Savitribai Phule Pune University

(Formerly University of Pune)

Post Graduate Program in Chemistry

(Faculty of Science and Technology)

Syllabi (As Per National Education Policy – 2020) for

M. Sc. Drug Chemistry Part – II

(For Colleges Affiliated to Savitribai Phule Pune University)

Approved by Board of Studies in Chemistry

To be implemented with the effect from Academic Year 2024 - 2025

M. Sc. Drug Chemistry Part II Programme Structure

SEMESTER III

Sr. No.	Course	Course Code	Major Core/ Major elective	Credits
1.	Drug Discovery and Development	CHD-601 MJ	Major Core	4T
2.	Spectroscopic Methods in Structure Determination	CHD-602 MJ	Major Core	4T
3.	Stereochemistry	CHD-603 MJ	Major Core	2T
4.	Synthesis of Heterocycles	CHD-604 MJP	Major Core	2P
5.	Solvent free Organic Synthesis	CHD-605 MJP	Major Core	2P
6.	Advanced Heterocyclic Chemistry	CHD-610 (A) MJ	Major elective (Any two)	4T
	Synthesis of Biologically active Molecules	CHD-610 (B) MJ		
	Microbiology and Immunology	CHD-610 (C) MJ		
7.	Research Project (RP)	CHD-631 RP	Research Project	4

SEMESTER IV

Sr. No.	Course	Course Code	Major Core/ Major elective	Credits
1.	Drug Design	CHD-651 MJ	Major Core	4T
2.	Advanced Medicinal Chemistry	CHD-652 MJ	Major Core	4T
3.	Ternary Mixture Separation	CHD-653 MJP	Major Core	2P
4.	Organic Synthesis by Named reactions	CHD-654 MJP	Major Core	2P
5.	Advanced Synthetic methods in Chemistry	CHD-660 (A) MJ	Major elective (Any two)	4T
	Organometallic reagents in Organic Synthesis	CHD-660 (B) MJ		
	Forensic Chemistry	CHD-660 (C) MJ		
6.	Research Project (RP)	CHD-681 RP	Research Project	6

PROGRAM OUTCOMES (POs):

PO No.	PO Statement After completing the Programme Master of Science in Drug Chemistry, students will be able to	Knowledge and Skill
PO-1	Learn the terms, theories, assumptions, methods, principles, theory statements, and classification.	Disciplinary knowledge
PO-2	Fixed out the problem and resolved it using theories and practical knowledge.	Critical thinking & Problem-solving
PO-3	Inculcate his knowledge for carrying projects and advanced research-related skills.	Research related skill
PO-4	Actively participate in the team on case studies and field-based situations.	Cooperation/Teamwork
PO-5	Analyse and interpret ideas, evidence, and experiences with learned scientific reasoning	Scientific reasoning
PO-6	Aware and implement the subject facts that can be applied to personal and social development	Reflective thinking
PO-7	Use digital literacy to retrieve and evaluate subject-related information	Information/Digitally literacy:
PO-8	Get moral and ethical values for society as well as in research	Moral and ethical awareness
PO-9	Give analytical reasoning to interpret research data.	Analytical Reasoning
PO-10	Improve their managerial skills and abilities in subject-related activities.	Leadership readiness/qualities
PO-11	Inculcate continuous learning habits through all available resources.	Lifelong readiness/qualities

PROGRAM SPECIFIC OUTCOMES (PSOs):

PO No.	Programme Specific Outcome Statement After completing the Programme Master of Science in Drug Chemistry, students will be able to
PSO-1	Demonstrate proficiency in advanced terms, theories, principles, and techniques of chemistry through different courses, laboratory experiments, and research projects.
PSO-2	Develop a foundational understanding of research methodologies, including literature review, hypothesis formulation, experimental design, data analysis, and interpretation.
PSO-3	Acquire hands-on experience with advanced chemistry-related equipment.
PSO-4	Apply modern research techniques to investigate complex chemical phenomena and solve practical problems.
PSO-5	Demonstrate competence in quality assurance and quality control practices essential for industry.

CHD-601 MJ: Drug Discovery and Development

Course type: Major **No. of Credits: 4**

Course Outcomes

After the completion of this course, students will be able to

CO1: Acquire advanced knowledge of the general stages of modern drug discovery.

CO2: Learn the Strategies used in drug discovery.

CO3: Apply acquired knowledge of Screening of Lead compounds in research.

CO4: Discuss the Sources of drugs.

CO:5: Evaluate the pre-clinical testing and clinical trials.

CO6: Discuss the concept regarding drug development.

Course Content

Section I	
Drug Discovery 1] Introduction to drugs, concept, terminology, history of drugs, classification of drugs, need of drug, generic drugs, drug discovery and stages in modern drug discovery. 2] Strategies used in drug discovery, lead discovery, pharmacophore identification, lead development, bioassay and types of bioassay. 3] Screening of lead compounds. 4] Sources of drugs: plants, microbial, animals, minerals, marine, toxins, synthetic and semisynthetic etc.	**16 Hours**
Drug targets Drugs and drug target overview and examples: 1] Proteins (enzyme, receptor, ion channels etc.) 2] Carbohydrates, 3] Lipids and 4] Nucleic acids.	**6 Hours**
Introduction to the different systems of medicines History, basic principles: Ayurveda, Siddha, Unani, Homeopathy, Chinese and Allopathy.	**6 Hours**
Pharmacokinetics and Pharmacodynamics of drug action	**2 Hours**

Pharmacokinetics and Pharmacodynamics of drug action, journey of drug, drug absorption, drug distribution, drug metabolism, drug excretion.	
Section II	
Drug Development 1] Toxicological evaluation of new drugs, repurposed drugs, parameters used in toxicological evaluation of new drugs, individual toxicity studies. 2] Preclinical testing and clinical trials. 3] Bioavailability of drugs, types, factors affecting on bioavailability and bioequivalence.	**11 Hours**
Pharmaceutical aspects 1] Routes of drug administration. 2] Formulation of dosage forms, types of dosage forms: a) Solid (granules, tablets, capsules and powder), b) Semisolid (gel, ointments and creams) c) Liquid (solutions, syrups and elixir), d) Sterile (parenteral/ injectable), e) Gaseous (spray, inhaler) f) Biological (vaccines).	**12 Hours**
Industrial aspects 1] Journey from R and D to plant, QA, QC, scale up process, pilot plant, good manufacturing practices (GMP), food and drug administration (FDA), 2] Documentation, Pharmacopeia (Indian Pharmacopeia, British Pharmacopeia and United States Pharmacopeia) 3] Industrial hygiene and safety, good laboratory practices (GLP)	**07 Hours**

References

1. Medicinal Chemistry: An Introduction by Gareth Thomas, 2nd Edn., Wiley, 2013.
2. An Introduction to Medicinal Chemistry by Graham L. Patrick, 6th Edn., Oxford University press, 2017.
3. Introduction to Medicinal Chemistry, How Drugs Act and Why by Alex Gringauz, 1st Edn., Wiley-VCH, 1996.
4. Comprehensive Medicinal Chemistry Vol-I, edited by C. Hansch, Pergamon press, 1990.
5. Principle of Drug Action: The Basis of Pharmacology (A Wiley biomedical-health publication) by Goldstein A., 2nd Edn., Wiley-Blackwell, 1974.
6. Dissolution, Bioavailability and Bioequivalence by H. M. Abdou, 1st Edn., Mack publication, 1989.
7. Indian Pharmacopoeia, volumes I to IV, 9th Edn., 2022.

8. British Pharmacopoeia, volumes I to VI, 11th Edn., 2024.
9. United States Pharmacopeia, volumes I to II, 2015.
10. Ansel's Pharmaceutical Dosage forms and Drug Delivery System by, L. V. Allen Jr., H. C. Ansel, 10th Edn., Wolters Kluwer Health, 2013.
11. Organic Chemistry of Drug Design and Drug Action by R. B. Silverman and M. W. Halladay, 3rd Edn., Academic Press Inc, 2014.
12. Burger's Medicinal Chemistry and Drug Discovery, edited by Donald J. Abraham, volumes I to IV, 6th Edn., Wiley Inter Science, 2003.

CHD-602 MJ: Spectroscopic Methods in Structure Determination

Course type: Major **No. of Credits: 4**

Course Outcomes

After the completion of this course, students will be able to-

CO1: Learn the fundamental knowledge of ^{1}H NMR, ^{13}C NMR and Mass Spectral techniques.

CO2: Acquire advanced knowledge of ^{1}H NMR, ^{13}C NMR and Mass Spectral techniques.

