamines –formation and applications, Ref. 3 **[8L]**
3. Reactions of carbenes and nitrenes Ref.3 Vol B **[6L]**

References:

1. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
2. Advanced organic chemistry by J. March, 6th Ed.
3. Advanced organic chemistry. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)

Additional Study Material: Organic Reaction Mechanism
https://nptel.ac.in/courses/104/101/104101005/
https://nptel.ac.in/courses/104/101/104101115/

PSCHO-232: Structure Determination of Organic Compounds by Spectroscopic Methods (4 Credits, 60 Hours)

Learning Outcome

1. Understand the principle, working and application of Nuclear magnetic resonance spectroscopy.
2. Understand the use of chemical shifts and coupling constant values in structure determination.
3. Understand the principle, working and application of Mass spectrometry.
4. Understand the structure elucidation using combined spectroscopic data.

Section-I: NMR Spectroscopy (2 Credits, 30 Hours)

1. Recapitulation: UV-Visible and IR spectroscopy [2L]

2. NMR in Stereochemistry Determination: Homotopic, enantiotopic and diastereotopic protons, Chemical and Magnetic equivalence; First and second order splitting, Complex multiplicity patterns and coupling constants in asymmetric compounds; Simplification of complex spectra, NOE, Diastereomerism, Atrop or axial chirality, % Enantiomeric excess, chiral NMR solvents etc in structure elucidation. **[12 L]**

3. ^{13}C NMR spectroscopy - APT, DEPT and INEPT **[6 L]**

4. ^{15}N, ^{19}F, ^{29}Si and ^{31}P NMR spectroscopy

Fundamentals and applications in structure elucidation of organic compounds, catalysts and biomolecules. (**Self learning and for internal assessment only).**

5. 2D NMR spectroscopy in structure elucidation: (a) Homonuclear: COSY, TOCSY, 2D-INADEQUATE, 2D- ADEQUATE, NOESY, ROESY (b) Heteronuclear: HSQC, HMQC, HMBC **[10 L]**

Section-II: Mass Spectrometry (2 Credits, 30 Hours)

1. Mass Spectrometry: Principle, ionization methods like EI, CI, ES, MALDI and FAB-Fragmentation of typical organic compounds, stability of fragments, Rearrangements, factors affecting fragmentation, ion analysis, ion abundance, High-Resolution mass spectrometry in determination of molecular formula. **[8 L]**

2. Applications of Mass Spectrometry: Determination of the elemental composition, Isotopic Abundance in structure establishment; Analysis of Biomolecules: Proteins and Peptides, Oligonucleotides and Oligosaccharides **[8 L]**

3. Problems solving: Structure elucidation using UV, IR, 1D (1H and13C) NMR and 2D NMR (1H-1H, 13C- 1H COSY /HETCOR only), APT, DEPT and MS data as well as spectra. **[14 L]**

References:

1. Spectrometric Identification of Organic Compounds by R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.

2. One- and Two-dimensional NMR Spectroscopy by Atta-Ur-Rehman, Elsevier (1989).

3. Organic Structure Analysis-Phillip Crews, Rodriguez, Jaspars by Oxford University Press (1998).

4. Organic Structural Spectroscopy by Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).

5. Organic Structures from Spectra by Field L.D. Kalman J.R. and Sternhell S. 4th Ed. John Wiley and Sons Ltd.

6. Mass Spectrometry Basics by Christopher G. Herbert Robert A.W. Johnstone

7. Mass Spectrometry Principles and Applications by Edmond de Hoffmann and Vincent Stroobant.

PSCHO-233: Stereochemistry and Asymmetric Synthesis of Organic Compounds (4 Credits, 60 Hours)

Learning Outcome:
1. Understand the stereochemistry, reactivity and conformational effects of six membered rings.
2. Understand the stereochemistry, shapes of rings other than six membered rings.
3. Understand the role various resolution methods, stereoselective synthesis and asymmetric synthesis.
4. Understand the stereochemistry of polymer chain.

Section I- Stereochemistry (2 Credits, 30 Hours)

1. Conformations of polysubstituted cyclohexane, six membered rings with SP2 carbon, heterocycles with N and O, anomeric effect, stereochemical principles involved in reactions of six membered rings and other than six membered rings, concept of I- Strain. *(**Ref.** 1, 2, 3, 4, 5, 6)* **[10 L]**

2. A) Stereochemistry of fused and bridged ring systems: Nomenclature, synthesis; stereochemical aspects of Perhydrophenanthrene, Perhydroanthracene, hydrindane, Steroids; Bridged system (bi, tri and polycyclo system) including heteroatoms, Bredt's Rule. **(*Ref.-1, 2, 3, 4, 5, 6)*.**

