Table 4: Course of study for M. Pharm (Pharmaceutical Chemistry)

Semester I

Course Code	**Course**	**Credit Hours**	**Credit Points**	**Hrs./wk**	**Marks**
MPC 101T	Modern Pharmaceutical Analytical Techniques	4	4	4	100
MPC 1012T	Advanced Organic Chemistry -I	4	4	4	100
MPC 103T	Advanced Medicinal chemistry	4	4	4	100
MPC 104T	Chemistry of Natural Products	4	4	4	100
MPC 105P	Pharmaceutical Chemistry Practical I	12	6	12	150
-	Seminar/Assignment	7	4	7	100
Total		**35**	**26**	**35**	**650**

Semester II

Course Code	Course	Credit Hours	Credit Points	Hrs./wk	Marks
MPC 201T	Advanced Spectral Analysis	4	4	4	100
MPC 202T	Advanced Organic Chemistry -II	4	4	4	100
MPC 203T	Computer-Aided Drug Design	4	4	4	100
MPC 204T	Pharmaceutical Process Chemistry	4	4	4	100
MPC 205P	Pharmaceutical Chemistry Practical II	12	6	12	150
-	Seminar/Assignment	7	4	7	100
Total		35	26	35	650

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PHARMACEUTICALCHEMISTRY(MPC)

MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES (MPC 101T)

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 about chemicals and excipients

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

	THEORY	60 Hrs
1.	a. UV-Visible spectroscopy: Introduction, Theory, Laws, Instrumentation associated with UV-Visible spectroscopy, Choice of solvents and solvent effect and Applications of UV-Visible spectroscopy, Difference/ Derivative spectroscopy. b. 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. c. Spectroflourimetry: Theory of Fluorescence, Factors affecting fluorescence (Characterestics of drugs that can be analysed by flourimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer. d. Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.	10 Hrs
2	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 13C NMR. Applications of NMR spectroscopy.	10 Hrs

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3	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 and Applications of Mass spectroscopy.	10 Hrs
4	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	10 Hrs
5	a.Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following: a) Paper electrophoresis b) Gel electrophoresis c) Capillary electrophoresis d) Zone electrophoresis e) Moving boundary electrophoresis f) Iso electric focusing b) X ray Crystallography: Production of X rays, Different X ray methods, Bragg's law, Rotating crystal technique, X ray powder technique, Types of crystals and applications of X-ray diffraction.	10 Hrs
6	a. Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry. b. 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	10 Hrs

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

REFERENCES

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

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ADVANCED ORGANIC CHEMISTRY - I
(MPC 102T)

Scope

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

Objectives

Upon completion of course, the student shall be to understand

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

THEORY 60 Hrs

1. Basic Aspects of Organic Chemistry: 12 Hrs
   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.

   Addition reactions

   a) Nucleophilic uni- and bimolecular reactions (SN1 and SN2)
   b) Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)
   c) Rearrangement reaction

2 Study of mechanism and synthetic applications of following named Reactions: 12 Hrs

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

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3 Synthetic Reagents & Applications: 12 Hrs

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

Protecting groups

a. Role of protection in organic synthesis
b. Protection for the hydroxyl group, including 1,2-and1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals
c. Protection for the Carbonyl Group: Acetals and Ketals
d. Protection for the Carboxyl Group: amides and hydrazides, esters
e. Protection for the Amino Group and Amino acids: carbamates and amides

4 Heterocyclic Chemistry: 12 Hrs

Organic Name reactions with their respective mechanism and application involved in synthesis of drugs containing five, six membered and fused hetrocyclics such as Debus-Radziszewski imidazole synthesis, Knorr Pyrazole Synthesis Pinner Pyrimidine Synthesis, Combes Quinoline Synthesis, Bernthsen Acridine Synthesis, Smiles rearrangement and Traube purine synthesis.

Synthesis of few representative drugs containing these hetrocyclic nucleus such as Ketoconazole, Metronidazole, Miconazole, celecoxib, antipyrin, Metamizole sodium, Terconazole, Alprazolam, Triamterene, Sulfamerazine, Trimethoprim, Hydroxychloroquine, Quinine, Chloroquine, Quinacrine, Amsacrine, Prochlorpherazine, Promazine, Chlorpromazine,Theophylline , Mercaptopurine and Thioguanine.

5 Synthon approach and retrosynthesis applications 12 Hrs

i. Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules. Functional group interconvertion and addition (FGI and FGA)
ii. C -X disconnections; C-C disconnections - alcohols and carbonyl 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.

