

# Scheme and Syllabus

## M. Pharmacy Pharmaceutical Chemistry

Batch 2017 onwards



# PTU

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By  
Board of Studies Pharmacy  
Department of Academics

### First Semester

Course Code	Course Name	L	P	Marks			Credits
				Internal	External	Total	
MPC101T	Modern Pharmaceutical Analytical Techniques	4	-	25	75	100	4
MPC102T	Advanced Organic Chemistry -I	4	-	25	75	100	4
MPC103T	Advanced Medicinal Chemistry	4	-	25	75	100	4
MPC104T	Chemistry of Natural Products	4		25	75	100	4
MPC105P	Pharmaceutical Chemistry Practical I	-	12	50	100	150	6
-	Seminar/Assignment <sup>#</sup>	-	7	-	-	100	4
<b>Total</b>		<b>16</b>	<b>19</b>	<b>150</b>	<b>400</b>	<b>650</b>	<b>26</b>

- # Minimum five seminar/assignment each of 20 marks per semester

### Second Semester

Course Code	Course Name	L	P	Marks			Credits
				Internal	External	Total	
MPC201T	Advanced Spectral Analysis	4	-	25	75	100	4
MPC202T	Advanced Organic Chemistry -II	4	-	25	75	100	4
MPC203T	Computer Aided Drug Design	4	-	25	75	100	4
MPC204T	Pharmaceutical Process Chemistry	4		25	75	100	4
MPC205P	Pharmaceutical Chemistry Practical II	-	12	50	100	150	6
-	Seminar/Assignment <sup>#</sup>	-	7	-	-	100	4
<b>Total</b>		<b>16</b>	<b>19</b>	<b>150</b>	<b>400</b>	<b>650</b>	<b>26</b>

- # Minimum five seminar/assignment each of 20 marks per semester

### Third Semester

Course Code	Course Name	L	P	Marks			Credits
				Internal	External	Total	
MRM301T	Research Methodology & Biostatistics*	4	-	25	75	100	4
-	Journal Club	1	-	25	-	25	1
-	Discussion / Presentation (Proposal Presentation)	2	-	50	-	50	2
-	Research Work*	-	28	-	350	350	14
<b>Total</b>		<b>7</b>	<b>28</b>	<b>100</b>	<b>425</b>	<b>525</b>	<b>21</b>

- \*Non -University Exam

### Fourth Semester

Course Code	Course Name	L	P	Marks			Credits
				Internal	External	Total	
-	Journal Club	1	-	25	-	25	1
-	Research Work	-	31	-	400	400	16
-	Discussion/Final Presentation	3	-	75	-	75	3
-	Co-curricular Activities	-	-	Satisfactory/Unsatisfactory			2*
<b>Total</b>		<b>4</b>	<b>31</b>	<b>100</b>	<b>400</b>	<b>500</b>	<b>22</b>

*\*Note: Required credit points 02 for satisfactory; Less than 02 credit points unsatisfactory*

**\*Credits not included towards calculation of CGPA**

### Semester Wise Credits Distribution

Semester	Credit Points
I	26
II	26
III	21
IV	20
Co-curricular Activities (Attending Conference, Scientific Presentations & Other Scholarly Activities)	02*
<b>Total Credit Points</b>	<b>93 + 2* = 95</b>

- \*Credit Points for Co-curricular Activities
- \*Credits not included towards calculation of CGPA
- \*The credit points assigned for extracurricular and or co-curricular activities shall be given by the Principals of the colleges and the same shall be submitted to the University

## **Guidelines for Awarding Credit Points for Co-curricular Activities**

<b>Name of the Activity</b>	<b>Maximum Credit Points</b>
Participation in National Level Seminar/ Conference/ Workshop/ Symposium/ Training Programs (related to the specialization of the student) OR Academic Award/Research Award from State Level/National Agencies	02
Participation in International Level Seminar/ Conference/ Workshop/ Symposium / Training Programs (related to the specialization of the student) #	02
Academic Award/Research Award from International Agencies	02
Research / Review Publication in National Journals (Indexed in Scopus / Web of Science)*	01
Research / Review Publication in International Journals (Indexed in Scopus / Web of Science)*\$	02

- #International Conference held even in India will be considered for award of Credit Points.
- \*Only those research / review publications will be considered which have been published during the tenure of M. Pharm. Course.
- \$ International Journal: The Editorial Board outside India.