CO3: Apply the knowledge of ^{1}H NMR, ^{13}C NMR and Mass Spectral techniques for structure determination.

CO4: Discuss probable spectral signals.

CO5: Interpret different types of spectra.

CO6: Deduce the structure of the unknown compound using ^{1}H NMR, ^{13}C NMR and Mass Spectra.

Course Content

Section I	
^{1}H NMR Spectroscopy **Recapitulation:** shielding and deshielding, Chemical shift, factors influencing chemical shift, Chemical and magnetic shift equivalence. **Chemical shift(δ)**: correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei (oxygen and nitrogen); **Spin-spin splitting:** (n+1) rule, origin of spin-spin splitting, pascal triangle. **Coupling Constant (J):** Mechanism of coupling, Type (Geminal, vicinal coupling, long range and W coupling), factors effecting geminal and vicinal coupling constant; **Spin System:** classification of spin system, spin notations (A_2, AB, AX, AB_2, AX_2, ABC, ABX, AMX, A_2B_2, A_2X_2), complex spin-spin interaction between two, three and four nuclei (First Order Spectra and Second order spectra); **Simplification of complex spectra:** nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, chiral resolving agent, Nuclear	**16 Hours**

Overhauser Effect (NOE), resonance of other nuclei like ^{31}P, ^{19}F. Problems and Assignment of PMR signal.	
^{13}C NMR Spectroscopy **Recapitulation:** ^{13}C Nucleus, Chemical Shift and factor affecting ^{13}C NMR; **Types of ^{13}C NMR Spectra:** proton coupled (spin-spin splitting), Proton decoupled, Off resonance; **Pulse sequence:** spin and magnetization vector, DEPT, APT and NOE; **Coupling constants:** Homo nuclear (^{13}C-^{13}C) and Hetero nuclear (^{13}C-^{1}H, ^{13}C-^{19}F, ^{13}C-^{31}P). Problem and Assignment of ^{13}C NMR signal	**14 Hours**
Section II	
Mass Spectrometry Instrumentation, **various methods of ionization:** Gas phase ionization (electron impact and Chemical) Desorption ionization (field desorption, FAB, Plasma, Laser), Evaporative ionization (Thermospray and Electrospray mass spectrometry); **Detectors:** Quadrupole mass filter, time of flight (TOF); **EI mass spectra interpretation:** intensity of molecular ion peak, base peak, fragment ion peak and isotope peak (M+1, M+2); Nitrogen Rule, Fragmentation Pattern and McLafferty rearrangement. **Fragmentation of functional groups:** Hydrocarbons, Ether, Aldehyde, Ketone, Carboxylic Acid, Ester, Amide, Sulphur and halogen compound. **Application of Mass spectrometry:** Molecular formula determination (Rule of 13).	**12 Hours**
Correlation Spectrometry: 2D NMR Pulse sequence in 1D and 2D spectra, type of 2D (Homo and Hetero nuclear); **2D in structure determination:** 1H-1H Correlation spectroscopy (COSY), Double Quantum Filtered COSY (1H-1H), Heteronuclear Correlation (HETCOR, HMQC and HMBC); **Applications:** INADEQUATE, Totally correlated spectroscopy (TOCSY), NOESY and ROESY experiments.	**8 Hours**
Structure Elucidation 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.	**10 Hours**

A] Organic molecules B] Drug molecules: 1) Vitamin C, 2) Thienamycin, 3) Clavulanic acid and 4) Geraniol	

References

1. Introduction to Spectroscopy by D. L. Pavia, G. M. Lampman and G. S. Kriz, 3rd Edn. Harcourt College Publishers, 2001.
2. Spectrometric Identification of Organic Compounds by R. M. Silverstein and F. X. Webster, D. J. Kiemle and D. L. Bryce, 8th Edn., John Wiley and Sons, 2014.
3. Spectroscopic Methods in Organic Chemistry by D. H. Williams and I. Fleming, 4th Edn., Mc Graw Hill, 2007.
4. One and Two Dimensional NMR spectroscopy by Atta-Ur-Rehman, 1st Edn., Elsevier, 1989.
5. Organic Structures from Spectra by L. D Field, S. Sternhell, and J. R. Kalman, 4th Edn., John Wiley and sons Ltd., 2008.
6. Spectroscopic Identification of Organic Compounds by M. Silverstein, G. C. Bassler, and T. C. Morril, 7th Edn., John Wiley, 1991.
7. Spectroscopy of organic molecule by P. S. Kalsi, 7th Edn., New Edge International Pvt. Ltd., 2016.
8. Absorption spectroscopy of organic molecules by V. M. Parikh
9. Organic structure Analysis by Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998).
10. Organic structural Spectroscopy by Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice Hall (1998).
11. Introduction to NMR spectroscopy by R. J. Abrahm, J. Fisher and P. loftus, Wiley.
12. Structure determination of Organic compounds by E. Pretsch, P. Buhlman, and C. Affolter, Springer (2005).
13. High-Resolution NMR Techniques in Organic Synthesis by Claridge, 3rd Ed., Wiley, 2016.

CHD-603 MJ: Stereochemistry

Course type: Major **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to-

CO1: Learn the stereochemistry principles governing six-membered rings.

CO2: Gain advanced knowledge about the shapes, reactivity, and conformational effects of rings other than six-membered rings.

CO3: Apply the significance of stereoselective synthesis and asymmetric synthesis in drug design.

CO4: Examine the stereochemistry principles applicable to drug molecules.

CO5: Evaluate the shapes, reactivity, and conformational effects of fused rings and bridged ring systems.

CO6: Create synthetic and industrial applications based on deduced principles.

Course Content

Stereochemistry of six membered rings Relation to physical properties, conformation and chemical reactivity, conformational effects in six membered rings containing unsaturation. Conformations of polysubstituted cyclohexane, six membered rings with SP2 carbon, heterocycleswith N and O, anomeric effect.	**5 Hours**
Stereochemistry of 1) Rings other than six membered rings: Small rings, Medium rings, Large rings, concept of I strain, transannular effects. 2) Fused rings and bridged rings: Nomenclature, synthesis; stereochemical aspects of Decalin, Perhydrophenanthrene, Perhydroanthracene, hydrindane, Steroids; Bridged system (bi, tri and polycyclo system) including heteroatoms, Bredt' rule.	**8 Hours**
Stereochemistry of Drug molecules a) Saquinavir (HIV protease inhibitor) b) Abiraterone (drug for prostate cancer) c) R- and S-enantiomers of Ibuprofen (non-steroidal anti-inflammatory)	**3 Hours**
Principles and applications of asymmetric synthesis Stereoselectivity in cyclic compounds, enantio-selectivity, diastereo-selectivity, enatiomeric and diastereomeric excess, stereoselective aldol reactions. Cram's	**14 Hours**

rule, Felkin Anh rule, Cram's chelate model, Asymmetric synthesis, use of chiral auxiliaries, chiral reagents and catalysts, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation. Synthetic and Industrial applications.	

References

1. Stereochemistry of Carbon Compounds by E. L. Eliel, Tata McGraw Hill Education, 1962.
2. Stereochemistry of Carbon Compounds by E. L. Eliel and S. H. Wilen, Wiley.
3. Organic Chemistry by J. Clayden, N. Greeves, S. Warren and P. Wothers, 1st Edn., Wiley, 2008.
4. Stereochemistry of Organic Compounds: Principles and Applications by D. Nasipuri, 3rd Edn., New Edge International Publishers, 2018.
5. Stereochemistry: Conformation and Mechanism by P. S. Kalsi, 11th Edn., New Edge International Publishers, 2022.
6. Stereochemistry with Applications to Organic Reaction by Jagdamba Singh, 1st Edn., New Edge International Pvt. Ltd., 2020.
7. Topics in Stereochemistry by Norman L. Allinger and Ernest L. Eliel, Volume 2, Wiley, 1967.
8. Topics in Stereochemistry by Ernest L. Eliel and Norman L. Allinger, Volume 8, Wiley, 1974.
9. Additional Study Material: Stereochemistry
   https://nptel.ac.in/content/syllabus_pdf/104105086.pdf
   https://nptel.ac.in/courses/104/105/104105086/

CHD-604 MJP: Synthesis of Heterocycles

Course type: Major **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to-

CO1: Understand the fundamental concepts of heterocyclic chemistry.

CO2: Explain the fundamental principles and applications of heterocyclic chemistry.

CO3: Perform laboratory experiments and submit detailed lab reports.

