Maharashtra Education Society's

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 NEP-2020

Level 6.5 (Chemistry)

To be implemented from Academic Year 2024-2025

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

Preamble:

Taking into consideration the rapid changes in science and technology and new approaches in different areas of Chemistry and related subjects, Board of studies in Chemistry after a thorough discussion with the teachers of Chemistry from Abasaheb Garware College and experts from industry as well as other Academic institutions has prepared the syllabus of M.Sc. II Semester - III and Semester- IV (w.e.f. 2024-25) Chemistry course under the Choice Based Credit System (CBCS). The model curriculum as developed by UGC is used as a guideline for the present syllabus.

Program Outcomes:

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 chemistry in natural products isolations, green chemistry, synthesis etc. and also to develop interdisciplinary approach of the subject

Eligibility: Students should be completed PG Diploma with 22 credits / 4 year of UG

MSc-II Organic Chemistry NEP structure

Level/ Degree	Semester	Course Type	Course Code	Course Name	Credits	No. of L to be conducted
6.5 PG Degree (After 1 year Diploma / 4 year UG)	III	Major Core	CHO-601-MJ	Structure Determination of Organic Compounds by Spectroscopic Methods	4	60
			CHO-602-MJ	Stereochemistry and Asymmetric Synthesis of Organic Compounds.	4	60
			CHO-603-MJ	Organic Reaction Mechanism	2	30
			CHO-604-MJP	Solvent free organic synthesis and Ternary Mixture Separation	4	120
		Major elective	CHO-611-MJ	**A)** Designing Organic Synthesis and Photochemistry & Pericyclic Reactions **OR** **B)** Protection - De-protection, Chiron approach and Carbohydrate Chemistry	4	60
		Research Project	CHO-631-RP	Research Project	4	120
	IV	Major Core	CHO-651-MJ	Chemistry of Natural Products and Biogenesis	4	60
			CHO-652-MJ	Organometallic Reagents in Organic Synthesis	4	60
			CHO-653-MJP	Convergent and two stage Organic Synthesis	4	120
		Major elective	CHO-661-MJ	**A)** Medicinal Chemistry **OR** **B)** Applied Organic Chemistry	4	60
		Research Project	CHO-681-RP	Research Project	6	180

SEMESTER-III

MAJOR CORE

Course code and Title: CHO-601-MJ Structure Determination of Organic Compounds by Spectroscopic Methods (4 Credits, 60 Hours)

Learning Outcomes: After completion of the course, students would be able to
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. **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. **[14 Hours]**
2. **^{13}C NMR spectroscopy:** APT, DEPT and INEPT **[06 Hours]**
3. **^{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).**
4. **2D NMR:** spectroscopy in structure elucidation: (a) Homonuclear: COSY, TOCSY, 2D-INADEQUATE, 2D- ADEQUATE, NOESY, ROESY (b) Heteronuclear: HSQC, HMQC, HMBC **[10 Hours]**

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. **[12 Hours]**
2. **Applications of Mass Spectrometry:** Determination of the elemental composition, Isotopic Abundance in structure establishment. **[04 Hours]**
3. **Problems solving:** Structure elucidation using UV, IR, 1D (^{1}H and^{13}C) NMR and 2D-NMR (^{1}H-^{1}H, ^{13}C- ^{1}H COSY /HETCOR only), APT, DEPT and MS data as well as spectra. **[14 Hours]**

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.

Course code and Title: CHO-602-MJ Stereochemistry and Asymmetric Synthesis of Organic Compounds (4 Credits, 60 Hours)

Learning Outcomes: After completion of the course, students would be able to
1. Understand the stereochemistry, reactivity and conformational effects of 6 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 diastereoselective and enantioselective transformations

Section-I: Stereochemistry (2 Credits, 30 Hours)

1. Conformations of polysubstituted cyclohexane, six membered rings with SP^2 carbon, heterocycles with N and O, anomeric effect, stereochemical principles involved in reactions of six membered rings and other than six membered rings, five membered, medium rings, transannular effects , concept of I- Strain. (Ref. 1, 2, 3, 4, 5, 6) **[06 Hours]**