2. B) Conformations of following compounds with justification of each: cis and trans - 1,3- and l,4-di-t-butyl-cyclohexanes; Cis-4-di-t-butyl-cis-2,5-dihydroxycyclohexane; Twistane; bicyclo- [2.2.2]octane; Trans-anti-trans-Perhydro-anthracene and the lactone; cyclohexane-l,4-dione; 1,2,2,6,6-penta-methyl-4-hydroxy-4-phenylpiperidine; ψ-tropine; 2-hydroxy-2-phenyl quinolizidine; 4-t-butyl-4-methyl-l,3-dioxane; cis- and trans-2,5-di-t-butyl-l,3-dithianes;cis-2,5-di-t-butyl-l,3,2-dioxaphosphorinan-2-one (Ref. 1, 7, 8) **[10 L]**

3. Determination of configuration, Cram's rule, Cram's cycle model, Cram's dipolar model, Felkin-Anh Model; Resolution and analysis of stereomers - formation of racemization and methods of resolution. (Ref. 1, 2, 4), Stereochemistry of a polymer chain – Types and examples of Tacticity (Ref. 7), **[10 L]**

4. Decalols, Decalones, Octahydronaphthalenes, decahydroquinolines
(Self-learning and for internal assessment only)

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
5. Stereochemistry of organic compounds-P. S. Kalsi
6. Organic stereochemistry – Jagdamba Singh
7. Topics in Stereochemistry (Volume 2) By Norman L. Allinger and Ernest L. Eliel.
8. Topics in Stereochemistry (Volume 8) By Ernest L. Eliel and Norman L. Allinger.
Additional Study Material: Stereochemistry
https://nptel.ac.in/content/syllabus_pdf/104105086.pdf
https://nptel.ac.in/courses/104/105/104105086/

Section II- Asymmetric Synthesis (2 Credits, 30 Hours)

1. Introduction of Asymmetric Synthesis, Chirol pool and Chiral auxillaries. **[6 L]**
2. Asymmetric Organocatalysis **[6 L]**
3. Asymmetric Aldol Reaction, Enantioselective, diastereoselective and double diastereo-selective Aldol reactions. **[6 L]**

4. Transition Metal-Catalyzed Homogeneous Asymmetric Hydrogenation **[6 L]**
5. Transition Metal-Catalyzed Homogeneous Asymmetric Hydroxylation and Epoxidation **[6 L]**
6. Asymmetric Phase-Transfer and Ion Pair Catalysis (Self learning)

References:

1. Catalytic Asymmetric Synthesis, 3rd ed,Ed: I. Ojima, John Wiley & Sons, New Jersey, 2010
2. Catalysis in Asymmetric Synthesis by Vittorio Caprio and Jonathan M. J. Williams
3. Angew. Chem. Int. Edn. 2008, 47, 4638–4660.
4. Principles and Applications of Asymmetric Synthesis by Guo-Qiang Lin, Yue-Ming Li, Albert S. C. Chan, A John Wiley & Sons, Inc., Publication.
5. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers 2nd. Ed.
Additional Study material: Catalytic Asymmetric Synthesis
https://nptel.ac.in/content/syllabus_pdf/104103067.pdf
https://nptel.ac.in/courses/104/103/104103067/

PSCHOELE:234 (A): Protection - De-protection, Chiron approach and Carbohydrate Chemistry OR PSCHOELE:234 (B): Designing Organic Syntheses and Heterocyclic Chemistry (4 Credits, 60 Hours)

PSCHOELE:234 (A): Protection - De-protection, Chiron approach and Carbohydrate (4 Credits, 60 Hours)

Learning Outcome
1. Use and applications of protecting and deprotecting reagent.
2. Understand the concept of chiron approach.
3. Learn the basics of carbohydrates, synthesis and its application.

Section I: Protection - De-protection, Chiron approach (2 Credits, 30 Hours)

1. Protection and de-protection of functional group in organic synthesis: Hydroxyl group-alkyl ether, benzyl ether,acyl, PMB, Trityl, TMS, TBDMS, THP, MOM, MEM, MIP ether; Diol - Acetone,Cyclohexanone; Amines- Benzyl, Acyl, CBZ, BOC, FMOC, Carboxyl group-Ester, DCCI, DIPCDI; Ketone and aldehydes- Glycol, Thioglycol, Ketal, Acetal; Othroesters as protecting groups, Protection de-protection approach - In Solid phase synthesis of polypeptide; polynucleotide, cyclitols, and amino-sugars. (Ref. 1, 2, 3, 4) **[15 L]**
2. Chiron approach: a) Introduction, b) The concept of chiral templates and chirons wherein the carbon skeleton is the chiral precursor, c) Utilization of the basic concepts in synthesis of (S) Propanediol, (R) and (S) – Epichlorohydrin, L (+)-Alanine, (-) Multistratin, (-) Pentenomycin and (-) Shikimic acid (Ref. 2, 5, 6, 7). [**15 L**]

Section - II: Carbohydrate Chemistry (2 Credits, 30 Hours)

