DEPARTMENT OF PHARMACY GURU GHASIDAS VISHWAVIDYALAYA, BILASPUR (C.G.) (A CENTRAL UNIVERSITY)

M.PHARM. (PHARMACEUTICAL CHEMISTRY) (W.E.F. SESSION 2020-21)

Course of study for M. Pharm. (Pharmaceutical Chemistry)

Course	Course	Credit	Credit	Hrs./w k	Marks
Code	Course	Hours	Points		111611115
		Semester			
MPC101T	Modern	4	4	4	100
	Pharmaceutical	-	-		
	Analytical Techniques				
MPC102T	Advanced Organic	4	4	4	100
	Chemistry – I				
MPC103T	Advanced Medicinal	4	4	4	100
	chemistry				
MPC104T	Chemistry of Natural	4	4	4	100
	Product				
MPC105P	Pharmaceutical	12	6	12	150
	Chemistry Practical I				
-	Seminar/Assignment	7	4	7	100
	Total	35	26	35	650
		Semester	II		
1 ED C201 E				1 4	100
MPC201T	Advanced Spectral Analysis	4	4	4	100
MPC202T	Advanced Organic	4	4	4	100
	Chemistry –II				
MPC203T	Computer Aided Drug	4	4	4	100
MPC204T	Design Pharmaceutical	4	4	4	100
MFC2041		4	4	4	100
MPC205P	Process Chemistry Pharmaceutical	12	6	12	150
WII C203F	Chemistry Practical II	12	U	12	150
	Seminar/Assignment	7	4	7	100
	Total	35	26	35	650
	Total	33	20	33	0.50

Schemes for internal assessments and end semester examinations (Pharmaceutical Chemistry-MPC)

Course	Course			ssessment	<u> </u>	End	Semester	Total
	Course	111	iternai A	ssessmem				
Code				1.5	.		xams	Marks
		Continu		al Exams	Total	Marks	Duration	
		ous	Marks	Duration				
		Mode						
			emester	1	T	T	1	1
MPC101T	Modern Pharmaceutical	10	15	1 Hr	25	75	3 Hrs	100
	Analytical Techniques							
MPC102T	Advanced Organic	10	15	1 Hr	25	75	3 Hrs	100
	Chemistry – I							
MPC103T	Advanced Medicinal	10	15	1 Hr	25	75	3 Hrs	100
	chemistry							
MPC104T	Chemistry of Natural	10	15	1 Hr	25	75	3 Hrs	100
	Product							
MPC105P	Pharmaceutical	20	30	6 Hrs	50	100	6 Hrs	150
	Chemistry Practical I							
-	Seminar/Assignment	_	-	-	-	-	-	100
			•			•	Total	650
		Se	mester l	Ι				
MPC201T	Advanced Spectral	10	15	1 Hr	25	75	3 Hrs	100
	Analysis							
MPC202T	Advanced Organic	10	15	1 Hr	25	75	3 Hrs	100
	Chemistry –II							
MPC203T	Computer Aided Drug	10	15	1 Hr	25	75	3 Hrs	100
	Design							
MPC204T	Pharmaceutical Process	10	15	1 Hr	25	75	3 Hrs	100
	Chemistry							
MPC205P	Pharmaceutical	20	30	6 Hrs	50	100	6 Hrs	150
	Chemistry Practical II							
_	Seminar/Assignment	_	_	_	_	_	_	100
	Somman, 1 1001 Similarit		1		l	I	Total	650
							1 Otal	050

Course of study for M. Pharm. III Semester (Common for All Specializations)

Course Code	Course	Credit Hours	Credit Points
MRM 301T	Research	4	4
	Methodology and		
	Biostatistics*		
-	Journal club	1	1
-	Discussion /	2	2
	Presentation (Proposal		
	Presentation)		
-	Research Work	28	14
	Total	35	21

^{*}Non University Examination

Course of study for M. Pharm. IV Semester (Common for All Specializations)

Course Code	Course	Credit Hours	Credit Points
-	Journal club	1	1
-	Research Work	31	16
-	Discussion / Final	3	3
	Presentation		
	Total	35	20

Semester wise credits distribution

Semester	Credit Points
I	26
II	26
III	21
IV	20
Co-curricular Activities (Attending	Minimum=02
Conference, Scientific Presentations and	Maximum=07*
Other Scholarly Activities)	
Total Credit Points	Minimum=95
	Maximum=100*

 $[*]Credit\ Points\ for\ Co-curricular\ Activities$

Schemes for internal assessments and end semester examinations (Semester III & IV)

Course Code	Course	In	ternal A	ssessment		Semester kams	Total Marks	
		Continu	Session	al Exams	Total	Marks	Duration	
		ous	Marks	Duration				
		Mode						
		Se	mester I	II				
MRM30	Research Methodology	10	15	1 Hr	25	75	3 Hrs	100
1T	and Biostatistics*							
-	Journal club	-	-	-	25	-	-	25
-	Discussion /	-	-	-	50	-	-	50
	Presentation (Proposal							
	Presentation)							
-	Research work*	-	-	-	-	350	1 hr	350
	<u> </u>						Total	525
		Se	mester I	V				
_	Journal club -		-	-	25	-	-	25
_	Discussion / -		-	-	50	-	-	50
	Presentation							
	(Proposal							
	Presentation)							
-	Research work and -		-	-	-	400	1 hr	400
	Colloquium							
	<u>-</u>		•		•		Total	475