2. A) Stereochemistry of fused and bridged ring systems: Nomenclature, synthesis; stereochemical aspects of Perhydrophenanthrene, Perhydroanthracene, hydrindane, Steroids; Bridged system (bi, tri and polycyclic system) including heteroatoms, Bredt's Rule. (Ref.-1, 2, 3, 4, 5, 6) **[06 Hours]**

B) Stereoselectivity in cyclic compounds: Introduction, Stereochemical control in six membered rings, Reactions on small rings, Regio-chemical control in cyclohexene epoxides, Stereoselectivity in bicyclic compounds, Fused bicyclic compounds, Spirocyclic compounds, Reactions with cyclic intermediates or cyclic transition states. (Ref. 3, Chapter 33) Further reading (Ref. 1, 7, 8) **[08 Hours]**

3. Diastereoselectivity: stereospecific and stereoselective reactions, diastereoselective iodo-lactonistion, stereoselective epoxidation, prochirality, nucleophilic additions to carbonyl compounds Cram's rule, Cram's dipolar model, Felkin-Anh Model; chelate Model diastereoselective reactions in acyclic alkenes and diastereo aldol reactions. (Ref. 3, Chapter 33) **[10 Hours]**

4. Decalols, Decalones, Octahydro naphthalenes, 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
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. Principles and applications of asymmetric synthesis: concept of enantiomeric excess and diastereomeric excess. chiral resolution and its limitations, use of chiral pool, chiral auxillaries. chiral reagents and catalyst for asymmetric inductions, asymmetric organo-catalysis, asymmetric Diels Alder reaction, asymmetric aldol reaction, Enantioselective, diastereoselective Aldol reactions. Transition Metal-Catalyzed Homogeneous Asymmetric Hydrogenation, Transition Metal-Catalyzed Homogeneous Asymmetric dihydroxylation and Sharpless Asymmetric Epoxidation, Jacobsen and Shi epoxidation. Industrial applications. **[30 Hours]**

2. Asymmetric Phase-Transfer and Ion Pair Catalysis (*Self learning)

References:

1. Catalytic Asymmetric Synthesis, 3rd ed,Ed: I. Ojima, John Wiley & Sons, New Jersey,
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.
6. Principles and Applications of Asymmetric Synthesis by Guo-Qiang Lin, Yue-Ming Li, Albert S. C. Chan, A John Wiley & Sons, Inc., Publication
7. Additional Study Material : Catalytic Asymmetric Synthesis
https://nptel.ac.in/content/syllabus_pdf/104103067.pdf
https://nptel.ac.in/courses/104/103/104103067/

Course code and Title: CHO-603-MJ Organic Reaction Mechanism (2 Credits, 30 Hours)

Learning Outcomes: After completion of the course, students would be able to
1. Understand various methods for determining reaction mechanism.
2. Understanding of synthetic equivalents
3. Applications of carbanions, enamines, carbenes and nitrenes

1. Methods for determining Reaction Mechanisms
(Kinetic and non-kinetic methods) **[5 Hours]**

2. Enamines – formation and applications **[5 Hours]**

3. Carbanions- Formation, stability and related name reactions. **[8 Hours]**

4. Concepts of synthetic equivalents and Umpolung: benzoyl and acyl anion equivalents, dithianes, enol ethers and nitro compounds. **[4 Hours]**

5. 5-Membered rings: intramolecular SN2 reactions, intramolecular Michael and aldol condensation reactions, intramolecular Wittig olefination, ring expansion and contraction reactions, 1,3-dipolar cycloaddition reactions, Nazarov cyclization, arene-olefin photocycloaddition, radical cyclization reactions. **[8 Hours]**

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 and B, F. A. Carey and R. J. Sundberg, 5th Edition, Springer 2007)
4. A guidebook to mechanism in Organic Chemistry- Peter Sykes
5. Organic Chemistry-J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press David J. Hart "Organic Synthesis via Examination of Selected Natural Products" World Scientific, 2011
6. S. Warren, "Designing Organic Syntheses", John Wiley & Sons 2009.
7. R. O. C. Norman and J. M. Coxon "Principles of Organic Synthesis" Nelson Thornes, Third Edition, 2005.
8. K. C. Nicolaou, E. J. Sorenson, "Classics in Total Synthesis, I, II and III"
9. B. M. Trost and I. Fleming, "Comprehensive Organic Synthesis",Pergamon Press, 1992.
10. W. Carruthers, "Some Modern Methods in Organic Synthesis", Cambridge University Press 1989.

