

ROYAL SCHOOL OF PHARMACY (RSP)

Master of Pharmacy (M. Pharm)

SYLLABUS

&

COURSE STRUCTURE

M. Pharm. (Pharmaceutical Chemistry)

PCI Syllabus 2016

M. PHARM. (PHARMACEUTICAL CHEMISTRY)

Programme Structure

	Semester-I							
Sl. No	. Subject Code	Names of subjects	L	Т	Р	С	ТСР	
	Core Subjects							
1	MPC101T	Modern Pharmaceutical Analytical Techniques	3	1	0	4	4	
2	MPC102T	Advanced Organic Chemistry-I	3	1	0	4	4	
3	MPC103T	Advanced Medicinal Chemistry	3	1	0	4	4	
4	MPC104T	Chemistry of Natural Products	3	1	0	4	4	
5	MPC105P	Pharmaceutical Chemistry Practical I	0	0	12	6	12	
6	MPC106S	Seminar / Assignment	0	0	7	4	7	
		TOTAL	12	4	19	26	35	

		Semester-II					
Sl. No.	Subject Code	Names of subjects	L	Τ	Р	С	ТСР
		Core Subjects					
1	MPC201T	Advanced Spectral Analysis	3	1	0	4	4
2	MPC202T	Advanced Organic Chemistry-II	3	1	0	4	4
3.	MPC203T	Computer Aided Drug Design	3	1	0	4	4
4.	MPC204T	Pharmaceutical Process Chemistry	3	1	0	4	4
5.	MPC205P	Pharmaceutical Chemistry Practical II	0	0	12	6	12
6.	MPC206S	Seminar / Assignment	0	0	7	4	7
		TOTAL	12	4	19	26	35

	Semester III							
Sl. No.	Subject Code	Names of subjects	L	Т	Р	С	ТСР	
	Core Subjects							
1	MRM301T	Research Methodology and Biostatistics	3	1	0	4	4	
2	MPC302S	Journal Club	0	0	1	1	1	
3	MPC303P	Discussion / Presentation (Proposal Presentation)	0	0	2	2	2	
4	MPC304P	Research Work	0	0	28	14	28	
		TOTAL	3	1	31	21	35	

	Semester IV							
Sl. No.	Subject Code	Names of subjects	L	Т	Р	С	ТСР	
	Core Subjects							
1	MPC401S	Journal Club	0	0	1	1	1	
2	MPC402P	Research Work	0	0	31	16	31	
3	MPC403P	Discussion / Final Presentation	0	0	3	3	3	
4	MPC404S	Co-curricular Activities						
		TOTAL	0	0	35	20	35	

Table-1: Semester wise credits distribution

Semester	Credit Points
Ι	26
II	26
III	21
IV	20
Co-curricular Activities	Minimum = 02 /
(a) Participation in National Level	Maximum = 07
Seminar/Conference/Workshop/Symposium/Training	
Programs (related to the specialization of the student - 01)	
(b) Research / Review Publication in National Journals	
(Indexed in Scopus / Web of Science – 01)	
Total Credit Points	Minimum = 95
	Maximum = 100

Scheme of Evaluation

Theory Papers (T):

- Internal assessment: 25%
- End Term Examination:75%

Practical Papers (P):

- Internal assessment: 30%
- End Term Examination: 70%

Internal assessment : Continuous mode

The marks allocated for Continuous mode of Internal Assessment shall be awarded as per the scheme given below:

Theory	
Criteria	Maximum Marks
Attendance (Refer Table–3)	8
Student–Teacher interaction	2
Total	10
Practical	
Attendance (Refer Table–3)	10
Based on Practical Records, Regular viva-voce, etc.	10
Total	20

Table-2: Scheme for awarding internal assessment: Continuous mode

Table-3: Guidelines for the allotment of marks for attendance

Percentage of Attendance	Theory	Practical
95-100	8	10
90-94	6	7.5
85-89	4	5
80-84	2	2.5
Less than 80	0	0

Paper I / Subject Name: MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES (MPC 101T)

L-T-P-C – 4-0-0-4 Credit Units:4 Scheme of Evaluation:(T)

Objective: 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.

Course Outcome: Upon completion of the course, the student shall be able to:

CO1: Understand the operation and applications of modern analytical instruments used in drug analysis, including UV-Visible, IR, Spectrofluorimetry, flame emission, and atomic absorption spectroscopy.

CO2: Understand the principles of NMR and mass spectroscopy and learn to interpret data for identifying organic compounds.

CO3: Understand chromatographic separation processes and apply them to the analysis of pharmaceutical compounds, gaining practical skills in chromatography and electrophoresis techniques.

CO4: Explore X-ray crystallography and immunological assays (RIA, ELISA) for characterizing and quantifying biological compounds. Develop skills in drug analysis using advanced techniques, and learn to interpret NMR, Mass, and IR spectra for identifying and characterizing organic compounds.