CO4: Analyze data, interpret the results, and present their findings in lab reports and presentations.

CO5: Develop the ability to design synthetic routes for the construction of various heterocyclic frameworks, considering efficiency, yield, and sustainability.

CO6: Enhance their problem-solving and critical thinking skills.

Course Content

Note: The students must perform at least twelve (12) experiments and their spectral characterization.

1. Synthesis of Benzotriazole from O-Phenylenediamine
2. Synthesis of 4, 5 Diphenyl Imidazole from Benzil
3. Synthesis of 3, 5 Dimethyl Isoxazole from Acetylacetone
4. Synthesis of 7-Hydroxy-4-Methyl Coumarin from Resorcinol
5. Synthesis of Benzimidazole from O-Phenylenediamine
6. Synthesis of 1-Phenyl-3-Methylpyrazol-5-One from Ethyl Acetoacetate
7. Synthesis of 3,5 Diethoxycarbonyl-2,4 Dimethyl Pyrrole from Ethyl Acetoacetate
8. Synthesis of 2-Phenyl indole from Acetophenone
9. Synthesis of Quinoline from Aniline
10. Synthesis of Dihydropyrimidone from Urea
11. Synthesis of 1,2,3,4 tetrahyracarbazole from cyclohexanone
12. Synthesis of 3, 5 Dimethyl Pyrazole from Acetyl acetone
13. Synthesis of 2, 5 dioxopiperazine from Glycine
14. Synthesis 4-benzylidene 2-phenyl oxazol-5-one from hippuric acid

References

1. Practical Organic Chemistry by F. G. Mann and B. C. Saunders, 4th Edn., Pearson, 2009.
2. Practical Heterocylic Chemistry, A. D. Fitton and R. K. Smalley, Academic Press, 2013.
3. Vogel's Text book of Practical Organic Chemistry, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, 5th Edn., Pearson, 2003.
4. Organic Synthesis Collective, Volume I to XII, edited by J. B. Freeman, W. E. Noland, A. H. Blatt, N. Rabjohn, H. E. Baumgarten and C. K. Zercher, Wiley, 2015.
5. Macroscale and Microscale organic experiments by K. L. Williamson and K. M. Masters, 5th Edn., Books/Cole, 2016.
6. The Systematic Identification of Organic Compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin, 8th Edn., Wiley, 2004.
7. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis by V. K. Ahluwalia and Renu Aggarwal, Sangam Books Ltd., 2001.

CHD-605 MJP: Solvent free organic synthesis

Course type: Major **No. of Credits: 2**

Course Outcomes

After the completion of this course, student will be able to-

CO1: Learn the concept of solvent-free organic synthesis.

CO2: Understand various synthetic strategies.

CO3: apply the gained knowledge in solvent-free organic synthesis.

CO4: analyse different synthesis and purification techniques.

CO5: evaluate the solvent-free synthesis methods.

CO6: design a plan for different solvent-free organic synthesis.

Course Content

Note: The students must perform at least fifteen (15) experiments and their spectral characterization.

1. Synthesis of dihydropyrimidinone from benzaldehyde and urea.
2. Synthesis of coumarin from *p*-cresol / resorcinol.
3. Synthesis of calix [4] resorcinarene from resorcinol.
4. Synthesis of Ethyl acetoacetate from ethyl acetate.
5. Synthesis of 2,6 di bromo 4-nitrophenol from 4-nitrophenol.
6. Bromination of Cinnamic acid using Sodium bromide and sodium bromate.
7. Synthesis of L, L cysteine from L-Cysteine using iodine catalyst.
8. Synthesis of Benzilic acid from Benzil.
9. Synthesis of 2,4 Dimethyl 3,4-benzo[b] [1,4] diazepine from acetylacetone and O-phenylenediamine
10. Synthesis of 1, 1 bis-2 napthol from 2-napthol.
11. Base catalysed aldol condensation using LiOH/H2O.
12. Ecofriendly nitration of phenol and its derivative using Calcium nitrate.
13. Synthesis of Diels -Alder adduct by using Anthracene.
14. Benzilic acid from benzoin (Benzilic acid rearrangement)
15. Benzopinacolone from Benzopinacol using iodine

16. Synthesis of catecholfrom salicyaldehyde
17. Synthesis of phenyl hydrazone derivative of acetophenone
18. Synthesis of methyl phenyl sulphoxide from by oxidation of methyl phenyl sulphide
19. Synthesis of substituted chalcone from acetophenone and p-chlorobenzaldehyde
20. Synthesis of diphenylsulphide from thiophenol in presence of MnO_2

References

1. Solvent-free Organic Synthesis by Koichi Tanaka (Copyright © 2009 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, ISBN: 978-3-527-32264-)
2. Additional Study Material: https://nptel.ac.in/courses/104/106/104106108/
3. Practical Organic Chemistry by F. G. Mann and B. C. Saunders, 4th Edn., Pearson, 2009.
4. Practical Heterocylic Chemistry, A. D. Fitton and R. K. Smalley, Academic Press, 2013.
5. Vogel's Text book of Practical Organic Chemistry, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, 5th Edn., Pearson, 2003.
6. Organic Synthesis Collective, Volume I to XII, edited by J. B. Freeman, W. E. Noland, A. H. Blatt, N. Rabjohn, H. E. Baumgarten and C. K. Zercher, Wiley, 2015.
7. Macroscale and Microscale organic experiments by K. L. Williamson and K. M. Masters, 5th Edn., Books/Cole, 2016.
8. The Systematic Identification of Organic Compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin, 8th Edn., Wiley, 2004.
9. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis by V. K. Ahluwalia and Renu Aggarwal, Sangam Books Ltd., 2001.

CHD-610 (A) MJ: Advanced Heterocyclic Chemistry

OR

CHD-610 (B) MJ: Synthesis of Biologically active Molecules

OR

CHD-610 (C) MJ: Microbiology and Immunology

Course type: Major elective (Any Two) **No. of Credits: 4**

CHD-610 (A) MJ: Advanced Heterocyclic Chemistry

Course type: Major elective **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to

CO1: Recall the systematic nomenclature rules for heterocyclic compounds.

CO2: Explain the structural differences between monocyclic, fused, and bridged heterocycles.

CO3: Develop synthetic pathways for the preparation of condensed heterocycles based on their structural characteristics and reactivity patterns.

CO4: Analyse the reactivity patterns of heterocycles with more than one heteroatom.

CO5: Evaluate the effectiveness of different synthetic routes for the preparation of heterocyclic compounds, considering factors such as yield, selectivity, and environmental impact.

CO6: Design novel heterocyclic compounds with specific functional groups for potential applications in drug discovery or materials science.

Course Content

Recapitulation: **Nomenclature and structure of Heterocyclic Compounds** Systematic nomenclature (Hantzsch-Widman System) for monocyclic, fused and bridged heterocycles.	**1 Hour**
Five membered Heterocyclic Compounds Structure, Nomenclature, Aromaticity, reactivity, synthesis and reactions of Pyrrole, Thiophene and Furan.	**3 Hours**

Condensed five membered heterocycles Structure, Nomenclature, Aromaticity, reactivity, synthesis and reactions of Indole, Benzofuran and Benzothiophene	**4 Hours**
Condensed six membered heterocycles Structure, Nomenclature, Aromaticity, reactivity, synthesis and reactions of Quinoline, Isoquinoline, Coumarins and Chromones.	**8 Hours**
Heterocycles having more than one hetero atom Structure, Nomenclature, Aromaticity, reactivity, synthesis and reactions of Five membered, condensed five members, six membered and condensed six membered heterocycles with more than one heteroatom- Oxazole, imidazole, Thiazole, pyrazole, isothiazole, triazole (1,2,3-triazole, 1,2,4- triazole), oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.	**10 Hours**
Pyridine and Pyrimidine Structure, Nomenclature, Aromaticity, reactivity, synthesis and reactions of Pyridine, Pyrimidine and Pyridine N oxide.	**4 Hours**
Additional study material: https://nptel.ac.in/content/syllabus_pdf/104105034.pdf https://nptel.ac.in/courses/104/105/104105034/	**------**

References

1. Heterocyclic Chemistry by John A. Joule, Keith Mills, 5th Edition, 2010,
2. Heterocyclic Chemistry by Gilchrist, T. L.,3rd ed.; Addison Wesley Longman: Edinburgh Gate
3. Principles of Modern Heterocyclic Chemistry by Paquette.
4. The Essence of heterocyclic Chemistry, A. R. Parikh, H. Parikh, R. Khunt, New Age Int. Publication.
5. Principles of Modern Heterocyclic Chemistry, L. A. Paquette, W. A. Benjamin, New York, 1968.
6. Name reactions in Heterocyclic Chemistry, Jie Jack Li, John Wiley and Sons Inc. Publication, 2005.
7. Comprehensive Heterocyclic Chemistry. The structure, reactions, synthesis and use of Heterocyclic compounds, (Ed. A.R. Katritzky and C. W. Rees). Vol 1-8, Pergamon Press, 1984.
8. Handbook of Heterocyclic Chemistry, A. R. Katritzky, Pergamon Press, 1985.