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

Course code and Title: CHO-604-MJP Solvent Free Organic Synthesis and Separation of Ternary mixture (4 Credits, 120 Hours)

Learning Outcomes: After completion of the course, students would be able to

1. Impart knowledge of basics of separation of organic ternary mixtures.
2. Make able to identify type and chemical nature of components of the mixture and separate solid, semi-solid and liquid organic mixtures.
3. Identify the elements and functional groups presents in the organic molecule.

Note: Students should separate minimum **12** ternary mixtures. Students should acquire **pre-experiment** (Reading MSDS, purification of compounds etc) and **post-experiment** skills (purification of components by different techniques, physical constants and identification using any chemical methods ie. derivatisation 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 6) (2 Credits, 6 P)

Separation of minimum **06** mixtures containing three components. The mixtures should also involve separation of nitrophenols, amino acids, low melting, 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 and analysis of three components.

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

Note: Batch size for practical should be of 08 students

Course code and Title: CHO-611-MJ A) Designing Organic Synthesis and Photochemistry & Pericyclic Reactions (4 Credits, 60 Hours)

Learning Outcomes: After completion of the course, students would be able to

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 and six membered ring and aromatic heterocyclic compounds

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

1. Disconnection approach and retrosynthetic analysis. Planning of multistep synthesis. Concepts of synthones, retrones and synthetic equivalents. Generation of structural complexity using tandem and cascade processes. Selectivities in synthesis: Chemo selectivity, regioselectivity, stereoselectivity, atom selectivity. **[04 Hours]**
2. Concept of Protecting Functional Groups: Protection of NH groups, Protection of OH group of alcohols, Protection of diols as acetals, Protection of carbonyl groups in aldehydes and ketones, Protection of carboxyl group, Protection of double bonds, Protection of triple bonds. **[04 Hours]**
3. Umpolung concept: Logical and illogical disconnection, different umpolung reagents ex. 1,3 dithiane **[04 Hours]**
4. **Concepts of Retrosynthesis:** Introduction to disconnection, One group disconnection, Disconnections of Simple Alcohols, Compounds Derived from Alcohols, Disconnections of Simple Olefins, Disconnections of Aryl Ketones, Control in disconnections, Disconnections of Simple Ketones and Acids, Two group disconnection. (a) β-Hydroxy Carbonyl compounds (b) α,β-Unsaturated Carbonyl Compounds, (c) 1,3-Dicarbonyl Compounds, frame. (d) 1,5-Dicarbonyl (a) Use of the Mannich Reaction, Illogical two group disconnection, 1,2-Dioxygenation Pattern, (a) α-Hydroxy Carbonyl Compounds, (b) 1,2-Diols, (c) 'Illogical' Electrophiles, The 1,4-Dioxygenation Pattern. (a) 1,4-Dicarbonyl Compounds (b) γ-Hydroxy Carbonyl Compounds, (c) Other 'Illogical' Synthons, (d). 1,6-Dicarbonyl Compounds, Synthesis of Lactones, Retrosynthetic approach by pericyclic reactions, Retrosynthesis of aliphatic and aromatic heterocyclic compounds ***Ref***.-1, 2, 4). **[08 Hours]**
5. **Application of Retrosynthetic Approach:** Retrosynthesis and synthesis of following Molecules: Strychnine, Reserpine, Thienamycin, Asteltoxin, Menthol **Ref**-3 **[10 Hours]**

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: Photochemistry & Pericyclic Reactions (2 Credits, 30 Hours)