^{*}Non University Examination

M. PHARM. (Pharmaceutical Chemistry)

Programme Outcomes

Postgraduate students will be able to:

- **PO1: Fundamentals on advanced analytical instrumental techniques:** UV-Visible, IR, Spectro-flourimetry, Flame emission and Atomic absorption spectroscopy, NMR spectroscopy, Mass Spectroscopy, Chromatography, Electrophoresis and Immunological assays methods.
- **PO2:** Knowledge about advances in organic chemistry: retrosynthesis, Organic intermediates, Nucleophilic reaction, electrophilic reactions, green chemistry, Peptide Chemistry, stereochemistry and asymmetric synthesis.
- **PO3:** Study of mechanism and synthetic applications OF compounds: Ugi reaction, Brook rearrangement, Ullmann coupling reactions, Ozonolysis and Michael addition reaction, Synthetic Reagents & Applications, Wilkinson reagent, Witting reagent. Osmium tetroxide, Benzotriazol-1-yloxy) tris (dimethylamino) phosphonium hexafluoro-phosphate (BOP).
- **PO4:** Advances in the field of medicinal chemistry: drug discovery, lead discovery; identification, validation of drug targets, Receptors, artificial enzymes, Prodrug Design and Analog design, Stereochemistry and Drug action, Rational Design of Enzyme Inhibitors, Peptidomimetics.
- **PO5:** Advanced knowledge and skills of pharmaceutical industries: Stages of scale up process, Impurities in API, Unit operation Extraction, Distillation, Filteration, evaporation, crystallization, Unit process Nitration, Halogenation, oxidation, Reduction, Fermentation, Industrial safety, OHSAS 1800, ISO 14001.
- **PO6:** Advanced knowledge about chemistry of medicinal compounds from natural origin: Drugs Affecting the Central Nervous System, Anticancer Drugs, Cardiovascular Drugs Neuromuscular Blocking Drugs, Anti-malarial drugs, Alkaloids, flavonoids, steroids, terpenoids, vitamins, Structural Characterization of natural compounds.
- **PO7:** Advanced knowledge about computer assisted drug design: CADD in drug discovery, Quantitative Structure Activity Relationships, Molecular Modeling and Docking, Pharmacophore Mapping and Virtual Screening, In Silico Drug Design and Virtual Screening Techniques.
- **PO8:** Knowledge about Research Methodology & Biostatistics: review of literature, strategies to eliminate errors/bias, values in medical ethics, CPCSEA guidelines for laboratory animal facility, Declaration of Helsinki.

First Semester

MODERN PHARMACEUTICAL ANALYTICAL TECHENIQUES (MPC 101T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC101T	3	1	-	4 hours	25	75	100	4

Scope

This subject deals with various advanced analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are NMR, Mass spectrometer, IR, HPLC, GC etc.

Objectives

After completion of course student is able to know, Chemicals and Excipients

- The analysis of various drugs in single and combination dosage forms
- Theoretical and practical skills of the instruments

THEORY 60 Hrs

- a. UV-Visible spectroscopy: Introduction, Theory, Laws, 10
 Instrumentation associated with UV-Visible spectroscopy, Choice Hrs
 of solvents and solvent effect and Applications of UV-Visible
 spectroscopy, Difference/ Derivative spectroscopy.
 - 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.
 - c. Spectroflourimetry: Theory of Fluorescence, Factors affecting fluorescence (Characteristics of drugs that can be analysed by flourimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.
 - d. Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.
- 2 NMR spectroscopy: Quantum numbers and their role in NMR, 10 Principle, Instrumentation, Solvent requirement in NMR, Hrs Relaxation process. NMR signals in various compounds, shift. Chemical shift, **Factors** influencing chemical Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and 13C NMR. Applications of NMR spectroscopy.
- 3 Mass Spectroscopy: Principle, Theory, Instrumentation of Mass 10

Spectroscopy, Different types of ionization like electron impact, Hrs 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.