1. Basics of Carbohydrates: Introduction of sugars, structures of monosaccharides, triose, tetrose, pentose, hexose, D/L forms of aldoses and ketoses in Fisher projections, cyclic hemiacetal forms of monosaccharides, representation of monosaccharide structure (Fisher, Zig-zag, Mills, Haworth projection and Chair conformation), The structure of Glucose, the anomeric configuration, mutarotation (D-Glucose), Conformations of monosaccharides, the anomeric effect. Modified monosaccharides, Alditols, Cyclitols, Nomenclature of monosaccharides, Cyclic forms of the α and β-D-aldoses. **[14 L]**
2. Synthesis of Glycosides: glycosyldonar acceptor concept, general methods for glycosyl bond formation: Glycosyl halides, Trichloroacetimides, Glycals and Glycal derivatives,

Thioglycosides, Phosphites, n-Pentyl glycosides, SulfoxidesDiazarines, Alkylation of reducing sugars **[8 L]**

3. Mannosides, Synthesis of 2-Deoxy Sugars, Orthogonal strategy in Oligosaccharide synthesis, Effect of protecting groups on glycosylation stereoselectivity and coupling efficiency, Intramolecular glycosylation, Total synthesis of natural products: Oligosaccharides and Glycoconjugates. (Ref. 5, 8, 9, 10, 11, 12) **[8 L]**

References:

1. Greene's protective groups in organic synthesis – Peter G. M. Wuts and Theodor R. A. Green 4th Edn. Wiley-India
2. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
3. Modern organic synthesis-An introduction- George S. Zweifel, Michael H. Nantz.
4. Advanced Organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007)
5. Chiron Approach in organic synthesis – S. Hanessianh
6. Organic Chemistry – R. P. Morrison and R. N. Boyd
7. Organic Chemistry – I. L. Finar, volume II.
8. Essentials of Carbohydrate Chemistry and Biology: Thisbe K. Lindhorst, WILEY-VCH, 2000, Chapter 3.
9. Monosaccharide's: Their Chemistry and their Roles in Natural Products: Peter M. Collins, Robert J. Ferrier: John Wiley & Sons, 1995.
10. Carbohydrate in Chemistry and Biology: Part 1 Chemistry of Saccharides Vol.1. WILEY-VCH, 2000.
11. The Organic Chemistry of Sugars; By: Daniel E. Levy Peter Fugedi
Publication: Taylor & Francis, Published on 2006
12. Handbook of Chemical Glycosylation by Alexei V. Demchenko, Wiley VCH, 2008

PSCHOELE:234 (B): Designing Organic Syntheses and Heterocyclic Chemistry (4 Credits, 60 Hours)

Learning Outcome

1. Understand the concepts of retrosynthesis and its applications.
2. Different applications of heterocyclic reactions.
3. Synthetic strategy involved in preparation of heterocyclic compounds.
4. Study of three, four, six membered ring and aromatic heterocyclic compounds

Section I: Designing Organic Syntheses (2 Credits, 30 Hours)

1. Concepts of Retrosynthesis: Retrosynthetic analysis, disconnection approach, Synthons, multiple step synthesis, functional group intercoversion, Illogical two group interconversion, C-C disconnection, Donor and acceptor Synthons, two group disconnection, 1,5 related functional group disconnection, Umpolung, convergent synthesis, special methods for small rings, Heteroatom and Heterocyclic compounds, problems, (***Ref.***-1, 2, 4). **[15 L]**

2. Application of Retrosynthetic Approach: Retrosynthesis and synthesis of following Molecules: Strychnine, Reserpine, Thienamycin, Asteltoxin **Ref**-3 **[15 L]**

References:

1. Designing Organic Syntheses by Stuart Warren
2. Organic Chemistry from Retrosynthesis to Asymmetric Synthesis, by Vitomir Sunjic, Springer; 1st ed. 2016 edition
3. Classics in Total Synthesis by K.C. Nicolaou and E.J.Sorensen

Additional Study material: NPTEL Lecture:
A Study Guide in Organic Retrosynthesis: Problem Solving Approach
(https://nptel.ac.in/content/syllabus_pdf/104105087.pdf)

Section II: Advanced Heterocyclic Chemistry (2 Credits, 30 Hours)

1. Systematic nomenclature (Hantzsch-Widman System) for monocyclic, fused and bridged heterocycles. Tautomerism in aromatic heterocycles. Strain-bond angle, torsional strains and their consequences in small ring heterocycles. **[6 L]**

2. Synthesis and reactions of Three and four membered heterocylces: Aziridines, Oxiranes, Thirienes, Azetidines, Oxitanes and Thietanes **[6L]**

3. Common Methods in Ring Synthesis of Aromatic Heterocyclic Systems: Typical ring synthesis involving C – Heteroatom, C – C bond formations, Electrocyclic processes in heterocyclic Synthesis: 1,3 -dipolar cycloaddition producing five - membered heterocycles, Nitrenes in heterocyclic synthesis, Palladium catalysis in the synthesis of Benzo - Fused heterocycles, Fischer synthesis, Epoxidation, Use of Sulphur Ylides, Azides for small rings **[10L]**

4. Synthesis and reactions of Six membered and benzo-fused six membered heterocycles: Pyridine, Pyridine N-oxide, Pyrazine, Pyridazine, Pyrimidine, Quinazoline, Quinoxaline, Quinoline **[8L]**