Module	Topics (if applicable)/Course Content	Hours				
I.	UV-Visible spectroscopy: Introduction, Theory, Laws, Instrumentation associated	15 hrs				
	with UV-Visible spectroscopy, Choice of solvents and solvent effect and					
	Applications of UV-Visible spectroscopy, Difference/ Derivative spectroscopy.					
	IR spectroscopy: Theory, Modes of Molecular vibrations, Sample handling,					
	Instrumentation of Dispersive and Fourier-Transform IR Spectrometer, Factors					
	affecting vibrational frequencies and Applications of IR spectroscopy, Data					
	Interpretation.					
	Spectroflourimetry: Theory of Fluorescence, Factors affecting fluorescence					
	(Characteristics of drugs that can be analysed by fluorimetry), Quenchers,					
	Instrumentation and Applications of fluorescence spectrophotometer.					
	Flame emission spectroscopy and atomic absorption spectroscopy: Principle,					
	Instrumentation, Interferences and Applications.					
II.	NMR spectroscopy: Quantum numbers and their role in NMR, Principle,	15 hrs				
	Instrumentation, Solvent requirement in NMR, Relaxation process, NMR signals in					
	various compounds, Chemical shift, Factors influencing chemical shift, Spin-Spin					

 applications of X-ray diffraction. Potentiometry: Principle, working, Ion selective Electrodes and 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, pharmaceutical applications. Differential Thermal Analysis (DTA): Principle, instrumentation and advantages and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). TGA: Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications. 	60 hrs
 Potentiometry: Principle, working, Ion selective Electrodes and 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, pharmaceutical applications. Differential Thermal Analysis (DTA): Principle, instrumentation and advantages and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). TGA: Principle, instrumentation, factors affecting results, advantage and 	
Potentiometry: Principle, working, Ion selective Electrodes and 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, pharmaceutical applications. Differential Thermal Analysis (DTA): Principle, instrumentation and advantages and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA).	
 Potentiometry: Principle, working, Ion selective Electrodes and 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, pharmaceutical applications. Differential Thermal Analysis (DTA): Principle, instrumentation and advantages and disadvantages, pharmaceutical applications, derivative differential thermal 	
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Potentiometry: Principle, working, Ion selective Electrodes and 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, pharmaceutical applications.	
Potentiometry: Principle, working, Ion selective Electrodes and 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	
Potentiometry: Principle, working, Ion selective Electrodes and 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	
Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry. Thermal Techniques: Principle, thermal transitions and Instrumentation (Heat flux and power-compensation and designs), Modulated DSC, Hyper DSC, experimental	
Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry. Thermal Techniques: Principle, thermal transitions and Instrumentation (Heat flux	
Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry.	
Potentiometry: Principle, working, Ion selective Electrodes and Application of	
law, Rotating crystal technique, X ray powder technique, Types of crystals and	
X ray Crystallography: Production of X rays, Different X ray methods, Bragg's	
electrophoresis e) Moving boundary electrophoresis f) Iso electric focusing	
a) Paper electrophoresis b) Gel electrophoresis c) Capillary electrophoresis d) Zone	
separation and applications of the following:	
Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting	15 hrs
i. Gel Chromatography	
f. High Performance Liquid chromatography	
e. Gas chromatography	
a. Thin Layer chromatography	
interpretation and applications of the following:	
parameters, factors affecting resolution, isolation of drug from excipients, data	
Chromatography: Principle, apparatus, instrumentation, chromatographic	15 hrs
and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy.	
APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation	
Different types of ionization like electron impact, chemical, field, FAB and MALDI,	
	 APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy. Chromatography: Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation 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 Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following: a) Paper electrophoresis b) Gel electrophoresis c) Capillary electrophoresis d) Zone

- 1. Instrumental methods of analysis Willards, 7th edition, CBS publishers.
- 2. Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
- 3. Pharmaceutical Analysis Modern Methods Part B J W Munson, Vol 11, Marcel. Dekker Series.
- 4. Spectroscopy of Organic Compounds, 2nd edn., P.S/Kalsi, Wiley estern Ltd., Delhi.
- 5. Textbook of Pharmaceutical Analysis, KA.Connors, 3rd Edition, John Wiley & Sons, 1982.

Reference Books:

- 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, 5th edition, Eastern press, Bangalore, 1998.
- Practical Pharmaceutical Chemistry Beckett and Stenlake, Vol II, 4th edition, CBS Publishers, New Delhi, 1997.
- 4. Organic Spectroscopy William Kemp, 3rd edition, ELBS, 1991.

Teaching Learning Process and Assessment Methods:

Unit No.	Course Learning Outcomes	Teaching and Learning Activity	Assessment Tasks
I.	CO1: Students will understand and apply principles of UV-Visible, IR, and Spectrofluorimetry, as well as flame emission and atomic absorption spectroscopy in drug analysis.	Traditional teaching, PPT	Class tests, assignments, MCQs
П.	CO2: Students will understand the principles of ionization and mass fragmentation and learn to interpret Mass and NMR spectroscopy data.	Traditional teaching, PPT	Class tests, assignments, MCQs
III.	CO3: Students will gain practical skills in chromatography and electrophoresis techniques for the separation and analysis of compounds.	Traditional teaching, PPT	Class tests, assignments, MCQs
IV.	CO4: Students will explore X-ray crystallography methods and immunological assays (RIA, ELISA) for the characterization and quantification of biological compounds.	Traditional teaching, PPT	Class tests, assignments, MCQs

Paper II / Subject Name: ADVANCED ORGANIC CHEMISTRY- I (MPC 102T)

L-T-P-C - 4-0-0-4	Credit Units:4	Scheme of Evaluation:(T)
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Objective: 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.

Course Outcome: Upon completion of the course the student will be able to

CO1: Concept on organic chemistry, retrosynthesis and various name reactions and their significances.

CO2: Understand the disconnection concept to develop synthetic routes for target molecules.

CO3: Develop the understanding for different catalysts in organic reactions and importance of different heterocyclic compounds in the synthesis of drugs.