- 4 Chromatography: Principle, apparatus, instrumentation, 10 chromatographic parameters, factors affecting resolution, isolation Hrs of drug from excipients, data interpretation and applications of the following:
 - a) Thin Layer chromatography
 - b) High Performance Thin Layer Chromatography
 - c) Ion exchange chromatography
 - d) Column chromatography
 - e) Gas chromatography
 - f) High Performance Liquid chromatography
 - g) Ultra High-Performance Liquid chromatography
 - h) Affinity chromatography
 - i) Gel Chromatography
- 5 a. Electrophoresis: Principle, Instrumentation, Working 10 conditions, factors affecting separation and applications of the Hrs following:
 - a) Paper electrophoresis b) Gel electrophoresis c) Capillary electrophoresis d) Zone electrophoresis e) Moving boundary electrophoresis f) Iso electric focusing
 - b. X-ray Crystallography: Production of X rays, Different X ray methods, Bragg's law, Rotating crystal technique, X ray powder technique, Types of crystals and applications of X-ray diffraction.
- a. Potentiometry: Principle, working, Ion selective Electrodes 10
 and Application of potentiometry.
 - Thermal Techniques: Principle, thermal transitions Instrumentation (Heat flux and power-compensation and designs), Modulated DSC, Hyper DSC, experimental parameters experimental conditions, calibration, preparation, heating cooling rates, resolution, source of errors) and their influence, disadvantages, advantage pharmaceutical and applications. Differential Thermal Analysis (DTA): Principle, instrumentation disadvantages, pharmaceutical advantage and applications, derivative differential thermal analysis (DDTA). TGA: Principle. instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications.

REFERENCES

- 1. Spectrometric Identification of Organic compounds Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.
- 2. Principles of Instrumental Analysis Doglas A Skoog, F. James Holler, Timothy A. Nieman, 5 th edition, Eastern press, Bangalore, 1998.
- 3. Instrumental methods of analysis Willards, 7th edition, CBS publishers.
- 4. Practical Pharmaceutical Chemistry Beckett and Stenlake, Vol II, 4th edition, CBS Publishers, New Delhi, 1997.
- 5. Organic Spectroscopy William Kemp, 3rd edition, ELBS, 1991.
- 6. Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
- 7. Pharmaceutical Analysis Modern Methods Part B J W Munson, Vol 11, Marcel. Dekker Series
- 8. Spectroscopy of Organic Compounds, 2nd edn., P.S/Kalsi, Wiley estern Ltd., Delhi.
- 9. Textbook of Pharmaceutical Analysis, KA. Connors, 3rd Edition, John Wiley & Sons, 1982.

Course Outcomes

After completion of course student is able to know-

CO1. The identification, characterisation, and quantification of drugs using a variety of sophisticated analytical instrumental techniques including instruments such as mass spectrometers, IR, HPLC, GC, etc are the topics covered in this course.

CO2. The analysis of different drugs in both single and multiple dose versions

CO3.Theoretical and practical instrument knowledge.

Course Outcomes and their mapping with Programme Outcomes:

CO	PO										
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8			
CO1	3										
CO2	3										
CO3	3										

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

ADVANCED ORGANIC CHEMISTRY – I (MPC 102T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC102T	3	1	1	4 hours	25	75	100	4

Scope

The subject is designed to provide in-depth knowledge about advances in organic chemistry, different techniques of organic synthesis and their applications to process chemistry as well as drug discovery.

Objectives

Upon completion of course, the student shall be to understand

- The principles and applications of retrosynthesis
- The mechanism & applications of various named reactions
- The concept of disconnection to develop synthetic routes for small target molecule.
- The various catalysts used in organic reactions.
- The chemistry of heterocyclic compounds

THEORY 60 Hrs

- 1 Basic Aspects of Organic Chemistry:
 - 1. Organic intermediates: Carbocations, carbanions, free Hrs radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications.

12

- 2. Types of reaction mechanisms and methods of determining them,
- 3. Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations.

Addition reactions

- a) Nucleophilic uni- and bimolecular reactions (SN1 and SN2)
- b) Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)
- c) Rearrangement reaction
- 2 Study of mechanism and synthetic applications of following 12 named Reactions: Hrs Ugi reaction, Brook rearrangement, Ullmann coupling reactions, Reaction, Doebner-Miller Reaction. Dieckmann Sandmeyer Reaction. Mitsunobu reaction, Mannich reaction, Vilsmeyer-Haack Reaction, Sharpless asymmetric epoxidation, Baeyer-Villiger oxidation, Shapiro & Suzuki reaction, Ozonolysis and Michael addition reaction
- 3 Synthetic Reagents & Applications: 12 Aluminiumisopropoxide, N-bromosuccinamide, diazomethane, reagent, dicyclohexylcarbodimide, Wilkinson Witting reagent. Osmium tetroxide. titanium chloride. diazopropane, diethyl azodicarboxylate. Triphenylphosphine, Benzotriazol-1-yloxy) tris (dimethylamino) phosphonium hexafluoro-phosphate (BOP). Protecting groups
 - a. Role of protection in organic synthesis

- b. Protection for the hydroxyl group, including 1,2-and1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals
- c. Protection for the Carbonyl Group: Acetals and Ketals
- d. Protection for the Carboxyl Group: amides and hydrazides, esters
- e. Protection for the Amino Group and Amino acids: carbamates and amides
- 4 Heterocyclic Chemistry:

12

Organic Name reactions with their respective mechanism and Hrs 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.

representative Synthesis of few drugs containing these such hetrocyclic nucleus 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.