Self Learning: Isoquinoline, Indoles

References:

1. Heterocyclic Chemistry by T. Gilchrist.
2. An Introduction to the Chemistry of Heterocyclic Compounds by RM Acheson.
3. Heterocyclic Chemistry by J A Joule and K. Mills.
4. Principles of Modern Heterocyclic Chemistry by A Paquette.
5. Heterocyclic Chemistry by J A Joule and Smith.
6. Handbook of Heterocyclic Chemistry by A R Katritzky

Additional Study Material: Heterocyclic Chemistry
https://nptel.ac.in/content/syllabus_pdf/104105034.pdf
https://nptel.ac.in/courses/104/105/104105034/

PSCHOP-235: Practical-I: Solvent Free Organic Synthesis and Ternary mixture Separation (4 Credits, 120 Hours)

Learning Outcome

1. Understand different name reactions using green method.
2. Learn monitoring of reactions, purification and characterization of products
3. Understand the separation technique of ternary mixture and the analysis of separated components.

Note: The students should perform any **(12)** Syntheses from the following list. Students should acquire **pre-experiment** (Reading MSDS, purification of reactants and reagents, mechanism, stoichiometry etc) and **post-experiment** skills (work-up, isolation and purification of products, physical constants characterization using any spectroscopic methods etc.)

Section-I Solvent Free Organic Synthesis (Any 12) (2 Credits, 12 P)

A) Solvent Free Carbon–Carbon Bond Formation

1. Pinacol coupling reaction (Page 36)
2. Knoevenagel condensation (Page 40)
3. Dieckmann condensation (Page 42)
4. Knoevenagel condensation, 3-carboxycoumarin (Page 45)
5. Biginelli reaction (Page 46)
6. Claisen reaction (Page 47)
7. Pechmann reaction (Page 50)

8. calix [4] resorcinarene (Page 50)
B) **Solvent-Free C–N Bond Formation**
1. azomethine synthesis (Page 213)
C) **Solvent-Free C–X Bond Formation**
1. Cinnamic acid/ stilbene halogenations (Page 319)
2. Phenol bromination using , *N*-bromosuccinimide (Page 320)
D) **Solvent-Free N–N Bond Formation**
1. Beckmann rearrangement (Page 346)
E) **Other Solvent-Free Reactions**
1. D-mannitol protection using phenylboronic acid (Page 388)
2. Baeyer-Villiger reaction
3. Alumina-supported permanganate oxidation (Page 15)
4. Iodine catalysed S-S bond formation of Cystine (Page 28)
G) Solvent free supramolecular assembly formation
1. Caffeine and oxalic acid (Page 420)
2. Isovaleraldehyde and pyrogallol

Reference:
Solvent-free Organic Synthesis by Koichi Tanaka (Copyright © 2009 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, ISBN: 978-3-527-32264-)
Additional Study Material: https://nptel.ac.in/courses/104/106/104106108/

Section-II: Separation of Ternary Mixture (Any 12) (2 Credits, 12 P)

Separation of minimum **12** mixtures containing three components. The mixtures should also involve separation of nitrophenols, amino acids, low boiling and water soluble and insoluble compounds solids and liquids with **multifunctional groups**. The mixture separation should be carried out on micro-scale using ether or water.

The students should be able to
1. Understand and employ concept of type determination and separation
2. Meticulously record physical constants
3. Perform micro scale chemical elemental analysis
4. Perform qualitative estimation of functional groups
5. Recrystallize /distill the separated compounds
6. Extend these skills to organic synthesis
7. Conduct Ternary Mixture for external examination
8. Conduct solvent free organic synthesis for internal examination

Semester IV

PSCHO- 241: Chemistry of Natural Products and Biogenesis (4 Credits, 60 Hours)

Learning Outcome
1. Understanding and planning of total synthesis of natural products.
2. Study of different methods of longifolene synthesis.
3. To know the building blocks and construction mechanism in biogenesis.

Section I: Chemistry of Natural Products (2 Credits, 30 Hours)

1. Understanding and planning of total synthesis while maintaining the stereochemistry. A case study: Longifolene – (All Nine syntheses from Advanced Organic Chemistry Carey, Sundberg; Part B). **[12 L]**

2. Total Synthesis of
i. Hirsutellone B (Angew. Chem. Int. Ed. 2009, 48, 6870 –6874.) **[9 L]**
ii. Ribisins A and B: (J. Org. Chem. 2019, 84, 15165−15172) **[9 L]**
iii. Subincanadine E: (*For Self-Learning) (J. Org. Chem. 2017, 82, 11126-11133) [12 L]

Section II: Biogenesis: The Building Blocks and Construction Mechanism (2 Credits, 30 Hours)

