# **CENTRAL UNIVERSITY OF PUNJAB**



# M.Sc. Chemical Sciences (Medicinal Chemistry)

Batch- 2025-27

# Department of Pharmaceutical Sciences and Natural Products

# Graduate attributes for M. Sc. Chemical Sciences (Medicinal Chemistry) Research

Graduates will have quality-conscious service providing attribute by adopting the knowledge of spectral analysis and chromatographic techniques in manufacturing and R & D of drugs. They will be able to implement the role of Computer-Aided Drug Design (CADD) in the modern drug discovery & development process and its applicability in higher studies and at the industrial level. They will be able to apply the knowledge of medicinal chemistry for the development of synthetic methodologies, including green chemistry, peptide chemistry, retro-synthesis for making the drugs affordable to the public. They will have the ability to create, select and apply appropriate techniques, resources and modern analytical tools to identify, formulate, and solve problems of medicinal chemistry and will develop attribute to become self-reliant in Active Pharmaceutical Ingredients (APIs) by the development of scale-up of APIs and intermediates, unit operations and industrial safety guidelines. Moreover, the program will help them make their career in academic, research, and industry.

#### **Course Structure**

#### SEMESTER 1

S. No.	Paper Code	Course Title	Course Type	L	Т	P	Cr
1.	MCMC.401	Advanced Organic Chemistry-I	DSC	4	0	0	4
2.	MCMC.402	Organic Chemistry-I (Practical)	SEC	0	0	6	3
3.	MCMC.403	Modern Spectral and Chromatography Techniques	DSC	4	0	0	4
4.	MCMC.404	Advanced Medicinal Chemistry-I	DSC	4	0	0	4
5.	XXX	Interdisciplinary Course	IDC	2	0	0	2
6.	MCMC.405	Entrepreneurship Course	EC	2	0	0	2
7.	XXX	Individualized Education Plan/ Tutorial	-	0	0	0	N. Cr
	Opt ar	y one course from following elec	tives				
8.	MCMC.406	Chemistry of Natural Products					
9.	MCMC.407	Quantum Chemistry	DSE	3	0	0	3
10.	MCMC.408	Inorganic Chemistry-1	DOE				
11.	MCMC.409	Physical Chemistry – I					
		Total		19	0	6	22

DSC: Discipline Specific Core Course, DSE: Discipline Specific elective course,

**SEC**: Skill Enhancement Course

L: Lectures T: Tutorial P: Practical Cr: Credits

**MOOC:** MOOC may be taken up 40% of the total credit (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match minimum 70%.

#### SEMESTER II

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr			
1.	MCMC.421	Advanced Organic Chemistry-II	DSC 4 0		0	4				
2.	MCMC.516	Organic Chemistry-II (Practical)	SEC	0	0	6	3			
3.	MCMC.517	Computer Aided Drug Design	AEC	2	0	0	2			
4.	MCMC.518	Advanced Spectral Analysis	DSC	4	0	0	4			
5.	XXX	Value Added Course	VAC	2	0	0	2			
6.	XXX	Indivisualized Education Plan/ Tutorials	-	2	0	0	N. Cr			
	Opt any Course from following electives									
7.	MCMC.519	Green Chemistry	DSE	3	0	0	3			
8.	MCMC.520	Nuclear Chemistry								
9.	MCMC.521	Advanced Medicinal Chemistry-II								
		Total		15	0	6	18			

**DSC:** Discipline Specific Core Course, **DSE**: Discipline Specific elective course,

SEC: Skill Enhancement Course, AEC: Ability Enhancement Courses

L: Lectures T: Tutorial P: Practical Cr: Credits

**MOOC:** MOOC may be taken up 40% of the total credit (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match minimum 70%.

# Multiple Entry/Exit scheme (After Second Semester)

Post-Graduate Diploma will be awarded as per NEP 2020 in multiple entry/exit scheme for students leaving the course after the end of first year (Second Semester) of M.Sc. Chemical Sciences (Medicinal Chemistry) programmes, provided students have to opt any one of the following 4 credit skill-based course.

have to op	t any one of the fo	ollowing 4 credit skill-based course.						
		MOOC Course						
1.	MCMC.526	Analytical Techniques	SB 4		0	0	4	
2.	MCMC.527	Introduction to Computer Network and Internet Protocols		4	0	0	4	
3.	MCMC.528	Solid and Hazardous Waste Management	SB	4	0	0	4	
4.	MCMC.529	Fundamentals of Bioinformatics	SB	4	0	0	4	
		Training						
5.	MCMC.530	Training at National Labs/Research Institutes/Central Instrumental Laboratory Facility of University/Industry for two months, subject to the submission of report for evaluation	SB	4	0	O	4	
		Lab rotation						
6.	MCMC.531	Lab rotation of two months within and the other relevant departments of the University.	SB	4	0	0	4	
	Publication							
7.	MCMC.532	One publication in an International repute journal indexed in Scopus/Web of Science.	SB	4	0	0	4	

# SEMESTER III

S. No.	Paper Code	Course Title	L	T	P	Cr
1.	MCMC. 599-1	Dissertation/Internship/Apprenticeship	0	0	40	20

# **SEMESTER IV**

	Paper Code	Course Title	L	T	P	Cr
1.	MCMC. 599-2	Dissertation/Internship/Apprenticeship	0	0	40	20

#### **Examination Pattern**

Core, Discipline Elective, Compulsory Interdisciplinary Foundation, Course, Value Added Entrepreneurship, Innovation and ski development Courses						
	Marks Evaluation		Marks	Evaluation		
Internal	25	Various methods	-	-		
Assessment						
Mid-semester	25	Descriptive	50	Descriptive (70%)		
test (MST)				Objective (30%)		
End-semester 50		Descriptive (70%) 50 Descr		Descriptive (70%)		
test (EST)		Objective (30%)		Objective (30%)		

**Objective Questions-** one-word/sentence answers, fill-in the blanks, MCQs', and matching

**Descriptive Questions**- Short answer and essay type questions

**Internal assessment**- any two or more of the given methods: Surprise Tests, open book examination, assignments, term paper, etc.).

#### **Evaluation Criteria for Practical**

Item	Practical Note book and continuous evaluation	Synopsis	Performance	Viva
	continuous evaluation			voce
Marks	40	10	20	30

#### **Evaluation Criteria for Dissertation**

Dissertation (Fourth Semester)						
	Marks	Evaluation				
Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce				
External expert, HoD and senior-most faculty of the department		Dissertation report (30), presentation (10), final viva-voce (10)				

Evaluation pattern similar to fourth semester dissertation will apply for internship where supervisor will award 50% marks and external co-supervisor, HoD and senior-most faculty will award 50% marks.

#### Semester 1

Course Title: Advanced Organic Chemistry-I

Paper Code: MCMC.401

Course Hours: 60h

# L T P Credits 4 0 0 4

#### **Learning Outcomes:**

After completing this course, the learner will be able to:

CLO1: Describe and understand basic chemistry of elimination and addition reactions

CLO2: Describe disconnection approaches applied on synthetic strategies and mechanism prediction.

CLO3: Describe nomenclature and synthetic methodologies of heterocyclic systems

Units/Hours	Content	Mapping
		with course
		learning
		outcomes
Unit 1	Basic Aspects of Organic Chemistry: Organic	CLO1
15 Hours	intermediates: Carbocations, carbanions, free radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications. Types of reaction mechanisms and methods of determining them, Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations.  Learning activities: Learner will be engaged in Molecular models to explain the stability of organic intermediates	
Unit 2 15 Hours	Addition reactions a) Nucleophilic uni- and bimolecular reactions (SN1 and SN2) b) Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule) c) Rearrangement reaction  Learning activities: Learner will be engaged in Molecular models to explain the stereochemistry in elimination reactions	CLO1

Unit 3 15 Hours	Synthetic methodologies: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, Importance of the order of events in organic synthesis. One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 & 1,5- difunctional compounds, One group C-C disconnections, alcohol and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis, Two group C-C disconnections, Diels-Alder reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5-difunctionalised compounds.	
	<b>Learning activities:</b> Learner will be engaged in Group discussion to explain disconnection approaches in synthesis	
Unit 4 15 Hours	Heterocyclic chemistry: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles, Aromatic heterocycle, Nonaromatic heterocycle: Bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles and their synthesis  (a) Three-membered and four-membered heterocycles: synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.  (b) Five membered heterocycles containing two heteroatoms (S,N,O): Diazoles, imidazole, pyrazole,oxazoles and thiazoles.	CLO3

(c) Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles.

(d)Six-membered heterocycles with heteroatom: Synthesis and reactions of

pyrylium salts and pyrones, coumarins, chromones, pyridine, pyrimidine, etc.