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2. "Mechanism and Structure in Organic Chemistry", ES Gould, Hold Rinchart and Winston, New York.
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4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Pearson Education Lts, Dorling Kindersley 9India) Pvt. Ltd.,.
5. A guide to mechanisms in Organic Chemistry, Peter Skyes (Orient Longman, New Delhi).
6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.
7. Combinational Chemistry – Synthesis and applications – Stephen R Wilson & Anthony W Czarnik, Wiley – Blackwell.
8. Carey, Organic Chemistry, 5th Edition (Viva Books Pvt. Ltd.)
9. Organic Synthesis – The Disconnection Approach, S. Warren, Wily India
10. Principles of Organic Synthesis, ROC Norman and JM Coxan, Nelson Thorns.
11. Organic Synthesis – Special Techniques. VK Ahluwalia and R Agarwal, Narosa Publishers.
12. Organic Reaction Mechanisms IVth Edtn, VK Ahluwalia and RK Parashar, Narosa Publishers.

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ADVANCED MEDICINAL CHEMISTRY
(MPC 103T)

Scope

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

Objectives

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

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

THEORY 60 Hrs

1. Drug discovery: Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets. 12 Hrs

   Biological drug targets: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes.

2 Prodrug Design and Analog design: 12 Hrs

   a) 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.

   b) Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.

   c) Analog Design: Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid analogs,

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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.

3 a) Medicinal chemistry aspects of the following class of drugs 12 Hrs

Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs:

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

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

4 Rational Design of Enzyme Inhibitors 12 Hrs

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.

5 Peptidomimetics 12 Hrs

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.

REFERENCES

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2. 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. Comprehensive Medicinal Chemistry - Corwin and Hansch.
4. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore

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5. Introduction to Quantitative Drug Design by Y.C. Martin.
6. Principles of Medicinal Chemistry by William Foye, 7th Edition, Ippincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
7. Drug Design Volumes by Arienes, Academic Press, Elsevier Publishers, Noida, Uttar Pradesh..
8. Principles of Drug Design by Smith.
9. The Organic Chemistry of the Drug Design and Drug action by Richard B.Silverman, II Edition, Elsevier Publishers, New Delhi.
10. An Introduction to Medicinal Chemistry, Graham L.Patrick, III Edition, Oxford University Press, USA.
11. Biopharmaceutics and pharmacokinetics, DM.Brahmankar, Sunil B. Jaiswal II Edition, 2014, Vallabh Prakashan, New Delhi.
12. Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, First edition, Wiley publishers.

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CHEMISTRY OF NATURAL PRODUCTS
(MPC 104T)

Scope

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

Objectives

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

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

THEORY 60 Hrs

1. Study of Natural products as leads for new pharmaceuticals for the following class of drugs — 12 Hrs
   a) Drugs Affecting the Central Nervous System: Morphine Alkaloids
   b) Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide
   c) Cardiovascular Drugs: Lovastatin, Teprotide and Dicoumarol
   d) Neuromuscular Blocking Drugs: Curare alkaloids
   e) Anti-malarial drugs and Analogues
   f) Chemistry of macrolid antibiotics (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and β - Lactam antibiotics (Cephalosporins and Carbapenem)
2. a) Alkaloids — 12 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.

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b) Flavonoids

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

c) Steroids

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

3	a) Terpenoids 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) carotinoids (β carotene). b) Vitamins Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin.	12 Hrs
4	a). 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 b). Active constituent of certain crude drugs used in Indigenous system Diabetic therapy – Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum; Liver dysfunction – Phyllanthus niruri; Antitumor – Curcuma longa Linn.	12 Hrs
5	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.	12 Hrs

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4. Chemistry of natural products Vol I onwards IWPAC.
5. Natural Product Chemistry Nakanishi Gggolo, University Science Books, California.
6. Natural Product Chemistry "A laboratory guide" – Rapheal Khan.
7. The Alkaloid Chemistry and Physiology by RHF Manske, Academic Press.
8. Introduction to molecular Phytochemistry – CHJ Wells, Chapmannstall.
9. Organic Chemistry of Natural Products Vol I and II by Gurdeep and Chatwall, Himalaya Publishing House.
10. Organic Chemistry of Natural Products Vol I and II by O.P. Agarwal, Krishan Prakashan.
11. Organic Chemistry Vol I and II by I.L. Finar, Pearson education.
12. Elements of Biotechnology by P.K. Gupta, Rastogi Publishers.
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14. Biotechnology by Purohit and Mathur, Agro-Bios, 13th edition.
15. Phytochemical methods of Harborne, Springer, Netherlands.
16. Burger's Medicinal Chemistry.

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PHARMACEUTICAL CHEMISTRY PRACTICAL - I
(MPC 105P)

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

To perform the following reactions of synthetic importance

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

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