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

Course Code	Course	Credit Hours	Credit Points	Hrs./wk	Marks
SEMESTER I					
MPAT101T	Modern Pharmaceutical Analytical Techniques	4	4	4	100
MPC1012T	Advanced Organic Chemistry – I	4	4	4	100
MPC103T	Advanced Medicinal Chemistry	4	4	4	100
MPC104T	Chemistry of Natural Products	4	4	4	100
MPC105P	Pharmaceutical Chemistry Practical I	12	6	12	150
-	Seminar / Assignment	7	4	7	100
	Total	**35**	**26**	**35**	**650**
SEMESTER II					
MPC201T	Advanced Spectral Analysis	4	4	4	100
MPC202T	Advanced Organic Chemistry –II	4	4	4	100
MPC203T	Computer Aided Drug Design	4	4	4	100
MPC204T	Pharmaceutical Process Chemistry	4	4	4	100
MPC205P	Pharmaceutical Chemistry Practical II	12	6	12	150
-	Seminar / Assignment	7	4	7	100
	Total	**35**	**26**	**35**	**650**

Common subjects for all specializations except for Pharmaceutical Regulatory Affairs (MRA) and Pharmacy Practice (MPP)

MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES (Theory) (MPAT101T) **60 hours**

Scope

This subject deals with various advanced analytical instrumental techniques for identification, characterization and quantification of drugs.

Instruments dealt are UV, IR, NMR, Mass spectrometer, HPLC, GC etc.

Simple structure elucidation problems may be included based on UV-IR-NMR data.

Objectives

Upon completion of the course the student shall be able to

- Analytical techniques for identification, characterization and quantification of drugs
- Theoretical and practical skills of instrument handling and use.
- Structural Elucidation of organic compounds using spectroscopic tools

UNIT-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.

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. **10 hrs**

c) **Spectroflourimetry:** Theory of Fluorescence, Factors affecting fluorescence, Quenchers, Instrumentation and Applications of fluorescence spectroscopy.

d) **Flame emission spectroscopy and Atomic absorption spectroscopy:** Principle, Instrumentation, Interferences and Applications.

UNIT-II

- **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**

UNIT-III

- **Mass Spectrometry:** Principle, Theory, Instrumentation of Mass Spectrometry, 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 spectrometry **12 hrs**
- **Simple structure elucidation problems based on UV, IR, NMR and Mass data.**

UNIT-IV

Chromatography: Principle, instrumentation, chromatographic parameters, factors affecting resolution and applications of the following: **10 hrs**

a) High Performance Liquid chromatography
b) High Performance Thin Layer Chromatography
c) Ion exchange chromatography

d) Gas chromatography
e) Ultra High Performance Liquid chromatography
f) Affinity chromatography
g) Gel Chromatography

UNIT-V

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

10 hrs

b) **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.

UNIT - VI

Thermal Techniques:

a) **Thermogravimetric analysis (TGA):** Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications.
b) **Differential scanning calorimetry (DSC):** 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.
c) **Differential Thermal Analysis (DTA):** Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA).

08 hrs

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 A and B - J W Munson, Volume 11, Marcel Dekker Series
8. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, Cengage Learning, 2008.
9. Solving spectroscopy problems: A basic approach by Nazma Inamdar (Career publications).

PHARMACEUTICAL CHEMISTRY (MPC)

ADVANCED ORGANIC CHEMISTRY - I (MPC 102T)	60 Hrs
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	
UNIT-I **a) 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: reactions, mechanisms and their relative reactivity and orientations. **b) Addition reactions** • **Nucleophilic uni– and bimolecular reactions (SN1 and SN2)** • **Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)** • **Rearrangement reactions**	**10 Hrs**
UNIT-II **Study of mechanism and synthetic applications of following name reactions** **1) Important Name reactions:** Ullmann coupling reactions, Dieckmann reaction, Doebner-Miller reaction, Sandmeyer reaction, Mitsunobu reaction, Mannich reaction, Vilsmeyer-Haack reaction, Sharpless asymmetric epoxidation, Shapiro & Suzuki reaction, Ozonolysis, Michael addition reaction **2) Multi-component synthesis:** Ugi reaction, Biginelli reaction, Hantzsch reaction, Passerini reaction and Strecker synthesis.	**12 Hrs**
UNIT-III **a) Synthetic Reagents & Applications** 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). **b) Protecting groups** i. Role of protection in organic synthesis ii. Protection for the hydroxyl group, including 1,2–and1,3–diols: ethers, esters, carbonates, cyclic acetals & ketals iii. Protection for the Carbonyl Group: Acetals and Ketals iv. Protection for the Carboxyl Group: amides and hydrazides,	**12 Hrs**

esters v. Protection for the Amino Group and Amino acids: carbamates and amides	
UNIT-IV • **Heterocyclic Chemistry** 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, Celecoxib, Metamizole sodium, Antipyrine, Alprazolam, Triamterene, Sulfamerazine, Hydroxychloroquine, Quinacrine, Amsacrine, Prochlorpherazine, Promazine, Theophylline , Mercaptopurine.	**14 Hrs**
UNIT-V **Synthon approach and retrosynthesis applications** 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.	**12 Hrs**