**Learning activities:** Learner will be engaged in using ball and stick models and web mediated activity to explain heterocyclic Chemistry

#### Suggested Readings:

- 1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press.
- 2. Finar, I.L., (2012). Organic Chemistry Vol. 1, Pearson Education, UK.
- 3. Mc Murry J., (2015). Organic Chemistry, Asian Book Pvt. Ltd, New Delhi
- 4. Smith, M. B. (2013). March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure. John Wiley & Sons.
- 5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., New Delhi-110002.
- 6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., New Delhi.
- 7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
- 8. Kalsi, P.S., (2010). Organic Reactions and Their Mechanisms. New Age International Pub., New Delhi.
- 9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
- 10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India. New Delhi.
- 11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
- 12. Eliel, E. L., & Wilen, S. H. (2008). Stereochemistry of organic compounds. John Wiley & Sons.
- 13. Carey, F. A., Guiliano, R. M. (2012). Organic Chemistry. McGraw Hill.
- 14. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
- 15. Solomons, T. W. G., Fryhle, C. B., Snyder, S. A. (2017). Solomons' Organic Chemistry. John Willey & Sons.
- 16. Acheson, R.M. (1976). An Introduction to the Chemistry of Heterocyclic Compounds, Wiley India Pvt. Ltd.

- 17. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
- 18. Warren, S., (2010). *Organic Synthesis: The Synthon Approach*. John Wiley & Sons, New York,
- 19. Warren, S., (2010). Designing Organic Synthesis: A Disconnection Approach. John Wiley & Sons, New York.

## The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Team teaching
- Tutorial
- Self-learning

- PPT
- YouTube
- Google drive
- Google meet

Course Title: Organic Chemistry -I (Practical)

L	T	P	Credits
0	0	6	3

Paper Code: MCMC.402 Course Hours: 90h

#### **Learning Outcomes:**

After completing this course, the learner will be able to:

CLO1: Interpret stereochemistry of organic compounds

CLO2: Explain the handling, storage and disposal of hazardous chemicals and their Material safety data sheets (MSDS)

CLO3: Monitor the progress of chemical reactions by thin layer chromatography

CLO4: Purify a given organic compound through crystallization, fractional distillation or column chromatography

Practical	Content/Title	Mapping course learning outcome	with
1.	Awareness to various glassware and plasticwares used in the organic synthesis.	CLO1	
2.	Demonstration of Stereochemical aspects of the compounds through molecular models	CLO1	
3.	Awareness to handling, storage and disposal of hazardous chemicals and their Material safety data sheets (MSDS)	CLO2	
4.	Thin layer chromatography: Monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the $R_{\rm f}$ values of known standards, preparative TLC for separation of mixtures		
5.	Purification of a given organic compound through crystallization, fractional distillation or column chromatography	CLO4	
6.	Organic Synthesis: Single or multi- steps synthesis of organic compounds. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, etc. should be paid attention. TLC should be used to monitor the reaction. (attempt any five)  a) Synthesis of an anticancer stilbene via Wittig reaction b) Synthesis of chalcones via Claisen-Schmidt condensation. c) Preparation of vanillyl alcohol from vanillin	CLO4	

- d) Reduction of 3-nitroacetophone using NaBH<sub>4</sub>/LiAlH<sub>4</sub>
- e) Preparation of bromohydrin from methylstyrene
- f) Preparation of aniline from nitrobenzene
- g) Synthesis of ethyl *N*-butyl acetoacetate by A.E.E. condensation
- h) Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.
- i) Preparation of Iodoxybenzoic acid (IBX) and its application in oxidation.
- j) Preparation of pyridine chlorochromate (PCC) and its application in oxidation.
- k) Multistep synthesis of phenytoin.

#### Suggested Readings:

- 1. Adams, R., Johnson, J.R., Wilcox, C.F. (1970). Laboratory Experiments in Organic Chemistry, The Macmillan Limited, London.
- 2. Mann, F. G. (2009). Practical Organic Chemistry. Pearson Education India.
- 3. Pasto, D.P., Johnson, C., Miller, M. (2010). Experiments and Techniques in Organic Chemistry, Prentice Hall.
- 4. Roberts, R.M., Gilbert, J.C., Rodewald, L.B., Wingrove, A.S. (1969). *An Introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
- 5. Vogel, A.I. (latest edition). Text Book of Practical Organic Chemistry, Pearson
- 6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments*, *Heath*, D. C & Co., Lexington, MA.
- 7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
- 8. Young, J. A. (Ed.). (1991). *Improving Safety in the Cemical Laboratory: a Practical Guide*. Wiley.
- 9. Zercher, C. A. (2010). Organic Syntheses. John Wiley & Sons.
- 10. Leonard, J., Lygo, B., Procter, G. (2013). *Advanced Practical Organic Chemistry*. CRC Press.

# The following are some of the modes of classroom transaction

- Experimentation
- Group discussion
- Demonstration
- Self-learning

- PPT
- Google classroom
- Google meet

Course Title: Modern Spectral and Chromatography

Techniques

Paper Code: MCMC.403

Course Hours: 60h

L	Т	P	Credits
4	0	0	4

#### **Learning Outcomes**

After completing this course, the learner will be able to:

CLO1: Conceptualize general principle and theory of UV-Vis and IR and spectroflourimetry

CLO2: Describe the concept and instrumentation of NMR and Mass techniques

CLO3: Separate different constituents of mixture by chromatographic techniques

CLO4: Explain the Principle, thermal transitions and Instrumentation of DSC, DTA

and TGA

Units/Hours	Content	Mapping
		with course
		learning
		outcome
Unit I	UV-Visible spectroscopy	CLO1
15 Hours	Introduction, Theory, Laws, Instrumentation	
	associated with UV-Visible spectroscopy, Choice of	
	solvents and solvent effect and Applications of UV-	
	Visible spectroscopy, Difference/ Derivative	
	spectroscopy.	
	IR spectroscopy	
	Theory, Modes of Molecular vibrations, Sample	
	handling, Instrumentation of Dispersive and	
	Fourier- Transform IR Spectrometer, Factors	
	affecting vibrational frequencies and applications of	
	IR spectroscopy, Data Interpretation, Theory of NIR.	
	Spectroflourimetry Theory of Elegender Boots and Elegender Boots a	
	Theory of Fluorescence, Factors affecting	
	fluorescence, Quenchers, Applications of	
	fluorescence spectrophotometer, Instrumentation	
	<b>Learning activities:</b> Learner will be provided	
	hands on training to different instruments like	
	UV, IR and spectroflourimetry.	
Unit 2	NMR spectroscopy	CLO2
15 Hours		
10 110415	Quantum numbers and their role in NMR, Principle,	
	Instrumentation, Solvent requirement in NMR,	

	D 1 (1 3734D 1 1 1 1			
	Relaxation process, NMR signals in various compounds, Chemical shift, Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and <sup>13</sup> C NMR, Applications of NMR spectroscopy			
	Mass Spectroscopy			
	<ul> <li>Principle, Theory, Instrumentation of Mass Spectroscopy, Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy.</li> </ul>			
	<b>Learning activities:</b> Learner will be provided NMR and mass spectra for the characterization of compounds.			
Unit 3	Chromatography	CLO3		
15 Hours	Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following: Thin Layer chromatography, High Performance Thin Layer Chromatography, Ion exchange chromatography, Column chromatography, Gas chromatography, High Performance Liquid chromatography, Ultra High-Performance Liquid chromatography, Affinity chromatography, Gel Chromatography			
	<b>Learning activities:</b> Learner will be provided experience of chromatography by using different techniques like TLC, Column, HPLC, HPTLC and GC.			
Unit 4	Thermal Techniques	CLO4		
15 Hours	Principle, thermal transitions and Instrumentation (Heat flux and power-compensation and designs), Modulated DSC, Hyper DSC, experimental parameters (sample preparation, experimental conditions, calibration, heating and cooling rates, resolution, source of errors) and their influence, advantage and disadvantages, pharmaceutical applications. Differential Thermal Analysis (DTA):			

Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). TGA: Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications

**Learning activities:** Learner will be provided Web based learning to explain thermal techniques

# Suggested readings

- 1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). Spectrometric Identification of Organic Compounds. John Wiley & Sons.
- 2. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2018). Principles of Instrumental Analysis. Singapore: Cengage Learning Asia Pte Ltd.
- 3. Willard, H. H. (2012). Instrumental methods of analysis. New Delhi: CBS.
- 4. Beckett, A. H., & Stenlake, J. B. (Eds.). (1988). Practical Pharmaceutical Chemistry: Part II, A&C Black.
- 5. Kemp, W. (1991). Organic Spectroscopy (pp. 42-51). London: Macmillan.
- 6. Sethi, P. D. (1985). *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. Unique Publishers.
- 7. Munson, J. W. (Ed.). (1984). Pharmaceutical Analysis: Modern Methods (Vol. 11). CRC Press.
- 8. Kalsi, P. S. (2007). Spectroscopy of Organic Compounds. New Age International.
- 9. Connors, K. A. (2007). A Textbook of Pharmaceutical Analysis. John Wiley & Sons.
- 10. McHale, J. L. (2017). Molecular Spectroscopy. CRC Press.
- **11.** Kromidas, S. (2017). *The HPLC Expert Possibilities and Limitations of Modern High Performance Liquid Chromatography*. John Wiley and Sons.