Modules	Topics (if applicable) & Course Contents	Period
I.	 Basic aspects of organic Chemistry 1. Organic intermediates: Carbocations, carbanions, free radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications. 2. Types of reaction mechanisms and methods of determining them. 3. Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations. 4. Addition reactions: a) Nucleophilic uni- and bimolecular reactions (SN1 and SN2) b) Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule) c) Rearrangement reaction. 5. Study of mechanism and synthetic applications of following named reactions: 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. 	24 hrs
П.	Synthetic Reagents & Applications:Aluminium isopropoxide, N-bromosuccinamide, diazomethane,dicyclohexylcarbodimide, Wilkinson reagent, Witting reagent. Osmiumtetroxide, titanium chloride, diazopropane, diethyl azodicarboxylate,Triphenylphosphine, Benzotriazol-1-yloxy) tris (dimethylamino) phosphoniumhexafluoro-phosphate (BOP).Protecting groups:	12 hrs

	TOTAL	60 hours			
	compounds; 1,2-, 1,3-, 1,4-, 1,5-, 1,6-difunctionalized compounds iii. Strategies for synthesis of three, four, five and six-membered ring.				
IV.	ii. C-X disconnections; C-C disconnections – alcohols and carbonyl				
	(FGI and FGA)	12 hrs			
	for dissection of molecules. Functional group interconvertion and addition				
	i. Basic principles, terminologies and advantages of retrosynthesis; guidelines				
	Synthon approach and retrosynthesis applications				
	and Thioguanine.				
	Prochlorpherazine, Promazine, Chlorpromazine, Theophylline, Mercaptopurine				
	Hydroxychloroquine, Quinine, Chloroquine, Quinacrine, Amsacrine,				
	sodium, Terconazole, Alprazolam, Triamterene, Sulfamerazine, Trimethoprim,				
	Synthesis of few representative drugs containing these hetrocyclic nucleus such as Ketoconazole, Metronidazole, Miconazole, celecoxib, antipyrin, Metamizole	12 hrs			
	synthesis.				
	Bernthsen Acridine Synthesis, Smiles rearrangement and Traube purine				
	Synthesis Pinner Pyrimidine Synthesis, Combes Quinoline Synthesis,				
111.	hetrocyclics such as Debus-Radziszewski imidazole synthesis, Knorr Pyrazole				
III.	involved in synthesis of drugs containing five, six membered and fused				
	Organic Name reactions with their respective mechanism and application				
	Heterocyclic Chemistry:				
	e) Protection for the Amino Group and Amino acids: carbamates and amides				
	c) Protection for the Carbonyl Group: Acetals and Ketalsd) Protection for the Carboxyl Group: amides and hydrazides, esters				
	 b) Protection for the hydroxyl group, including 1,2- and 1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals c) Protection for the Carbonyl Group: Acetals and Ketals 				
	a) Role of protection in organic synthesis				

- 1. Advanced Organic chemistry, Reaction, Mechanisms and Structure", J March, John Wiley and Sons, New York.
- 2. Morrison and Boyd, Organic Chemistry, 7th Edition, 2010

Reference Books:

- 1. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.
- 2. Combinational Chemistry Synthesis and applications Stephen R Wilson & Anthony W Czarnik, Wiley Blackwell.
- 3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers., Oxford University Press 2001

Journals

- 1. Journal of Chemistry Part A7B
- 2. The Journal of Organic Chemistry, ACS Publications

Teaching Learning Process and Assessment Methods

Unit No.	Course Learning Outcomes	Teaching and Learning Activity	Assessment Tasks
I., II.	CO1: Concept on organic chemistry, retrosynthesis and various name reaction.	Classroom lectures though online resources, Educational Software's, digital simulations, concept videos, practical demonstrations, case- based presentations, scientific report discussions (Research articles, research reports etc.)	Seminar, quiz, assignments, journal club, problem-based assignments, report writing, Internal assessments (Sessional exams), continuous evaluation) and End Sem Examinations.
III.	CO2: Understand the disconnection concept to develop synthetic routes for target molecules	Classroom lectures though online resources, Educational Software's, digital simulations, concept videos, practical demonstrations, case- based presentations, scientific report discussions (Research articles, research reports etc.)	Seminar, quiz, assignments, journal club, problem-based assignments, report writing, Internal assessments (Sessional exams), continuous evaluation) and End Sem Examinations.
IV.	CO3: Develop the understanding for different catalysts in organic reaction and importance of different heterocyclic compounds	Classroom lectures though online resources, Educational Software's, digital simulations, concept videos, practical demonstrations, case- based presentations, scientific report discussions (Research articles, research reports.	Seminar, quiz, assignments, journal club, problem-based assignments, report writing, Internal assessments (Sessional exams), continuous evaluation) and End Sem Examinations.

L-T-P-C - 4-0-0-4	Credit Units: 4	Scheme of Evaluation: (T)
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Objective: 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.

Course Outcome: At completion of this course, it is expected that students will be able to understand.

CO1: Different stages of drug discovery.

CO2: Role of medicinal chemistry in drug research.

CO3: Different techniques for drug discovery.

CO4: Various strategies to design and develop new drug like molecules for biological targets and peptidomimetics.