5 Synthon approach and retrosynthesis applications

12

- Basic principles, terminologies and advantages of Hrs retrosynthesis; guidelines for dissection of molecules.
 Functional group interconvertion and addition (FGI and FGA)
- I. C-X disconnections; C-C disconnections alcohols and carbonyl compounds; 1,2-, 1,3-,1,4-, 1,5-, 1,6-difunctionalized compounds
- 1. Strategies for synthesis of three, four, five and six-membered ring.

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, New York.
- 3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers., Oxford University Press 2001.
- 4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Pearson Education Lts, Dorling Kindersley 9India) 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, 5 th 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, Nelson Thorns.
- 11. Organic Synthesis Special Techniques. VK Ahluwalia and R Agarwal, Narosa Publishers.
- 12. Organic Reaction Mechanisms IV th Edtn, VK Ahluwalia and RK Parashar, Narosa Publishers

Course outcomes

After completion of course student is able to know-

- **CO1.** The goal of the study is to give students in-depth knowledge of recent developments in organic chemistry, various methods of organic synthesis, and how these methods can be used to process chemistry and drug discovery.
- CO2. Study the fundamentals and uses of retrosynthesis. Study various named reactions mechanisms and applications. Knowledge of different catalysts that are employed in organic processes and understanding chemistry of heterocyclic compounds.

Course Outcomes and their mapping with Programme Outcomes:

CO		PO										
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8				
CO1			3									
CO2			3									

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

ADVANCED MEDICINAL CHEMISTRY (MPC 103T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC103T	3	1	-	4 hours	25	75	100	4

Scope

The subject is designed to impart knowledge about recent advances in the field of medicinal chemistry at the molecular level including different techniques for the rational drug design.

Objectives

At completion of this course it is expected that students will be able to understand

Different stages of drug discovery

- · Role of medicinal chemistry in drug research
- Different techniques for drug discovery
- Various strategies to design and develop new drug like molecules for biological targets
- Peptidomimetics

3

THEORY 60 Hrs

- 1. Stages drug Drug discovery: of discovery. lead discovery: 12 identification, validation and diversity of drug targets. Hrs Biological drug targets: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes.
- 2 Prodrug Design and Analog design:

- 12
- a) Prodrug design: Basic concept, Carrier linked prodrugs/ Hrs 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.
- b) Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.
- c) Analog Design: Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid alteration of chain branching, changes in ring size, ring design position isomers, of stereo isomers isomers. fragments of a lead molecule. geometric variation in inter atomic distance.
- a) Medicinal chemistry aspects of the following class of drugs
 12
 Systematic study, SAR, Mechanism of action and synthesis of new Hrs generation molecules of following class of drugs:
 - a) Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, 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,

Enantio selectivity in drug adsorption, metabolism, distribution and elimination.

4 Rational Design of Enzyme Inhibitors 12 Enzyme kinetics & Principles of Enzyme inhibitors, Enzyme Hrs inhibitors in medicine, Enzyme inhibitors in basic research, rational design of non-covalently and covalently binding enzyme inhibitors.

5 Peptidomimetics

12

Therapeutic values of Peptidomimetics, design of Hrs peptidomimetics by manipulation of the amino acids, modification of the peptide backbone, incorporating conformational constraints locally or globally. Chemistry of prostaglandins, leukotrienes and thromboxones.

REFERENCES

- 1. Medicinal Chemistry by Burger, Vol I -VI.
- 2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12 th Edition, 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 Moore 80
- 5. Introduction to Quantitative Drug Design by Y.C. Martin.
- 6. Principles of Medicinal Chemistry by William Foye, 7th Edition, Ippincott 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, II Edition, Elsevier Publishers, New Delhi.
- 10. An Introduction to Medicinal Chemistry, Graham L.Patrick, III Edition, Oxford University Press, USA.
- 11. Biopharmaceutics and pharmacokinetics, DM.Brahmankar, Sunil B. Jaiswal II Edition, 2014, Vallabh Prakashan, New Delhi.
- 12. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, First edition, Wiley publishers.

Course outcomes

After completion of course student is able to know-

CO1. The course is intended to teach students about recent developments in medicinal chemistry at the molecular level, including various methods for rational drug design.

CO2. Study different phases of drug discovery, medicinal chemistry's role in drug research, different methods for design and developing novel drug-like compounds for biological targets.

Course Outcomes and their mapping with Programme Outcomes:

СО			PSO								
CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3
CO1				3							
CO2				3							

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

CHEMISTRY OF NATURAL PRODUCTS (MPC 104T)

Sub Code	${f L}$	T	P	Duration	IA	ESE	Total	Credits
MPC104T	3	1	-	4 hours	25	75	100	4

Scope

The subject is designed to provide detail knowledge about chemistry of medicinal compounds from natural origin and general methods of structural elucidation of such compounds. It also emphasizes on isolation, purification and characterization of medicinal compounds from natural origin.