# The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Tutorial
- Self-learning

- PPT
- YouTube
- Google drive
- Google mee

Course Title: Advanced Medicinal Chemistry-I

Paper Code: MCMC.404

Course Hours: 60h

L	T	P	Credits
4	0	0	4

## **Learning Outcomes**

After completing this course, the learner will be able to:

CLO1: Interpret basics concepts of drugs, their effects and screening.

CLO2: Describe drugs interaction with various types of enzymes and receptors

CLO3: Conceptualize the process of drug discovery and its progress

Units/Hours	Content	Mapping with course
		learning
		outcome
Unit 1	<b>History of drug discovery</b> Introduction, Drug	CLO1
15 Hours	discoveries, Recent trends in drug discovery, Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets	
	<b>Learning activities:</b> Learner will be engaged in group discussion to explain history of drug discovery	
Unit 2	Drug discovery:	CLO2
15 Hours	Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets  Biological drug targets Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonist vs antagonists, artificial enzymes.  Measurement and expression of drug effects  Introduction, In-vitro experiments, Ex-vivo experiments, In-vivo experiments.  Learning activities: Learner will be explained about drug interaction and target through molecular modeling studies	
Unit 3 15 Hours	Prodrug Design and Analog design Prodrug design	CLO3

Carrier linked Basic concept, prodrugs/ Bioprecursors, Prodrugs of functional group, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action. of prodrug design Rationale and practical consideration of prodrug design. Combating drug resistance Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance. **Analog Design** Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid analogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance. Learning activities: Learner will be engaged in Web based training to familiarize with prodrug and analog design Unit 4 CLO3 Medicinal chemistry aspects of the following class 15 Hours of drugs, Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs: a). Anti-hypertensive drugs, Psychoactive drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Antineoplastic and Antiviral agents. b). Stereochemistry and Drug action: Realization that stereo selectivity is a pre-requisite for evolution. Role of chirality in selective and specific therapeutic agents. Case studies, enantioselectivity in drug adsorption, metabolism, distribution and elimination. Learning activities: Learner will be engaged in Group discussion to explain SAR, Mechanism of action and synthesis of drugs

#### Suggested Readings:

- 1. Foye, W. C. (2019). Principles of Medicinal Chemistry, Publisher: Wolters Kluwer.
- 2. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry.
- 3. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press.
- 4. Patrick, G.L. (2017). An Introduction to Medicinal Chemistry, Publisher: Oxford university Press, UK.
- 5. Singh, H., Kapoor, V.K. (1996). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
- 6. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis.
- 7. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
- 8. Wolff, M E, Ed., (Latest Edition). Burger's Medicinal Chemistry and Drug Discovery John Wiley and Sons, New York.
- 9. Ferrant, E., (2011). New Synthetic Technologies In Medicinal Chemistry. Royal Chemical Society.
- 10. Medicinal Chemistry by Burger, Vol I –VI.
- 11. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12<sup>th</sup> Edition, (2004). Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt. Ltd, New Delhi.
- 12. Comprehensive Medicinal Chemistry Corwin and Hansch.
- 13. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore

# The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Team teaching

- Molecular Models
- PPT
- YouTube
- Software for *In silico* study
- Google meet

Course Title: Entrepreneurship Course

Paper Code: MCMC. 405

Course Hours: 30h

L	Т	P	Credits
2	0	0	2

**Learning Outcomes:** After completing this course, the learner will be able to:

CLO1: Understand the basic concepts of skill entrepreneur, entrepreneurship and its importance.

CLO2: Aware of the issues, challenges and opportunities in skill entrepreneurship.

CLO3: Develop capabilities of preparing proposals for starting small Pharmaceutical businesses.

CLO4: Know the availability of various institutional supports for making a new start-up for Drug Discovery.

Units/Hours	Content	Mapping
		with course
		learning
		outcome
Unit 1	Introduction to entrepreneur and	CLO1
6 Hours	entrepreneurship; Characteristics of an	
	entrepreneur; Characteristics of entrepreneurship;	
	entrepreneurial traits and skills; innovation and	
	entrepreneurship; Types of entrepreneurial	
	ventures; enterprise and society in Indian context;	
	Importance of women entrepreneurship	
	<b>Learning activities:</b> Learner will be engaged in	
	Group discussion to explain the concept of	
	entrepreneurship	
Unit 2	Promotion of a venture - Why to start a small	CLO2
8 Hours	business; How to start a small business;	
	opportunity analysis, external environmental	
	analysis, legal requirements for establishing a new	
	unit, raising of funds, and establishing the venture	
	- Project report preparation – format for a	
	preliminary project report, format for a	
	detailed/final project report.	

	Learning activities: Learner will interact with	
	Entrepreneurs to understand how to start small	
	business	
Unit 3	Launching and Organising an Enterprise in	CLO1, CLO2
10 Hours	Medicinal and Process Chemistry: Environment	
	scanning - Information, sources, schemes of	
	assistance, problems. Enterprise selection, market	
	assessment, enterprise feasibility study, Resource	
	mobilisation - finance, technology, raw material,	
	site and manpower. Costing and marketing	
	management and quality control. Feedback,	
	monitoring and evaluation.	
	Learning activities: Learner will be engaged in	
	Group discussion to explain about resource	
	mobilization, costing and marketing management	
Unit 4	Introduction to Intellectual Property Rights:	CLO3, CLO4
6 Hours	Importance of IPR, Patentable and non-patentable,	
	Trade Secrets, Know-how agreements, Types of	
	inventions protected by a patent, Need for a patent,	
	Preparing Project Proposal to Start On New	
	Enterprise Project work in Drug Design development – Feasibility report; Planning, resource	
	mobilisation and implementation.	
	<b>Learning activities:</b> Learner will be engaged to	
	prepare project proposal to start new enterprise	

#### Suggested Readings:

- 1. Arora, Renu (2008). Entrepreneurship and Small Business, Dhanpat Rai & Sons Publications.
- 2. Chandra, Prasaaan (2018). *Project Preparation, Appraisal, Implementation*, Tata Mc-Graw Hills.
- 3. Desai, Vasant (2019). *Management of a Small-Scale Industry*, Himalaya Publishing House.
- 4. Jain, P. C. (2015). Handbook of New Entrepreneurs, Oxford University Press.
- 5. Srivastava, S. B. (2009). A Practical Guide to Industrial Entrepreneurs, Sultan Chand & Sons.
- 6. Akhauri, M.M.P. (1990): Entrepreneurship for Women in India, NIESBUD, New Delhi.

- 7. Hisrich, R.D & Brush, C.G. (1996) The Women Entrepreneurs, D.C. Health & Co., Toranto.
- 8. Hisrich, R.D. and Peters, M.P. (1995): Entrepreneurship Starting, Developing and Managing a New Enterprise, Richard D., Inwin, INC, USA.
- 9. Meredith, G.G. et al (1982): Practice of Entrepreneurship, ILO, Geneva.
- 10. Patel, V.C. (1987): Women Entrepreneurship Developing New Entrepreneurs, Ahmedabad EDII.
- Douglas, F.S. etal (2010). The case for entrepreneurship in R&D In the Pharmaceutical industry. Nature Reviews Drug Discovery, 6, 683-689
- 12. Shorr, R.R.G. (2008). Entrepreneurship in Pharmaceutical and Biological Drug Discovery and Development. In: Madhavan, G., Oakley, B., Kun, L. (eds) Career Development in Bioengineering and Biotechnology. Series in Biomedical Engineering. Springer, New York, NY.

#### The following are some of the modes of classroom transaction

- Group discussion
- Lecture
- Demonstration
- Team teaching

- PPT
- YouTube
- Google drive
- Google meet

# **Discipline Specific Elective courses**

**Course Title: Chemistry of Natural Products** 

Paper Code: MCMC.406

Course Hours: 45h

L	T	P	Credits
3	0	0	3

#### **Learning Outcomes**

After completing this course, the learner will be able to:

CLO1: Describe categories, synthesis and biosynthesis of terpenoids

CLO2: Conceptualize the nomenclature, synthesis and structure of alkaloids

CLO3: Explain the occurrence, nomenclature and structural investigation of steroids

CLO4: Describe the isolation, purification and structural investigation of flavonoids

Units/Hours	Content	Mapping with course learning outcome
Unit 1	Terpenoids and carotenoids: Classification,	CLO1
10 Hours	nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and $\beta$ -Carotene Learning activities: Learner will be engaged in molecular models to explain the structure and stereochemistry of terpenoids.	
Unit 2	<b>Alkaloids:</b> Definition, nomenclature and	CLO2
10 Hours	physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine and Morphine  Learning activities: Learner will be able to explain chemical tests for the identification of plant alkaloids	
Unit3	Steroids: Occurrence, nomenclature, basic	CLO3
10 Hours	skeleton and stereochemistry, Structure	

	determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids  Learning activities: Learner will be engaged in molecular models to explain the structure and stereochemistry of steroids.	
Unit 4 15 Hours	Flavonoids: Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin Chemistry of Carbohydrates Introduction, classification, configuration and conformation, reactions of monosaccharides; oxidation, reduction, osazone formation, chain shortening and chain lengthening, mutarotation, Structure elucidation and chemistry of Glucose  Learning activities: Learner will be provided spectral data for the identification of abovementioned natural compounds.	CLO4

#### **Suggested Readings**

- 1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2013). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.
- 2. Bhat, S.V., Nagasampagi, B.A., Sivakumar, M. (2005), *Chemistry of Natural Products*. Narosa Publishing House, New Delhi.
- 3. Brahamchari, G. (2009). *Natural Product: Chemistry, Biochemistry and Pharmacology*. Narosa Publishing House, New Delhi.
- 4. Cseke, L.J. (2009). *Natural Products from plants*. CRC Press, Taylor and Francis, US.
- 5. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Willey & Sons, UK.
- 6. Finar, I.L. (2006). Organic Chemistry: Stereochemistry and the Chemistry of Natural Products. Dorling Kindersley Pvt. Ltd., India.
- 7. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs*. Birkhauser Verlay.
- 8. Thomson, R.H. (2008). The Chemistry of Natural Products, Springer.
- 9. Singh, J., Ali, S. M., Singh, J. (2010) Natural Products Chemistry. Pragati Books.
- 10. Xu, R., Ye, Y., Zhao, W., (2011). *Introduction to Natural Products Chemistry*. CRC Press.
- 11. Rehman, A., (2015). Studies in Natural Products Chemistry, Elsevier Books.