### **Academic Work**

The department / teaching staff of respective courses shall maintain a regular record of attendance in Theory, Practical, Seminar, Assignment, Journal Club, and Discussion with the supervisor, Research work presentation and Dissertation.

### **Program Committee**

1. M. Pharm. Programme shall have a Programme Committee constituted by the Head of the Institution in consultation with all the Heads of the departments.
2. The composition of the Programme Committee shall be as follows:
  - a. A teacher at the cadre of Professor shall be the Chairperson
  - b. One Teacher from each M. Pharm. Specialization
  - c. Four student representatives (two from each academic year), nominated by the Head of the Institution
3. Duties of the Programme Committee:
  - a. Periodically review the progress of the classes.
  - b. Discuss the problems concerning curriculum, syllabus and the conduct of classes.
  - c. Discussing with the course teachers on the nature and scope of assessment for the course and the same shall be announced to the students at the beginning of respective semesters.

### **Sessional Exams**

- ❖ Two sessional exams shall be conducted for each theory/practical course.
- ❖ The average marks of two sessional exams shall be computed for internal assessment.
- ❖ Sessional exam shall be **conducted for 30 marks** for theory and shall be **computed for 15 marks**.
- ❖ Sessional exam for practical shall be **conducted for 40 marks** and shall be **computed for 30 marks**.

### **Question Paper Pattern for Theory Sessional Examinations**

Multiple Choice Questions (MCQs)	10 x 1 = 10
<b>OR</b>	<b>OR</b>
Objective Type Questions (5 x 2) (Answer all the questions)	05 x 2 = 10
Short Answers (Answer 2 out of 3)	2 x 5 = 10
Long Answers (Answer 1 out of 2)	1 x 10 = 10
<b>Total</b>	<b>30 Marks</b>

### **Question Paper Pattern for Practical Sessional Examinations**

Synopsis	10
Experiments	25
Viva voce	05
<b>Total</b>	<b>40 Marks</b>

### Internal Assessment

- ❖ The internal assessment will have two components i.e. **Continuous Mode** and **Sessional Exams**

1. Theory Courses having Internal of 25 Marks the scheme of internal award is:

- Sessional Exams: 15 Marks
- Continuous Mode: 10 Marks

#### Continuous Mode Scheme

Criteria	Maximum Marks
*Attendance (as per table given below)	08
Student – Teacher interaction	02
<b>Total</b>	<b>10</b>

2. Practical Courses having Internal of 50 Marks the scheme of internal award is:

- Sessional Exams: 30 Marks
- Continuous Mode: 20 Marks

#### Continuous Mode Scheme

Criteria	Maximum Marks
*Attendance (as per table given below)	10
Based on Practical Records, Regular viva voce, etc.	10
<b>Total</b>	<b>20</b>

#### **\*Guidelines for the Allotment of Marks for Attendance**

Percentage of Attendance	Theory (Maximum Marks 08)	Practical (Maximum Marks 10)
95 – 100	08	10
90 – 94	06	7.5
85 – 89	04	5
80 – 84	02	2.5
Less than 80	0	0

# **1<sup>st</sup> SEMESTER**

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC101T	Modern Pharmaceutical Analytical Techniques	4	-	25	75	1	3	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

1. About chemicals and excipients.
2. The analysis of various drugs in single and combination dosage forms.
3. Theoretical and practical skills of the instruments.