Modules	Topics (if applicable) & Course Contents	Periods
I.	Drug discovery Stages of drug discovery, lead discovery; identification, validation, and diversity of drug targets.	16 hrs
	Biological drug targets: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes.	
	Prodrug design: Basic concept, Carrier linked prodrugs/Bio precursors, 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.	
Ш.	Prodrug Design and Analog design: Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.	16 hrs
	Analog Design: Introduction, Classical & Non classical, Bio isosteric 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. Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs: Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs.	
III.	Medicinal chemistry aspects of the following class of drugsSystematic study, SAR, Mechanism of action and synthesis of new generationmolecules of following class of drugs:	12 hrs

CholSterepre-retherametalIV.RatioEnzymedicovalPeptiThera	 k H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & inergic agents, Antineoplastic and Antiviral agents. cochemistry and Drug action: Realization that stereo selectivity is a equisite for evolution. Role of chirality in selective and specific peutic agents. Case studies, Enantio selectivity in drug adsorption, bolism, distribution, and elimination. Donal Design of Enzyme Inhibitors me kinetics & Principles of Enzyme inhibitors, Enzyme inhibitors in cine, Enzyme inhibitors in basic research, rational design of non-ently and covalently binding enzyme inhibitors. idomimetics apeutic values of Peptidomimetics, design of peptidomimetics by pulation of the amino acids modification of the pentide backbone. 	16 hrs
incor	pulation of the amino acids, modification of the peptide backbone, porating conformational constraints locally or globally. Chemistry of	
prostaglandins, leukotrienes and thromboxones. TOTAL		

- 1. Comprehensive Medicinal Chemistry Corwin and Hansch.
- Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore.
- 3. Introduction to Quantitative Drug Design by Y.C. Martin.
- Principles of Medicinal Chemistry by William Foye, 7th Edition, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt. Ltd, New Delhi.
- 5. Drug Design Volumes by Arienes, Academic Press, Elsevier Publishers, Noida, Uttar Pradesh.
- 6. Principles of Drug Design by Smith.
- 7. An Introduction to Medicinal Chemistry, Graham L.Patrick, III Edition, Oxford University Press, USA.
- 8. Biopharmaceutics and pharmacokinetics, D.M. Brahmankar, Sunil B. Jaiswal II Edition, 2014, Vallabh Prakashan, New Delhi.

Reference Books:

- 1. Medicinal Chemistry by Burger, Vol I –VI.
- Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12th Edition, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt. Ltd, New Delhi.
- 3. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, II Edition, Elsevier Publishers, New Delhi.
- 4. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, First edition, Wiley publishers.

Teaching Learning Process and Assessment Methods

Unit No.	Course Learning Outcomes	Teaching and Learning	Assessment Tasks
110.	Gutcomes	Activity	
I.	CO1: Students will be able to understand the stages of drug discovery, lead discovery; identification, validation, and diversity of drug target.	Traditional chalk and board teaching and power point presentations.	Unit assessment by multiple choice questions (MCQ), internal assessments, regular question answer session, seminar.
II.	CO2: Students will be able to understand how to combat drug resistance, analog design and SAR studies of some important classes of drugs.	Traditional chalk and board teaching, power point presentations.	MCQs, regular discussions, internal assessments, seminar.
III.	CO2, CO3: Students will be able to understand the SAR, Mechanism of action and synthesis of new generation molecules of some important classes of drugs.	Traditional teaching and regular discussions and power point presentations.	Test and MCQs, assignments, internal assessments, seminar.
IV.	CO4: Students will be able to understand the Rational Design of Enzyme Inhibitors, Peptidomimetics	Class conduction using board and power point presentation.	Test and MCQs, assignments, internal assessments, Seminar.

Paper IV / Subject Name: CHEMISTRY OF NATURAL PRODUCTS (Theory)

(MPC	104T)
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L-T-P-C – 4-0-0-4 Credit Units: 4 Scheme of Evaluation: (Г)	
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Objective: 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.

Course Outcome: Upon completion of this course the student should be able to

CO1: Understand the different types of natural compounds and their chemistry and medicinal importance.

CO2: Understand the importance of natural compounds as lead molecules for new drug discovery.

CO3: Understand the concept of rDNA technology tool for new drug discovery.

CO4: Study the general methods of structural elucidation of compounds of natural origin and know the isolation, purification and characterization of simple chemical constituents from natural source.

Modules	Topics (if applicable) & Course Contents	Periods
I.	Study of Natural products as leads for new	12 hrs
	pharmaceuticals 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 macrolide antibiotics (Erythromycin,	
	Azithromycin, Roxithromycin, and Clarithromycin) and	
	β-Lactam antibiotics (Cephalosporins and Carbapenem)	
II.	a) Alkaloids	12 hrs
	General introduction, classification, isolation, purification, molecular modification and biological activity of alkaloids, general methods of structural determination of alkaloids, structural elucidation and stereochemistry of ephedrine, morphine, ergot, emetine	
	and reserpine.	
	b) Flavonoids	

Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin. c) 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). 18 hrs III. a) Terpenoids 18 hrs Classification, isolation, isoprene rule and general methods of structural elucidation of Terpenoids; Structural clucidation of drugs belonging to mono (citral, menthol, camphor), di(retinol, Phytol, taxol) and triterpenoids (Squalene, Ginsenoside) carotinoids (β carotene). 18 hrs b) Vitamins Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin. 6 c) Recombinant DNA technology and drug discovery rDNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. 18 hrs IV. a) 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. 18 hrs b) Structural Characterization of natural compounds Structural Characterization of natural compounds 60 hours			1
 III. a) Terpenoids Classification, isolation, isoprene rule and general methods of structural elucidation of Terpenoids; Structural elucidation of drugs belonging to mono (citral, menthol, camphor), di(retinol, Phytol, taxol) and triterpenoids (Squalene, Ginsenoside) carotinoids (β carotene). b) Vitamins Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin. c) Recombinant DNA technology and drug discovery rDNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, Clinical application and recent advances in gene therapy, principles of RNA & DNA estimation. IV. a) Active constituent of certain crude drugs used in Indigenous system Diabetic therapy – Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graecum; Liver dysfunction – Phyllanthus niruri; Antitumor – Curcuma longa Linn. b) Structural Characterization of natural compounds 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. 		 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 	
 Classification, isolation, isoprene rule and general methods of structural elucidation of Terpenoids; Structural elucidation of drugs belonging to mono (citral, menthol, camphor), di(retinol, Phytol, taxol) and triterpenoids (Squalene, Ginsenoside) carotinoids (β carotene). b) Vitamins Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin. c) Recombinant DNA technology and drug discovery rDNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, Clinical application and recent advances in gene therapy, principles of RNA & DNA estimation. IV. a) 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. b) 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. 	ш		10 hm
 Indigenous system Diabetic therapy – Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum; Liver dysfunction – Phyllanthus niruri; Antitumor – Curcuma longa Linn. b) Structural Characterization of natural compounds 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. 	111.	 Classification, isolation, isoprene rule and general methods of structural elucidation of Terpenoids; Structural elucidation of drugs belonging to mono (citral, menthol, camphor), di(retinol, Phytol, taxol) and triterpenoids (Squalene, Ginsenoside) carotinoids (β carotene). b) Vitamins Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin. c) Recombinant DNA technology and drug discovery rDNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, Clinical application and recent advances in gene therapy, principles of RNA & 	18 hrs
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TOTAL 60 hours		 Indigenous system Diabetic therapy – Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum; Liver dysfunction – Phyllanthus niruri; Antitumor – Curcuma longa Linn. b) Structural Characterization of natural compounds 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. 	
		TOTAL	60 hours

- 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 W ells, 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. Elements of Biotechnology by P.K. Gupta, Rastogi Publishers.
- 12. Biotechnology by Purohit and Mathur, Agro-Bios, 13th edition.

Reference Books:

- 1. Organic Chemistry Vol I and II by I.L. Finar, Pearson education.
- 2. Pharmaceutical Biotechnology by S.P. Vyas and V.K. Dixit, CBS Publishers.
- 3. Phytochemical methods of Harborne, Springer, Netherlands.
- 4. Burger's Medicinal Chemistry.

Teaching Learning Process and Assessment Methods

Unit No.	Course Learning Outcomes	Teaching and Learning Activity	Assessment Tasks
I.	CO1: Students will learn the different types of natural products as leads for new pharmaceuticals.	Teaching will be conducted both through black board mode and power point presentation mode.	Oral questions will be asked in the class. Students will be given to prepare power point presentation on the assigned topics related to the class teachings.
II.	CO2: Students will understand the importance of natural compounds as lead molecules for new drug discovery.	Teaching will be conducted both through black board mode and power point presentation mode.	Unit assessment by multiple choice questions (MCQs), internal assessments, Question answer sessions.
III.	CO3: Understand the concept of rDNA technology tool for new drug discovery.	Traditional teaching and regular discussion and power point presentations.	Regular question answer sessions, and Unit-test for internal assessment
IV.	CO2, CO4: Study the general methods of structural elucidation of compounds and know the isolation, purification and characterization of simple chemical constituents from natural source.	Class conduction using board and power point presentation.	Class tests, Quiz, Assignments.

PHARMACEUTICAL CHEMISTRY PRACTICAL I (MPC105P)

12 Hours/Week

Modules	s Topics (if applicable) & Course Contents			
I.	 Analysis of Pharmacopoeial compounds and their formulations by UV Vis spectrophotometer, RNA & DNA estimation. Simultaneous estimation of multi component containing formulations by UV spectrophotometry. Experiments based on Column chromatography. Experiments based on HPLC. Experiments based on Gas Chromatography. Estimation of riboflavin/quinine sulphate by fluorimetry. Estimation of sodium/potassium by flame photometry. 	12 hrs/wk		
П.	 To perform the following reactions of synthetic importance 8. Purification of organic solvents, column chromatography. 9. Claisen-schimidt reaction. 10. Benzyllic acid rearrangement. 11. Beckmann rearrangement. 12. Hoffmann rearrangement. 13. Mannich reaction. 	12 hrs/wk		
III.	14. Synthesis of medicinally important compounds involving more than one step along with purification and Characterization using TLC, melting point and IR spectroscopy (4 experiments)	12 hrs/wk		
IV.	 15. Estimation of elements and functional groups in organic natural compounds. 16. 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. 17. Some typical degradation reactions to be carried on selected plant constituents. 	12 hrs/wk		
TOTAL 18				

Paper I / Subject Name: ADVANCED SPECTRAL ANALYSIS (MPC 201T)

L-T-P-C – 4-0-0-4 Credit Units: 4 Scheme of Evaluation: (T)

Objective: 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.

Course Outcome: At completion of this course, it is expected that students will be able to understand

CO1: Interpretation of the UV, IR, and NMR spectra of various organic compounds.

CO2: Interpretation of the Mass spectra of various organic compounds.

CO3: Theoretical and practical skills of the hyphenated instruments.

CO4: Identification of organic compounds.