9. Chemistry of Heterocycles, Theophil Eicher, Siegfried Hauptmann, Wiley VCH, 2003.
10. Heterocyclic Chemistry by R. K. Bansal, New Age International Publishers (P) Ltd., 2005.
11. An Introduction to the Chemistry of Heterocyclic Compounds by RM Acheson, 3rd Edn., Wiley 2008.

OR

CHD-610 (B) MJ: Synthesis of Biologically Active Molecules

Course type: Major elective **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to,

CO1: Learn the fundamental aspects and knowledge of biologically active molecules.

CO2: Understand pathways and biogenesis and their laboratory synthesis.

CO3: Apply the knowledge of basic as well as advanced reactions and new reagents in the synthesis.

CO4: Discuss the functional group transformations in their synthesis.

CO5: Interpret the logical retrosynthetic analysis.

CO6: Deduce the correct mechanism including stereochemistry

Course Content

1] An Introduction to Total Synthesis Importance of total synthesis; Challenges in multistep synthesis; Merits and demerits of divergent and convergent synthesis; Need and criteria of protection and deprotection; importance of chemo/ regio /stereo-selectivity in synthesis.	**3 Hours**
2] Total synthesis of **a) Oseltamivir** i] Journal of American Chemical Society 1997, 119, 681-690 (Scheme 2 and 3), doi.org/10.1021/ja963036t. ii] Pharmaceutical Industry in Swizerland; Chemia 2004, 58, 621-629, doi.org/10.2533/000942904777677605.	

b) Atorvastatin i] Alexander Domling et al. Medicinal Chemistry Letters. 2019, 10, 389-392, doi:10.1021/acsmedchemlett.8b00579.	**27 Hours**
c) Brevisamide i] J. S. Yadav et al. European Journal of Organic Chemistry, 2016, 13, 2300-2307. ii] Olugbeminiyi O. Fadeyi and Craig W. Lindsley, Organic Letters 2009, 11(17), 3950-3952, doi.org/10.1021/ol9015755.	
d) Prostaglandin F2α i] Classics in total synthesis by K. C. Nicolaou and E. J. Sorensen. ii] Advanced Organic Chemistry; Part B: Carey and Sundberg.	
e) Estrone and Mifepristone i] Classics in total synthesis by K. C. Nicolaou and E. J. Sorensen. ii] Advanced Organic Chemistry; Part B: Carey and Sundberg.	

References

1. a) Virtual textbook of organic chemistry; William Revsch, Prof. Emeritus, Michigan state university;
   b) Organic Chemistry; Clayden, Greeves, Warren and Wothers.
   c) Advanced Organic Chemistry; Part B: Carey and Sundberg.
2. a) i] Journal of American Chemical Society 1997, 119, 681-690 (Scheme 2 and 3), doi.org/10.1021/ja963036t.
   ii] Pharmaceutical Industry in Swizerland; Chemia 2004, 58, 621-629, doi.org/10.2533/000942904777677605.
   b) i] Alexander Domling et al. Medicinal Chemistry Letters. 2019, 10, 389-392, doi:10.1021/acsmedchemlett.8b00579.
   c) i] J. S. Yadav et al. European Journal of Organic Chemistry, 2016, 13, 2300-2307.
   ii] Olugbeminiyi O. Fadeyi and Craig W. Lindsley. Organic Letters 2009, 11(17), 3950- 3952, doi.org/10.1021/ol9015755.
   d) i] Classics in total synthesis by K. C. Nicolaou and E. J. Sorensen.
   ii] Advanced Organic Chemistry; Part B: Carey and Sundberg.
   e) i] Classics in total synthesis by K. C. Nicolaou and E. J. Sorensen.
   ii] Advanced Organic Chemistry; Part B: Carey and Sundberg.

OR

CHD-610 (C) MJ: Microbiology and Immunology

Course type: Major elective **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to,

CO1: gain a knowledge of Microbes.

CO2: understand the concept of primary and secondary screening.

CO3: apply the knowledge of Microbial Drug Development, Immunology and Immunopharmacology

CO4: analyze the different effluent treatments.

CO5: Learn an Overview of the immune system.

CO6: Design Diagnostic techniques.

Course Content

Microbial Drug Development 1] Introduction to Microbiology and Classification of Microbes. 2] Screening of Microbes fermentation process, the concept of primary and secondary screening, characterization of ideal industrial strains, Microbia1growth, kinetics, Isolation and Improvement of Individualmicroorganism. 3] Fermenter designing, Media designing, antimicrobial assays; Down Stream process and effluent treatment (Microbial and Chemical)	**12 Hours**
Immunology and Immunopharmacology 1]Overview of the immune system and its role, three lines of defense, Types of immunity – active, passive, cell mediated and humoral immunity. 2] Antigen and antibody, organs of immune system (Primary and secondary). Adaptive and innate Immunity. 3]Immune responseand the underlying mechanisms, Hypersensitivity, immunodeficiency, Autoimmunity,Immunization, Immunosuppressant's, Immunomodulators, 4]Immunological techniques: Agglutination reaction (Haemogluttination, bacterial agglutination), Precipitation reaction (single and double	**18 Hours**

Immunodiffusion) 5] Diagnostic techniques: i)Enzyme Linked Immunoassay (ELISA), ii)Radioimmunoassay (RIA) and iii)Fluorescence-Activated Cell Sorting(FACS)	

References

1. Principles of Medicinal Chemistry including Proteomics S. Rangnathan and Jerad Suresh 2011CBS press
2. Statistical Methods in Biology-Norman Bailey (1995) Cambridge
3. Molecular Modeling, Principles and applications -Andrew Leach (Longman) 1998.
4. Comprehensive Medicinal Chemistry vol.4 Corwin Hansch (1990) pergaman press.
5. Organic Chemistry of drug design and drug action by R. B. Silverman 2nd Ed. (2004)Elsevier
6. Basic and Chemical Immunology-Stites (1987) Prentice Hall.

CHD-631 RP Research Project

Course type: Research Project **No. of Credits: 4**

Course Outcomes

At the end of the course, students will be able to -

1. understand key concepts and principles relevant to the research topic.
2. learn diverse research methodologies proficiently.
3. write and communicate research findings persuasively through various mediums in the form of project report
4. analyze and synthesize scholarly literature effectively.
5. evaluate research findings and methodologies critically.
6. design and execute original research projects independently.

Following guidelines should be followed for the conduction and evaluation of research project.

- Each student will perform project separately.
- Project working hours should be 30 hours for each credit.
- Choose a topic that aligns with your interests and career goals, but also consider its feasibility within the available resources and time frame.
- Consult with faculty members, advisors, or mentors to identify a research area that has potential for contribution to the field of chemistry.
- Adhere to ethical principles and standards in all aspects of your research.
- Project report must be written systematically and presented in bound form: The project will consist of name page, certificate, content, summary of project followed by introduction, literature survey (recently published research papers must be included), experimental techniques, results and discussion, conclusions, Appendix consisting of i) references, ii) standard spectra / data if any and iii) safety precautions.
- 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 and discuss results and conclusions in details (10-15 min.) which will be followed by question-answer session (5-7 min). It is open type of examination.

- Students are encouraged to participate in national and international conferences and other project competitions.
- For conducting research study in M.Sc. Chemistry, it is highly recommended to follow the journals given below or any other journal from reputed publication.