### Module 01

**10 Hour**

#### UV-Visible Spectroscopy

- Introduction, Theory, Laws, and Instrumentation associated with UV-Visible spectroscopy
- Choice of solvents and solvent effect
- 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
- Applications of IR spectroscopy, data interpretation

#### Spectrofluorimetry

- Theory of Fluorescence
- Factors affecting fluorescence (characteristics of drugs that can be analysed by fluorimetry), Quenchers, Instrumentation
- Applications of fluorescence spectrophotometer

#### Flame Emission Spectroscopy and Atomic Absorption Spectroscopy

- Principle, Instrumentation, Interferences and Applications

### Module 02

**10 Hours**

#### NMR Spectroscopy

- Quantum numbers and their role in NMR
- Principle, Instrumentation, Solvent requirement in NMR
- Relaxation process, NMR signals in various compounds
- Chemical shift, Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance
- Brief outline of principles of FT-NMR and <sup>13</sup>C NMR



- Applications of NMR spectroscopy

**Module 03**

**10 Hours**

**Mass Spectroscopy**

- Principle, Theory, Instrumentation of Mass Spectroscopy
- Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight
- Mass fragmentation and its rules
- Meta stable ions
- Isotopic peaks
- Applications of Mass spectroscopy

**Module 04**

**10Hours**

**Chromatography**

Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following:

- Thin Layer chromatography
- Ion exchange chromatography
- Column chromatography
- Gas chromatography
- High Performance Liquid chromatography
- Ultra High Performance Liquid chromatography
- Affinity chromatography
- Gel Chromatography

**Module 05**

**10Hours**

**Electrophoresis**

Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following:

- Paper electrophoresis
- Gel electrophoresis
- Capillary electrophoresis
- Zone electrophoresis
- Moving boundary electrophoresis
- Isoelectric focusing

**X ray Crystallography**

- Production of X rays
- Different X ray diffraction methods
- Bragg's law, Rotating crystal technique, X ray powder technique
- Types of crystals and applications of X-ray diffraction

**Module 06**

**10 Hours**

**Potentiometry**

- Principle, working, ion selective electrodes
- Application of potentiometry

**Thermal Techniques**

- Principle, thermal transitions and instrumentation (Heat flux and power-compensation and designs)
- Modulated DSC, Hyper DSC
- Experimental parameters (sample preparation, experimental conditions, calibration, heating and cooling rates, resolution, source of errors) and their influence
- Advantage and disadvantages
- Pharmaceutical applications

**Differential Thermal Analysis (DTA)**

- Principle, instrumentation
- Advantage and disadvantages
- Pharmaceutical applications
- Derivative differential thermal analysis (DDTA)

**TGA**

- Principle, instrumentation
- Factors affecting results
- Advantage and disadvantages
- Pharmaceutical applications

**Recommended Books (Latest editions)**

1. Spectrometric Identification of Organic Compounds - Robert M Silverstein, John Wiley & Sons.
2. Principles of Instrumental Analysis - Douglas A Skoog, F. James Holler, Timothy A. Nieman, Eastern press, Bangalore.
3. Instrumental methods of analysis – Willards, CBS publishers.
4. Practical Pharmaceutical Chemistry – Beckett and Stenlake, Vol II, CBS Publishers, New Delhi.
5. Organic Spectroscopy - William Kemp, ELBS.
6. Quantitative Analysis of Drugs in Pharmaceutical formulation - P D Sethi, CBS Publishers, New Delhi.
7. Pharmaceutical Analysis- Modern methods – Part B - J W Munson, Volume 11, Marcel Dekker Series.
8. Spectroscopy of Organic Compounds, P.S. Kalsi, Wiley Estern Ltd., Delhi.
9. Textbook of Pharmaceutical Analysis, K. A. Connors, John Wiley & Sons.