1. Terpenoids: Mono-, Sesqui-, Di-, tri-terpenoids and cholesterol, *Ref.- 1, 2, 3* **[8 L]**
2. Alkaloids: Derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan. *Ref.- 1, 2, 3* **[8 L]**
3. The Shikimate pathway: Cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids and terpenoid quinones. *Ref.- 1, 2, 3* **[8 L]**
3. A case study: Alkaloids isolated from the Roots of ***Piper nigrum,*** *Ref. -4, 5* **[6 L]**
References:
1. Natural Product Biosynthesis: Chemical Logic and Enzymatic Machinery by Christopher T Walsh, Yi Tang
2. From Biosynthesis to Total Synthesis: Strategies and Tactics for Natural Products- Editor Alexandros L. Zografo
3. Medicinal Natural Products: A Biosynthetic Approach, 3rd Edition By Paul M. Dewick
4. J. Nat. Prod. 2004, 67, 1005-1009.
5. J. Org. Chem. 2005, 70, 4, 1164–1176

PSCHO-242: Organometallic Reagents in Organic Synthesis (4 Credits, 60 Hours)

Learning Outcomes
1. Use of Transition metal complexes in organic synthesis.
2. Knowledge of name reactions in synthesis
3. Different application of name reactions
4. Use of organo Boron and Silicon reagents in organic synthesis.

Section-I: (2 Credits, 30 Hours)

1. Transition metal complexes in organic synthesis; Pd, Ni, Ru, Rh and Cu only (C-C, C-N, C-O bond formation reactions with catalytic cycle, ligand and % mole concepts) **[22 L]**
2. C=C formation reactions: Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions. **[8 L]**

Section-II: (2 Credits, 30 Hours)

1. Multi-component reactions: Ugi, Passerini, Biginelli and Mannich reaction **[4 L]**
2. Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization **[4 L]**
3. Click chemistry: criterion for click reaction, Sharpless azides cycloadditions.
Click reactions in synthesis of bioconjugates (sugars and proteins) **[8 L]**
4. Metathesis: Schrock and Grubbs catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, application in polymerization and synthesis of small organic molecules. **[8 L]**
5. Organo Boron and Silicon reagents in organic synthesis. **[6 L]**
6. Other important reactions: Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction. [*Self Learning]

References:
1. C–N bond forming cross-coupling reactions: an overview: by Jitender Bariwalab and Erik Van der Eycken Chem. Soc. Rev., 2013, 42, 9283
2. Iron Catalysis in Organic Synthesis Chem. Rev. 2015, 115, 3170–3387.
3. Recent advances in homogeneous nickel catalysis Nature 2014, Vol 509, Page 299-309.
4. Ruthenium-Catalyzed Reactions for Organic Synthesis Chem. Rev. 1998, 98, 2599-2660.
5. Organic Synthesis Involving Iridium-Catalyzed Oxidation Chem. Rev. 2011, 111, 1825–1845.
6. Aerobic Copper-Catalyzed Organic Reactions Chem. Rev. 2013, 113, 6234−6458.
7. Transition Metals for Organic Synthesis Volume 1 Edited by M. Beller and C. Bolm WILEY-VCH Verlag GmbH & Co. KGaA ISBN: 3-527-30613-7
8. Multicomponent Reactions Edited by Jieping Zhu, Hugues Bienayme WILEY-VCH Verlag GmbH & Co. KGaA
9. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press),
10. Some modern methods of organic synthesis – W. Carruthers (Cambridge)
11. Organic synthesis – Michael B. Smith
12. Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007).
13. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako
14. Name Reactions Jie Jack Li (Fourth Expanded Edition), Page No: 1-582.
15. Organic Synthesis Using Transition Metals, by Roderick Bates, Second Edition, A John Wiley & Sons, Ltd., Publication.

PSCHOELE-243 (A): Concepts and Applications of Medicinal Chemistry OR PSCHOELE-243 (B): Applied Organic Chemistry (4 Credits, 60 Hours)

PSCHOELE-243 (A): Concepts and Applications of Medicinal Chemistry (4 Credits, 60 Hours)

Learning Outcome

1. Student should understand the various biomolecules and medicines.
2. To understand concept of drug and different sources of drugs.
3. Student should able to learn drug designing and development.
4. To know about bioassays and toxicological evaluation of new drugs.
5. Student should understand structure and activity relationship.
6. To know about Pharmacokinetics and Pharmacodynamics of drug action.

Section-I: (2 Credits, 30 Hours)

1. Introduction to Biomolecules: Peptides and proteins, Proteins as biological catalyst Nucleic acids, Metabolism, Chemistry of cofactors/coenzymes, Chemistry of TPP, PLP, Folic Acid and other vitamins, Principle of drug design, Chemistry of diseases and Drug development, Proton pump inhibitors and Problem solving. **[10 L]**

2. Introduction to medicinal Chemistry. History, drug targets, Drug discovery, design and development, Case Study: Design of Oxamniquine. **[6 L]**

Additional study material: NPTEL lecture: Organic Chemistry in Biology and Drug Development (full course) https://nptel.ac.in/content/syllabus_pdf/104105120.pdf) https://nptel.ac.in/courses/104/105/104105120/

3. Peptides, sequencing and applications in therapeutics, Solution phase and solid phase peptide synthesis and Modern techniques for biomolecules and disease diagnosis. **[8 L]**