Objectives

At completion of this course it is expected that students will be able to understand-

- Different types of natural compounds and their chemistry and medicinal importance
- The importance of natural compounds as lead molecules for new drug discovery
- The concept of rDNA technology tool for new drug discovery
- General methods of structural elucidation of compounds of natural origin
- Isolation, purification and characterization of simple chemical constituents from natural source

THEORY 60 Hrs

- Study of Natural products as leads for new pharmaceuticals 12 for the following class of drugs
 - a) Drugs Affecting the Central Nervous System: Morphine Alkaloids
 - b) Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide
 - c) Cardiovascular Drugs: Lovastatin, Teprotide and Dicoumarol

- d) Neuromuscular Blocking Drugs: Curare alkaloids
- e) Anti-malarial drugs and Analogues
- f) Chemistry of macrolid antibiotics (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and β Lactam antibiotics (Cephalosporins and Carbapenem)
- 2 a) Alkaloids

12

General introduction. classification, isolation, purification. molecular modification and biological activity of alkaloids, general methods of structural determination of alkaloids, elucidation and stereochemistry of ephedrine, morphine, emetine and reserpine.

b) Flavonoids

Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin.

c) 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).

3 a) Terpenoids

12

Classification, isolation, isoprene rule and general methods of structural hreelucidation of Terpenoids; Structural elucidation of drugs belonging to mono (citral, menthol, camphor), di(retinol, Phytol, taxol) and tri terpenoids (Squalene, Ginsenoside) carotinoids (\$\beta\$ carotene).

b) Vitamins

Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin.

- 12 4 a) Recombinant DNA technology and drug discovery rDNA hybridoma technology, New pharmaceuticals technology, hrs derived from biotechnology; Oligonucleotide therapy. Gene therapy: Clinical application recent Introduction, and advances gene therapy, principles of RNA & DNA estimation
 - crude Active of certain b) constituent drugs used in Gymnema Indigenous Diabetic system therapy sylvestre. Salacia reticulate, Pterocarpus marsupiam, Swertia chirata. Trigonella foenum graccum; Liver dysfunction - Phyllanthus niruri; Antitumor - Curcuma longa Linn.
- 5 Structural Characterization of natural compounds 12 Structural characterization of natural compounds using IR, hrs

1HNMR, 13CNMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides.

REFERENCES

- 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, 13 th edition.
- 15. Phytochemical methods of Harborne, Springer, Netherlands.
- 16. Burger's Medicinal Chemistry.

Course outcomes

After completion of course student is able to know-

CO1. The goal of the topic is to give students in-depth knowledge of the chemistry of drugs with natural sources as well as the general approaches to determining their structural details.

CO2. To learn about separation, purification, and characterisation of pharmaceutical substances of natural origins.

CO2. The idea of using rDNA technology as a tool for finding novel drugs. Methods for elucidating natural chemical structures in general.

Course Outcomes and their mapping with Programme Outcomes:

СО		PO										
CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8				
CO1						3						
CO2						3						
CO3												

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

PHARMACEUTICAL CHEMISTRY PRACTICAL – I (MPC 105P)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC105P	-	-	12	12 Hrs.	50	100	150	6

- 1. Analysis of Pharmacopeial compounds and their formulations by UV Vis spectrophotometer, RNA & DNA estimation
- 2. Simultaneous estimation of multi component containing formulations by UV spectrophotometry
- 3. Experiments based on Column chromatography
- 4. Experiments based on HPLC
- 5. Experiments based on Gas Chromatography
- 6. Estimation of riboflavin/quinine sulphate by fluorimetry
- 7. Estimation of sodium/potassium by flame photometry

To perform the following reactions of synthetic importance

- 1. Purification of organic solvents, column chromatography
- 2. Claisen-schimidt reaction.
- 3. Benzyllic acid rearrangement.
- 4. Beckmann rearrangement.
- 5. Hoffmann rearrangement
- 6. Mannich reaction
- 7. Synthesis of medicinally important compounds involving more than one step along with purification and Characterization using TLC, melting point and IR spectroscopy (4 experiments)
- 8. Estimation of elements and functional groups in organic natural compounds
- 9. Isolation, characterization like melting point, mixed melting point, molecular weight determination, functional group analysis, co-chromatographic technique for identification of isolated compounds and interpretation of UV and IR data.
- 10. Some typical degradation reactions to be carried on selected plant constituents

Course outcomes

After completion of course student is able to know-

CO1. Analysis of Pharmacopeial compounds and their formulations by UV Vis spectrophotometer, RNA & DNA estimation.

CO2. Experiments based on Column chromatography, HPLC, Gas chromatography.

CO3. To perform reactions of synthetic importance

Course Outcomes and their mapping with Programme Outcomes:

CO		PO									
CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8			
CO1	3										
CO2	3										

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

Second Semester

ADVANCED SPECTRAL ANALYSIS (MPC 201T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC201T	3	1	-	4 hours	25	75	100	4

Scope

This subject deals with various hyphenated analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are LC-MS, GC-MS, ATR-IR, DSC etc.