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC102T	Advanced Organic Chemistry - I	4	-	25	75	1	3	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 the course, student shall be able to understand

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

### Module 01

**12Hours**

#### Basic Aspects of Organic Chemistry

- Organic intermediates: carbocations, carbanions, free radicals, carbenes and nitrenes.
- Their method of formation, stability and synthetic applications
- Types of reaction mechanisms and methods of determining them
- Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations

#### Addition Reactions

- Nucleophilic uni-molecular and bimolecular reactions (SN1 and SN2)
- Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)
- Rearrangement Reaction

### Module 02

**12Hours**

#### 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, Vilsmeier-Haack Reaction, Sharpless asymmetric epoxidation, Baeyer-Villiger oxidation, Shapiro & Suzuki reaction, Ozonolysis and Michael addition reaction

### Module 03

**12Hours**

#### Synthetic Reagents and Applications

- Aluminiumisopropoxide, N-bromosuccinamide, diazomethane, dicyclohexylcarbodiimide, Wilkinson reagent, Wittig reagent, Osmium tetroxide, titanium chloride, diazopropane, diethyl azodicarboxylate, Triphenylphosphine, Benzotriazol-1-yloxy) tris (dimethylamino) phosphonium hexafluoro-phosphate (BOP)

#### Protecting Groups

- Role of protection in organic synthesis
- Protection for the hydroxyl group, including 1,2-and 1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals
- Protection for the Carbonyl Group: Acetal and Ketals
- Protection for the Carboxyl Group: amides and hydrazides, esters
- Protection for the Amino Group and Amino acids: carbamates and amides

#### **Module 04**

**12Hours**

##### **Heterocyclic Chemistry**

- Organic Name reactions with their respective mechanism and application involved in synthesis of drugs containing five, six membered and fused heterocyclics such as Debus-Radziszewski imidazole synthesis, Knorr Pyrazole Synthesis, Pinner Pyrimidine Synthesis, Combes Quinoline Synthesis, Berntsen Acridine Synthesis, Smiles rearrangement and Traube purine synthesis
- Synthesis of few representative drugs containing these heterocyclic nucleus such as Ketoconazole, Metronidazole, Miconazole, celecoxib, antipyrin, Metamizole sodium, Terconazole, Alprazolam, Triamterene, Sulfamerazine, Trimethoprim, Hydroxychloroquine, Quinine, Chloroquine, Quinacrine, Amsacrine, Prochlorperazine, Promazine, Chlorpromazine, Theophylline, Mercaptopurine and Thioguanine

#### **Module 05**

**12Hours**

##### **Synthon Approach and Retrosynthesis Applications**

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

##### **Recommended Books (Latest editions)**

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 Wothers, Oxford University Press.
4. Organic Chemistry Vol I and II. I.L. Finar. ELBS, Pearson Education Lts, Dorling Kindersley India Pvt. Ltd.
5. A guide to mechanisms in Organic Chemistry, Peter Skyes (Orient Longman, New Delhi).
6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.

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

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC103T	Advanced Medicinal Chemistry	4	-	25	75	1	3	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:** Upon completion of the course, student shall be able to understand

1. Different stages of drug discovery.
2. Role of medicinal chemistry in drug research.
3. Different techniques for drug discovery.
4. Various strategies to design and develop new drug like molecules for biological targets.
5. Peptidomimetics.

### **Module 01**

**12 Hours**

#### **Drug Discovery**

- Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets

#### **Biological Drug Targets**

- Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes

### **Module 02**

**12 Hours**

#### **Pro-drug Design and Analog Design**

- Prodrug design: Basic concept, Carrier linked prodrugs/ Bioprecursors, Prodrugs of functional group, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and distribution, site-specific drug delivery and sustained drug action. Rationale of prodrug design and practical consideration of prodrug design
- Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance
- Analog design: Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid analogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance

### **Module 03**

**12 Hours**

#### **Medicinal Chemistry Aspects of the Following Class of Drugs**

#### **Systematic Study, SAR, Mechanism of Action and Synthesis of New Generation Molecules of Following Class of Drugs**

- Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, Antineoplastic and Antiviral agents

### **Stereochemistry and Drug Action**

- Realization that stereo selectivity is a pre-requisite for evolution
- Role of chirality in selective and specific therapeutic agents
- Case studies, Enantio selectivity in drug adsorption, metabolism, distribution and elimination

### **Module 04**

**12 Hours**

#### **Rational Design of Enzyme Inhibitors**

- Enzyme kinetics & Principles of enzyme inhibitors, Enzyme inhibitors in medicine, Enzyme inhibitors in basic research, rational design of non-covalently and covalently binding enzyme inhibitors

