# **CENTRAL UNIVERSITY OF PUNJAB**



Master of Pharmacy
(Pharmaceutical Chemistry)

**Session - 2024-26** 

Department of Pharmaceutical Sciences and Natural Products

# **Course structure for M. Pharm. (Pharmaceutical Chemistry)**

Course Code	Name of the course	Credit hours	Credit points	Hrs/ wk	Marks
		Hours	points	WK	
	SEMESTER I				
MPC101T	Modern Pharmaceutical Analytical Techniques	4	4	4	100
MPC102T	Advanced Organic Chemistry–I	4	4	4	100
MPC103T	Advanced Medicinal Chemistry	4	4	4	100
MPC104T	Chemistry of Natural Products	4	4	4	100
MPC105P	Pharmaceutical Chemistry Practical-I	12	6	12	150
MPC106S	Seminar/Assignment	7	4	7	100
	Total	35	26	35	650
	SEMESTER II				
MPC201T	Advanced Spectral Analysis	4	4	4	100
MPC202T	Advanced Organic Chemistry – II	4	4	4	100
MPC203T	Computer Aided Drug Design	4	4	4	100
MPC204T	Pharmaceutical Process Chemistry	4	4	4	100
MPC205P	Pharmaceutical Chemistry Practical-II	12	6	12	150
MPC206S	Seminar/Assignment	7	4	7	100
XXX	Inter-Disciplinary Course (or through MOOC)	2	2	2	50
	Total	37	28	37	700
	SEMESTER III	-			
MRM 301T	Research Methodology & Biostatistics	4	4	4	100
MPC302T	Journal club	1	1	1	25
MPC303T	Discussion/ Presentation (Proposal Presentation)	2	2	-	50
MPC599	Research Work	28	14	-	350
	Total	35	21	5	525
	SEMESTER IV				
MPC401T	Journal club	1	1	1	25
MPC402T	Discussion / Presentation	3	3	-	75
MPC599	Research Work, thesis and viva-voce#	31	16	-	400
	Total	35	20	1	500

<sup>\*</sup>To be evaluated by external expert

## **Examination pattern**

Core, Discipline Elective, Compulsory Foundation,		Value Entrepre Innovati	ciplinary Course, Added, eneurship, ion and skill ment Courses		
	Marks	Evaluation	Marks	Evaluation	
Internal Assessment	25	Various methods	-	-	
Mid-semester test	25	Descriptive	50	Descriptive (70%)	
(MST)				Objective (30%)	
End-semester test	50	Descriptive (70%)	50	Descriptive (70%)	
(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	Synopsis	Performance	Practical continuous 6	Note evaluation	book	and	Viva voce
Marks	20	50	>	50			30

Thesis/Disserta	Thesis/Dissertation Proposal (Third		Thesis/Dissertat	tion (Four	rth Semester)
Semester)					
	Marks	Evaluation		Marks	Evaluation
Supervisor	200	Dissertation	Supervisor	200	Continuous assessment
		proposal and			(regularity in work, mid-
		presentation			term evaluation)
					dissertation report,
					presentation, final viva-
					voce
HoD and	150	Dissertation	External	200	Dissertation report (100),
senior-most		proposal and	expert, HoD		presentation (50), final
faculty of the		presentation	and senior-		viva-voce (50)
department			most faculty of		
			the department		

Evaluation pattern similar to third and fourth semester dissertation will apply for internship

### Graduate attributes for M. Pharm. in Pharmaceutical Chemistry

After completing a Master of Pharmacy in Pharmaceutical Chemistry; the graduates will have a quality conscious service providing attitude by adopting the knowledge of spectral analysis and chromatographic techniques in manufacturing and Research & Development of drugs. They will have a perspective to develop efficacious, safe, and affordable drugs in a reasonable time using transformative digital technologies and will be able to implement Computer Aided Drug Design principles in modern drug discovery and development process in higher studies and at the industrial level. They will be able to apply the knowledge of chemistry for the development of synthetic methodologies including peptide chemistry, retro-synthesis and green chemistry for making the drugs affordable to the public and will be having an attribute to become self- reliant in APIs by the development of scale-up of APIs and intermediates, unit operations and industrial safety guidelines. The graduates will have a positive attitude to implement the sustainable development goals to make the planet safe for the next generations by implementing a circular economy and a philosophy to comprehend the socioeconomy of medicines and make the world healthy. This program will also help graduates make careers in industry, government organizations or institutions of higher learning.

#### Semester 1

Course Title: Modern Pharmaceutical Analytical

**Techniques** 

Paper Code: MPC101T 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, theory and applications of UV-Vis, IR and spectroflourimetry

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

CLO3: Separate different constituents of mixture by chromatographic techniques

CLO4: Conceptualize general principle and theory of electrophoresis and X-ray crystallography with handling of instruments.

CLO5: Explain the Principle, thermal transitions and Instrumentation of DSC, DTA and TGA

Units/Hours	Content	Mapping
		with course
		learning
		outcomes
Unit 1	UV-Visible Spectroscopy	CLO1
10 Hours	<ul> <li>Introduction, Theory, Laws, and Instrumentation associated with UV-Visible spectroscopy</li> <li>Choice of solvents and solvent effect</li> <li>Applications of UV- Visible spectroscopy</li> <li>Difference/ Derivative spectroscopy</li> <li>Theory, Modes of Molecular vibrations, Sample handling</li> <li>Instrumentation of Dispersive and Fourier - Transform IR Spectrometer</li> <li>Factors affecting vibrational frequencies</li> <li>Applications of IR spectroscopy, data interpretation</li> <li>Spectroflourimetry</li> <li>Theory of Fluorescence</li> <li>Factors affecting fluorescence (characteristics of drugs that can be analysed by flourimetry), Quenchers, Instrumentation</li> <li>Applications of fluorescence spectrophotometer</li> </ul>	

	Flame Emission Spectroscopy and Atomic Absorption Spectroscopy  • Principle, Instrumentation, Interferences and Applications.  Learning activities: Learner will be engaged in hands on training on different instruments like UV, IR and spectrophotometer.	
Unit 2	NMR Spectroscopy	CLO2
10 Hours	<ul> <li>Quantum numbers and their role in NMR</li> <li>Principle, Instrumentation, Solvent requirement in NMR • Relaxation process, NMR signals in various compounds</li> <li>Chemical shift, Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance</li> <li>Brief outline of principles of FT-NMR and 13C NMR</li> <li>Applications of NMR spectroscopy</li> <li>Learning activities: Learner will be familiarized with the instrument and</li> </ul>	
	provided NMR for the characterization of	
TT '4 O	compounds.	CT CC
Unit 3 10 Hours	<ul> <li>Mass Spectroscopy</li> <li>Principle, Theory, Instrumentation of Mass Spectroscopy</li> <li>Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight</li> <li>Mass fragmentation and its rules</li> <li>Meta stable ions</li> <li>Isotopic peaks</li> <li>Applications of Mass spectroscopy</li> <li>Learning activities: Learner will be provided mass spectra for the characterization of compounds.</li> </ul>	CLO2
Unit 4	Chromatography	CLO3
10 Hours	Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following:  • Thin Layer chromatography  • Ion exchange chromatography  • Column chromatography	