Additional study material: NPTEL lecture (only 3 topics): Essentials of Biomolecules: Nucleic Acids and Peptides https://nptel.ac.in/content/syllabus_pdf/104103121.pdf

https://nptel.ac.in/courses/104/103/104103121/

4. Pharmacokinetics and Pharmacodynamics of drug: Drug absorption, distribution, metabolism, elimination and toxicity, drug metabolism, biotransformation, Drug receptor interactions, Hansch Equation and significance of terms involved in it. **[6 L]**

Section II: (2 Credits, 30 Hours)

1. Structure and activity Relationship: QSAR, Applications of SAR and QSAR in drug design, physio-chemical parameters lipophilicity, partition coefficient, electronic ionization constant, Case Study: Statins **[14 L]**

2. Introduction, Developments, SAR, Mode of action, limitations and adverse effect of Anti-infective Agents, Beta lactam antibacterial agents (Penicillins, Cephalosporins), Tetracyclins, Macrolides, Chloramphenicol, Polyenes, Amphotrecin-B, Azoles, Amantadine, Acyclovir, Quinine, Quinolines, Quinolones, Refamycine, Sulphonamides [**16 L]**

References:

1. Medicinal Chemistry and Drug Discovery by Burger
2. Introduction to Medicinal Chemistry by Grham and Patrick
3. Introduction to Drug Design by J. R. Dimmock and S.S. Pandeya
4. The Organic Chemistry of Drug Design and Drug Action, 3rd Edition, R. B. Silverman, Academic Press, 2014
5. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F Dorge, 12th Edition, 2010
6. Chemistry of Heterocycles by T. Eicher and S. Hauptmann, Thieme

PSCHOELE-243 (B): Applied Organic Chemistry (4 Credits, 60 Hours)

Learning Outcome

1. Learn the covalent organic frameworks and organic electroluminescent materials
2. Concept of supramolecular chemistry
3. Application of supramolecular chemistry in drug synthesis

Section-I: (2 Credits, 30 Hours)

1. Covalent Organic Frameworks: Structures, Synthesis, and Applications. [15 L]
(Ref: Review article by Maria S. Lohse and Thomas Bein ***Adv. Funct. Mater***. 2018, 28(33), 1705553.)

2. Organic Electroluminescent Materials, [15 L]
(Ref: Review article by L.S. Hunga and C. H. Chen ***Materials Science and Engineering*** 2002, R 39, 143–222)

Section –II: (2 Credits, 30 Hours)

1. Supramolecular Organic Compounds [10 L]
(Ref: Review by Matthew C. T. Fyfe and J. Fraser Stoddart ***Accounts of Chemical*** *Research* 1997, 30 (10), 393-401.)
(Ref: Review article by Wei Chen and et al. ***Chem. Soc. Rev.***, **2015**, *44*, 2998-3022)

2. Molecular Machines [20 L]

References:

1. Review article by David A. Leigh and et al. *Chem. Rev.* 2015, *115*, 10081−10206.
2. Redox-Gated Tristable Molecular Brakes of Geared Rotation*. J. Org. Chem*., 2017, 82(10), 5354-5366.
3. Massimo Baroncini, Serena Silvi, Alberto Credi. *Chem. Rev.* 2020, *120* (1), 200-268).

References:
1. The Chemistry of Metal–Organic Frameworks- Wiley Online. Print ISBN: 9783527338740, Online ISBN:9783527693078, DOI:10.1002/9783527693078
2. Covalent Organic Frameworks - 1st Edition - Atsushi Nagai, ISBN 9789814800877, Published January 24, 2020 by Jenny Stanford Publishing.

PSCHOP-244: Practical-II: Project (4 Credits, 120 Hours)

Learning Outcome

1. Students will Learn Referencing
2. To know about various scientific databases
3. Understand applications of various characterization techniques
4. Learn how to write project report
5. Learn presentation skills

1. Students should carry out a small research project.
2. This should make them familiar with
i. Literature survey, research methodologies
ii. Data Analysis
iii. Column and TLC chromatographic techniques
iv. Characterization of the products by analytical and spectral methods.
3. Project report must be written and submitted in a proper format as follows;
i) Certificate (Signed by Project guide and Head of the Department)
ii) Certificates for Poster/Paper presented in conferences (if any)
iii) Self declaration certificate for plagiarism
iv) Introduction (not more than 6 pages)
v) Results and Discussions
vi) Experimental Section
vii) Conclusion
viii) References (Use ACS format)
ix) Spectroscopic or other relevant supporting data
x) Acknowledgement
4. Interdisciplinary projects shall be encouraged; however there must be some organic chemistry component.
5. Students should spend enough time for the project works (at least 8 hours per week for 15 weeks)
6. 100 % students should undertake projects.
7. If student is performing project in another institute, for such a student, internal mentor must be allotted and he will be responsible for internal assessment of a student. In this case student has to obtain certificate from both external and internal mentor. Systematic record of attendance of project students must be maintained by a mentor. Project will be evaluated jointly by three examiners and there will not be any practical performance during the examination. Typically, student has to present his practical work, discuss results and conclusions in details (20-30 min.) which will be followed by question-answer session (20 min). It is open type of examination.