### **Module 05**

**12 Hours**

#### **Peptidomimetics**

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

#### **Recommended Books (Latest editions)**

1. Medicinal Chemistry by Burger, Vol I–VI.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt. Ltd, New Delhi.
3. Comprehensive Medicinal Chemistry – Corwin and Hansch.
4. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moor.
5. Introduction to Quantitative Drug Design by Y.C. Martin.
6. Principles of Medicinal Chemistry by William Foye, 7th Edition, Lippincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
7. Drug Design Volumes by Arienes, Academic Press, Elsevier Publishers, Noida, Uttar Pradesh.
8. Principles of Drug Design by Smith.
9. The Organic Chemistry of the Drug Design and Drug action by Richard B.Silverman, Elsevier Publishers, New Delhi.
10. An Introduction to Medicinal Chemistry, Graham L.Patrick, Oxford University Press, USA.
11. Biopharmaceutics and pharmacokinetics, DM.Brahmankar, Sunil B. Jaiswal, Vallabh Prakashan, New Delhi.
12. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, Wiley publishers.

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC104T	Chemistry of Natural Products	4	-	25	75	1	3	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:** Upon completion of the course, it is expected that the students will be able to understand

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

### Module 01

**12 Hours**

#### Study of Natural Products as Leads for New Pharmaceuticals for the Following Class of Drugs

- Drugs affecting the Central Nervous System: Morphine Alkaloids
- Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide
- Cardiovascular Drugs: Lovastatin, Teprotide and Dicoumarol
- Neuromuscular Blocking Drugs: Curare alkaloids
- Anti-malarial drugs and Analogues
- Chemistry of macrolid antibiotics (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and  $\beta$  - Lactam antibiotics (Cephalosporins and Carbapenem)

### Module 02

**12 Hours**

#### Alkaloids

- 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

#### Flavonoids

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

#### Steroids

- General introduction, chemistry of sterols, sapogenin and cardiac glycosides
- Stereochemistry and nomenclature of steroids, chemistry of contraceptive agents male & female sex hormones (Testosterone, Estradiol, Progesterone), adrenocorticoids (Cortisone), contraceptive agents and steroids (Vit – D)



**Module 03**

**12 Hours**

**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 tri terpenoids (Squalene, Ginsenoside) carotenoids ( $\beta$  carotene)

**Vitamins**

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

**Module 04**

**12 Hours**

**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

**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

**Module 05**

**12 Hours**

**Structural Characterization of Natural Compounds**

- Structural characterization of natural compounds using IR,  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides

**Recommended Books (Latest editions)**

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, Chapmanstall.
9. Organic Chemistry of Natural Products Vol I and II by Gurdeep and Chatwall, Himalaya Publishing House.

10. Organic Chemistry of Natural Products Vol I and II by O.P. Agarwal, Krishan Prakashan.
11. Organic Chemistry Vol I and II by I.L. Finar, Pearson education.
12. Elements of Biotechnology by P.K. Gupta, Rastogi Publishers.
13. Pharmaceutical Biotechnology by S.P.Vyas and V.K.Dixit, CBS Publishers.
14. Biotechnology by Purohit and Mathur, Agro-Bios.
15. Phytochemical methods of Harborne, Springer, Netherlands.
16. Burger's Medicinal Chemistry.

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC105P	Pharmaceutical Chemistry Practical - I	-	12	50	100	6	6	6

1. Analysis of Pharmacopoeial 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
8. To perform the following reactions of synthetic importance:
  - a. Purification of organic solvents, column chromatography
  - b. Claisen-schimidt reaction
  - c. Benzylic acid rearrangement
  - d. Beckmann rearrangement
  - e. Hoffmann rearrangement
  - f. Mannich reaction
  - g. Synthesis of medicinally important compounds involving more than one step along with purification and Characterization using TLC, melting point and IR spectroscopy (4 experiments)
  - h. Estimation of elements and functional groups in organic natural compounds
  - i. 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.
  - j. Some typical degradation reactions to be carried on selected plant constituents

# **2<sup>nd</sup> SEMESTER**

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC201T	Advanced Spectral Analysis	4	-	25	75	1	3	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:** Upon completion of the course, student shall be able to understand

1. Interpretation of the NMR, Mass and IR spectra of various organic compounds.
2. Theoretical and practical skills of the hyphenated instruments.
3. Identification of organic compounds.