	- Coa almomata smambra	
	• Gas chromatography	
	High Performance Liquid chromatography	
	•Ultra-High Performance Liquid	
	chromatography	
	Affinity chromatography	
	Gel Chromatography	
	<b>Learning activities:</b> Learner will be familiarized	
	and trained in different chromatographic	
	techniques like TLC, Column, HPLC, HPTLC	
	and GC for the purification and characterization	
	of compounds.	
Unit 5	Electrophoresis	CLO4
10 Hours	Principle, Instrumentation, working conditions,	
	factors affecting separation and applications of	
	the following:	
	• Paper electrophoresis	
	• Gel electrophoresis	
	Capillary electrophoresis	
	• Zone electrophoresis	
	Moving boundary electrophoresis	
	• Isoelectric focusing	
	X ray Crystallography	
	Production of X rays	
	Different X ray diffraction methods	
	• Bragg's law, Rotating crystal technique, X ray	
	powder technique	
	• Types of crystals and applications of X-ray	
	diffraction	
	Y	
	<b>Learning activities:</b> Learner will be provided	
	conceptual learning based on electrophoresis as	
	well as handling of instruments.	
Unit 6	Potentiometry	CL05
10 Hours	• Principle, working, ion selective electrodes	
	• Application of potentiometry	
	Thermal Techniques	
	• 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      Dharma soutised ambientions	
	• Pharmaceutical applications	
	Differential Thermal Analysis (DTA)	
	Principle, instrumentation	

- 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

#### **REFERENCES**

- 1. Spectrometric Identification of Organic compounds Robert M Silverstein, 8<sup>th</sup> edition, John Wiley & Sons, 2015.
- 2 Principles of Instrumental Analysis Doglas A Skoog, F. James Holler, Timothy A. Nieman, 6<sup>th</sup> edition, Cengage, 2014.
- 3. Instrumental methods of analysis Willards, 7<sup>th</sup> edition, CBS publisher, 2004.
- 4. Practical Pharmaceutical Chemistry Beckett and Stenlake, Vol II, 4<sup>th</sup> edition, CBS Publishers, New Delhi, 2007.
- 5. Organic Spectroscopy William Kemp, 3<sup>rd</sup> edition, ELBS, 2008.
- 6 Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, 3<sup>rd</sup> edition, CBS Publishers, New Delhi, 2007.
- 7. Pharmaceutical Analysis Modern Methods Part B J W Munson, Vol 11, Marcel, Dekker Series 1984 (Reprint 2012)
- 8 Spectroscopy of Organic Compounds, 6th edn., P. S. Kalsi, Wiley Eastern Ltd., Delhi, 2016.
- 9. Textbook of Pharmaceutical Analysis, KA. Connors, 3<sup>rd</sup> Edition, John Wiley & Sons, 2007.
- 10. Introduction to spectroscopy. 4<sup>th</sup> Edition, Pavia DL, Lampman GM, Kriz GS, Vyvyan JA.; Cengage Learning, 2008
- 11. Pharmaceutical quality by design: a practical approach. Schlindwein WS, Gibson M, editors. John Wiley & Sons; 2018.

Course Title: Advanced Organic Chemistry - I

Paper Code: MPC102T 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: Through understating of the chemistry and mechanism of various named reactions having application in synthetic and medicinal chemistry.

CLO3: Understanding of chemistry and applications of various synthetic reagents including the protecting groups and various organic transformations.

CLO4: Describe nomenclature and synthetic methodologies of heterocyclic systems

CLO5: Describe disconnection approaches applied on synthetic strategies and mechanism prediction

Units/Hours	Content	Mapping with course learning outcomes
Unit 1	Basic Aspects of Organic Chemistry:	CLO1
12 Hours	<ol> <li>Organic intermediates: Carbocations, carbanions, free radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications.</li> <li>Types of reaction mechanisms and methods of determining them,</li> <li>Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations w.r.t addition, substitution, elimination and rearrangement reactions.</li> <li>Chemistry of enolates</li> </ol> Learning activities: Learner will be engaged in molecular models to explain the structure stability and conformation of organic	
	intermediates to explain the stereochemistry in organic transformations and knowledge of reaction mechanisms.	
Unit 2 10 Hours	Study of Mechanism and Synthetic Applications of Following Named Reactions	CLO2

	• Ugi reaction, Brook rearrangement, Ullmann coupling reactions, Dieckmann	
	Reaction, Doebner-Miller Reaction,	
	Sandmeyer Reaction, Mitsunobu reaction,	
	Mannich reaction, Vilsmeyer-Haack	
	Reaction, Sharpless asymmetric	
	epoxidation, Baeyer-Villiger oxidation,	
	Shapiro & Suzuki reaction, Ozonolysis and	
	Michael addition reaction.	
	<b>Learning activities:</b> Learner will be	
	engaged hand on training in some of the	
	named reactions with applications in	
	organic and drug synthesis.	
TT 1/ 0		<b>GT 63</b>
Unit 3	Synthetic Reagents and Applications	CLO3
12 Hours	Aluminiumisopropoxide, N-  hromosupoinamida diagomethana	
	bromosuccinamide, diazomethane, dicyclohexylcarbodimide, Wilkinson reagent,	
	Witting reagent, Osmium tetroxide, titanium	
	chloride, diazopropane, diethyl	
	azodicarboxylate, Triphenylphosphine,	
	Benzotriazol-1-yloxy) tris (dimethylamino)	
	phosphonium hexafluoro-phosphate (BOP)	
	Protecting Groups	
	• Role of protection in organic synthesis	
	• Protection for the hydroxyl group, including	
	1,2-and1,3-diols: ethers, esters, carbonates,	
	<ul><li>cyclic acetals &amp; ketals</li><li>Protection for the Carbonyl Group: Acetal and</li></ul>	
	Ketals	
	Protection for the Carboxyl Group: amides and	
	hydrazides, esters	
	• Protection for the Amino Group and Amino	
	acids: carbamates and amides	
	<b>Learning activities:</b> Learner will be	
	engaged in performing experiments using	
	various the synthetic reagents and	
	protection of various functional groups.	
Unit 4	Heterocyclic chemistry:	CLO4
12 Hours	• Organic Name reactions with their respective	
	mechanism and application involved in	
	synthesis of drugs containing five, six membered	
	and fused hetrocyclics such as Debus	
	Radziszewski imidazole synthesis, Knorr	
	Pyrazole Synthesis, Pinner Pyrimidine	
	Synthesis, Combes Quinoline Synthesis,	