1. **Journal of the American Chemical Society (JACS)**
   Publisher: American Chemical Society (ACS)
   Focus: Comprehensive coverage of all fields of chemistry, known for high-impact research.
2. **Angewandte Chemie International Edition**
   Publisher: Wiley-VCH on behalf of the German Chemical Society (GDCh)
   Focus: Broad coverage of all chemistry fields, emphasizing novel and significant research.
3. **Chemical Science**
   Publisher: Royal Society of Chemistry (RSC)
   Focus: Cutting-edge research across chemical sciences, open access.
4. **Nature Chemistry**
   Publisher: Nature Publishing Group
   Focus: Multidisciplinary and high-impact research across all areas of chemistry.
5. **Journal of Organic Chemistry (JOC)**
   Publisher: American Chemical Society (ACS)
   Focus: Specialized in organic chemistry, including synthesis and mechanisms.
6. **Inorganic Chemistry**
   Publisher: American Chemical Society (ACS)
   Focus: Research on inorganic and organometallic compounds.
7. **Analytical Chemistry**
   Publisher: American Chemical Society (ACS)
   Focus: Developments and applications in analytical techniques and methodologies.
8. **Physical Chemistry Chemical Physics (PCCP)**
   Publisher: Royal Society of Chemistry (RSC)
   Focus: Physical chemistry, chemical physics, and biophysical chemistry.
9. **Chemical Communications (ChemComm)**

Publisher: Royal Society of Chemistry (RSC)

Focus: Rapid publication of high-quality communications across all chemical sciences.

10. Accounts of Chemical Research

Publisher: American Chemical Society (ACS)

Focus: Comprehensive reviews and accounts of current research topics in chemistry.

11. Chemical Society Reviews

Publisher: Royal Society of Chemistry (RSC)

Focus: The journal publishes high-quality, authoritative, and state-of-the-art reviews across all areas of chemical science. It covers comprehensive and critical reviews on a broad range of topics in chemistry, including emerging and interdisciplinary fields.

CHD-651 MJ: Drug Design

Course type: Major **No. of Credits: 4**

Course Outcomes

After the completion of this course, students will be able to

CO1: Learn various types of receptors and their superfamilies.

CO2: Know the physicochemical properties of pharmacologically active compounds.

CO3: Examine case studies of potent drugs.

CO4: Distinguish between different novel methods used in synthesis.

CO5: Assess the different methods of drug design.

CO6: Create a summary of different methods of drug design.

Course Content

Section I	
Membrane and Receptors 1] Structure of cell membrane, receptors structure, functions and the mechanism of drug action (receptor response), classifications. 2] Types of membrane bound receptors: GPCR, ion channels receptor, kinase linked receptor and their signal transduction mechanism. 3] Design of agonists and antagonists as drugs, receptor theories, models and their types.	**10 Hours**
Quantitative structure activity relationship (QSAR) 1] Physicochemical principles of Drug action, SAR, line of best, drug receptor interactions, description of physicochemical parameters and their calculation; hydrophobicity, electronic factor and steric factor. 2] Quantitative structure activity relationship (QSAR), Hansch equation, Craig's plot, Topliss scheme, bioisosteres, Free Wilson approach. 3]3D QSAR, COMFA, COMSIA and QSAR study of Aspirin.	**10 Hours**
Molecular Biology 1] Recombinant technology, r-DNA products (vaccines, enzymes, hormones), genes, genetic engineering and protein engineering. 2] Hybridoma technology, monoclonal antibodies and biotechnology in production of biologicals as drugs.	**10 Hours**

3] Human gene therapy, Antisense technology, therapeutic agents, an overview of genomics and proteomics.	
Section II	
Combinatorial Chemistry and high throughput Screening 1] Combinatorial Chemistry, concept, need, uses, Solid phase peptide synthesis, need, uses and examples. 2] Parallel synthesis, Mix and split method, principle, example, SPOS, MAOS and Microfluidics. 3] Planning and designing a compound library and Deconvolution. 4] High throughput screening.	**8 Hours**
Computer Aided Drug Design (CADD) 1] Basic concepts of Computational chemistry like Quantum Mechanics, Molecular Mechanics and Force fields. 2] Energy minimization, Conformational search (local and global energy minima, molecular dynamics, stepwise bond rotation and Monte Carlo method). 3] Ligand based drug design, Receptor based drug design. 4] Analog approach, pharmacophore mapping. Molecular modelling, Docking (manual and automatic), De Novo drug design and Virtual Screening. 5] Bioinformatics, Cheminformatics, applications of Bioinformatics, use of Bioinformatics in drug design.	**12 Hours**
Case studies and Strategies 1] Case studies on drug design: Statin, Artemisinin, ACE inhibitors, Oxamniquine. (From the book An Introduction to Medicinal Chemistry by Graham L. Patrick, 6th Edn., Oxford University press, 2017). 2] Current Developments in a] Vaccines: Covishield and Covaxin. b] Monoclonal antibody: Trastuzumab and Rituximab. 3] Drug designs based on pharmacokinetics, Pro-drug Design, Design of enzyme inhibitors.	**10 Hours**

References

1. An Introduction to Medicinal Chemistry by Graham L. Patrick, 6th Edn., Oxford University press, 2017.
2. Medicinal Chemistry: An Introduction by Gareth Thomas, 2nd Edn., Wiley, 2013.
3. Burger's Medicinal Chemistry and Drug Discovery, edited by Donald J. Abraham, volumes I to IV, 6th Edn., Wiley Inter Science, 2003.
4. Comprehensive Medicinal Chemistry Vol-I, edited by C. Hansch, Pergamon press, 1990.
5. Organic Chemistry of Drug Design and Drug Action by R. B. Silverman and M. W. Halladay, 3rd Edn., Academic Press Inc, 2014.
6. Smith and William's Introduction to the Principles of Drug Design and Action by H. John Smith, 4th Edn., CRC press, 2005.
7. Molecular Modelling: Principles and applications by Andrew R. Leach, 1st Edn., Prentice Hall, 1996.
8. Lehninger Principles of Biochemistry sixth Edn. by D. L. Nelson and M. M. Cox, 6th Edn., W. H. Freeman publisher, 2013.
9. Burger's Medicinal Chemistry and Drug Discovery, edited by Donald J. Abraham volumes I to IV, 6th Edn., John Wiley Interscience.
10. Introduction to Medicinal Chemistry, How Drugs Act and Why by Alex Gringauz, 1st Edn., Wiley-VCH, 1996.
11. Principle of Drug Action: The Basis of Pharmacology (A Wiley biomedical-health publication) by Goldstein A., 2nd Edn., Wiley-Blackwell, 1974.

CHD-652 MJ: Advanced Medicinal Chemistry

Course type: Major **No. of Credits: 4**

Course Outcomes

After the completion of this course, students will be able to

CO1: Identify the mode of action of different antibiotics.

CO2: Recognize the physicochemical properties of pharmacologically active compounds.

CO3: Differentiate the diseases caused by various pathogens and their treatment.

CO4: Categorize different novel methods of synthesis.

CO5: Relate the concept of Chemotherapy of cancer and different approaches to treat cancer.

CO6: Summarize the functioning of the CNS, CVS, Gastrointestinal, and Endocrine systems, their coordination, systemic diseases, and treatments.

Course Content

Section I

Antimicrobial therapy Developments, structure activity relationship (SAR), mechanism of action, uses, doses and side effects of following classes of drugs: **1] Antibacterial**: 1) Quinolones and Fluoroquinolones 2) Sulfonamides. **2] Antibiotics**: 1) Beta lactam antibiotics: a) Penicillins, b) Cephalosporins c) Carbapenems and d) Monobactams. 2) Aminoglycosides, 3) Macrolides, 4) Chloramphenicol, 5) Tetracyclines, 6) Peptides and 7) Polyene antibiotics. **3] Antifungal**: 1) Polyene membrane disruptors 2) Ergosterol biosynthesis inhibitors 3) Drugs acting through other mechanism: Flucytosine, Griseofulvin. **4] Antiviral**: a) DNA virus: i) DNA polymerase inhibitors ii) Tubulin polymerization inhibitors and iii) Antisense therapy b) RNA virus: i) Reverse transcriptase inhibitors, ii) Protease inhibitors, iii)Ion channel disruptors and iv) Neuraminidase inhibitors c) Broad spectrum antiviral agents: i) Cytidine triphosphate synthetase inhibitors ii) S- adenosylhomocysteine hydrolase inhibitors **5] Antimalarial**: Types of malaria, Causetive agent, symptoms and. life cycle of malarial parasite.	**20 Hours**