Objectives

At completion of this course it is expected that students will be able to understand-

- Interpretation of the NMR, Mass and IR spectra of various organic compounds
- Theoretical and practical skills of the hyphenated instruments
- Identification of organic compounds

THEORY 60Hrs

1. UV and IR spectroscopy:

- 12
- Wood ward Fieser rule for 1,3– butadienes, cyclic dienes and α , Hrs β -carbonyl compounds and interpretation compounds of enones. ATR-IR, IR Interpretation of organic compounds.
- 2 NMR spectroscopy:

12

- 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE Hrs techniques, Interpretation of organic compounds.
- 3 Mass Spectroscopy

12

- Mass fragmentation and its rules, Fragmentation of important Hrs functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, Mc Lafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.
- 4 Chromatography:

12

Principle, Instrumentation and Applications of the following: Hrs 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 critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion Chromatography) k) Flash chromatograph

- 5 1. Thermalmethods of analysis 12
 Introduction, principle, instrumentation and application of DSC, Hrs
 DTA and TGA.
 - 2. Raman Spectroscopy
 Introduction, Principle, Instrumentation and Applications.
 - 3. Radio immuno assay
 Biological standardization , bioassay, ELISA, Radioimmuno
 assay of digitalis and insulin.

RFERENCES

- 1. Spectrometric Identification of Organic compounds Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.
- 2. Principles of Instrumental Analysis Doglas A Skoog, F. James Holler, Timothy A. Nieman, 5 th edition, Eastern press, Bangalore, 1998.
- 3. Instrumental methods of analysis Willards, 7 th edition, CBS publishers.
- 4. Organic Spectroscopy William Kemp, 3 rd edition, ELBS, 1991.
- 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, 3 rd Edition, CBS Publishers, New Delhi, 1997.
- 7. Pharmaceutical Analysis- Modern methods Part B J W Munson, Volume 11, Marcel Dekker

Course outcomes

After completion of course student is able to know-

CO1. Various hyphenated analytical instrumental approaches for drug identification, characterisation, and quantification and working with LC-MS, GC-MS, FT-IR, DSC and other instruments are covered in this subject.

Course Outcomes and their mapping with Programme Outcomes:

CO		PO									
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8			
CO1	3										

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

ADVANCED ORGANIC CHEMISTRY – II (MPC 202T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC202T	3	1	-	4 hours	25	75	100	4

Scope

The subject is designed to provide in-depth knowledge about advances in organic chemistry, different techniques of organic synthesis and their applications to process chemistry as well as drug discovery.

Objectives

Upon completion of course, the student shall able to understand

- The principles and applications of Green chemistry
- The concept of peptide chemistry.
- The various catalysts used in organic reactions
- The concept of stereochemistry and asymmetric synthesis.

THEORY 60 Hrs

1. Green Chemistry:

a. Introduction, principles of green chemistry

- 12 Hrs
- b. Microwave assisted reactions: Merit and demerits of its use. increased reaction rates, mechanism, superheating effects effects solvents microwave. of in microwave assisted synthesis, microwave technology in process optimization, applications in various organic reactions and heterocycles synthesis
- c. Ultrasound assisted reactions: Types of sonochemical reactions, homogenous, heterogeneous liquid-liquid and liquid-solid reactions, synthetic applications
- d. Continuous flow reactors: Working principle, advantages and synthetic applications

2 Chemistry of peptides

12

a. Coupling reactions in peptide synthesis

- Hrs
- b. Principles of solid phase peptide synthesis, t-BOC and FMOC protocols, various solid supports linkers: and Activation procedures, bond formation, peptide deprotection and low and high HF cleavage cleavage from resin, 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, overactivation and side reactions of individual amino acids.

3 Photochemical Reactions

12

Basic principles of photochemical reactions. Photo-oxidation, Hrs photo-addition and photo-fragmentation.

Pericyclic reactions

Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigmatrophic rearrangement reactions with examples.

4 Catalysis:

12

- a. Types of catalysis, heterogeneous and homogenous catalysis, Hrs 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
- 5 Stereochemistry & Asymmetric Synthesis

12

- a. Basic concepts in stereochemistry optical activity, specific Hrs 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.
- b. Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation and Stereo selective synthesis with examples.

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, New York.
- 3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers., Oxford University Press 2001.
- 4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Sixth ed., 1995.
- 5. Carey, Organic chemistry, 5th edition (Viva Books Pvt. Ltd.)
- 6. Organic synthesis-the disconnection approach, S. Warren, Wily India
- 7. Principles of organic synthesis, ROCNorman and JMCoxan, 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 outcomes

After completion of course student is able to know-

CO1. To study the concept peptide chemistry.

CO2. Green chemistry principles and applications. To study the ideas of stereochemistry and asymmetric synthesis.

Course Outcomes and their mapping with Programme Outcomes:

CO	PO									
CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8		
CO1		3								
CO2		3								

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

COMPUTER AIDED DRUG DESIGN (MPC 203T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC203T	3	1	-	4 hours	25	75	100	4

Scope

The subject is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design.