Learning outcomes:

1. Students should able to understand free radicals' formation, stability and reactivity and there use for the basic understanding in writing probable reaction mechanisms.
2. Students should able to write MO diagram for various olefinic compounds and should able to predict the products, the stereochemistry as well as should able to understand the preferred reaction pathways.
3. Students should able to calculate λmax of organic compounds containing more than one and less than four conjugated systems. Students should able to correlate IR bands with functional groups using numerical data as well as spectral data.
4. Students should able to solve 1H-NMR problems and to draw the 1H-NMR

1) Photochemistry (15 Hours)

Principles of Photochemistry, photochemistry of carbonyl compounds, alkenes, dienes, and aromatic compounds, photo rearrangements, Barton reaction, Patrno Buchi [2+2] cycloaddition reaction, photo redox reactions

Self-Learning; Photochemistry of Vision

2) Pericyclic Reactions (15 hours)

Electro cyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Analysis by correlation diagrams, FMO approach, ene reactions, 1, 3-dipolar additions.

Self-Learning: Group transfer reactions

References:

1. Advanced Organic Chemistry, Part A by F. A. Carey and R. J. Sundberg
2. Excited states in Organic Chemistry by J.A. Barltrop and J.D.Coyle
3. Organic photochemistry: A visual approach by Jan Kopecky
4. Conservation of orbital symmetry by R. B. Woodward and R. Hoffmann
5. Orbital Symmetry: A problem solving approach- R. E. Lehr and A. P. Marchand
6. Pericyclic Reactions By A. P. Marchand, Roland E. Lehr
7. Organic reactions and orbital symmetry, 2nd Ed. T. L. Gilchrist and R. C. Storr
8. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming
9. Pericyclic Reactions by Ian Fleming
10. Pericyclic Reactions by A Mechanistic and Problem-Solving Approach by Sunil Kumar Vinod Kumar S.P. Singh
11. Essentials of Pericyclic and Photochemical Reactions by Dinda and Biswanath

Course code and Title: CHO-611E-MJ B) Protection - De-protection, Chiron approach and Carbohydrate Chemistry (4 Credits, 60 Hours)

Learning Outcomes: After completion of the course, students would be able to

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; Othro-esters as protecting groups, Protection de-protection approach - In Solid phase synthesis of polypeptide; polynucleotide, cyclitols, and amino-sugars. (Ref. 1, 2, 3, 4) **[15 Hours]**

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 Hours]**

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 Hours]**

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 **[08 Hours]**
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: Oligo saccharides and Glycoconjugates. (Ref. 5, 8, 9, 10, 11, 12) **[08 Hours]**

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

Course code and Title: CHO-631-RP Research Project

(4 Credits, 120 Hours)

Learning Outcomes:

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 (10 min). It is open type of examination.

NOTE: 30 mins per student workload should be calculated for staff

SEMESTER-IV

MAJOR CORE

Course code and Title: CHO-651-MJ Chemistry of Natural Products and Biogenesis (4 Credits, 60 Hours)

Learning Outcomes: After completion of the course, students would be able to
1. Understanding and planning of total synthesis of natural products.
2. Study of different routes of longifolene retrosynthesis and 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). **[14 Hours]**
2. Total Synthesis of
i. Hirsutellone B (Angew. Chem. Int. Ed. 2009, 48, 6870 –6874.) **[08 Hours]**
ii. Ribisins A and B: (J. Org. Chem. 2019, 84, 15165–15172) **[08 Hours]**
iii. Subincanadine E: (*For Self-Learning) (J. Org. Chem. 2017, 82, 11126-11133)

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

1. Introduction to biogenesis: Distinctions between primary and secondary metabolism, are defined, basic building blocks used in the biosynthesis of secondary natural products. The chemistry of building blocks according to chemical mechanism, including alkylation reactions, Wagner–Meerwein rearrangements, aldol and Claisen reactions, Schiff base formation and Mannich reactions, transaminations, decarboxylations, oxidation and reduction reactions, phenolic oxidative coupling, and glycosylations **[06 Hours]**
2. Terpenes: The mevalonate pathway and the recently discovered mevalonate-independent pathway via deoxyxylulose phosphate. Terpenoids classification, Biogenesis of hemiterpenes, monoterpenes and the variants irregular monoterpenes and iridoids, sesquiterpenes, diterpenes, sesterterpenes, triterpenes, tetraterpenes, and higher terpenoids. Structures are rationalized through extensive use of carbocation mechanisms and subsequent Wagner–Meerwein rearrangements.