	Bernthsen Acridine Synthesis, Smiles	
	rearrangement and Traube purine synthesis.	
	Synthesis of few representative drugs	
	containing these hetrocyclic nucleus such as	
	Ketoconazole, Metronidazole, Miconazole,	
	celecoxib, antipyrin, Metamizole sodium,	
	Terconazole, Alprazolam, Triamterene,	
	Sulfamerazine, Trimethoprim,	
	Hydroxychloroquine, Quinine, Chloroquine,	
	Quinacrine, Amsacrine, Prochlorpherazine,	
	Promazine, Chlorpromazine, Theophylline ,	
	Mercaptopurine and Thioguanine.	
	Learning activities: Learner will be	
	engaged in performing the synthesis and characterization of some of the	
	representative heterocyclic compounds as	
	well as drugs based on these heterocycles.	
Unit 5	Synthon Approach and Retrosynthesis	CLO5
10		
12 Hours	Applications	
12 Hours	<ul><li>Applications</li><li>Basic principles, terminologies and</li></ul>	
12 Hours		
12 Hours	Basic principles, terminologies and	
12 Hours	Basic principles, terminologies and advantages of retrosynthesis; guidelines for	
12 Hours	Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> <li>C- X disconnections; C- C disconnections -</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> <li>C- X disconnections; C- C disconnections – alcohols and carbonyl compounds; 1,2-, 1,3-</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> <li>C- X disconnections; C- C disconnections – alcohols and carbonyl compounds; 1,2-, 1,3-,1,4-, 1,5-, 1,6- difunctionalized compounds</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> <li>C- X disconnections; C- C disconnections – alcohols and carbonyl compounds; 1,2-, 1,3-,1,4-, 1,5-, 1,6- difunctionalized compounds</li> <li>Strategies for synthesis of three, four, five and</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> <li>C- X disconnections; C- C disconnections – alcohols and carbonyl compounds; 1,2-, 1,3-,1,4-, 1,5-, 1,6- difunctionalized compounds</li> <li>Strategies for synthesis of three, four, five and</li> </ul>	
12 Hours	<ul> <li>Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules</li> <li>Functional group interconversion and addition (FGI and FGA)</li> <li>C- X disconnections; C- C disconnections – alcohols and carbonyl compounds; 1,2-, 1,3-,1,4-, 1,5-, 1,6- difunctionalized compounds</li> <li>Strategies for synthesis of three, four, five and six- membered ring</li> </ul>	

## Suggested Readings:

- 1. Advanced Organic chemistry, Reaction, Mechanisms and Structure. J March, John Wiley and Sons, New York.
- 2. Mechanism and Structure in Organic Chemistry. ES Gould, Hold Rinchart and Winston, New York.
- 3. Organic Chemistry. Clayden, Greeves, Warren and Woihers, Oxford University Press.
- 4. Organic Chemistry Vol I and II. I.L. Finar. ELBS, Pearson Education Lts, Dorling Kindersley India Pvt. Ltd.
- 5. A guide to mechanisms in Organic Chemistry, Peter Skyes (Orient Longman, New Delhi).

- 6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.
- 7. Combinational Chemistry Synthesis and applications Stephen R Wilson & Anthony W Czarnik, Wiley Blackwell.
- 8. Carey, Organic Chemistry, 5th Edition (Viva Books Pvt. Ltd.).
- 9. Organic Synthesis The Disconnection Approach, S. Warren, Wily India.
- 10. Principles of Organic Synthesis, ROC Norman and JM Coxan, NelsonThorns.
- 11. Organic Synthesis- Special Techniques. VK Ahluwalia and R Agarwal, Narosa Publishers.
- 12. Organic Reaction Mechanisms. VK Ahluwalia and RK Parashar, Narosa Publishers

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

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

#### **Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

Course Title: Advanced Medicinal Chemistry

Paper Code: MPC103T 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 drugs interaction with various types of enzymes and receptors

CLO2: Conceptualize the process of drug discovery and its progress

CLO3: Rational design and synthesis of covalent and non-covalent inhibitors as drug candidates in medicinal chemistry

CLO4: Knowledge of peptidomimetic design and understanding of coupling procedures for its synthesis including stereochemical aspects and backbone modification.

Units/Hours	Content	Mapping
		with course
	400	learning
		outcome
Unit 1	Drug Discovery	CLO1
12 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, agonists vs antagonists,	
	artificial enzymes.	
	3	
	<b>Learning activities:</b> Learner will be explained	
	about drug interaction and target through	
	molecular modeling studies	
Unit 2	Prodrug Design and Analog design	CLO2
12 Hours	Prodrug design	
	Basic concept, Carrier linked 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. Rationale of prodrug	
	design 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.		
	<b>Learning activities:</b> Learner will be engaged		
	in learning the methods and concepts used for		
	prodrug design, drug targeting and		
	modification of lead compounds in wet lab as		
	well as using in silico tools to optimize their		
Unit 3	biological and physical properties.	CLO2	
12 Hours	Medicinal chemistry aspects of the following class of drugs	0202	
	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.		
	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.		
	<b>Learning activities:</b> Learner will be engaged in		
	Group discussion to explain SAR, Mechanism of		
	1 1		
	action and given hands on training for the		
Unit 4 12 Hours	action and given hands on training for the	CLO3	
	action and given hands on training for the		

	inhibitors, Enzyme inhibitors in medicine, Enzyme inhibitors in basic research, rational design of non-covalently and covalently binding enzyme inhibitors.		
	<b>Learning activities:</b> Learner will be engaged in performing experiments to determine the enzyme kinetics and <i>in silico</i> design of enzyme inhibitors having applications in medicinal chemistry.		
Unit 5	Peptidomimetics	CLO4	
12 Hours	<ul> <li>Therapeutic values of Peptidomimetics, design of peptidomimetics by manipulation of the amino acids, modification of the peptide backbone, incorporating conformational constraints locally or globally</li> <li>Chemistry of prostaglandins, leukotrienes and thromboxones</li> </ul>		
	<b>Learning activities:</b> Learner will be engaged in in performing coupling experiments, amino acid synthesis, stereochemistry of biomolecules and <i>in silico</i> experiments for design of peptidomimetics.		