Objectives

At completion of this course it is expected that students will be able to understand

- Role of CADD in drug discovery
- Different CADD techniques and their applications
- Various strategies to design and develop new drug like molecules.
- Working with molecular modeling softwares to design new drug molecules
- The in silico virtual screening protocols

Theory 60 Hrs

Introduction to Computer Aided Drug Design (CADD)
 History, different techniques and applications.

12 Hrs

Quantitative Structure Activity Relationships: Basics

History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi-substituent constant), steric effects

	(Taft steric and MR parameters) Experimental and theoretical	
	approaches for the determination of these physicochemical	
	parameters.	
2	Quantitative Structure Activity Relationships: Applications	12
	Hansch analysis, Free Wilson analysis and relationship between	Hrs
	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.	
3	Molecular Modeling and Docking	12
	a) Molecular and Quantum Mechanics in drug design.	Hrs
	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)	
4	Molecular Properties and Drug Design	12
	a) Prediction and analysis of ADMET properties of new molecules and its	Hrs
	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 modeling and generation of 3D-structure of protein.	
5	Pharmacophore Mapping and Virtual Screening	12
	Concept of pharmacophore, pharmacophore mapping,	Hrs

REFERENCES

identification

modeling;

mapping.

of

based

Conformational

1. Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers.

search

and

features

used

Pharmacophore

and

in

base

Pharmacophore

pharmacophore

screening,

Pharmacophore

In Silico Drug Design and Virtual Screening Techniques

methods

structure based In-silico virtual screening protocols.

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, 1975, 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, lippincott Williams & Wilkins.
- 9. Comprehensive Medicinal Chemistry Corwin and Hansch, Pergamon Publishers.

Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore

Course outcomes

After completion of course student is able to know-

CO1. The course is intended to teach students about the state-of-the-art techniques used in computer-assisted drug discovery currently.

CO2. The function of CADD in drug development.

CO3. Different methods for designing and developing novel compounds.

CO4. Creating novel drug molecules using molecular modelling software.

Course Outcomes and their mapping with Programme Outcomes:

СО		PO									
CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8			
CO1							3				
CO2							3				
CO3							3				
CO4							3				

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

PHARMACEUTICAL PROCESS CHEMISTRY (MPC 204T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPC204T	3	1	-	4 hours	25	75	100	4

Scope

Process chemistry is often described as scale up reactions, taking them from small quantities created in the research lab to the larger quantities that are needed for further testing and then to even larger quantities required for commercial production. The goal of a process chemist is to develop synthetic routes that are safe, cost-effective, environmentally friendly, and efficient. The subject is designed

to impart knowledge on the development and optimization of a synthetic route/s and the pilot plant procedure for the manufacture of Active Pharmaceutical Ingredients (APIs) and new chemical entities (NCEs) for the drug development phase.

Objectives

At completion of this course it is expected that students will be able to understand

- The strategies of scale up process of apis and intermediates
- The various unit operations and various reactions in process chemistry

Theory 60 Hrs

1. Process chemistry

12

Introduction, Synthetic strategy

Hrs

Stages of scale up process: Bench, pilot and large scale process.

In-process 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

2 Unit operations

12

- a) Extraction: Liquid equilibria, extraction with reflux, Hrs extraction with agitation, counter current extraction.
- b) Filtration: Theory of filtration, pressure and vacuum filtration, centrifugal filtration,
- c) Distillation: azeotropic and steam distillation
- d) Evaporation: Types of evaporators, factors affecting evaporation.
- e) Crystallization: Crystallization from aqueous, nonaqueous solutions factors affecting crystallization, nucleation. Principle and Preparation general methods of of polymorphs, hydrates, solvates and amorphous APIs.

3 Unit Processes – I

12

- a) Nitration: Nitrating agents, Aromatic nitration, kinetics Hrs and mechanism of aromatic nitration, process equipment for technical nitration, mixed acid for nitration,
- b) Halogenation: Kinetics of halogenations, types of halogenations, catalytic halogenations. Case study on industrial halogenation process.
- c) Oxidation: Introduction, of oxidative reactions, types Liquid phase oxidation with oxidizing Nonmetallic agents. Oxidizing H_2O_2 , sodium hypochlorite, agents such as Oxygen gas, ozonolysis.

4 Unit Processes – II 12

- a) Reduction: Catalytic hydrogenation, Heterogeneous Hrs and homogeneous catalyst; Hydrogen transfer reactions. hydrides. Case reduction Metal study on industrial process.
- b) Fermentation: Aerobic and anaerobic fermentation.

 Production of
 - i. Antibiotics; Penicillin and Streptomycin,
 - ii. Vitamins: B2 and B12
 - iii. Statins: Lovastatin, Simvastatin
- c) Reaction progress kinetic analysis
 - i. Streamlining reaction steps, route selection,
 - ii. Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up.
- 5 Industrial Safety

12

- a) MSDS (Material Safety Data Sheet), hazard labels of Hrs chemicals and Personal Protection Equipment (PPE)
- b) Fire hazards, types of fire & fire extinguishers
- c) Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001 (Environmental Management System), Effluents and its management

REFERENCES

- 1. Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever-Changing Climate-An Overview; K. Gadamasetti, CRC Press.
- 2. Pharmaceutical Manufacturing Encyclopedia, 3 rd edition, Volume 2.
- 3. Medicinal Chemistry by Burger, 6 th 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 outcomes

After completion of course student is able to know-

CO1. To study the techniques for scaling up the production of intermediates and APIs.