PSCHOELE-245: Practical-III: A) Convergent and Divergent Organic Syntheses (24 P) OR B) Isolation of Natural Products (4 Credits, 12 P)

Learning Outcome

1. Students will learn convergent, divergent syntheses and its applications.
2. Use of various synthetic strategies in synthesis.
3. Understand various extraction techniques for isolation of natural product.
4. Learn purification of natural product and its characterization by different spectroscopic methods.

A) Convergent and Divergent Organic Syntheses (2 Credits, 24 P)

Note: Any **3** sets should be conducted from the following convergent and divergent synthesis sets.
Students should acquire pre-experiment (Reading MSDS, purification of reactants and reagents, mechanism, stoichiometry etc) and post-experiment skills (work-up, isolation and purification of products, physical constants characterization using any spectroscopic methods etc.)

SET-I

A) Convergent Synthesis 1 (Three Stage Synthesis)
1. Stage I: Anisole to 4-nitro anisole to 4-amino anisole (2 steps)
2. Stage II: Toluene to 4-nitro toluene to 3-acyl nitro toluene (2 steps)
3. Stage III: Synthesis of N-(1-(2-methyl-5-nitrophenyl) ethyl) aniline from 4-amino anisole, 3-acyl nitro toluene and SBH (One pot synthesis: MCR)
B) Divergent Synthesis 1 (5 Single Stage Synthesis from Acetyl acetone):
1. Acetyl acetone to Pyrimidine
2. Acetyl acetone to 2,4-dimethyl-1H-benzo[b][1,4]diazepine
3. Acetyl acetone to Pyrazole
4. Acetyl acetone with 1mmol benzaldehyde to 3-benzylidenepentane-2,4-dione
5. Acetyl acetone with 3 mmol benzaldehyde into 3-benzylidene-6-phenylhex-5-ene-2,4-dione

SET-II

A) Convergent Synthesis 2(Three Stage Synthesis)
1. Stage I: 4-Nitro toluene to 4-amino toluene (Reduction by using Sn/HCl)
2. Stage II: Phenol into 2-hydroxy benzaldehyde (Reimer-Tiemann reaction)
3. Stage III: Synthesis of amidoalkyl-2-naphthols from β-Naphthol,4-amino toluene and of 2-hydroxy benzaldehyde (One pot synthesis: MCR)
B) Divergent Synthesis (5 Single Stage Synthesis from β-Naphthol)
1. β-Naphthol to Synthetic dye (By diazonium coupling)
2. β-Naphthol to 6-Bromo-2-naphthol (Bromination reaction)
3. β-Naphthol to β-Naphthyl methyl ether (Methylation reaction)
4. β-Naphthol to temperature dependent sulfonation (Sulfonation reaction)
5. β-Naphthol to (±) Binol then Resolution of Binol (Resolution technique)

SET-III

A) Convergent Synthesis-3 (Three Stage Synthesis)
1. Stage I: Salicylic acid to 5-Chloro-2-hydroxybenzoic acid
2. Stage II: o- Anisidine to 2-methoxy-4-nitroaniline
3. Stage III: Synthesis of 5-chloro-2-hydroxy-N-(2-methoxy-4-nitrophenyl) benzamide from 5-Chloro-2-hydroxybenzoic acid, -methoxy-4-nitroaniline (One pot synthesis: MCR)
B) Divergent Synthesis-3 (5 Single Stage Synthesis from Salysaldehyde)
1. Salicylaldehyde to Salicylaldehyde phenylhydrazone
2. Salicylaldehyde with malononitrile to 2-iminochromene by intramolecular cyclization.
3. Salicylaldehyde to 2-hydroxy-3,5-dinitrobenzaldehyde
4. Salicylaldehyde to o-Formyl phenoxy acetic acid

5. Salicylaldehyde to catechol

SET-IV

A) Convergent Synthesis- 4 (Three Stage Synthesis)

1. Stage I: Benzene to acetophenone (F.C acylation)

2. Stage II: 4-Nitrochlorobenzene into 4-amino chlorobenzene (Reduction by using hydrazine)

3. Stage III: Quinoline synthesis by using acetophenone, 4-amino chloro benzene and styrene (One pot synthesis: [3 + 2 + 1] cycloaddition reaction)

B) Divergent Synthesis-4 (5 Single Stage Synthesis from Acetophenone)

1. Acetophenone to Ethyl benzene by Wolf Kishner reduction

2. Acetophenone to m-Nitro acetophenone by nitration

3. Acetophenone to Chalcone using aromatic aldehyde

4. Acetophenone into Schiff base using aromatic amine

5. Acetophenone to Benzoic acid and Iodoform

References:

1. Practical organic chemistry by Mann and Saunders

2. Text book of practical organic chemistry –by Vogel

3. The synthesis, identification of organic compounds –Ralph L. Shriner, Christine K.F.

4. Hermann, Terence C. Morrill and David Y. Curtin

OR B) Isolation of Natural Products (Any 12)

Unit I: Isolation of pigments from the natural products

1. Orange Marigold
2. Rose
3. Sunflower
4. Hibiscus
5. Any colored flowers/fruits available in the local area **(only one is allowed).**

Note: Students should be able to collect reasonable quantities of color pigments to do the characterization (Physical Constant, Elemental analysis functional group test etc) and should also form the appropriate derivative. They are encouraged to use these pigments for developing food grade natural colors from lesser-known plant sources.