## Suggested Readings:

- 1. Medicinal Chemistry by Burger, Vol I -VI.
- 2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt. Ltd, New Delhi.
- 3. Comprehensive Medicinal Chemistry Corwin and Hansch.
- 4. Computational and structural approaches to drug design edited by Robert M Stroud and Janet.

F Moor.

- 5. Introduction to Quantitative Drug Design by Y.C. Martin.
- 6. Principles of Medicinal Chemistry by William Foye, 7th Edition, Lippincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
- 7. Drug Design Volumes by Arienes, Academic Press, Elsevier Publishers, Noida, Uttar Pradesh.
- 8. Principles of Drug Design by Smith.
- 9. The Organic Chemistry of the Drug Design and Drug action by Richard B.Silverman, Elsevier

Publishers, New Delhi.

- 10. An Introduction to Medicinal Chemistry, Graham L.Patrick, Oxford University Press, USA.
- 11. Biopharmaceutics and pharmacokinetics, DM.Brahmankar, Sunil B. Jaiswal, Vallabh Prakashan, New Delhi.
- 12. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, Wiley publishers.

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

- Lecture
- Group discussion
- Demonstration
- Team teaching

## **Transaction Mode**

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



**Course Title: Chemistry of Natural Products** 

Paper Code: MPC104T Course Hours: 60h

L	T	P	Credits
4	0	0	4

## **Learning Outcomes**

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

CLO1: Understand chemistry and structural modifications of natural leads for drug discovery and development

CLO2: Conceptualize the nomenclature, synthesis and structure of alkaloids steroids

CLO3: Describe categories, synthesis and biosynthesis of terpenoids and vitamins

CLO3: Understand and apply modern biotechnological methods, scientific principles and technologies in drug discovery/ hands on participation in laboratory

CLO5: Explain the structural characterization of natural products using advanced spectroscopic techniques

Units/Hours	Content	Mapping with course learning outcome
Unit 1	Study of Natural Products as Leads for New	CLO1
12 Hours	Pharmaceuticals for the Following Class of Drugs	
	• Drugs affecting the Central Nervous System: Morphine Alkaloids	
	• Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide	
	Cardiovascular Drugs: Lovastatin, Teprotide and	
	Dicoumarol	
	<ul><li>Neuromuscular Blocking Drugs: Curare alkaloids</li><li>Anti-malarial drugs and Analogues</li></ul>	
	• Chemistry of macrolid antibiotics (Erythromycin,	
	Azithromycin, Roxithromycin, and Clarithromycin) and	
	β - Lactam antibiotics (Cephalosporins and	
	Carbapenem)	
	Learning activities- Learner will be engaged in	
	understanding principles and methodologies involved in	
TT 11 0	drug discovery and development from natural resources	GT 00
Unit 2 12 Hours	Alkaloids	CLO2
12 Hours	• General introduction, classification, isolation,	
	purification, molecular modification and biological	
	activity of alkaloids	
	General methods of structural determination of	
	alkaloids	10

·		
	Structural elucidation and stereochemistry of	
	ephedrine, morphine, ergot, emetine and reserpine	
	Flavonoids	
	• Introduction, isolation and purification of	
	flavonoids	
	• General methods of structural determination of	
	flavonoids	
	• Structural elucidation of quercetin	
	Steroids	
	General introduction, chemistry of sterols,	
	sapogenin and cardiac glycosides	
	• Stereochemistry and nomenclature of steroids,	
	chemistry of contraceptive agents male & female sex	
	hormones (Testosterone, Estradiol, Progesterone),	
	adrenocorticoids (Cortisone), contraceptive agents	
	and steroids (Vit – D) <b>Learning activities-</b> Learner will be able to explain	
	and perform various chemical tests for the	
	identification of plant alkaloids to explain the	
	structure and stereochemistry of steroids using ball	
	and stick model.	
Unit 3	Terpenoids	CLO3
12 Hours	Classification, isolation, isoprene rule and general	J200
12 110415	methods of structural elucidation of Terpenoids	
	Structural elucidation of drugs belonging to mono	
	(citral, menthol, camphor), di(retinol, Phytol, taxol) and	
	tri terpenoids (Squalene, Ginsenoside) carotinoids (β	
	carotene)	
	Vitamins	
	• Chemistry and Physiological significance of Vitamin A,	
	B1, B2, B12, C, E, Folic acid and Niacin.	
	<b>Learning activities-</b> Learner will be engaged in	
	molecular models to explain the structure and	
	stereochemistry of terpenoids, perform various	
	identification tests to confirm their presence and	
	<u> </u>	
	familiarize with the use of various spectral techniques for l	
	familiarize with the use of various spectral techniques for the structure elucidation of terpenoids based drugs.	
Unit 4	the structure elucidation of terpenoids based drugs.	CLO3
Unit 4 12 Hours	the structure elucidation of terpenoids based drugs. <b>a.</b> Chemistry of Carbohydrates	CLO3
Unit 4 12 Hours	the structure elucidation of terpenoids based drugs.  a. Chemistry of Carbohydrates Introduction, classification, configuration and	CLO3
	the structure elucidation of terpenoids based drugs.  a. Chemistry of Carbohydrates  Introduction, classification, configuration and conformation, reactions of monosaccharides;	CLO3
	the structure elucidation of terpenoids based drugs.  a. Chemistry of Carbohydrates  Introduction, classification, configuration and conformation, reactions of monosaccharides; oxidation, reduction, osazone formation, chain	CLO3
	the structure elucidation of terpenoids based drugs.  a. Chemistry of Carbohydrates  Introduction, classification, configuration and conformation, reactions of monosaccharides; oxidation, reduction, osazone formation, chain shortening and chain lengthening, mutarotation.	CLO3
	the structure elucidation of terpenoids based drugs.  a. 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	CLO3
	the structure elucidation of terpenoids based drugs.  a. 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  b. Active Constituent of Certain Crude Drugs Used in	CLO3
	the structure elucidation of terpenoids based drugs.  a. 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 b. Active Constituent of Certain Crude Drugs Used in Indigenous System	CLO3
	the structure elucidation of terpenoids based drugs.  a. 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  b. Active Constituent of Certain Crude Drugs Used in Indigenous System  • Diabetic Therapy: Gymnema sylvestre, Salacia	CLO3
	a. 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 b. Active Constituent of Certain Crude Drugs Used in Indigenous System  • Diabetic Therapy: Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata,	CLO3
	<ul> <li>the structure elucidation of terpenoids based drugs.</li> <li>a. 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         b. Active Constituent of Certain Crude Drugs Used in Indigenous System         Diabetic Therapy: Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum     </li> </ul>	CLO3
	the structure elucidation of terpenoids based drugs.  a. 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 b. Active Constituent of Certain Crude Drugs Used in Indigenous System  • Diabetic Therapy: Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum  • Liver dysfunction: Phyllanthus niruri	CLO3
	a. 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 b. Active Constituent of Certain Crude Drugs Used in Indigenous System  • Diabetic Therapy: Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum  • Liver dysfunction: Phyllanthus niruri  • Antitumor: Curcuma longa Linn.	CLO3
	the structure elucidation of terpenoids based drugs.  a. 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 b. Active Constituent of Certain Crude Drugs Used in Indigenous System  • Diabetic Therapy: Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum  • Liver dysfunction: Phyllanthus niruri	<b>CLO3</b>