CO2. Process chemistry's various unit operations and reactions.

Course Outcomes and their mapping with Programme Outcomes:

CO		PO									
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8			
CO1					3						
CO2					3						

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

PHARMACEUTICAL CHEMISTRY PRACTICALS – II (MPC 205P)

Sub Code	${f L}$	T	P	Duration	IA	ESE	Total	Credits
MPC205P	1	-	12	12 hours	50	100	150	6

- Synthesis of organic compounds by adapting different approaches involving (3 experiments)
 - 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)
- 4. Comparison of absorption spectra by UV and Wood ward Fieser rule
- 5. Interpretation of organic compounds by FT-IR
- 6. Interpretation of organic compounds by NMR
- 7. Interpretation of organic compounds by MS
- 8. Determination of purity by DSC in pharmaceuticals
- 9. Identification of organic compounds using FT-IR, NMR, CNMR and Mass spectra

- 10. To carry out the preparation of following organic compounds
- 11. Preparation of 4-chlorobenzhydrylpiperazine. (an intermediate for cetirizine HCl).
- 12. Preparation of 4-iodotolene from p-toluidine.
- 13. NaBH4 reduction of vanillin to vanillyl alcohol
- 14. Preparation of umbelliferone by Pechhman reaction
- 15. Preparation of triphenyl imidazole
- 16. To perform the Microwave irradiated reactions of synthetic importance (Any two)
- 17. Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- 18. Calculation of ADMET properties of drug molecules and its analysis using softwares
 - Pharmacophore modeling
- 19. 2D-QSAR based experiments
- 20. 3D-QSAR based experiments
- 21. Docking study based experiment
- 22. Virtual screening based experimentSynthesis of organic compounds by adapting different approaches involving (3 experiments)
 - a) Oxidation
 - b) Reduction/hydrogenation
 - c) Nitration
- 23. Comparative study of synthesis of APIs/intermediates by different synthetic routes (2 experiments)
- 24. Assignments on regulatory requirements in API (2 experiments)
- 25. Comparison of absorption spectra by UV and Wood ward Fieser rule
- 26. Interpretation of organic compounds by FT-IR
- 27. Interpretation of organic compounds by NMR
- 28. Interpretation of organic compounds by MS
- 29. Determination of purity by DSC in pharmaceuticals
- 30. Identification of organic compounds using FT-IR, NMR, CNMR and Mass spectra
- 31. To carry out the preparation of following organic compounds
- 32. Preparation of 4-chlorobenzhydrylpiperazine. (an intermediate for cetirizine HCl).
- 33. Preparation of 4-iodotolene from p-toluidine.
- 34. NaBH₄ reduction of vanillin to vanillyl alcohol
- 35. Preparation of umbelliferone by Pechhman reaction
- 36. Preparation of triphenyl imidazole

- 37. To perform the Microwave irradiated reactions of synthetic importance (Any two)
- 38. Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- 39. Calculation of ADMET properties of drug molecules and its analysis using softwares

Pharmacophore modeling

- 40. 2D-QSAR based experiments
- 41. 3D-QSAR based experiments
- 42. Docking study based experiment

Virtual screening based experiment

Course outcomes

After completion of course student is able to know-

- **CO1.** Synthesis of organic compounds by adopting nitration, oxidation, reduction
- CO2. Interpretation of organic compounds by FT-IR, NMR, MS.

CO3. To perform 2D-QSAR based experiments,3D-QSAR based experiments, docking study-based experiment, Virtual screening-based experiment.

Course Outcomes and their mapping with Programme Outcomes:

СО	PO									
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8		
CO1		3								
CO2	3									
CO3							3			

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

Third Semester

RESEARCH METHODOLOGY & BIOSTATISTICS (MRM 301T)

Sub Code	L	T	P	Duration	IA	ESE	Total	Credits
MPM301T	3	1	-	4 hours	25	75	100	4

UNIT - I

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.

UNIT - II

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.

UNIT - III

Medical Research: History, values in medical ethics, autonomy, 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.

UNIT - IV

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.

UNIT - V

Declaration of Helsinki: History, introduction, basic principles for all medical research, and additional principles for medical research combined with medical care.

Course outcomes

After completion of course student is able to know-

CO1. Student will gain knowledge of general research methodology, review of literature, biostatics.

CO2. They will know about values of medical ethics.

CO3. CPCSEA guidelines for laboratory animal facility

Course Outcomes and their mapping with Programme Outcomes:

СО		PO										
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8				
CO1								3				
CO2								3				
CO3								3				

Weightage: 1-Sightly; 2-Moderately; 3-Strongly