Modules	Topics (if applicable) & Course Contents	Periods
I.	UV and IR spectroscopy	15 hrs
	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.	
	NMR spectroscopy	
	1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE	
	techniques, Interpretation of organic compounds.	
II.	Mass Spectroscopy	15 hrs
	Mass fragmentation and its rules, Fragmentation of important	
	functional groups like alcohols, amines, carbonyl groups and alkanes,	
	Meta stable ions, Mc Lafferty rearrangement, Ring rule, Isotopic	
	peaks, Interpretation of organic compounds.	
III.	Chromatography	15 hrs
	Principle, Instrumentation and Applications of the following:	
	a) GC-MS b) GC-AAS c) LC-MS d) LC-FTIR e) LC-NMR f) CEMS	
	g) High Performance Thin Layer chromatography h) Super critical	
	fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion	
	Chromatography) k) Flash chromatography	
IV.	Thermal methods of analysis	15 hrs
	Introduction, principle, instrumentation, and application of DSC,	
	DTA and TGA.	

Raman Spectroscopy	
Introduction, Principle, Instrumentation and Applications.	
Radio immuno assay	
Biological standardization, bioassay, ELISA, Radioimmuno assay of	
digitalis and insulin.	
TOTAL	60 hours

- 1. Organic Spectroscopy William Kemp, 3rd edition, ELBS, 1991.
- 2. Quantitative analysis of pharmaceutical formulations by HPTLC P D Sethi, CBS Publishers, New Delhi.
- 3. Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
- 4. Pharmaceutical Analysis- Modern methods Part B J W Munson, Volume 11, Marcel Dekker Series 87.

Reference Books:

- 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, 5th edition, Eastern press, Bangalore, 1998.
- 3. Instrumental methods of analysis Willards, 7th edition, CBS publishers.

Unit	Course Learning	Teaching and Learning	Assessment Tasks
No.	Outcomes	Activity	
I.	CO1, CO4: Students will be	Traditional chalk and board	Unit assessment by
	able to understand the different	teaching and power point	multiple choice
	types of spectroscopies such as	presentations.	questions (MCQ),
	UV, IR, NMR spectroscopy,		internal assessments,
	and Interpretation of organic		regular question answer
	compounds.		session, seminar.
II.	CO2, CO4: Students will be	Traditional chalk and board	MCQs, regular
	able to understand about mass	teaching, power point	discussions, internal
	spectrometry and Interpretation	presentations.	assessments, seminar.
	of organic compounds.		
III.	CO3: Students will be able to	Traditional teaching and	Test and MCQs,
	understand various	regular discussions and	assignments, internal
	chromatographic techniques	power point presentation	assessments, seminar.
	and their principle,		
	instrumentation, and		
	applications.		
IV.	CO4: Students will be able to	Class conduction using	Test and MCQs,
	understand thermal methods of	board and power point	assignments, internal
	analysis, Raman spectroscopy,	presentation.	assessments, seminar.
	and Radio immune assays.		

Teaching Learning Process and Assessment Methods

Paper II / Subject Name: ADVANCED ORGANIC CHEMISTRY-II (MPC 202T)

L-T-P-C – 4-0-0-4	Credit Units: 4	Scheme of Evaluation: (T)
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Objective: 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.

Course Outcome: At completion of this course, it is expected that students will be able to understand

CO1: The principles and applications of Green chemistry.

CO2: The concept of peptide chemistry.

- **CO3:** The various catalysts used in organic reactions.
- CO4: The concept of stereochemistry and asymmetric synthesis.

Modules	Topics (if applicable) & Course Contents	Periods		
I.	Green Chemistry	15 hrs		
	Introduction, principles of green chemistry.			
	Microwave assisted reactions			
	Merit 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			
	heterocycles synthesis.			
	Ultrasound assisted reactions			
	Types of sonochemical reactions, homogenous, heterogeneous			
	liquid-liquid and liquid-solid reactions, synthetic applications.			
	Continuous flow reactors			
	Working principle, advantages, and synthetic applications.			
II.	Chemistry of peptides	15 hrs		
	Coupling reactions in peptide synthesis.			
	• Principles of solid phase peptide synthesis, t-BOC and FMOC			
	protocols, various solid supports and linkers: Activation			
	procedures, peptide bond formation, deprotection and			
	cleavage from resin, low and high HF cleavage protocols,			
	formation of free peptides and peptide amides, purification and			
	case studies, site-specific chemical modifications of peptides.			

trocyclic reaction and sigmatrophic rearrangement reactions in examples. Types of catalysis, heterogeneous and homogenous catalysis, advantages, and disadvantages. Heterogeneous catalysis – preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs. 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. Transition-metal and Organo-catalysis in organic synthesis: Metal-catalyzed reactions. Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction. Phase transfer catalysis - theory and applications reochemistry & Asymmetric Synthesis 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. Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation and Stereo selective synthesis with examples.	12 hrs
h examples. alysis Types of catalysis, heterogeneous and homogenous catalysis, advantages, and disadvantages. Heterogeneous catalysis – preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs. 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. Transition-metal and Organo-catalysis in organic synthesis: Metal-catalyzed reactions. Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction. Phase transfer catalysis - theory and applications reochemistry & Asymmetric Synthesis 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. Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure	12 hrs
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trooxialia reaction and giamatrachia reamon compart reactions	
otochemical Reactions	18 hrs
overactivation and side reactions of individual amino acids.	
reactions initiated by proton abstraction, protonation,	
Side reactions in peptide synthesis: Deletion peptides, side	
synthesis with any two case studies.	
	Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, overactivation and side reactions of individual amino acids.