#### The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Tutorial

- PPT
- YouTube
- Google meet

Course Title: Quantum Chemistry

**L T P Credits** 3 0 0 3

Paper Code: MCMC.407 Course Hours: 45 h

#### **Learning Outcomes**

After completing this course, the learner will be able to:

CLO1: Describe quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry

CLO2: Explain Electronic and Hamiltonian operators for molecules.

CLO3: Utilize Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.

CLO4: Conceptualize Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle

Units/Hours	Content	Mapping with course learning outcome
Unit 1 10 Hours	<b>Fundamental Background:</b> Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor, Particle in a Ring, Hydrogen Atom.	CLO1, CLO2
	<b>Learning activities:</b> Learner will apply Schrodinger equation for particle in 1D and 3D	
Unit 2 10 Hours	<b>Approximate Methods:</b> Perturbation theory for non-degenerate and degenerate states and its applications, Variation theorem and its application. <b>Learning activities:</b> Web based approach will be used to explain perturbation and variation theory	CLO1
Unit 3 10 Hours	Angular Momentum: Ordinary angular momentum, Eigen functions and Eigen values for angular momentum, Addition of angular momenta, Spin, Anti-symmetry and Pauli exclusion principle.  Electronic Structure of Atoms: Electronic	CLO3
	configuration, Russell-Saunders terms and	

	Coupling Schemes, Magnetic Effects: Spin-orbit Coupling and Zeeman Splitting, the self-consistent field method, Hartree-Fock SCF method for	
	molecules.	
	<b>Learning activities:</b> Learner will apply Angular momentum and Pauli exclusion principle to	
	solve numerical problems	
Unit 4	Born-Oppenheimer Approximation: LCAO-MO	CLO4
15 Hours	and VB treatments of the H <sub>2</sub> <sup>+</sup> and H <sub>2</sub> , Hybridization	
	and valence MOs of H <sub>2</sub> O and NH <sub>3</sub> . Huckel Theory of	
	acyclic and cyclic conjugated systems, Bond Order	
	and Charge Density Calculations.	
	<b>Learning activities:</b> Learner will be engaged in web-based learning to explain Born-Oppenhelmer approximation concept	

#### Suggested Readings:

- 1. Levine, I.N. Quantum Chemistry, 2016, Pearson Educ., Inc. New Delhi.
- 2. Chandra, A.K. 1994, Introductory Quantum Chemistry, Tata McGraw Hill.
- 3. Prasad, R.K., 2009, Quantum Chemistry, New Age Science.
- 4. Mc Quarrie, D. A. (2011). Quantum Chemistry. Viva Publishers.
- 5. Murrell, J.N. Kettle S.F.A. and Tedder, J. M. Valence Theory, 1965, John Wiley.
- 6. Lowe, J. P. and Peterson, K. 2006, Quantum Chemistry, Academic Press.

# The following are some of the modes of classroom transaction

- Demonstration
- Group discussion
- Lecture
- Self-learning

- Google meet
- PPT

Course Title: Inorganic Chemistry - I

Paper Code: MCMC.408 Total Contact Hours: 45 h

L	Т	Р	Credits
3	0	0	3

#### **Learning Outcome:**

On completion of this course the student's will able to:

**CLO1:** Reaction mechanism, formation constant and stability of the coordination complexes.

**CLO2:** Interpret the electronic properties. **CLO3:** Interpret the magnetic properties.

Units/ hours	Content	Mapping with course learning outcome
Unit-1 10 Hours	Metal-Ligand Equilibria in Solution: Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of formation constants by spectrophotometry and potentiometric (pH) methods.	CLO1
	Group Discussion among the students on the stability of metal complex formation	
Unit-2 10 Hours	Reaction Mechanisms of Transition Metal Complexes: Introduction, potential energy diagram and reactivity of metal complexes, ligand substitution reactions, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere.  Demonstration of reactions mechanism of metal complexes.	CLO1

IInit-3	Electronic Absorption spectra of Metal	CLO2
Unit-3 15 Hours	<b>Electronic Absorption spectra of Metal Complexes:</b> Ligand field theory, nephelauxetic effect, Jahn-Teller effects, spin orbital (LS) coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of p <sup>n</sup> , d <sup>n</sup> , f <sup>n</sup> ions, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters () energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. selection rules of electronic transitions, relaxation of the selection rule in centrosymmetric and noncentrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths.  Classroom discussion on interpretation of LS coupling and various energy level diagrams through brainstorming	CLO2
Unit-4 10 Hours	Magnetic properties: magnetic properties of transition metal complexes, effects of L-S coupling on magnetic properties, quenching of orbital angular momentum by crystal fields in complexes in terms of splitting, temperature independent paramagnetism (TIP).  Hands-on experience of metal complexes for magnetic properties by using Gouy's Balance.	CLO3

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

## **Suggested Readings**

- 1. Cotton, F. A., and Wilkinson, G., Murillo, C. A., Bochmann, M.(1999). *Advanced Inorganic Chemistry* (6th Edition). New York: Wiley.
- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
- 3. Greenwood, N. N., and Earnshaw, A. (2012). Chemistry of the Elements. Elsevier.
- 4. Miessler, G. L. and Tarr, D. A. (2011) Inorganic Chemistry, Pearson Education.
- 5. Atkins, P. (2010). Shriver and Atkins' Inorganic Chemistry. Oxford University Press, USA.

- 6. Dutta, R. L., and Syamal, A. (1993). *Elements of Magnetochemistry*. Affiliated East- West Press.
- 7. Drago, R. S. (1992) *Physical Methods for Chemists*. Saunders College Publishing.
- 8. Lee, J. D. Concise Inorganic Chemistry: Fifth Edition (2012). Elsevier.
- 9. Kent, B. Inorganic Chemistry: Reactions, Structures and Mechanisms (12 June 2019), NY Research Press.
- 10. Close, D. Principles of Inorganic Chemistry (19 June 2019), Larsen and Keller Education

# The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Team teaching

- PPT
- Google meet
- YouTube

Course Title: Physical Chemistry-I

Paper Code: MCMC. 409 Total Contact Hours: 45

L	Т	Р	Credits
3	0	0	3

**Learning Outcome:** After the completion of the course students will be able to:

**CLO1:** Interpret and solve the Schrodinger equation for various systems, particle in a boundary model, Electronic and Hamiltonian operators for molecules.

**CLO2:** Explain the quantum chemical description of angular momentum and term symbols for a one and many-electron systems.

**CLO3:** Relate the Born- Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle with the atomic and molecular phenomena.

**CLO4:** Explain the statistical aspects of system and relate the classical thermodynamics to quantum mechanics.

**CLO5:** Apprehend and apply partition function in the deduction of thermodynamic properties of chemical systems.

Units/ hours	Content	Mapping with CLOs
Unit 1 11 Hours	Fundamental Background: Review of essential mathematical concepts required for quantum chemistry, Postulates of quantum mechanics, Eigen values and Eigen functions, operators, Schrodinger equation.  Translational, Rotational and Vibrational Motions: - Free particle and particle in a box and its application, one-dimensional harmonic oscillator and rigid rotor, particle in a ring, particle on a sphere.  Problem solving approach to determine Eigen values and Eigen function using corresponding operator and Schrodinger equation.  Brainstorming on defining and solving Schrodinger equation for different systems like particle in a box, rigid rotator, simple harmonic oscillator.	CLO1