	performing and handling various techniques/ experiments used in the isolation of active constituents of crude drugs including their characterization. Perform various experiments for the synthesis and functional group analysis in sugars including their stereochemical aspects.		
Unit 5	Structural Characterization of Natural Compounds CLO5		
12 Hours	• Structural characterization of natural compounds using IR, 1HNMR, 13CNMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides.  Learning activities: Learner will be provided spectral data for the identification of above-mentioned natural compounds		

### Suggested Readings

- 1. Modern Methods of Plant Analysis, Peech and M.V.Tracey, Springer –Verlag, Berlin, Heidelberg.
- 2. Phytochemistry Vol. I and II by Miller, Jan Nostrant Rein Hld.
- 3. Recent advances in Phytochemistry Vol. I to IV Scikel Runeckles, Springer Science & Business Media.
- 4. Chemistry of natural products Vol I onwards IWPAC.
- 5. Natural Product Chemistry Nakanishi Gggolo, University Science Books, California.
- 6. Natural Product Chemistry "A laboratory guide" Rapheal Khan.
- 7. The Alkaloid Chemistry and Physiology by RHF Manske, Academic Press.
- 8. Introduction to molecular Phytochemistry CHJ Wells, Chapmannstall.
- 9. Organic Chemistry of Natural Products Vol I and II by Gurdeep and Chatwall, Himalaya Publishing House.
- 10. Organic Chemistry of Natural Products Vol I and II by O.P. Agarwal, Krishan Prakashan.
- 11. Organic Chemistry Vol I and II by I.L. Finar, Pearson education.
- 12. Elements of Biotechnology by P.K. Gupta, Rastogi Publishers.
- 13. Pharmaceutical Biotechnology by S.P.Vyas and V.K.Dixit, CBS Publishers.
- 14. Biotechnology by Purohit and Mathur, Agro-Bios.
- 15. Phytochemical methods of Harborne, Springer, Netherlands.
- 16. Burger's Medicinal Chemistry.

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

- Lecture
- Group discussion
- Demonstration
- Tutorial

#### **Transaction Mode**

- PPT
- YouTube
- Google meet

Course Title: Organic Synthesis -I (Practical)

L	T	P	Credits
0	0	12	6

Paper Code: CMC 507 Course Hours: 60h

### **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 with course learning outcome	1
1.	Analysis of Pharmacopoeial compounds and their formulations by UV Vis spectrophotometer, RNA & DNA estimation	CLO1	
2.	Simultaneous estimation of multi component containing formulations by UV spectrophotometry	CLO1	
3.	Experiments based on Column chromatography	CLO2	
4.	Experiments based on HPLC	CLO3	
5.	Experiments based on Gas Chromatography	CLO4	
6.	Estimation of riboflavin/quinine sulphate by fluorimetry		
7.	Estimation of sodium/potassium by flame photometry	CLO4	
8.	8. To perform the following reactions of synthetic importance: a. Purification of organic solvents, column chromatography b. Claisen-schimidt reaction c. Benzyllic acid rearrangement d. Beckmann rearrangement e. Hoffmann rearrangement f. Mannich reaction g. Synthesis of medicinally important compounds involving more than one step along with purification and Characterization using TLC, melting point and IR spectroscopy (4 experiments) h. Estimation of elements and functional groups in organic natural compounds	CLO4	

n	Isolation, characterization like melting point, mixed nelting point, molecular weight etermination, functional group analysis, co-
cl ic	hromatographic technique for dentification of isolated compounds and description of UV and IR data.
j.	Some typical degradation reactions to be carried on elected plant constituents

### 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

#### **Transaction Mode**

- PPT
- YouTube
- Google drive
- Google meet

Course Title: Seminar/Assignment

Paper Code: MPC106S

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	L	T	P	Credits	Marks
	0	0	0	4	100

**Learning outcome:** Students who successfully complete this course will be able to

- Perform literature review on a given topic
- Prepare a report on a given topic
- Prepare a power point presentation on a given topic

### **Evaluation criteria:**

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

#### Semester -II

Course Title: Advanced Spectral Analysis

Paper Code: MPC201T Course Hours: 60hr

L	T	P	Credits
4	0	0	4

### **Learning Outcomes**

After completion of the course, student shall be able to understand:

CLO1: Conceptualize general principle and theory of UV-Vis, 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 with application of Raman spectroscopy and radio immunoassay

Units/Hours	Content	Mapping with		
		course		
		learning		
Unit 1	UV and IR spectroscopy:	CLO1		
12 Hours	Wood ward – Fieser rule for 1,3- butadienes, cyclic			
	dienes and α, β-carbonyl compounds and			
	interpretation compounds of enones.			
	ATR-IR, IR Interpretation of organic compounds			
	Learning activities: Learner will be provided			
	hands on training to different instruments like			
	UV, IR and spectroflourimetry.	GT 00		
Unit 2	NMR Spectroscopy: 1-D and 2-D NMR, NOESY and	CLO2		
11 Hours	COSY, HECTOR, INADEQUATE techniques,			
	Interpretation of organic compounds			
	Learning activities: Learner will be provided			
Unit 3	NMR for the characterization of compounds.	CLO2		
10 Hours	Mass Spectroscopy: Mass fragmentation and its	CLOZ		
10 Hours	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.			
	compositio.			
	<b>Learning activities:</b> Learner will be provided Mass			
	spectra for the characterization of compounds.			
Unit 4	Chromatography:	CLO3		
12 Hours	Principle, Instrumentation and Applications of the			

	following:	
	• GC-MS	
	• GC-AAS	
	• LC-FTIR	
	• LC-NMR	
	• CE-MS	
	High Performance Thin Layer chromatography	
	Super critical fluid chromatography	
	• Ion Chromatography	
	• I-EC (Ion- Exclusion Chromatography)	
	• Flash chromatography	
	Learning activities: Learner will be provided	
	experience of chromatography by using different	
	techniques like TLC, Column, HPLC, HPTLC and GC.	
Unit 5	-	CLO4
12 Hours	spectroscopic techniques using like UV, IR, Mass,	CLO4
12 110015	NMR ( <sup>1</sup> H and <sup>13</sup> C)	
	a. Carvove, Citral, Menthol	
	b. Luteolin, Kaempferol	
	c. Nicotine, Caffeine	
	d. Glycyrrhizin	
	Learning activities: Learner will be provided	
	spectral data of various natural and synthetic	
	compounds for their characterization and structure	
	elucidation using various spectroscopic techniques.	