Steroids biogenesis in detail, including stereochemistry and molecular shape. Examples cholesterol, steroidal saponins, cardioactive glycosides, phytosterols, vitamin D, bile acids, corticosteroids and their semi-synthesis, progestogens, oestrogens, and androgens. Biogenesis of taxol, vitamin A, **[10 Hours]**

3. **Alkaloids:** Biogenesis of Onithine based(pyrrolizidine), Lysine based (quinolizidine and indolizidine), Pyridine based, Tyrosine and modified tetrahydroisoquinoline based alkaloids, Phenethylisoquinoline and terpinoid tetrahydroisoquinoline (Amaryllidaceae alkaloids) anthranilic acid based, simple Indole and terpinoid indole **[08 Hours]**
4. **The Shikimate pathway:** Cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids and terpenoid quinones. **[06 Hours]**

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

Course code and Title: CHO-652-MJ Organometallic Reagents in Organic Synthesis (4 Credits, 60 Hours)

Learning Outcomes: After completion of the course, students would be able to

1. Use of Transition metal complexes in organic synthesis.
2. Role of metal in catalysis reactions
3. Concept of catalysis
4. Knowledge of name reactions in synthesis
5. Different application of name reactions
6. Use of organo boron and silicon reagents in organic synthesis.

Section-I: Transition Metals Complexes in Synthesis (2 Credits, 30 Hours)

1. Transition metal complexes in organic synthesis-Introduction-oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal,ligand and % mole concepts **[04 Hours]**
2. Transition metal complexes in C-C, C-N, C-O bond formation reactions with catalytic cycle:Pd, Ni, only **[10 Hours]**
3. Asymmetric transfer hydrogenation reactions:Ru, Rh only **[04 Hours]**
4. Aerobic Cu Catalyzed organic oxidation reaction **[04 Hours]**
5. C=C formation reactions: Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe, Tebbe's reagent and Peterson olefination reactions. **[08 Hours]**

Section II: (2 Credits, 30 Hours)

1. Multi-component reactions: Ugi, Passerini, Biginelli and Mannich reaction **[04 Hours]**
2. Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization **[04 Hours]**
3. Click chemistry: criterion for click reaction, Sharpless azidescycloadditions. Click reactions in synthesis of bioconjugates (sugars and proteins) **[08 Hours]**

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. **[08 Hours]**
5. Organo Boron and Silicon reagents in organic synthesis. **[06 Hours]**
6. Other important reactions: BaylisHilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction. (*Self Learning)

References:
1. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press),
2. Some modern methods of organic synthesis – W. Carruthers (Cambridge)
3. Organic Synthesis Using Transition Metals, by Roderick Bates, Second Edition, A John Wiley & Sons, Ltd., Publication.
4. Organic synthesis – Michael B. Smith
5. Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007).
6. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako
7. Recent advances in homogeneous nickel catalysis Nature 2014, Vol 509, Page 299- 309.
8. Ruthenium-Catalyzed Reactions for Organic Synthesis Chem. Rev. 1998, 98, 2599- 2660.
9. Aerobic Copper-Catalyzed Organic Reactions Chem. Rev. 2013, 113, 6234−6458.

Course code and Title: CHO-653-MJP Convergent and Two stage Organic Synthesis (4 Credits, 120 Hours)

Learning Outcomes: After completion of the course, students would be able to
1. Understand difference between linear and convergent synthesis.
2. Understand what is convergent synthesis and their advantages over linear synthesis.
3. Understand convergent synthesis of small molecules offers advantages in reducing the overall steps count of a sequence while increasing the overall yield.
4. Understand correlation between writing theory reactions and performing actual reactions in practical.