Unit 2	Angular Momentum: Ordinary angular	CLO2,
11 Hours	momentum, generalized angular momentum, Eigen functions and Eigen values for angular momentum, Ladder operator, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle, Slatter determinantal wave functions.  Electronic Structure of Atoms: Electronic configuration, term symbols and spectroscopic states, Russell-Saunders terms and J-J coupling schemes, Magnetic effects: spin-orbit coupling and Zeeman splitting.  Understanding multi-electron atom quantum evaluation through peer discussion and brainstorming sessions.	CLO3
Unit 3 12 Hours	Variation Methods: The variation theorem	CLO4
	and its application, linear variation principle. <b>Born-Oppenheimer Approximation:</b> LCAO-MO and VB treatments of the H2+ and H2, Shape of molecules, Hybridization and valence MOs of H2O and NH3. Determination of bond angle in sp³, sp² and sp, Huckel Theory of acyclic and cyclic conjugated systems, Bond order and charge density Application of Variation method and its uses in pi-HMO theory for acyclic and cyclic conjugated organic systems through peer learning. Application of MOT and VBT for H2 and H2+ system through demonstration.	
Unit 4 11 Hours	Classical Thermodynamics and Phase Transitions: Partial Molar Properties, Gibbs- Duhem equation, Chemical potential of liquids, Phase transition: Clausius-Clapeyron equation.  Statistical Thermodynamics: Statistical concepts and examples, Thermodynamic probability and entropy, Partition function, molar partition function, thermodynamic properties in terms of the molecular partition function for monoatomic gases, rotational, translational, vibrational, and electronic partition functions for diatomic molecules, calculation of equilibrium constants in terms of the partition function.	CLO5

Partition function and its correlation to classical thermodynamic evaluation through brainstorming session and peer learning

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

#### Suggested Readings

- 1. Levine, I.N. (2014) Quantum Chemistry. 7th ed. Pearson Education Inc.
- 2. Chandra, A.K. (2017) *Introductory Quantum Chemistry*. 4<sup>th</sup> ed. Tata Mcgraw-Hill.
- 3. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
- 4. Prasad, R.K., (2009) Quantum Chemistry. 4th Ed. New Age Science.
- 5. Murrell, J.N., Kettle S.F.A. and Tedder, J. M. (1965) *Valence Theory*. John Wiley Publishers.
- 6. Lowe, J. P. and Peterson, K., (2006). Quantum Chemistry. Academic Press.
- 7. Atkins, P., and Friedman, R. (2011). *Molecular Quantum Mechanics*, 5<sup>th</sup> edition, Oxford university press.
- 8. Drennan, C., Taylor, E. V., (2008) https://ocw.mit.edu/courses/chemistry/5-111- principles-of-chemical-science-fall-2008/index.htm
- 9. Griffin, R. G., Voorhis, T. V. (2007) https://ocw.mit.edu/courses/chemistry/5-111- principles-of-chemical-science-fall-2008/index.htm
- 10. Atkins, P., De Paula, J. and Keeler, J. (2018) Oxforda University Pressed.
- 11. McQuarrie, D. A. and Simon, J. D. (2019) *Physical Chemistry: A Molecular Approach*.
  Viva Books
- 12. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004) *Physical Chemistry*. Wiley- Interscience Publication.
- 13. Engel, T., Reid, P. and Hehre, W. (2012) *Physical Chemistry*. Pearson Education
- 14. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company Nash, L. K. (2012) *Elements of Statistical Thermodynamics*. *Dover Publication Inc.*
- 15. Laurendeau, N. M. (2005) Statistical Thermodynamics: Fundamentals and Applications. Cambridge University Press.
- 16. Hill, T. L. (1986) An Introduction to Statistical Thermodynamics. Dover Publications Inc.
- 17. Yu, T. H. (2020) Teaching Thermodynamics with the Quantum Volume J. Chem. Educ., 97 (3), 736-740 DOI: 10.1021/acs.jchemed.9b00742
- 18. Nelson, K. A., Bawendi, M. (2008) https://ocw.mit.edu/courses/chemistry/5-60-thermodynamics-kinetics-spring-2008/video-lectures.

- 19. Bhattacharyya, D. and Dawlaty, J. M. (2019) Teaching Entropy from Phase Space Perspective: Connecting the Statistical and Thermodynamic Views Using a Simple One-Dimensional Model *J. Chem. Educ.*, 96 (10), 2208-2216. DOI: 10.1021/acs.jchemed.9b00134
- 20. Halpern A. M. and Marzzacco, C. J. (2018) Using the Principles of Classical and Statistical Thermodynamics to Calculate the Melting and Boiling Points, Enthalpies and Entropies of Fusion and Vaporization of Water, and the Freezing Point Depression and Boiling Point Elevation of Ideal and Nonideal Aqueous Solutions, *J. Chem. Educ.*,95(12), 2205-2211. DOI: 10.1021/acs.jchemed.8b00561
- 21. Halpern A. M. and Marzzacco, C. J. (2018) Constructing the Phase Diagram of a Single-Component System Using Fundamental Principles of Thermodynamics and Statistical Mechanics: A Spreadsheet-Based Learning Experience for Students. *J. Chem. Educ.*, 95 (12), 2197-2204. DOI: 10.1021/acs.jchemed.8b00560

#### The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Team teaching

- PPT
- Google meet
- YouTube

# Semester -II

Course Title: Advanced Organic Chemistry-II

Paper Code: MCMC.421

Course Hours: 60h

L	T	P	Credits
4	0	0	4

# **Learning Outcomes**

After completing this course, the learner will be able to:

CLO1: Interpret the stereochemistry, spatial arrangement of atoms/groups and apply it on the course of reactions and mechanism prediction.

CLO2: Explain the chemical reactions in peptides

CLO3: Apply principle of photochemistry in various chemical transformations

Units/Hours	Content	Mapping
		with course
		learning
		outcome
Unit 1	Stereochemistry: IUPAC nomenclature of organic	CLO1
15 Hours	molecules, Elements of symmetry, Chirality,	
	Projection formulae [Fly wedge, Fischer, Newman	
	and Saw horse], Configurational and	
	conformational isomerism in acyclic and cyclic	
	compounds; Stereogenicity, stereoselectivity,	
	enantioselectivity, diastereoselectivity, racemic	
	mixture and their resolution, Configurational	
	notations of simple molecules, D/L, R/S, $E/Z$ and	
	cis/trans configurational notations, Threo and	
	erythro isomers, Methods of resolution, Optical	
	purity, Enantiotopic and diastereotopic atoms,	
	groups and faces, Stereospecific and stereoselective	
	synthesis, Asymmetric synthesis, Optical activity in	
	the absence of chiral carbon (biphenyls, allenes and	
	spiranes), Chirality due to helical shape,	
	Stereochemistry of the compounds containing	
	nitrogen, sulphur and phosphorus, Conformational	
	analysis of cyclic compounds such as cyclopentane,	
	cyclohexane, cyclohexanone derivatives, decalins,	
	1,2-; 1,3-, 1,4-disubstituted cyclohexane	
	derivatives and D-Glucose, Effect of conformation	
	on the course of rate of reactions, Effect of	

	conformation on reactivity, Conformation of sugars,	
	strain due to unavoidable crowding.	
	Learning activities: Learner will be engaged in	
	Molecular models and online modeling tools to	
Unit 2	explain the stereochemistry of compounds	CLO2
	Chemistry of peptides:	CLO2
15 Hours	a) Coupling reactions in peptide synthesis	
	b) Principles of solid phase peptides synthesis, t-BOC and FMOC protocols, various solid supports and linkers: Activation procedures, peptide and bond formation, deprotection and cleavage from resin, low and high HF cleavage protocols, formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides.	
	c) Segment and sequential strategies for solution phase peptide synthesis with any two case studies	
	d) Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over- activation and side reactions of individual amino acids ide reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over- activation and side reactions of individual amino acids.	
	<b>Learning activities:</b> Learner will be engaged in practical's involving coupling, protection/deprotection and coupling reactions for peptide synthesis.	
Unit 3	<b>Photochemistry:</b> Franck-Condon principle,	CLO3
15 Hours	Jablonski diagram, Singlet and triplet states,	
	Photosensitization, Quantum efficiency,	
	Photochemistry of carbonyl compounds, Norrish	
	type-I and type-II cleavages, Paterno-Buchi	
	reaction, Photoreduction, Di $\pi$ – methane	
	rearrangement. Photochemistry of aromatic	
	compounds, Photo-Fries reactions of anilides,	
	Photo-Fries rearrangement, Barton reaction Singlet	
	molecular oxygen reactions	
L	1 20	ı

	<b>Learning activities:</b> Learner will be engaged in web-based learning to explain photochemical reactions				
Unit 4	<b>Pericyclic Chemistry:</b> Main features of pericyclic	CLO3			
15 Hours	reactions, Classification of pericyclic reactions,				
	Thermal and photochemical pericyclic reactions.				
	Electrocyclic reactions: Conrotation and				
	disrotation, Electrocyclic closure and opening in 4n				
	and 4n+2 systems. Woodward-Hoffmann selection				
	rules for electrocyclic reactions. Explanation for the				
	mechanism of electrocyclic reactions by (i)				
	symmetry properties of HOMO of open chain				
	partner (ii) Conservation of orbital symmetry and				
	orbital symmetry correlation diagrams and (iii)				
	Huckel-Mobius aromatic and antiaromatic				
	transition state method. Examples of electrocyclic				
	reactions.				
	Cycloaddition reactions: Suprafacial and				
	antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$				
	cycloadditions. Cycloreversions. Stereochemical				
	aspects in supra-supra, supra-antara, antara-				
	supra and antara-antara $\pi^2$ + $\pi^2$ and $\pi^4$ + $\pi^2$				
	cycloadditions. Diels-Alder reaction. Woodward-				
	Hoffmann Selection rules for cycloaddition				
	reactions.				
	Sigmatropic reactions: [1,j] and [i,j] shifts;				
	Suprafacial and antarafacial shifts; Selection rules for [lj] shifts; Cope and Claisen rearrangements				
	<b>Learning activities:</b> Learner will be engaged in				
	web-based learning to explain cycloaddition,				
	electrocyclic and sigmatropic reactions.				