#### **REFERENCES:**

- 1. Spectrometric Identification of Organic compounds Robert M Silverstein, John Wiley & Sons.
- 2. Principles of Instrumental Analysis Doglas A Skoog, F. James Holler, Timothy A. Nieman, Eastern press, Bangalore.
- 3. Instrumental methods of analysis Willards, CBS publishers.
- 4. Organic Spectroscopy William Kemp, ELBS.
- 5. Quantitative analysis of Pharmaceutical formulations by HPTLC P D Sethi, CBS Publishers, New Delhi.
- 6. Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, CBS Publishers, New Delhi.
- 7. Pharmaceutical Analysis- Modern methods Part B J W Munson, Volume 11, Marcel Dekker Series

Course Title: Advanced Organic Chemistry-II

Paper Code: MPC 202T Course Hours: 60h

 L
 T
 P
 Credits

 4
 0
 4
 4

## **Learning Outcomes**

After completing this course, the student shall able to understand:

CLO1: The principles and applications of green chemistry.

CLO2: The concept of peptide chemistry.

CLO3: Apply principles of photochemistry and pericyclic reactions in various chemical transformations

CLO4: The various catalysts used in organic reactions.

CLO5: Describe the asymmetric synthesis, chiral resolution and apply it on the resolution of chiral drugs.

Unit/Hours	Content	Mapping with course learning outcome
Unit 1	Green Chemistry:	CLO1
12 Hours	<ul> <li>a. Introduction, principles of green chemistry</li> <li>b. Microwave assisted reactions: merits and demerits of its use, increased reaction rates, mechanism, superheating effects of microwave, effects of solvents in microwave assisted synthesis, microwave technology in process optimization, its applications in various organic reactions and heterocyclic synthesis.</li> <li>c. Ultrasound assisted reactions: types of sonochemical reactions, homogenous, heterogeneous liquid-liquid and liquid-solid reactions, synthetic application</li> <li>d. Continuous flow reactors: working principle, advantages and synthetic applications.</li> <li>Learning activities: Learner will be engaged in practical's using greener synthetic routes such as microwave assisted synthesis and ultrasound and sonication assisted reactions for the synthesis of various</li> </ul>	
	key intermediates and drug molecules.	
Unit-2	Chemistry of peptides:	CLO2
12 Hours	a) Coupling reactions in peptide synthesis	

	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	Photochemical reactions	CLO3		
12 Hours	<ul> <li>Basic principles of photochemical reactions.</li> </ul>			
	Pericyclic reactions			
	Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and Sigmatrophic rearrangement reactions with examples			
	<b>Learning activities:</b> Learner will be engaged in solving exercises related to the mechanism of photochemical and pericyclic chemistry including rearrangements reactions in these with suitable examples and their applications in organic and medicinal chemistry.			
Unit-4 12	Catalysis:			
Hours	a) Types of catalysis, heterogeneous and homogenous catalysis, advantages and disadvantages			
	b) Heterogeneous catalysis-preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs			
	c) Homogenous catalysis, hydrogenation, hydroformylation, hydrocyanation,			

	Wilkinson catalysts, chiral ligands and chiral induction, Ziegler- Natta catalysts, some examples of homogenous catalysis used in synthesis of drugs	
	d) Transition-metal and Organo-catalysis in organic synthesis: Metal-catalyzed reactions	
	e) Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction	
	f) Phase transfer catalysis - theory and applications	
	<b>Learning activities:</b> Learner will be familiarize with the science of catalysis, their synthetic applications in various key organic transformations and will be engaged in hand-on synthesis using various catalysts/phase transfer catalyst in some important organic transformations of organic and medicinal interests.	
	1	
Unit-5	Stereochemistry and Asymmetric Synthesis	CLO5
Unit-5 12 Hours	Stereochemistry and Asymmetric Synthesis  a) Basic concepts in stereochemistry – optical activity, specific rotation, racemates and resolution of racemates, the Cahn, Ingold, Prelog (CIP) sequence rule, meso compounds, pseudo asymmetric centres, axes of symmetry, Fischers D and L notation, cis-trans isomerism, E and Z notation.	CLO5
	a) Basic concepts in stereochemistry – optical activity, specific rotation, racemates and resolution of racemates, the Cahn, Ingold, Prelog (CIP) sequence rule, meso compounds, pseudo asymmetric centres, axes of symmetry, Fischers D and L notation, cis-trans isomerism, E and Z	CLO5

#### **REFERENCES:**

- 1. Advanced Organic chemistry, Reaction, mechanisms and structure, J March, John Wiley and sons, New York.
- 2. Mechanism and structure in organic chemistry, ES Gould, Hold Rinchart and Winston, NewYork.
- 3. Organic Chemistry Clayden, Greeves, Warren and Woihers., Oxford University Press.

- 4. Organic Chemistry" Vol I and II. I.L. Finar. ELBS.
- 5. Carey, Organic chemistry, Viva Books Pvt. Ltd.
- 6. Organic synthesis-the disconnection approach, S. Warren, Wily India.
- 7. Principles of organic synthesis, ROC Norman and JM Coxan, Nelson Thorns.
- 8. Organic synthesis- Special techniques VK Ahluwalia and R Aggarwal, Narosa Publishers.
- 9. Organic reaction mechanisms IV edtn, VK Ahluwalia and RK Parashar, Narosa Publishers

Course Title: Fundamentals of Computer Aided

**Drug Design** 

Paper Code: MPC203T Course Hours: 60h

T P Credits 0 4

## Learning outcome:

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

CLO1: Describe the role of CADD in drug discovery

CLO2: Different CADD techniques and their applications.

CLO3: Various strategies to design and develop new drug like molecules.