Unit II: Isolation of essential oils from the natural products

1. Ginger
2. Lemongrass
3. Garlic
4. Ajwain/ajowan/Trachyspermum ammi
5. Vekhand (achourus calamus) root
6. Any natural products available in the local area **(only one is allowed)**

Note: Students should be able to collect a reasonable quantity of essential oils to do the characterization (Physical Constant, Density, Elemental analysis functional group test) Should form the appropriate derivative. They are encouraged to use these essential oils for the development of the products like soap, perfumes etc.

Unit III: Isolation of medicinally important component from the natural products

1. Nimbin from Neem leave
2. Amyrin from Apati/Apta bark
3. Eujenol from Tulsi leaves
4. D-Galacturonic Acid from Jeshtamadh

5. Piper from Betel leaf
6. Any medicinally important plants available in the local area (only one is allowed)

At least one natural product should be isolated by using column chromatographic techniques (Use micro columns to avoid excess use of solvents)

Note: Students should be able to collect a reasonable quantities natural products to do the characterization (Physical Constant, solubility, Elemental analysis functional group test etc) and should also form the appropriate derivative. They are encouraged to study novel medicinal plants from their local area.

Important Notes for Practical Courses

- All experiments should be carried out on micro-scale and by considering stoichiometric quantities of reactants and reagents with the proper understanding of the mechanism.
- Post graduate departments should arrange at least one study visit to relevant industry/national research laboratory/premier academic institute.
- Students must read MSDS and should handle chemicals and reactions accordingly.
- The necessary reactions should be carried out in fume hood and appropriate safety measures should be taken during the laboratory experiments and projects.
- All reactions should be monitored using alumina coated TLC plates.
- Certified journals should be presented at the time of final examination.
- Project Students are encouraged to participate in AVISHKAR, national and international conferences and other project competitions.
- Teachers are encouraged to give the project ideas based on the societal needs.

Pattern of Question Paper

Examination: Each theory and practical course carry 100 marks equivalent to 4 credits. Each course will be evaluated with Continuous Assessment (CA) and College Assessment mechanism. Continuous assessment shall be of 30 marks (30%) while college evaluation shall be of 70 marks (70%). To pass the course, a student has to secure 40% mark in continuous assessment as well as college assessment i.e. 12 marks in continuous assessment and 28 marks in college assessment.

For Continuous assessment teacher must select variety of procedures for examination such as: i) Class test (not more than one for each course), ii) Term paper, iii) Group discussion, iv) Journal, v) Seminar presentation, vi) Group discussion, vii) assignment, viii) research project by individual student ix) An open book test, etc.

For theory and practical courses, end semester question papers will be set by the College and centralized assessment for theory and practical papers done as per the rules laid down by the College. Questions will be designed to test the conceptual knowledge and understanding of the basic and advanced concepts of the subject. There will be **two sections** for each paper and two experiments for each practical. Each section and each experiment will be of **35 marks** and the pattern of question paper shall be:

Internal Theory Examination

- Time: 1.30 hour
- Total Marks: **30**: 20 Marks Internal examination + 10 Marks assignments/seminar/class test
- Title of the questions:

  Section -I

  Q.1) Answer the following (any 2) (4M)

  Q.2) Attempt any two of the following (any 2) (6M)

  Section -II

  Q.3) Answer the following (any two) (4M)

  Q.4) Attempt any two of the following (any 2) (6M)
- All questions are compulsory
- Q.1 and Q.3 carries 2 marks each with three options and Q.2 and Q.4 carries 3 marks each with four options

External Theory Examination

- Time: 3 hours

- Total Marks: **70**
- Title of the questions:

  Section -I

  Q.1) Answer the following (any 5) (10M)

  Q.2) Attempt any three of the following (9M)

  Q.3) Attempt any four of the following (16M)

  Section-II

  Q.4) Answer the following (any 5) (10M)

  Q.5) Attempt any three of the following (9M)

  Q.6) Attempt any four of the following (16M)
- All questions are compulsory

  Q.1 and 4: any five out of seven, each question carries 2 Marks

  Q.2 and 5: any three out of five, each question carries 3 Marks

  Q.3 and 6: any four out of six, each question carries 4 Marks

Internal Practical Examination

Total Marks: **15**, 5 Marks for test + 5 Marks for Oral/seminar + 5 Marks for journal

External Practical Examination

Total Marks: **35**, 25 Marks for experiment + 10 Marks for Oral

[Note: In question paper setting wattage for each chapter will be proportional to number of theory lectures assigned to that chapter.]