Antimalarial agents: i) 4- substituted Quinolines ii) Artemisinins iii) 8- Amino Quinolines iv) Pyrimethamine and sulfadoxime **6] Antimycobacterial**: a) Antitubercular agents: i) Isoniazid ii) Antibiotics: Rifamycin, Streptomycin, Capriomycin, Canamycin, Clarithromycin, Azithromycin iii) Other Drugs: Pyrazinamide, Ethambutol, para amino Salicylic acid, Ethionamide b) Antileprotic agents: i) Sulphones ii) Antibiotics: Clofazimine, Rifampin c) Mycobacterium Avium Complex (MAC): i) Azithromycin ii) Clarithromycin iii) Leprostatic drugs.	
Cancer and its Chemotherapy 1] Cancer, Causes, Cell Cycle. 2] Diagnosis: Biopsy and positron emission tomography (PET). 3] Treatment with Various classes of drugs, mode of action and side effects: 1] DNA crosslinking agents: a) Alkylating agents b) Organometallics 2] Topoisomerase poisons 3] Antimetabolites 4] Antibiotics 5] Plant Products 6] Protein kinase inhibitors 7] Mitosis Inhibitors 8] Miscellaneous drug and hormonal drugs. 4] Developments in Immunotherapy: Introduction, need, types of immunotherapies: 1] Checkpoint inhibitors, 2] Chimeric antigen receptor (CAR) T-cell therapy, 3] Cytokines, 4] Immunomodulators, 5] Cancer vaccines, 6] Monoclonal antibodies and 7] Oncolytic viruses.	**10 Hours**
Section II	
Physiological Systems, Disorders and Treatment Functioning of following body systems and all classes of drugs. **1] Cardiovascular system and its disorders**: Hypertension, Heart Failure, Angina Pectoris, Arrhythmia, Myocardial Infarction, Ischemic heart diseases, Stroke etc.	**30 Hours**

2] Central Nervous System and CNS disorders: Antidepressants, Anticonvulsants. **3] Immune System Disorders**: Inflammation, Pain, Analgesics and anti-inflammatory agents. **4] Endocrine system and Hormonal therapy**: Diabetes and Management of Diabetes, Diseases related to growth hormone, Diseases related to thyroid hormone, Diseases related to adrenal gland hormone. **5] Gastrointestinal tract disorders and Drugs**: Hyperacidity, ulcer, nausea and vomiting.	

References

1. Foye's Principles of Medicinal Chemistry by Lemke, Williams, Riche and Zito, 7th, Edn., Lippincott Williams and Wilkins, 2012.
2. Burger's Medicinal Chemistry and Drug Discovery, edited by Donald J. Abraham, volumes I to IV, 6th Edn., Wiley Inter Science, 2003.
3. Comprehensive Medicinal Chemistry Vol-I, edited by C. Hansch, Pergamon press, 1990.
4. Selective Toxicity the physicochemical basis of therapy by A. Albert, Chapman Hall, 1985.
5. Principle of Drug Action: The Basis of Pharmacology (A Wiley biomedical-health publication) by Goldstein A., 2nd Edn., Wiley-Blackwell, 1974.
6. Organic Chemistry of Drug Design and Drug Action by R. B. Silverman and M. W. Halladay, 3rd Edn., Academic Press Inc, 2014.
7. Human Anatomy and Physiology by Carolla, Harley and Noback, 2nd, Edn., 1992.
8. Medicinal Chemistry a Biochemical approach by Thomas Nogardy, 2nd, Edn., 1988.
9. Essentials of medical pharmacology by K. D. Tripathi, 8th, Edn., 2018.
10. Wilson and Gisvolds Textbook of Organic, Medicinal and Pharmaceutical Chemistry 12th, Edn., John M beale and John H Block, 2011, Lippincott Williams and Wilkins.
11. Goodman and Gilman's the pharmacological basis of Therapeutics by Brunton and Knollmann, 14th, Edn., 2022.
12. An Introduction to Medicinal Chemistry by Graham L. Patrick, 6th Edn., Oxford University press, 2017.
13. Smith and William's Introduction to the Principles of Drug Design and Action by H. John Smith, 4th Edn., CRC press, 2005.

14. Introduction to Medicinal Chemistry, How Drugs Act and Why by Alex Gringauz, 1st Edn., Wiley-VCH, 1996.
15. Medicinal Chemistry: An Introduction by Gareth Thomas, 2nd Edn., Wiley, 2013.

CHD-653 MJP: Ternary Mixture

Course type: Major **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to

CO1: Understand the concept of type determination and apply separation techniques.

CO2: Comprehend different purification techniques.

CO3: Accurately record and report physical constants.

CO4: Analyze microscale chemical elemental analysis.

CO5: Evaluate and execute qualitative estimation of functional groups.

CO6: create a report on ternary mixture separation.

Course Content

The students should perform the Separation of minimum **eight (8) mixtures** containing three components. The mixtures should also involve separation of nitrophenols, amino acids, low boiling and water soluble and insoluble compounds, solidsand liquids with multifunctional groups. The mixture separation should be carried out on micro-scale using ether.

References

1. Practical Organic Chemistry by F. G. Mann and B. C. Saunders, 4th Edn., Pearson, 2009.
2. Practical Heterocylic Chemistry, A. D. Fitton and R. K. Smalley, Academic Press, 2013.
3. Vogel's Text book of Practical Organic Chemistry, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, 5th Edn., Pearson, 2003.
4. Organic Synthesis Collective, Volume I to XII, edited by J. B. Freeman, W. E. Noland, A. H. Blatt, N. Rabjohn, H. E. Baumgarten and C. K. Zercher, Wiley, 2015.
5. Macroscale and Microscale organic experiments by K. L. Williamson and K. M. Masters, 5th Edn., Books/Cole, 2016.
6. The Systematic Identification of Organic Compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin, 8th Edn., Wiley, 2004.
7. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis by V. K. Ahluwalia and Renu Aggarwal, Sangam Books Ltd., 2001.

CHD-654 MJP: Organic synthesis by Named reactions

Course type: Major **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to

CO1: Learn the concept of type determination and separation technique.

CO2: Understand the different experimental techniques.

CO3: Perform micro-scale chemical elemental analysis.

CO4: Relate all named reactions according to their significance.

CO5: Evaluate different techniques based on their applications.

CO6: create a report on different named organic synthesis.

Course Content

Note: The students must perform at least twelve (12) experiments and their spectral characterization.

Named reactions:

1. Claisen Condensation: Acetoacetic-Ester Condensation
2. Biginelli Reaction: Synthesis of Dihydropyrimidinone from Benzaldehyde and Urea.
3. Cannizzaro reaction: Synthesis of Benzoic acid & Benzyl alcohol from Benzaldehyde.
4. Dakin reaction: Synthesis of catechol from Salicylaldehyde.
5. Darzen reaction: Synthesis of epoxy ester from ketone / aldehyde.
6. Sandmeyer reaction: Synthesis of *p*-chlorotoluene from *p*-toluidine.
7. Jones Oxidation: Synthesis of Benzil from Hydrobenzoin.
8. Wolff-kishner: Synthesis of Ethylbenzene from Acetophenone.
9. Pinacol synthesis (Photochemical reaction):Synthesis of Benzopinacol from Benzophenone.
10. Pechmann reaction: Synthesis of Coumarin from *p*-cresol / Resorcinol.
11. Vilsmeier Haack formylation: Synthesis of 2-methoxy Naphthaldehyde from 2-methoxy Naphthalene.
12. Perkin reaction: Synthesis of cinnamic acid from Benzaldehyde.
13. Fischer Esterification Synthesis: a. Ethyl benzoate from Benzoic acid.
    b. Diethyl adipate from Adipic acid.
14. Friedel Craft acylation: Synthesis of 4-methyl benzophenone from Toluene.

15. Dieckmann condensation: Synthesis of ethyl -2-oxocyclopentane carboxylate from diethyl adipate.
16. Grignard reaction: Synthesis of Triphenyl carbinol from Ethyl Benzoate.
17. Wittig reaction: Synthesis of ethyl cinnamate from Benzaldehyde.

Named rearrangements:

1. Pinacol Rearrangement: Synthesis of Benzopinacolone from Benzopinacol.
2. Beckmann Rearrangement: Synthesis of Benzanilide from Benzophenone.
3. Hoffman Rearrangement: Synthesis of Aniline from Benzamide.
4. Benzil Benzilic acid Rearrangement: Synthesis of Benzilic acid from Benzil.
5. Fries rearrangement: Synthesis of Resacetophenone from Resorcinol.
6. Baeyer Villiger rearrangement: Synthesis of Phenyl benzoate from Benzophenone.