CLO4: Working with molecular modeling software to design new drug molecules.

		with course learning outcome
Unit 1 12 Hours	Introduction to Computer Aided Drug Design (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, pi-substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physiochemical parameters.  Learning activities: Learner will be engaged in group discussion to explain 2D-QSAR, 3D-QSAR and importance of statistical parameters.	CLO1
Unit 2	importance of statistical parameters  Quantitative structure Activity Relationships:	CLO1
12 Hours	Applications 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.	
	<b>Learning activities:</b> Learner will be engaged in group discussion to explain 2D-QSAR, 3D-QSAR and importance of statistical parameter	
Unit 3 12 Hours	Molecular Modeling and Docking:  a) Molecular and Quantum Mechanics in drug design. 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	CLO2

	doolsing Agents acting on engames such as DUED						
	docking. Agents acting on enzymes such as DHFR,						
	HMG-CoA reductase and HIV protease, choline esterase						
	(AchE & BchE)						
	<b>Learning activities:</b> Learner will be engaged in						
	molecular modeling of compounds.						
Unit 4	Molecular Properties and Drug Design:	CLO3					
12 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.						
	Learning activities: Learner will study Molecular						
	model to explain interactions between ligand and						
	drug target						
Unit 5							
	Pharmacophore Mapping and Virtual Screening:	CLO2, CLO3					
12 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.						
	Learning activities: Learner will be engaged in						
	Pharmacophore band structure based <i>In-silico</i> virtual						
	screening protocols						

#### **REFERENCES:**

- 1. Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers.
- 2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor & Francis group.
- 3. Drug Design by Ariens Volume 1 to 10, Academic Press, Elsevier Publishers.
- 4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.
- 5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
- 6. Medicinal Chemistry by Burger, Wiley Publishing Co.
- 7. An Introduction to Medicinal Chemistry Graham L. Patrick, Oxford University Press.
- 8. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.
- 9. Comprehensive Medicinal Chemistry Corwin and Hansch, Pergamon Publishers.
- 10. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore.

**Course Title: Process Chemistry** 

Paper Code: MPC204T Course Hours: 60h

L	T	P	Credits
4	0	0	4

## Learning outcome:

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

CLO1: The strategies of scale up process of APIs and intermediate

CLO2: The various unit operations and various reactions in process chemistry

CLO3: Study the MSDS of hazardous chemicals

Units/Hours	Content	Mapping with course learning outcome
Unit 1 12 Hours	Process chemistry Introduction, Synthetic strategy, Stages of scale up process: Bench, pilot and large-scale process. Inprocess control and validation of large-scale process. Case studies of some scale up process of APIs. Impurities in API, types and their sources including genotoxic impurities  Learning activities: Learner will be provided	CLO1
Unit 2 12 Hours	Unit operations  Extraction: Liquid equilibria, extraction with reflux, extraction with agitation, counter current extraction.  Filtration: Theory of filtration, pressure and vacuum filtration, centrifugal filtration,  Distillation: azeotropic and steam distillation  Evaporation: Types of evaporators, factors affecting evaporation.  Crystallization: Crystallization from aqueous, non-aqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphous APIs.  Learning activities: Learner will be engaged in group discussion to understand Extraction, filtration, distillation, evaporation and crystallization processes	CLO2
Unit 3 12 Hours	Unit process- II Reduction Catalytic hydrogenation, Heterogeneous and homogeneous catalyst; Hydrogen transfer reactions, Metal hydrides Case study on industrial reduction process	CLO2

	Fermentation	
Unit 4 12 Hours	Unit Processes - III Reduction: Catalytic hydrogenation, Heterogeneous and homogeneous catalyst; Hydrogen transfer reactions, Metal hydrides. Case study on industrial reduction process. Fermentation: Aerobic and anaerobic fermentation. Production of Antibiotics; Penicillin and Streptomycin, Vitamins: B2 and B12 Statins: Lovastatin, Simvastatin Reaction progress kinetic analysis Streamlining reaction steps, route selection, Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up. Learning activities: Learner will be engaged in group discussion to understand unit processes for reduction, fermentation and reaction progress kinetic analysis	CLO2
Unit 5 12 Hours	Industrial Safety MSDS (Material Safety Data Sheet), hazard labels of chemicals and Personal Protection Equipment (PPE) Fire hazards, types of fire & fire extinguishers Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001(Environmental Management System), Effluents and its management  Learning activities: Learner will be provided Awareness about industrial safety protocols	CLO3

#### REFERENCES:

- 1. Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview; K. Gadamasetti, CRC Press.
- 2. Pharmaceutical Manufacturing Encyclopedia, 3rd edition, Volume 2.
- 3. Medicinal Chemistry by Burger, 6th edition, Volume 1-8.
- 4. W.L. McCabe, J.C Smith, Peter Harriott. Unit operations of chemical engineering, 7th edition, McGraw Hill
- 5. Polymorphism in Pharmaceutical Solids. Dekker Series Volume 95 Ed: H G Brittain (1999)
- 6. Regina M. Murphy: Introduction to Chemical Processes: Principles, Analysis, Synthesis
- 7. Peter J. Harrington: Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale-Up
- 8. P.H.Groggins: Unit processes in organic synthesis (MGH)
- 9. F.A.Henglein: Chemical Technology (Pergamon)
- 10.M.Gopal: Dryden's Outlines of Chemical Technology, WEP East-West Press
- 11. Clausen, Mattson: Principle of Industrial Chemistry, Wiley Publishing Co.,
- 12. Lowenheim & M.K. Moran: Industrial Chemicals
- 13.S.D. Shukla & G.N. Pandey: A text book of Chemical Technology Vol. II, Vikas Publishing House
- 14.J.K. Stille: Industrial Organic Chemistry (PH)
- 15. Shreve: Chemical Process, Mc Grawhill.
- 16.B.K.Sharma: Industrial Chemistry, Goel Publishing House
- 17.ICH Guidelines
- 18. United States Food and Drug Administration official website www.fda.gov

Course code	Course Title	Credits
MPC205P	Pharmaceutical	6
	Chemistry Practical- II	

- 1. Synthesis of organic compounds by adapting different approaches involving (3experiments) a) Oxidation
- b) Reduction/hydrogenation