# **Suggested Readings**

- 1. Morrin Acheson, R. (2008) An Introduction to the Chemistry of heterocyclic compounds. Wiley India Pvt. Ltd.
- 2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic Chemistry*. Oxford press.
- 3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., India.

- 4. Bansal, R. K., (2012). Organic Reaction Mechanism, New Age International (P) Ltd., New Delhi.
- 5. Bansal, R. K., (2007). *A Text Book of Organic Chemistry*, New Age International (P) Ltd., New Delhi.
- 6. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., New Delhi.
- 7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer*.
- 8. Finar, I. L., (2012). Organic Chemistry Vol. 1, Pearson Education, UK.
- 9. Gilchrist, T.L. (1997). Heterocyclic Chemistry, Longman, Prentice Hall, US.
- 10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles*, Springer Verlag, India.
- 11. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, New York.
- 12. Kalsi P. S., (2010). Organic Reactions and Their Mechanisms, New Age International Publication, New Delhi.
- 13.Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc, US.
- 14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
- 15. Mukherjee S. M., Singh S. P., (2009). Reaction Mechanism in Organic Chemistry, Macmillan India Ltd., New Delhi.
- 16.R. Katritzky, (2010). Handbook of Heterocyclic Chemistry Elsevier, UK.
- 17. Smith, M. B. (2013). March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure. John Wiley & Sons.
- 18. Sykes, P., (1997). A Guide Book to Mechanism in Organic Chemistry, Prentice Hall, US.
- 19. Norman, R.O.C.; Coxon, J.M. (1995). *Principles of Organic Synthesis*, Blackie Academic & Professional.
- 20. Warren, S., (2010). Organic Synthesis: The Synthon Approach. John Wiley & Sons, New York,
- 21. Warren, S., (2010). Designing Organic Synthesis: A Disconnection Approach. John Wiley & Sons, New York.
- 22. Corey E.J., Cheng Xue-Min, (1989) *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons,
- 23. Carey, F. A., Guiliano, R. M. (2012). Organic Chemistry. McGraw Hill.
- 24. Kofie, W., Caddick, S. (2016). *Problems in Advanced Organic Chemistry*. Auris Publishing.
- 25. Solomons, T. W. G., Fryhle, C. B., Snyder, S. A. (2017). Solomons' Organic Chemistry. John Willey & Sons.
- 26. Fleming (1999). Pericyclic Reactions, Oxford University Press, Oxford.

- Lecture
- Group discussion
- Demonstration
- Team teaching

- PPT
- Google meet
- YouTube

Course Title: Organic Chemistry-II (Practical)

Paper Code: MCMC.516

Course Hours: 90h

L	1	•	P	Credits
0	(	)	6	3

# **Learning Outcomes**

After completing this course, the learner will be able to:

CLO1: Differentiate mixture of *ortho* and *para* as well as cis/trans mixture by column chromatography

CLO2: Describe Multi-Step Synthesis of Organic Compounds

CLO3: Identify compounds via combined spectral interpretation of  $^1$ H,  $^{13}$ C NMR, IR, UV and Mass along with 2-D NMR spectra.

Practical	Content/Title	Mapping with course learning outcome
1.	Separation and purification of organic compounds by column chromatography: Separation of mixture of <i>ortho</i> and <i>para</i> mixture and cis/trans mixture. The column chromatography should be monitored by TLC.	CLO1
2.	<ul> <li>Multi-Step Synthesis of Organic Compounds: The Learning activities should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. (Any five)</li> <li>a) Synthesis of isoxazole derivatives via 1,3-dipolar cycloaddition.</li> <li>b) Synthesis of pyrazole derivatives from chalcones.</li> <li>c) Synthesis of an antihypertensive drug-propranolol via epoxide ring opening reaction.</li> <li>d) Synthesis of Diltiazem (a calcium channel blocker) via Darzen condensation, a key step in its synthesis.</li> <li>e) Protection and deprotection of alcohols and amines.</li> <li>f) Preparation of Triphenyl Carbinol from Bromobenzene (Grignard's reaction)</li> <li>g) Preparation of allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst under neat condition and their characterization through various spectroscopic techniques.</li> <li>h) Preparation of homoallyl alcohols via Barbier type reaction under aqueous condition using Indium as a catalyst.</li> </ul>	CLO2

	i) Suzuki reaction of 3,4-dimethoxy phenyl boronic acid with aryl halides using Pd(PPh <sub>3</sub> ) <sub>4</sub> as a catalyst.	
3.	Exercises on identification of compounds <i>via</i> combined spectral interpretation of <sup>1</sup> H, <sup>13</sup> C NMR, IR, UV and Mass along with 2-D NMR spectra.	

# **Suggested Readings**

- 1. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). Laboratory Experiments in Organic Chemistry, The Macmilan Limited, London.
- 2. Mann and Saunders. (2009). Practical organic chemistry, Pearson.
- 3. Pasto, D.P., Johnson, C., Miller, M. (2010). Experiments and Techniques in Organic Chemistry, Prentice Hall.
- 4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
- 5. Vogel, A.I. (Latest edition). (1989). Text book of practical organic chemistry, Pearson
- 6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments*, *Heath*, *D. C*and Co.,Lexington, MA.
- 7. Findeisen, M., (2013). 50 And More Essential NMR Experiments: A Detailed Guide. John Willey & Sons.

# The following are some of the modes of classroom transaction

- Experimentation
- Group discussion
- Demonstration
- Self-learning

- PPT
- YouTube
- Google drive
- Google meet

Course Title: Computer Aided Drug Design

Paper Code: MCMC.517

Course Hours: 30h

L	T	P	Credits
2	0	0	2

# Learning outcome:

After completing this course, the learner will be able to:

CLO1: Describe the role of CADD in drug discovery

CLO2: Work with molecular modelling software's to design new drug molecules

CLO3: Design and develop new drug like molecules

Units/Hours	Content	Mapping with course learning outcome
Unit 1	Introduction to Computer Aided Drug Design	CLO1
8 Hours	(CADD): History, different techniques and applications. Quantitative Structure Activity Relationships: Basics. History and development of QSAR: Physiochemical parameters and methods to calculate physiochemical parameters: Hammett equation and electronic parameters (sigma), lipoiphilicity effects and parameters (log P, pisubstituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physiochemical parameters. Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages: Deriving 2D-QSAR equations. 3D-QSAR approaches and contour map analysis. Statistical methods used in QSAR analysis and importance of statistical parameters.  Learning activities: Learner will be engaged in group discussion to explain 2D-QSAR, 3D-QSAR and importance of statistical parameters	
Unit 2 8 Hours	Molecular Modeling and Docking:  a) Molecular and Quantum Mechanics in drug design.	CLO2

	b) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation. c) Molecular docking and drug receptor interactions: rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AchE & BchE)  Learning activities: Learner will be engaged in molecular modeling of compounds	
Unit 3	Molecular Properties and Drug Design:	CLO3
7 Hours	a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design.	
	b) De novo drug design: Receptor/enzyme- interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design.	
	c) Homology modelling and generation of 3D-structure of protein.	
	<b>Learning activities:</b> Learner will study Molecular model to explain interactions between ligand and drug target	
Unit 4	Pharmacophore Mapping and Virtual Screening:	
7 Hours	Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore's modelling; Conformational search used in pharmacophore mapping. In-silico Drug Design and Virtual Screening Techniques. Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols.	CLO3
	<b>Learning activities:</b> Learner will be engaged in Pharmacophore band structure based <i>In-silico</i> virtual screening protocols	

# **Suggested Readings**

1. Ellis, G.P., West, G. B. (1983). *Progress in Medicinal Chemistry Series*. Elsevier Science.

- 2. Foye, W.O., Lemke, T. L., Williams, D. A. (2019). *Principles of Medicinal Chemistry*, Indian Ed. Waverly, Pvt. Ltd. New Delhi.
- 3. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
- 4. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II*), Nirali publication
- 5. Kulkarni, V. M., Bothra, K.G., (2008). Drug Design, Nirali Publication.
- 6. Lawton, G., Witty, D.R. (2011). Progress in Medicinal Chemistry Series. Volume 50.
- 7. Lednicer D., Laster A. M. (1998). The Organic Chemistry of Drug Synthesis(3 Volumes) John Wiley & Sons.
- 8. Lednicer, D. (2008). Strategies for Organic Drug Synthesis and Design. (7 volume) Publisher: John Wiley & Sons.
- 9. Lemke, T.L., Williams, D.A. (2012). Foye's Principles of Medicinal Chemistry.
- 10. Silverman R.B., (2014). Organic Chemistry of Drug Design and Drug Action, Publisher: Elsevier.
- 11. Wilson, C.O.; Block, J.H.; Gisvold, O.; Beale, J. M. Wilson and Gisvold's (2003) Textbook of Organic Medicinal and Pharmaceutical Chemistry. Lippincott Willaiams & Wikins.
- 12. Gore, M., & Jagtap, U. (2018). Computational Drug Discovery and Design. Springer Publishers.