- 1. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Sixth ed., 1995.
- 2. Carey, Organic chemistry, 5th edition (Viva Books Pvt. Ltd.)
- 3. Organic synthesis-the disconnection approach, S. Warren, Wily India
- 4. Principles of organic synthesis, ROCNorman and JMCoxan, Nelson thorns
- 5. Organic synthesis- Special techniques VK Ahluwalia and R Aggarwal, Narosa Publishers.
- 6. Organic reaction mechanisms IV edtn, VK Ahluwalia and RK Parashar, Narosa Publishers.

Reference Books:

- 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 2001.

Unit	Course Learning	Teaching and Learning	Assessment Tasks
No.	Outcomes	Activity	
I.	CO1: Students will be able to	Traditional chalk and	Unit assessment by
	understand about the green	board teaching and power	multiple choice
	chemistry, microwave assisted	point presentations.	questions (MCQs),
	reactions, ultrasound assisted		internal assessments,
	reactions, Continuous flow		regular question answer
	reactors.		session, seminar.
II.	CO2: Students will be able to	Traditional chalk and	MCQs, regular
	understand about Coupling	board teaching, power	discussions, internal
	reactions in peptide synthesis,	point presentations.	assessments, seminar.
	principles of solid phase		
	peptide synthesis, solution		
	phase peptide synthesis.		-
III.	CO3: Students will be able to	Traditional teaching and	-
	understand the basic principles	regular discussions and	assignments, internal
	of photochemical reactions.	power point	assessments, seminar.
	photo-oxidation, photo-	presentations.	
	addition, and photo-		
	fragmentation, types of		
	catalysis, heterogeneous and		
	homogenous catalysis,		
	advantages, and		
IV.	disadvantages. CO4: Students will be able to	Class conduction using	Test and MCQs,
1.	understand transition-metal	board and power point	assignments, internal
	and Organo-catalysis in	presentations.	assessments, seminar.
	organic synthesis: Metal-	presentations.	assessments, semmar.
	catalyzed reactions,		
	biocatalysis, Stereochemistry		
	& Asymmetric Synthesis.		
	& Asymmetric Synthesis.		

Teaching Learning Process and Assessment Methods

Paper III / Subject Name: COMPUTER AIDED DRUG DESIGN (MPC 203T)

L-T-P-C – 4-0-0-4 Credit Units: 4 Scheme of Evaluation: (T)

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

Course Outcome: At completion of this course, it is expected that students will be able to understand.

CO1: Role of CADD in drug discovery.

CO2: Different CADD techniques and their applications.

CO3: Various strategies to design and develop new drug like molecules.

CO4: Working with molecular modeling software's to design new drug molecules and the in silico virtual screening protocols.

Modules	Topics (if applicable) & Course Contents	Periods
I.	Introduction to Computer Aided Drug Design (CADD)	12 hrs
	History, different techniques and applications.	
	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.	
II.	Quantitative Structure Activity Relationships: Applications	12 hrs
	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.	
III.	Molecular Modeling and Docking	18 hrs
	 Molecular and Quantum Mechanics in drug design. 	
	• Energy Minimization Methods: comparison between global	
	minimum conformation and bioactive conformation.	
	• Molecular docking and drug receptor interactions: Rigid	
	docking, flexible docking and extra-precision docking.	

 Agents acting on enzymes such as DHFR, HMG reductase and HIV protease, choline esterase (AchE & B Prediction and analysis of ADMET properties of molecules and its importance in drug design. 	chE).
 IV. Molecular Properties and Drug Design De novo drug design: Receptor/enzyme-interaction and analysis, Receptor/enzyme cavity size prediction, prediction the functional components of cavities, Fragment based design. Homology modeling and generation of 3D-structure protein. 	cting drug
Pharmacophore Mapping and Virtual Screening Concept of pharmacophore, pharmacophore map identification of Pharmacophore features and Pharmacop modeling; Conformational search used in pharmacop 	bhore bhore
structure based In-silico virtual screening protocols.	
TOTAL	60 hours

- 1. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
- 2. Medicinal Chemistry by Burger, Wiley Publishing Co.
- 3. An Introduction to Medicinal Chemistry Graham L. Patrick, Oxford University Press.
- 4. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.
- 5. Comprehensive Medicinal Chemistry Corwin and Hansch, Pergamon Publishers.
- 6. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore.

Reference Books:

- 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, 1975, Elsevier Publishers.
- 4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.

Teaching Learning Process and Assess	nent Methods
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Unit	Course Learning	Teaching and	Assessment Tasks
No.	Outcomes	Learning	
		Activity	
I.	CO1, CO2: Students will be able to understand Computer Aided Drug Design (CADD) and the role of CADD in drug discovery.	Traditional chalk and board teaching and power point presentations.	Unit assessment by multiple choice questions (MCQ), internal assessments, regular question answer session, seminar.
II.	CO1, CO2: Students will be able to understand QSAR, 2D-QSAR, 3D- QSAR and the different CADD techniques and their applications.	Traditional chalk and board teaching, power point presentations.	MCQs, regular discussions, internal assessments, seminar.
III	CO3, CO4: Students will be able to understand the Various strategies to design and develop new drug like molecules.	Traditional teaching and regular discussions and power point presentations.	Test and MCQs, assignments, internal assessments, seminar.
IV	CO3, CO4: Students will be able to understand the working with molecular modeling softwares to design new drug Molecules and the <i>in silico</i> virtual screening protocols.	Class conduction using board and power point presentation.	Test and MCQs, assignments, internal assessments, Seminar.