#### c) Nitration

- 2. Comparative study of synthesis of APIs/intermediates by different synthetic routes (2 experiments)
- 3. Assignments on regulatory requirements in API (2 experiments) of absorption spectra by UV and Wood ward Fieser rule
- 4. Interpretation of organic compounds by FT-IR
- 5. Interpretation of organic compounds by NMR
- 6. Interpretation of organic compounds by MS
- 7. Determination of purity by DSC in pharmaceuticals
- 8. Identification of organic compounds using FT-IR, NMR, CNMR and Mass spectra
- 9. To carry out the preparation of following organic compounds
- 10. Preparation of 4-chlorobenzhydrylpiperazine (an intermediate for cetirizine HCl)
- 11. Preparation of 4-iodotolene from p-toluidine
- 12. NaBH4 reduction of vanillin to vanillyl alcohol
- 13. Preparation of umbelliferone by Pechhman reaction
- 14. Preparation of triphenyl imidazole
- 15. To perform the Microwave irradiated reactions of synthetic importance (Any two)
- 16. Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- 17. Calculation of ADMET properties of drug molecules and its analysis using softwares
- 18. Pharmacophore modelling
- 19. 2D-QSAR based experiments
- 20. 3D-QSAR based experiments
- 21. Docking study based experiment
- 22. Virtual screening based experiment

- PPT
- YouTube
- Google driveGoogle meet

Course Title: Seminar/Assignment

Paper Code: MPC106S

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	L	T	P	Credits	Marks
	0	0	0	4	100

**Learning outcome:** Students who successfully complete this course will be able to

- Perform literature review on a given topic
- Prepare a report on a given topic
- Prepare a power point presentation on a given topic

## Evaluation criteria:

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

## Semester III

Course Title: Research Methodology & Biostatistics

Paper Code: MRM301T Course Hours: 60h

5	L	T	P	Credits
	4	0	0	4

## **Learning Outcomes:**

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

CLO1: Define an appropriate research problem

CLO2: Understand and interpret commonly reported statistical measures and analysis of different types of data using statistical software's

CLO3: Develop skills for scholarly investigations, pursuit of discovery including principles in research in clinical practice

CLO4: To understand and promote the care of animals in biomedical/behavioral and breeding of animals for this purpose

CLO5: To understand principles and history of human care in medical research

Units/Hours	Content	Mapping with course learning outcome
Unit 1 12 Hours	General Research Methodology: Research, objective, requirements, practical difficulties, review of literature, study design, types of studies. Strategies to eliminate errors/bias, controls, randomization, crossover design, placebo, blinding techniques.  Learning activities: Learner will be engaged in literature search and study design	CLO1, CLO2
Unit 2 12 Hours	Biostatistics: Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, type of significance tests, parametric tests (students "t" test, ANOVA, Correlation coefficient, regression), non-parametric tests (wilcoxan rank tests, analysis of variance, correlation, chi square test), null hypothesis, P values, degree of freedom, interpretation of P values.  Learning activities: Learner will be engaged in Web based learning to explain concepts of biostatics in research problem and analysis of different type of statistical data	CLO2
Unit 3 12 Hours	<ul><li>Medical Research</li><li>History, values in medical ethics, autonomy,</li></ul>	CLO3

	beneficence, non-maleficence, double effect, conflicts between autonomy and beneficence/non-maleficence, euthanasia, informed consent, confidentiality, criticisms of orthodox medical ethics, importance of communication, control resolution, guidelines, ethics committees, cultural concerns, truth telling, online business practices, conflicts of interest, referral, vendor relationships, treatment of family members, sexual relationships, fatality  Learning activities: Learner will be engaged to get familiarize with terms related to medical research and ethics in medical research	
Unit 4 12 Hours	CDCSEA Cuidolines for Loborotomy Animal Escility	CLO4
	CPCSEA Guidelines for Laboratory Animal Facility	
	• Goals, veterinary care, quarantine, surveillance,	
	diagnosis, treatment and control of disease, personal hygiene, location of animal facilities to laboratories,	
	anesthesia, euthanasia, physical facilities,	
	environment, animal husbandry, record keeping,	
	SOPs, personnel and training, transport of lab animals	
	Learning activities: Learner will be engaged to	
	develop a comprehensive understanding of ethical	
	and practical consideration in care and use of animal in research settings.	
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Unit 5 12 Hours	Declaration of Helsinki	CLO5
12 110015	History, introduction, basic principles for all	
	medical research, and additional principles for medical research combined with medical care	
	Learning activities: Learner will be engaged in	
	understanding profound history and principles	
	applicable to medical research	

### Suggested Readings:

- 1. Gupta, S. (2005). Research methodology and statistical techniques, Deep & Deep Publications (p) Ltd. New Delhi.
- 2. Kothari, C. R. (2008.) *Research Methodology(s)*, New Age International (p) Limited.New Delhi
- 3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
- 4. Safe Science: Promoting a Culture of Safety in Academic Chemical Research; National Academic Press, <u>www.nap.edu</u>.
- 5. Creswell, D., & Creswell, J. W. (2017). Research Design: Qualitative, Quantitative, and Mixed Methods Approaches.

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

- Lecture
- Group discussion
- Demonstration

## **Transaction Mode**

- PPT
- YouTube
- Google drive

Course Title: Journal Club

Paper Code: MPC302T

L	T	P	Credits	Marks
0	0	0	1	25

Course Title: Discussion/ Presentation

(Proposal Presentation)

Paper Code: MPC303T

L	Т	P	Credits	Marks
0	0	0	2	50

Course Title: Research Work

Paper Code: MPC599

L	T	P	Credits	Marks
0	0	0	14	350

**Learning outcome:** Students who successfully complete this course will be able to

- Design a research problem and prepare synopsis
- Plan and execute experiments in the laboratory
- Interpret and analyze the results

#### Evaluation criteria:

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

## **Semester IV**

Course Title: Journal Club

Paper Code: MPC401T

L	T	P	Credits	Marks
0	0	0	1	25

Course Title: Discussion/ Presentation

Paper Code: MPC402T

L	T	P	Credits	Marks
0	0	0	3	75

Course Title: Research Work, Thesis and viva-voce

Paper Code: MPC599

L	T	P	Credit s	Marks
0	0	0	16	400

**Learning outcome:** Students who successfully complete this course will be able to

- Design a research problem and prepare synopsis
- Plan and execute experiments in the laboratory
- Interpret and analyze the results

#### **Evaluation criteria:**

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Thesis evaluation
- Viva-voce

## The following are some of the classroom transactional modes

- 1. Lecture
- 2. Demonstration
- 3. Lecture cum demonstration
- 4. Project method
- 5. Seminar
- 6. Group Discussion
- 7. Focused group discussion
- 8. Team teaching
- 9. Experimentation
- 10. Tutorial
- 11. Problem solving
- 12. Self-learning

## The following tools can be used in different transactional modes:

- $\bullet$  PPT
- Facebook
- WhatsApp
- Video
- Multimedia packages
- •TED Talks
- •google drive