References

1. Practical Organic Chemistry by F. G. Mann and B. C. Saunders, 4th Edn., Pearson, 2009.
2. Practical Heterocylic Chemistry, A. D. Fitton and R. K. Smalley, Academic Press, 2013.
3. Vogel's Text book of Practical Organic Chemistry, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, 5th Edn., Pearson, 2003.
4. Organic Synthesis Collective, Volume I to XII, edited by J. B. Freeman, W. E. Noland, A. H. Blatt, N. Rabjohn, H. E. Baumgarten and C. K. Zercher, Wiley, 2015.
5. Macroscale and Microscale organic experiments by K. L. Williamson and K. M. Masters, 5th Edn., Books/Cole, 2016.
6. The Systematic Identification of Organic Compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin, 8th Edn., Wiley, 2004.
7. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis by V. K. Ahluwalia and Renu Aggarwal, Sangam Books Ltd., 2001.

CHD-660(A) MJ: Advanced synthetic methods in chemistry

OR

CHD-660(B) MJ: Organometallic Reagents in Organic Synthesis

OR

CHD-660(C) MJ: Forensic Chemistry

Course type: Major elective (Any Two) **No. of Credits: 4**

CHD-660(A) MJ: Advanced synthetic methods in chemistry

Course type: Major elective **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to

CO1: Know the fundamental concepts of protection and deprotection.

CO2: Understand the significance of advanced synthetic methods.

CO3: Employ different techniques like protecting and deprotecting agents, the umpolung reagents, Multicomponent, Ring formation reactions and Click chemistry.

CO4: Analyze synthetic methods according to their physical and chemical properties.

CO5: Relate different advanced syntheses based on their applications.

CO6: Summarize the different advanced synthetic methods.

Course Content

Section I	
Protection and deprotection of functional groups **1] Hydroxyl group**: alkyl ether, benzyl ether, acyl, PMB, Trityl, TMS, TBDMS, THP, MOM, MEM and MIP ether. **2] Diol**: Acetone, Cyclohexanone, Cyclohexane amide and Acetamide. **3] Amines**: Benzyl, Acyl, CBZ, BOC and FMOC. **4] Carboxyl group**: Ester, DCCI and DIPCDI. **5] Ketone and aldehydes**: Glycol, Thioglycol, Ketal, Acetal; Othroesters as protecting groups, Protection deprotection approach - In Solid phase synthesis of polypeptide; polynucleotide.	**6 Hours**

Enamines in synthesis Stork enamine reaction, regioselectivity, synthetic applications of enamines.	**01 Hour**
Retrosynthesis Retrosynthetic analysis, disconnection approach, synthons, multiple step synthesis, functional group interconversion, logical and illogical two group disconnections, 1, 5 related functional group disconnection, Synthons, Umpolung, convergent synthesis, special methods for small rings, heterocyclic compounds, synthesis of target molecules.	**15 Hours**
Multicomponent, Ring formation reactions and Click chemistry **1] Multicomponent reactions**: Ugi, Passerini, Biginelli and Mannich reaction. **2] Ring Formation reactions**: Pausan-Khand, Bergman and Nazarov cyclization. **3] Other important reactions**: Mitsunobu reaction, Appel reaction, Woodward and Prevost reaction. **4] Click chemistry**: Criterion for click reaction, Sharpless azides cycloadditions. Click reactions in synthesis of bioconjugates (sugars and proteins)	**8 Hours**

References

1. Organic synthesis through disconnection approach by P. S. Kalsi – 2nd edition
2. Organic synthesis by M. B. Smith.
3. Designing Organic syntheses: A Programmed Introduction to the Synthon Approach by S. Warren, 1st Edn., Wiley, 1978.
4. Organic Synthesis: The Disconnection Approach by S. Warren and P. Wytt, Wiley, 2008.
5. Some Modern Methods of Organic Synthesis by W Carruthers and I. Coldham, 4th Edn., Cambridge, 2004.
6. Organic Chemistry by J. Clayden, N. Greeves, S. Warren, 2nd Edn., Oxford University Press, 2012.
7. Classics in Total Synthesis- Target, Strategies, methods Volume I and II by K. C. Nicolaou, E. J. Sorensen, 1st Edn., Wiley-VCH Verlag GmbH, 1996.
8. Modern Synthetic Reactions by H. O. House, 2nd Edn., Benjamin-Cummings Co., 1972.
9. The Organic Chemistry of Drug Synthesis by Daniel Lednicer, Lester A. Mitscher volume 3, 1st Edn., Wiley Interscience, 1985.
10. Additional Study material: NPTEL Lecture: A Study Guide in Organic Retrosynthesis: Problem Solving Approach (https://nptel.ac.in/content/syllabus_pdf/104105087.pdf)

OR

CHD-660(B) MJ: Organometallic Reagents in Organic Synthesis

Course type: Major elective **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to

CO1: Learn the basics of organometallic reagents.

CO2: Know the significance of organometallic reagents in Organic synthesis.

CO3: Employ different organometallic reagents like Mg, Li, Cu, Zn, Organoborane, and transition metal complexes in organic synthesis.

CO4: Categorize different reactions based on their chemical properties and reaction mechanism.

CO5: Assess the organometallic reagents and their application in the organic synthesis.

CO6: Make a summary of reactions that involve organometallic reagents.

Course Content

Section I	
Organometallic Reagents of Mg, Li, Cu and Zn in Synthesis Preparation of Organomagnesium, Organolithium, Organocuopper and organozinc reagent and their application in organic synthesis.	**4 Hours**
Organoborane Reagents in Organic Synthesis Applications of diborane and Organoborane reagents such as 9-BBN, Thexyl borane, Disiamy borane, Catechol borane and chiral Organoborane reagents in organic synthesis	**3 Hours**
Olefine Metathesis in synthesis Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closir (RCM) and ring opening (ROM) metathesis, applications.	**2 Hours**
Transition metal complexes in synthesis Application of Pd, Ni, Ru and Fe only (C-C, C-N, C-O bond formation reactions with catalytic cycle, ligand and % mole concepts) Introduction, Catalytic Cycle of Cross-coupling reactions, C-C, C-N, C-O bond formation reactions. catalytic cycle and examples of Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama,	**9 Hours**

Negishi, Buchwald-Hartwig, Noyori, Reppe, Oxo process and Wacker oxidation reaction.	
Alkene and alkyne formation reactions Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Boord olefination, Corey winter olefination, Tebbe olefination, Baylis Hilman, Eschenmoser-Tanabe fragmentation.	**5 Hours**
Multicomponent, Ring formation reactions and Click chemistry 1**] Multicomponent reactions**: Ugi, Passerini, Biginelli and Mannich reaction. **2] Ring Formation reactions**: Pausan-Khand, Bergman and Nazarov cyclization. **3] Other important reactions**: Mitsunobu reaction, Appel reaction, Woodward and Prevost reaction. **4] Click chemistry**: Criterion for click reaction, Sharpless azides cycloadditions. Click reactions in synthesis of bioconjugates (sugars and proteins)	**7 Hours**

References

1. Organic Chemistry by J. Clayden, N. Greeves and S. Warren, 2nd Edn., Oxford University Press, 2012.
2. Some modern methods of organic synthesis by W. Carruthers and I. Coldham, 4th Edn., Cambridge University Press, 2004.
3. Organic synthesis by Michael B. Smith, 4th Edn., Academic University Press, 2016.
4. Transition Metals for Organic Synthesis: Building Blocks and Fine Chemicals, Edited by M. Beller and C. Bolm, 2nd Edn., WILEY-VCH, 2005.
5. C–N bond forming cross-coupling reactions: an overview: by Jitender Bariwalab and Erik Van der Eycken, Chemical Society Reviews, 2013, 42, 9283-9303.
6. Multicomponent Reactions Edited by Jieping Zhu, Hugues Bienayme WILEY-VCH, 2005.
7. Advanced organic chemistry, Part B by F.A Carey and R. J. Sundberg, 5th Edn., Springer, 2008.
8. Strategic Applications of Named Reactions in Organic Synthesis by Laszlo Kurti and Barbara Czako, 1st Edn., Academic University Press, 2005.
9. Name Reactions: A Collection of Detailed Reaction Mechanism by Jie Jack Li, 5th expanded Edn., Springer, 2003.
10. Organic Synthesis Using Transition Metals by Roderick Bates, 2nd Edn., A John Wiley and Sons, Ltd., 2012.

11. The Organometallic Chemistry of the transition metals by Robert H. Crabtree, 6th Edn., Wiley Blackwell, 2014.
12. Organometallics in Organic Synthesis by J. M. Swan and D. C. Black (Chapman and Hall)
13. Ruthenium-Catalyzed Reactions for Organic Synthesis Chem. Rev. 1998, 98, 2599- 2660.
14. Guidebook to organic synthesis by R K Meckie, D M Smith and R A Atken
15. Organic synthesis by Robert E Ireland.