#### **Module 01**

**12 Hours**

##### **UV and IR spectroscopy**

- Wood ward – Fieser rule for 1,3- butadienes, cyclic dienes and  $\alpha$ ,  $\beta$ -carbonyl compounds and interpretation compounds of enones
- ATR-IR, IR Interpretation of organic compounds

#### **Module 02**

**12 Hours**

##### **NMR Spectroscopy**

- 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds

#### **Module 03**

**12 Hours**

##### **Mass Spectroscopy**

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

#### **Module 04**

**12 Hours**

##### **Chromatography**

Principle, Instrumentation and Applications of the following :

- GC-MS
- GC-AAS
- LC-MS
- LC-FTIR
- LC-NMR
- CE-MS
- High Performance Thin Layer chromatography
- Super critical fluid chromatography
- Ion Chromatography

- I-EC (Ion- Exclusion Chromatography)
- Flash chromatography

**Module 05**

**12 Hours**

**Thermal Methods of Analysis**

- 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

**Recommended Books (Latest editions)**

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

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC202T	Advanced Organic Chemistry - II	4	-	25	75	1	3	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 this course it is expected that students will be able understand

1. The principles and applications of Green chemistry.
2. The concept of peptide chemistry.
3. The various catalysts used in organic reactions.
4. The concept of stereochemistry and asymmetric synthesis.

### Module 01

**12 Hours**

#### Green Chemistry

- 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

### Module 02

**12 Hours**

#### Chemistry of Peptides

- 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
- Segment and sequential strategies for solution phase peptide synthesis with any two case studies
- Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over-activation and side reactions of individual amino acids

### Module 03

**12 Hours**

#### Photochemical Reactions

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

### **Pericyclic Reactions**

- Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction
- Sigmatropic rearrangement reactions with examples

### **Module 04**

**12 Hours**

#### **Catalysis**

- 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

### **Module 05**

**12 Hours**

#### **Stereochemistry & 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

#### **Recommended Books (Latest editions)**

1. Advanced Organic chemistry, Reaction, mechanisms and structure, J March, John Wiley and sons, New York.
2. Mechanism and structure in organic chemistry, ES Gould, Hold Rinchart and Winston, NewYork.
3. Organic Chemistry Clayden, Greeves, Warren and Woihers., Oxford University Press.
4. Organic Chemistry” Vol I and II. I.L. Finar. ELBS.
5. Carey, Organic chemistry, Viva Books Pvt. Ltd.
6. Organic synthesis-the disconnection approach, S. Warren, Wily India.
7. Principles of organic synthesis, ROC Norman and JM Coxan, Nelson Thorns.
8. Organic synthesis- Special techniques VK Ahluwalia and R Aggarwal, Narosa Publishers.
9. Organic reaction mechanisms IV edtn, VK Ahluwalia and RK Parashar, Narosa Publishers.



Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC203T	Computer Aided Drug Design	4	-	25	75	1	3	4

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

**Objectives:** Upon completion of this course, it is expected that students will be able to understand

1. Role of CADD in drug discovery.
2. Different CADD techniques and their applications.
3. Various strategies to design and develop new drug like molecules.
4. Working with molecular modeling software to design new drug molecules.