- Lecture
- Group discussion
- Demonstration
- Team teaching
- Tutorial
- Self-learning

- PPT
- YouTube
- Molecular modeling software
- Google drive
- Google meet

Course Title: Advanced Spectral Analysis

Paper Code: MCMC.518

Course Hours: 60h

L	T	P	Credits
4	0	0	4

# Learning outcome:

After completing this course, the learner will be able to:

CLO1: Describe the applications of UV, IR and Raman spectroscopy

CLO2: Explain the 1D and 2D NMR analysis of different compounds

CLO3: Conceptualize the different rules of mass fragmentation

CLO4: Describe chromatographic techniques for separation and quantification of drugs

Units/Hours	Content	Mapping with course learning outcome
Unit 1 15 Hours	<b>UV and IR spectroscopy:</b> Wood ward – Fisher rule for 1,3- butadienes, cyclic dienes and carbonyl compounds and interpretation compounds of enones.	CLO1
	<b>Infrared spectroscopy</b> : IR Interpretation of organic compounds, NIR Applications.	
	Raman Spectroscopy: Introduction, Principle, Instrumentation and Applications.	
	• Learner will calculate λmax for conjugated diene and enone derivatives	
Unit 2 15 Hours	<b>NMR spectroscopy:</b> 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds.	CLO2
	<b>Learning activities:</b> Learner will be provided spectra for the identification of compounds	
Unit 3 15 Hours	a. Mass Spectroscopy: Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, Mc Lafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.	CLO1, CLO2, CLO3

	b. Spectral Characterization of the following		
	compounds by spectroscopic techniques: UV,		
	IR, MS, NMR (1H, 13C) a) Carvone, Citral,		
	Menthol b) Luteolin, Kaempferol c) Nicotine,		
	Caffeine d) Glycyrrhizin		
	<b>Learning activities:</b> Students will develop		
	advanced skills in data interpretation and problem-		
	solving through the rigorous analysis of spectral		
	data acquired from UV, IR, MS, and NMR		
	experiments conducted on natural products.		
Unit 4	Chromatography: Principle, Instrumentation and CLO4		
15 Hours	Applications of the following: a) GC-MS b) GC-AAS		
	c) LC-MS d) LC-FTIR e) LC-NMR f) CE-MS g) High		
	Performance Thin Layer chromatography h) Super		
	Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion		
	Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion		
	Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion		
	Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion		
	Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion Chromatography) k) Flash chromatography		

#### Suggested Readings:

- 1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). Spectrometric Identification of Organic Compounds. John wiley & sons.
- 2. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
- 3. Willard, H. H., Merritt Jr, L. L., Dean, J. A., & Settle Jr, F. A. (1988). Instrumental Methods and Analysis.
- 4. Kemp, W. (1991). Organic Spectroscopy (pp. 42-51). London: Macmillan.
- 5. Sethi, P. D. (1996). HPTLC: High Performance Thin-layer Chromatography; Quantitative Analysis of Pharmaceutical Formulations. CBS Publishers & Distributors.
- 6. Sethi, P. D. (1985). Quantitative Analysis of Drugs in Pharmaceutical Formulations. CBS Publishers, New Delhi, 1997.
- 7. Munson, J. W. (Ed.). (1984). *Pharmaceutical Analysis: Modern Methods* (Vol. 11). CRC Press.
- 8. Findeisen, M., (2013). 50 And More Essential Nmr Experiments: A Detailed Guide. John Willey & Sons.
- 9. Kromidas, S. (2017). The Hplc Expert Possibilities and Limitations of Modern High Performance Liquid Chromatography. John Wiley and Sons

- Lecture
- Group discussion
- Demonstration
- Problem solving

- PPT
- YouTube
- Google meet

# **Discipline Specific Elective Course**

Course Title: Green Chemistry Paper Code: MCMC.519

Course Hours: 45h

L	T	P	Credits
3	0	0	3

## Learning outcome

After completing this course, the learner will be able to:

CLO1: Describe various aspects of green chemistry for sustainable development

CLO2: Utilize ionic liquids and solid supported reaction conditions to reduce or

eliminate use of volatile organic solvents

CLO3: Utilize MW and sonicator in organic synthesis

CLO4: Solid state and aqueous reactions

Units/Hours	Content	Mapping
		with course
		learning
		outcome
Unit 1	Introduction to green chemistry: History, need	CLO1
12 Hours	and goals. Green chemistry and sustainability,	
	dimensions of sustainability, limitations/obstacles	
	in pursuit of the goals of green chemistry.	
	Opportunities for the next generation of materials	
	designers to create a safer future. Basic principles	
	of green chemistry: Atom economy and scope,	
	Prevention/Minimization of hazardous/toxic	
	products, designing safer chemicals, Selection of	
	appropriate auxiliary substances (solvents,	
	separation agents etc.), use of renewable starting	
	materials, Avoidance of unnecessary derivatization-	
	careful use of blocking/protection groups. Use of	
	catalytic reagents (wherever possible) in preference	
	to stoichiometric reagents, designing biodegradable	
	products, Prevention of chemical accidents,	
	Strengthening/development of analytical	
	techniques to prevent and minimize the generation	
	of hazardous substances in chemical processes.	
	<b>Learning activities:</b> Learner will be engaged in Group discussion to explain Green Chemistry Principles	

Unit 2	Approaches to green synthesis: Basic principles	CLO2			
12 Hours	of green synthesis. Different approaches to green				
	synthesis, Use of green reagents in green synthesis: polymer supported reagents, polymer supported				
	peptide coupling reagents. Green catalysts, Phase-				
	transfer catalysts in green synthesis. Advantages of PTC, Reactions to green synthesis, Application of PTCs in C-alkylation, N-alkylation, S-alkylation.				
	Darzens reaction, Williamson's synthesis, Wittig reaction, Click Chemistry. Use of Crown ethers in				
	esterification, saponification, anhydride formation, aromatic substitution and elimination reactions.				
	Water and ionic liquids as green solvents.				
	Learning activities: Learner will be engaged in				
	Group discussion to explain the use of PTC and crown ethers				
Unit 3	Microwave induced and ultrasound assisted	CLO3			
12 Hours	<b>green synthesis:</b> Introduction to synthetic organic				
	transformation under microwave (i) Microwave				
	assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave solvent				
	free reactions Ultrasound assisted reactions: Introduction, substitution reactions, addition,				
	oxidation, reduction reactions. Biocatalysts in				
	organic synthesis: Introduction, Biochemical oxidation and reductions.				
	<b>Learning activities:</b> Learner will be engaged in Web based learning to Perform Microwave induced and ultrasound assisted reactions				
Unit 4	Organic synthesis in aqueous phase and in solid	CLO4			
9 Hours	state: Aqueous reactions. Solid state reactions (i) Solid				
	phase synthesis without using any solvent (ii) Solid supported synthesis				

# Suggested Readings:

- 1. Ahulwalia, V.K.; Kidwai M. (2004). New Trends in Green Chemistry, Springer
- 2. Anastas, P.T.; Warner J. C. (2000). *Green Chemistry, Theory and Practical*. Oxford University Press.
- 3. Grieco, P.A. (1997). Organic Synthesis in Water. Publisher: Kluwer Academic.
- 4. Matlack, A. (2010). Introduction to green chemistry. CRC Press.

- 5. Ahluwalia, V. K. (2011). *Green Chemistry: Greener Alternatives to Synthetic Organic Transformations*. Alpha Science International.
- 6. Torok, B.; Dransfield, T. (2018). *Green Chemistry: An Inclusive Approach*, Elsevier

- Lecture
- Group discussion
- Demonstration
- Self-learning

- PPT
- YouTube
- Google drive
- Google meet

**Course Title: Nuclear Chemistry** 

Paper Code: MCMC.520

Course Hours: 45h

L	Т	P	Credits
3	0	0	3

# Learning outcome:

After completing this course, the learner will be able to

CLO1: Explain the nuclear structure and its stability

CLO2: Describe nuclear reactions and different fission model CLO3: Explain reactor theory along with nuclear resources

CLO4: Describe interaction of gamma radiation

Units/Hours	Content	Mapping		
		with course		
		learning		
		outcome		
Unit 1	Nuclear Structure and Stability	CLO1		
11 Hours	Binding energy, empirical mass equation, nuclear			
	models, the liquid drop model, the shell model, the			
	Fermi gas model & collective nuclear model,			
	nuclear spin, parity & magnetic moments of odd			
	mass numbers nuclei.			
	<b>Learning activities:</b> Learner will be provided			
	models to explain structure and stability of			
	nucleus			
Unit 2	Nuclear reaction	CLO2		
11 Hours	Introduction, Production of projectiles, nuclear			
	cross section, nuclear dynamics, threshold energy			
	of nuclear reaction, Coulomb scattering, potential			
	barrier, potential well, formation of a compound			
	nucleus, Nuclear reactions, direct Nuclear			
	reactions, heavy ion induced nuclear reactions,			
	photonuclear reactions.			
	Nuclear fission			
	Liquid drop model of fission, fission barrier and			
	threshold, fission cross section, mass energy and			
	charge distribution of fission products, symmetric			
	and Asymmetric fission, decay chains and delayed			
	neutrons.			