Note: Any **2** sets should be conducted from the following convergent synthesis sets and any **6** two stage preparations. 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: Convergent Organic Synthesis (any three sets) (2 Credits, 60 Hours)

SET-I
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)

SET-II
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)

SET-III

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)

SET-IV

Convergent Synthesis- 4 (Three Stage Synthesis)

1. Stage I: Benzene to actophenone (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)

Section-II: Two Stage Organic Synthesis (any 6) (2 Credits, 60 Hours)

1. Benzaldehyde + Acetophenone-------- Benzalacetophenone-------- Epoxide
2. Cyclohexanone ---------Phenylhydrazone---------- 1, 2, 3, 4-tetrahydrocarbazole
3. 4-Nitrotoluene----- 4-Nitrobenzoic acid------ 4-Aminobenzoic acid
4. Benzophenone-------- Oxime ----------Benzanilide
5. Benzoin---------- Benzil ----------Benzilquinoxaline
6. Acetanilide ----------p-bromo acetanilide ----------p-bromoaniline
7. Benzyl cyanide-------- p-nitro benzyl cyanide ----------p-nitro phenyl acetic acid
8. Preparation of Wittig reagent followed by olefination
9. Preparation of PCC followed by oxidation

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

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.
- Students opting for the projects 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.

Course code and Title: CHO-661E-MJ A) Medicinal Chemistry (4 Credits, 120 Hours)

Learning Outcomes: After completion of the course, students would be able to
1. Understanding and basic concepts and applications of medicinal chemistry.
2. To know the drug design and development approach.
3. Pharmacokinetics and Pharmacodynamics of drug

Section-I (2 Credits, 30 Hours)

1. Introduction to medicinal Chemistry. History, drug targets, Drug discovery, design and development, Case Study: Design of Oxamniquine. **[06 Hours]**

2. Introduction to 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 Hours]**
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. **[07 Hours]**
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. **[07 Hours]**

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 Hours]**

2. Selected examples of drug mechanisms, selected examples of the following drugs: NSAI steroids, antibacterials, anticancer, antiulcer, drugs related to tropical diseases, antivirals, antihistamines. **[16 Hours]**

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

Course code and Title: CHO-661E-MJ B) Applied Organic Chemistry (4 Credits, 120 Hours)

Learning Outcomes: After completion of the course, students would be able to
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 Hours]**
(Ref: Review article by Maria S. Lohse and Thomas Bein ***Adv. Funct. Mater***. 2018, 28 (33), 1705553.)

2. Organic Electroluminescent Materials, [15 Hours]
(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 Hours]
(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 Hours]

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

Course code and Title: CHO-681-RP Research Project (6 Credits, 180 Hours)

Learning Outcomes:
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 12 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 (10 min). It is open type of examination.

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 50 marks (50%) while college evaluation shall be of 50 marks (50%). To pass the course, a student has to secure 40% mark in continuous assessment as well as college assessment i.e. 20 marks in continuous assessment and 20 marks in college assessment.

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

For theory and practical course, 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 one ternary mixture/two experiments for each practical. Each section and each experiment will be of **25 marks** .

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

M.Sc.-II Examination Semester Pattern

Internal Theory Examination

- Time: 1.30 hour
- Total Marks: **25**: 20 Marks Internal examination + 5 Marks assignment/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: 2 hours
- Total Marks: **50**
- Title of the questions:

  Section -I

  Q.1) Answer the following (any 7) (7M)

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

  Q.3) Attempt any four of the following (12M)

  Section-II

  Q.4) Answer the following (any 7) (7M)

  Q.5) Attempt any three of the following (6M)

  Q.6) Attempt any four of the following (12M)
- All questions are compulsory

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

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

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

Internal Practical Examination

Total Marks: **25**, 15 Marks for experiment + 5 Marks for Oral/seminar + 5 Marks for journal

External Practical Examination

Total Marks: **25**, 20 Marks for experiment + 5 Marks for Oral