Paper IV / Subject Name: PHARMACEUTICAL PROCESS CHEMISTRY (MPC 204T)

L-T-P-C – 4-0-0-4 Credit Units: 4 Scheme of Evaluation: (T)

Objective: 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.

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

CO1: The strategies of scale up process of APIs and intermediates.

CO2: The various unit operations in process chemistry.

CO3: The various reactions in process chemistry.

CO4: The various industrial safety management.

Modules	Topics (if applicable) & Course Contents	Periods
I.	Process chemistry Introduction, Synthetic strategy 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 AP Is. Impurities in API, types and their sources including genotoxic impurities	12 hrs
II.	 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. 	12 hrs

	• Crystallization: Crystallization from aqueous, non-aqueous		
	solutions factors affecting crystallization, nucleation. Principle		
	and general methods of P reparation of polymorphs, hydrates,		
	solvates and amorphous APIs.		
III.	Unit Processes-I	18 hrs	
	• Nitration: Nitrating agents, Aromatic nitration, kinetics and		
	mechanism of aromatic nitration, process equipment for		
	technical nitration, mixed acid for nitration.		
	• Halogenation : Kinetics of halogenations, types of		
	halogenations, catalytic halogenations. Case study on		
	industrial halogenation process.		
	• Oxidation: Introduction, types of oxidative reactions, Liquid		
	phase oxidation with oxidizing agents. Nonmetallic		
	Oxidizing agents such as H ₂ O ₂ , sodium hypochlorite, Oxygen		
	gas, ozonolysis.		
	Unit Processes-II		
	• 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		
IV.	Unit Processes-II	18 hrs	
	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.		
	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	60 hours	
TOTAL			

- 1. Process Chemistry in the Pharmaceutical Industry : Challenges in an Ever-Changing Climate-An Overview; K. Gadamasetti, CRC Press.
- 2. Medicinal Chemistry by Burger, 6 edition, Volume 1-8.
- 3. W.L. McCabe, J.C Smith, Peter Harriott. Unit operations of chemical engineering, 7th edition, McGraw Hill
- 4. Polymorphism in Pharmaceutical Solids. Dekker Series Volume 95 Ed: H G Brittain (1999)
- 5. Regina M. Murphy: Introduction to Chemical Processes: Principles, Analysis, Synthesis
- 6. Peter J. Harrington: Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale-Up
- 7. P. H. Groggins : Unit processes in organic synthesis (MGH)
- 8. F. A. Henglein : Chemical Technology (Pergamon)
- 9. M. Gopal : Dryden's Outlines of Chemical Technology, WEP East-West Press
- 10. Lowenheim & M.K. Moran: Industrial Chemicals
- 11. S.D. Shukla & G.N. Pandey: A text book of Chemical Technology Vol. II, Vikas Publishing House
- 12. J.K. Stille: Industrial Organic Chemistry (PH)

Reference Books:

- 1. Pharmaceutical Manufacturing Encyclopedia, 3 edition, Volume 2.
- 2. Clausen, Mattson : Principle of Industrial Chemistry, Wiley Publishing Co.
- 3. Shreve: Chemical Process, Mc Grawhill.
- 4. B. K. Sharma: Industrial Chemistry, Goel Publishing House
- 5. ICH Guidelines
- 6. United States Food and Drug Administration official website www.fda.gov

Unit	Course Learning	Teaching and Learning	Assessment Tasks	
No.	Outcomes	Activity		
I.	CO1: Students will be able to	Traditional chalk and board	Unit assessment by	
	understand about process	teaching and power point	multiple choice	
	chemistry, stages of scale up	presentations.	questions (MCQ),	
	process, case studies of scale up		internal assessments,	
	process of APIs and about the		regular question answer	
	impurities in API.		session, seminar.	
II.	CO2: Students will learn about	Traditional chalk and board	MCQs, regular	
	the various unit operations.	teaching, power point	discussions, internal	
		presentations.	assessments, seminar.	
III.	CO3: Students will learn about	Traditional teaching and	Test and MCQs,	
	the various unit processes.	regular discussions and	assignments, internal	
		power point presentation	assessments, seminar.	
IV.	CO3, CO4: Students will learn	Class conduction using	Test and MCQs,	
	about the various unit processes	board and power point	assignments, internal	
	and about industrial safety.	presentation.	assessments, seminar.	

Teaching Learning Process and Assessment Methods

PHARMACEUTICAL CHEMISTRY PRACTICALS – II (MPC 205P)

12 Hours/Week

Modules	Topics (if applicable) & Course Contents	Periods
I.	 Synthesis of organic compounds by adapting different approaches (3 experiments): a) Oxidation b) Reduction/hydrogenation c) Nitration Comparative study of synthesis of APIs/intermediates by different synthetic routes (2 experiments) 	12 hrs/wk
II.	 3. Assignments on regulatory requirements in API (2 experiments) 4. Comparison of absorption spectra by UV and Woodward-Fieser rule 5. Interpretation of organic compounds by FT-IR 6. Interpretation of organic compounds by NMR 7. Interpretation of organic compounds by MS 	12 hrs/wk
III.	 8. Determination of purity by DSC in pharmaceuticals 9. Identification of organic compounds using FT-IR, NMR, CNMR, and Mass spectra 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 	12 hrs/wk
IV.	 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 Pharmacophore modeling 18. 2D-QSAR based experiments 19. 3D-QSAR based experiments 20. Docking study-based experiment 21. Virtual screening-based experiment 	12 hrs/wk
	180 hours	