	<b>Learning activities:</b> Learner will be provided Web based learning to understand nuclear fission reactions	
Unit 3	Reactor Theory	CLO3
Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.  Nuclear Resources in India  Uranium and Thorium resources in India and their extractions, Heavy water manufacturing in India.		CLOS
	<b>Learning activities:</b> Learner will be engaged in group discussion to understand reactor theory and natural resources in India	
Unit 4	Elements of Radiation Chemistry	CLO4
12 Hours	Radiation Chemistry, Interaction of radiation with matter, Passage of neutrons through matter, Interaction of gamma radiation with matter, Units for measuring radiation absorption, Radiolysis of water, Free radicals in water radiolysis, Radiolysis of some aqueous solutions	
	<b>Learning activities:</b> Learner will be provided Web based learning to understand radiation chemistry and interaction of gamma radiation	

#### Suggested readings:

- 1. Friedlander, G., Kennedy, J. W., & Macias, E. S. (1981). *Nuclear and radiochemistry*. John Wiley & Sons.
- 2. Harvey, B. G. (1962). *Introduction to Nuclear Physics and Chemistry*. Soil Science, 94(4), 274.
- 3. Haissinsky, M. (1964). *Nuclear chemistry and its applications*. Addison-Wesley Pub. Co.
- 5. Choppin, G. R., Liljenzin, J. O., & Rydberg, J. (2002). *Radiochemistry and Nuclear Chemistry*. Butterworth-Heinemann.
- 6. Friedlander, G., Kennedy, J. W., & Macias, E. S. (1981). *Nuclear and Radiochemistry*. John Wiley & Sons.

- 7. Kanne, W. R. (1961). *Basic Principles of Nuclear Science and Reactors*. Journal of the American Chemical Society, 83(2), 508-508.
- 8. Darmstadter, J., Landsberg, H. H., & Morton, H. C. (1983). Energy, today and tomorrow: living with uncertainty. Prentice Hall.
- 9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
- 10. Arnikar, H. J. (1995). Essentials of nuclear chemistry (No. 1653). New Age International.
- 11. Cottingham, W. N., Greenwood, D. A., & Greenwood, D. A. (2001). *An Introduction to Nuclear Physics*. Cambridge University Press.

- Lecture
- Demonstration
- Tutorial
- Self-learning

- PPT
- YouTube

Course Title: Advanced Medicinal Chemistry-II

Paper Code: MCMC.521

Course Hours: 45h

# L T P Credits 3 0 0 3

# Learning outcome:

After completing this course, the learner will be able to:

CLO1: Interpret basics concepts of drugs, their effects and screening.

CLO2: Describe drugs interaction with various types of enzymes and receptors

CLO3: Conceptualize the mechanism of action and SAR studies of drug molecules.

Units/Hours	Content	Mapping with course learning outcome
Unit 1 10 Hours	Physicochemical and stereochemical aspects: In relation to biological activity, Drug receptor interaction, Adrenergic hormones and Drugs including biosynthesis, storage, release and metabolism of catecholamines (Adrenaline, Isoprenaline, Salbutamol, Amphetamine, Naphazoline), Cholinergics and Anticholinesterases including biosynthesis, storage and metabolism of acetylcholine (Methacholine Chloride, Neostigmine Bromide), Antiparkinsonism Drugs (Apomorphine).  Learning activities: Learner will be engaged in Web based learning to study Physicochemical	
Unit 2 10 Hours	Neuromuscular blocking agents: Gallamine Triethiodide, Succinylcholine chloride, Hypoglycaemic drugs (Tolbutamide), Thyroid hormones and Antithyroid drugs (L- Thyroxine, Propylthiouracil) Pancuronium, vecuronium, rocuronium, rapacuronium, dacuronium, malouètine, duador, dipyrandium, pipecuronium, chandonium. Anticoagulants and haemostatic agents: Warfarin, Phenindione, Oxytocics (includes discussion on Ergot alkaloids) (Ergometrine). Antihistamines including discussion on Sodium cromoglycate (Mepyramine, Diphenhydramine, Chlorpheniramine, Promethazine). Non-steroidal anti-inflammatory drugs and anti-gout drugs:	CLO2

	Indomethacin, Phenylbutazone, Allopurinol,	
	Probenecid.	
	<b>Learning activities:</b> Learner will be engaged in	
	Molecular modeling study to understand	
	neuromuscular blocking reagent	
Unit 3	General Anaesthetic Agents: Introduction,	CLO2
10 Hours	medicinal aspects of anaesthetics, mode of action,	
	gases and volatile liquid anaesthetics, intravenous	
	anaesthetics or fixed anaesthetics, toxicity of	
	general anaesthetics (Divinyl ether, Ethyl chloride,	
	Cyclopropane, Thiopentone Sodium).	
	Local Anaesthetic Agents: Introduction, Structure-	
	activity relationships, benzoic acid derivatives,	
	aminobenzoic acid derivatives, lidocaine	
	derivatives, miscellaneous, toxicity, mode of action	
	(Benzocaine, Procaine Hydrochloride, Lidocaine	
	Hydrochloride).	
	Learning activities: Learner will be engaged in	
	web-based study to understand aesthetic reagent	
Unit 4	Sedatives-Hypnotics: Introduction, classification of	CLO3
15 Hours	sedative-hypnotics, structure-activity	
	relationships, barbiturates, amides and imides,	
	alcohols and their carbamate derivatives,	
	aldehydes and their derivatives, mode of action,	
	pharmacological properties and side effects	
	(Barbitone, Phenobarbitone, Cyclobarbitone,	
	Pentobarbitone Sodium, Thiopentone Sodium),	
	non-barbiturates (Official drugs).	
	Anticonvulsants: Introduction, epilepsy and its	
	types, SAR, barbiturates (official products),	
	hydantoins, Oxazolidinediones, Succinamides;	
	miscellaneous drugs, (Phenytoin Sodium,	
	Troxidone), Antipsychotic agents: introduction,	
	SAR and drugs like chlorpromazine,	
	prochlorperazine, etc.	
	Learning activities: Learner will be engaged in	
	group discussion to understand the structures of	
	different sedatives and hypnotics and	
	anticonvulsants.	

## **Suggested Readings**

- 1. Delgado, J. N. and Remers W A, Ed. (2010). Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry, J. Lippincott Co., Philadelphia.
- 2. Foye, W. C. (2019). *Principles of Medicinal Chemistry*, Publisher: Wolter Kluwer.
- 3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, London.
- 4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, UK.
- 5. Patrick, G.L. (2017). An Introduction to Medicinal Chemistry, Oxford University PressUS.
- 6. Singh, H., Kapoor, V.K. (1996). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
- 7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis.
- 8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
- 9. Wolff, M E, Ed., (2010). Burger's Medicinal Chemistry and Drug Discovery John Wiley & Sons, New York.
- 10. Ferrant, E., (2011). *New Synthetic Technologies In Medicinal Chemistry*. Royal Chemical Society.

## The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Self-learning

- PPT
- YouTube
- Google drive
- Google meet

#### **Semester III**

**Course Title: Dissertation Part** 

Paper Code: MCMC. 599-1

L	T	P	Credits
0	0	40	20

# Learning outcome:

After completing this course, the learner will be able to:

CLO1: Designing of research problem and prepare synopsis

CLO2: Preparation of synopsis for Project

CLO3: Planning of experiments

#### Evaluation criteria:

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

Mapping with course learning outcome: CLO1, CLO2, CLO3

The following are some of the **modes of classroom transaction** 

- Lecture cum demonstration
- Project Method
- Seminar
- Group discussion

The following tools can be used in different transactional modes:

PPT Video Multimedia packages TED Talks google drive

#### **Software tools**

- Tracker
- ChemBioDraw
- Schrodingermaestro/AutoDck
- ppt
- BLAST
- Endnote

#### **Semester IV**

Course Title: Dissertation Part Paper Code: MCMC. 599-2

L	T	P	Credits
0	0	40	20

# Learning outcome:

After completing this course, the learner will be able to:

CLO1: Designing of research problem and prepare synopsis

CLO2: Preparation of synopsis for Project

CLO3: Planning of experiments

#### **Evaluation criteria:**

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

Mapping with course learning outcome: CLO1, CLO2, CLO3

The following are some of the **modes of classroom transaction** 

- Lecture cum demonstration
- Project Method
- Seminar
- Group discussion

The following tools can be used in different transactional modes:

TED Talks

google drive

PPT Video Multimedia packages

#### **Software tools**

- Tracker
- ChemBioDraw
- Schrodingermaestro/AutoDck
- ppt
- BLAST
- Endnote