OR

CHD-660(C) MJ: Forensic Chemistry

Course type: Major Elective **No. of Credits: 2**

Course Outcomes

After the completion of this course, students will be able to know the

CO1: know the fundamental principles and functions of forensic science.

CO2: Identify the illicit/abused drugs.

CO4: Classify the drugs according to their applications.

CO5: Relate the drugs based on their properties and applications.

CO6: create a summary of different concepts of forensic chemistry.

Course Content

Section I	
Introduction to Forensic Science Introduction, Need, Scope, Concepts and Significance of Forensic Science, History and Development of Forensic Science, Basic principles of Forensic Science, Frye case and Daubert standard.	**2 Hours**
General Drugs, Other Chemicals Introduction, Pharma drugs [barbiturates, benzodiazepine &other pharma drugs, **Drug abuse** in sports & Date rape drugs: Introduction, common prohibited substances, analytical approach, Forensic Pharmacological studies, Ingestion of drugs, absorption, distribution, metabolism, pathways of drug metabolism, drug metabolism and drug toxicity, excretion of drugs, detection of drugs on the basis of their Metabolic studies. **Solvent Abuse** chlorinated hydrocarbons, Aromatic hydrocarbons, alcohols, glycols, fuel and fuel additives: absorption, distribution, and metabolism, psychological & clinical effects.	**8 Hours**
Narcotic Drugs and Psychotropic Substances Introduction to narcotic drugs, Analysis of Narcotic Drugs and Psychotropic Substances, Classification of Narcotics and other drugs, Analytical techniques for identification of drugs. Characterization and synthesis of 1) Narcotics- heroin	**8 Hours**

and cocaine. 2) Stimulants- caffeine, amphetamines. 3) Depressants- Barbiturates, Benzodiazepines. Analysis of NDPS evidence by various procedures prescribed by U.N. Manual, DFS manual, spot tests, microcrystal tests, extraction methods, TLC, UV-Vis spectrophotometry, IR spectrophotometry, GC-HPLC, MS, GC-MS, NMR and XRD as exemplified by cocaine, cannabis, amphetamines, opiates and hallucinogens (LSD, psilocybine and mescaline), evidence handling & sampling techniques, clandestine laboratory investigation and designer drugs.	
Fingerprinting & Other Impressions Fingerprint **Fingerprinting:** Nature, Location, Classification, Types, Patterns of Fingerprints, Poroscopy & Edgeoscopy, Classification of Fingerprints: Henry's Classification, Single Digit Classification, Extended Henry's System, Types of Fingerprints [Latent, Patent and Plastic], Invisible Fingermarks development methods [Powder methods, Fuming methods, Chemical Methods, etc.] Recent techniques [Digital Imaging & Enhancement, Laser & other radiation-based techniques, Preservation and photography of fingerprints on various surfaces. Ridge counting, Ridge tracing, Minutiae Identification & Matching [Manual and Automated: AFIS]. **Palm Prints**: Nature, Location, Types, Classification, Development, Lifting, Evaluation, Analysis, Forensic Significance. **Footprints**: Importance, Gait pattern analysis, Evaluation and analysis of various casts. Electrostatic lifting of latent footprints and comparison with reference sample. Tyre marks / prints and skid marks and comparison with control samples. **Cheiloscopy:** Nature, location, collection and evaluation of lip print. **Ear prints**: Introduction, growth & development, evaluation and analysis of ear print.	**12 Hours**

References

1. https://epgp.inflibnet.ac.in. : Forensic Science Paper 01: General Forensic Science
2. https://epgp.inflibnet.ac.in.: Forensic Science Paper 03: Fingerprint and other impression
3. https://epgp.inflibnet.ac.in. : Forensic Science Paper 09: Drug of Abuse
4. Introduction to Forensic Science in Crime Investigation, Krishnamurthy, R., Selective & Scientific Books, New Delhi. 2011,

5. Fundamentals of Forensic Science, Houck, M.M & Siegel, J.A; Acadamic Press, London, 2006.
6. Forensic Science in Criminal Investigation & Trials, Sharma, B.R; Universal Publishing Co., New Delhi, 2003
7. Forensic Science in India- A vision for the Twenty First Century, Nanda B.B and Tewari, R.K; Select Publisher, New Delhi, 2001.
8. Analytical Spectroscopy 2nd Edn, G.R. Chatwal; Himalaya Publishing House New Delhi,2002.
9. Isolation and Identification of Drugs, Clark, E.G.C.; Vol. I and Vol. II, Academic Press, (1986).
10. Finger Prints Techniques, Moenssens:1975, Chitton Book Co., Philadelphia, New York.
11. Identification of Thumb Impression & Cross Examination of Finger Prints, Mehta, M. K.: 1980 N. M. Tripathi (P) Ltd. Bombay.
12. Finger Prints, Palms and Soles, Cummins & Midlo : The Blakiston office London 1943,
13. Footprints, Tracks and Trials. Sharma B. R.: Central Law Agency. Allahabad 1980.
14. Ear Identification, Forensic Identification series, Paramount Iannarelli, A V; (1989)
15. Law & Techniques Relating to Finger Prints, Foot Prints & Detection of Forgery, Central Law Agency, Saxena's : Saxena's Allahabd (Ed. A.K. Singla).
16. Fingerprint detection with lasers, Marcel Dekker, Menzel, E Roland; NY (1999)

CHD-681 RP Research Project

Course type: Research Project **No. of Credits: 6**

Course Outcomes

At the end of the course, students will be able to -

1. understand key concepts and principles relevant to the research topic.
2. learn diverse research methodologies proficiently.
3. write and communicate research findings persuasively through various mediums in the form of project report
4. analyze and synthesize scholarly literature effectively.
5. evaluate research findings and methodologies critically.
6. design and execute original research projects independently.

Following guidelines should be followed for the conduction and evaluation of research project.

- Each student will perform project separately.
- Project working hours should be 30 hours for each credit.
- Choose a topic that aligns with your interests and career goals, but also consider its feasibility within the available resources and time frame.
- Consult with faculty members, advisors, or mentors to identify a research area that has potential for contribution to the field of chemistry.
- Adhere to ethical principles and standards in all aspects of your research.
- Project report must be written systematically and presented in bound form: The project will consist of name page, certificate, content, summary of project followed by introduction, literature survey (recently published research papers must be included), experimental techniques, results and discussion, conclusions, Appendix consisting of i) references, ii) standard spectra / data if any and iii) safety precautions.
- 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 and 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.

- Students are encouraged to participate in national and international conferences and other project competitions.
- For conducting research study in M.Sc. Chemistry, it is highly recommended to follow the journals given below or any other journal from reputed publication.

1. **Journal of the American Chemical Society (JACS)**

   Publisher: American Chemical Society (ACS)

   Focus: Comprehensive coverage of all fields of chemistry, known for high-impact research.

12. **Angewandte Chemie International Edition**

    Publisher: Wiley-VCH on behalf of the German Chemical Society (GDCh)

    Focus: Broad coverage of all chemistry fields, emphasizing novel and significant research.

13. **Chemical Science**

    Publisher: Royal Society of Chemistry (RSC)

    Focus: Cutting-edge research across chemical sciences, open access.

14. **Nature Chemistry**

    Publisher: Nature Publishing Group

    Focus: Multidisciplinary and high-impact research across all areas of chemistry.

15. **Journal of Organic Chemistry (JOC)**

    Publisher: American Chemical Society (ACS)

    Focus: Specialized in organic chemistry, including synthesis and mechanisms.

16. **Inorganic Chemistry**

    Publisher: American Chemical Society (ACS)

    Focus: Research on inorganic and organometallic compounds.

17. **Analytical Chemistry**

    Publisher: American Chemical Society (ACS)

    Focus: Developments and applications in analytical techniques and methodologies.

18. **Physical Chemistry Chemical Physics (PCCP)**

    Publisher: Royal Society of Chemistry (RSC)

    Focus: Physical chemistry, chemical physics, and biophysical chemistry.

19. **Chemical Communications (ChemComm)**

Publisher: Royal Society of Chemistry (RSC)

Focus: Rapid publication of high-quality communications across all chemical sciences.

20. Accounts of Chemical Research

Publisher: American Chemical Society (ACS)

Focus: Comprehensive reviews and accounts of current research topics in chemistry.

21. Chemical Society Reviews

Publisher: Royal Society of Chemistry (RSC)

Focus: The journal publishes high-quality, authoritative, and state-of-the-art reviews across all areas of chemical science. It covers comprehensive and critical reviews on a broad range of topics in chemistry, including emerging and interdisciplinary fields.