#### **Module 01**

**12 Hours**

##### **Introduction to Computer Aided Drug Design (CADD)**

- 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

#### **Module 02**

**12 Hours**

##### **Quantitative Structure Activity Relationships**

- Applications Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages; Deriving 2D-QSAR equations
- 3D-QSAR approaches and contour map analysis
- Statistical methods used in QSAR analysis and importance of statistical parameters

#### **Module 03**

**12 Hours**

##### **Molecular Modeling and Docking**

- 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-CoA reductase and HIV protease, cholinesterase (AChE & BChE)

**Module 04**

**12 Hours**

**Molecular Properties and Drug Design**

- Prediction and analysis of ADMET properties of new molecules and its importance in drug design
- 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
- Homology modeling and generation of 3D-structure of protein

**Module 05**

**12 Hours**

**Pharmacophore Mapping and Virtual Screening**

- Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features
- Pharmacophore modelling: Conformational search used in pharmacophore mapping
- *In silico* drug design and virtual screening techniques
- Similarity based methods and Pharmacophore based screening
- Structure based *in-silico* virtual screening protocols

**Recommended Books (Latest editions)**

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

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC204T	Pharmaceutical Process Chemistry	4	-	25	75	1	3	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:** Upon completion of the course, the students shall be able to understand

1. The strategies of scale up process of APIs and intermediates.
2. The various unit operations and various reactions in process chemistry.

### Module 01

**12 Hours**

#### 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 APIs
- Impurities in API, types and their sources including genotoxic impurities

### Module 02

**12 Hours**

#### Unit Operations

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

### Module 03

**12 Hours**

#### Unit Processes - I

- 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
- Non-metallic Oxidizing agents such as H<sub>2</sub>O<sub>2</sub>, sodium hypochlorite, Oxygen gas, ozonolysis

#### **Module 04**

**12 Hours**

##### **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 (B<sub>2</sub> and B<sub>12</sub>), Statins (Lovastatin, Simvastatin)

##### **Reaction Progress Kinetic Analysis**

- Streamlining reaction steps, route selection
- Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up

#### **Module 05**

**12 Hours**

##### **Industrial Safety**

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

##### **Recommended Books (Latest editions)**

1. Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate- An Overview, K. Gadamasetti, CRC Press.
2. Pharmaceutical Manufacturing Encyclopedia, Volume 2.
3. Medicinal Chemistry by Burger, Volume 1-8.
4. W. L. McCabe, J.C Smith, Peter Harriett. Unit operations of chemical engineering, McGraw Hill.
5. Polymorphism in Pharmaceutical Solids .Dekker Series Volume 95 Ed: H G Brittain.
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](http://www.fda.gov).

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MPC205P	Pharmaceutical Chemistry Practical - II	-	12	50	100	6	6	6

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

# **3<sup>rd</sup> SEMESTER**

Course Code	Course Title	Teaching Load		Marks		Exam (hrs)		Credits
		L	P	Int.	Ext.	Int.	Ext.	
MRM301T	Research Methodology & Biostatistics	4	-	25	75	1	3	4

**Module 01**

**12 Hours**

**General Research Methodology**

- Research, objective, requirements, practical difficulties, review of literature, study design, types of studies, strategies to eliminate errors/bias, controls, randomization, crossover design, placebo, blinding techniques

**Module 02**

**12 Hours**

**Biostatistics**

- Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, type of significance tests, parametric tests (students “t” test, ANOVA, Correlation coefficient, regression), non-parametric tests (wilcoxon rank tests, analysis of variance, correlation, chi square test), null hypothesis, P values, degree of freedom, interpretation of P values

**Module 03**

**12 Hours**

**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

**Module 04**

**12 Hours**

**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

**Module 05**

**12 Hours**

**Declaration of Helsinki**

- History, introduction, basic principles for all medical research, and additional principles for medical research combined with medical care



**Recommended Books (Latest editions)**

1. Basic & Clinical Biostatistics, Beth Dawson and Robert G. Trapp. Lange Medical Books/McGraw-Hill Medical Publishing Division.
2. Research Methodology, R. Panneerselvam, PHI Learning Pvt. Limited, Delhi.
3. Methods in Biostatistics, B.K. Mahajan. JAYPEE Brothers Medical Publishers (P) Ltd.
4. CPCSEA Guidelines.
5. A Handbook of Applied Statistics in Pharmacology, Katsumi Kobayashi and K. Sadasivan Pillai. CRC Press, Taylor & Francis Group.