REFERENCES

1. "Advanced Organic chemistry, Reaction, Mechanisms and Structure", J March, John Wiley and Sons, New York.
2. "Mechanism and Structure in Organic Chemistry", ES Gould, Hold Rinchart and Winston, New York.
3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers. Oxford University Press 2001.
4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Pearson Education Lts, Dorling Kindersley 9India) Pvt. Ltd.
5. A guide to mechanisms in Organic Chemistry, Peter Skyes (Orient Longman, New Delhi).
6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.
7. Combinational Chemistry - Synthesis and applications - Stephen R Wilson & Anthony W Czarnik, Wiley - Blackwell.
8. Carey, Organic Chemistry, 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.

ADVANCED MEDICINAL CHEMISTRY (MPC 103T)	60 Hrs
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	
UNIT-I **a) Drug discovery**: Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets. **b) Biological drug targets**: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonist's vs antagonists, and artificial enzymes.	**12 Hrs**
UNIT-II **Medicinal Chemistry Aspects of following classess of drugs** **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, COX-1 & COX-2 inhibitors, Alzheimer's and Parkinson's disease, Antineoplastic and Antiviral agents. **b) Stereochemistry and Drug action**: Stereo selectivity as a pre–requisite for evolution, role of chirality in selective and specific therapeutic agents, Enantio selectivity in drug adsorption, metabolism, distribution and elimination with Case studies.	**16 Hrs**
UNIT-III **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.	**10 Hrs**
UNIT-IV **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.	**10 Hrs**
UNIT-V **Prodrug Design and Analog design** **a) Prodrug design**: Basic concept, Carrier linked prodrugs/ Bioprecursors, Prodrugs of functional group, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and	**12 Hrs**

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, 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.	

REFERENCES

1. Medicinal Chemistry by Burger, Vol I -VI.
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
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.

CHEMISTRY OF NATURAL PRODUCTS (MPC 104T)	60 Hrs
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	
UNIT-I **Study of Natural products as leads for new 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)	**12 Hrs**
UNIT-II **a) 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. **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).	**12 Hrs**
UNIT-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 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**

UNIT-IV **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**
UNIT-V **Structural Characterization of natural compounds** Structural characterization of natural compounds using IR, ^{1}H-NMR, ^{13}C-NMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit–D, Quercetin and Digitalis glycosides.	**12 Hrs**

REFERENCES

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

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

ADVANCED SPECTRAL ANALYSIS (MPC 201T)	60 Hrs
Scope This subject deals with various hyphenated analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are LC–MS, GC–MS, ATR–IR, DSC etc. **Objectives** At completion of this course it is expected that students will be able to understand - • Interpretation of the NMR, Mass and IR spectra of various organic compounds • Theoretical and practical skills of the hyphenated instruments • Identification of organic compounds	
UNIT-I **UV and IR spectroscopy** • Woodward - Fieser rule for 1,3– butadienes, cyclic dienes and α, β– carbonyl compounds and interpretation compounds of enones. • ATR–IR, Interpretation of IR Spectra of Organic Compound	**12 Hrs**
UNIT-II **NMR spectroscopy** 1–D and 2–D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds.	**12 Hrs**
UNIT-III **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.	**12 Hrs**
UNIT-IV **Chromatography:** Principle, Instrumentation and Applications of the following : a) GC–MS b) GC-AAS c) LC-MS d) LC-FTIR e) LC-NMR f) CE- MS g) Super critical fluid chromatography h) Flash chromatography i.) LC-MS/MS	**16 Hrs**
UNIT-V **a) Thermal methods of analysis** Interpretation of TGA, DTA and DSC spectras of drug and excipients **b)** Bioassay, ELISA, Radioimmuno assay of digitalisand insulin.	**8 Hrs**

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. Organic Spectroscopy – William Kemp, 3rd edition, ELBS, 1991.
5. Quantitative analysis of Pharmaceutical formulations by HPTLC – P D Sethi, CBS Publishers, New Delhi.

6. Quantitative Analysis of Drugs in Pharmaceutical formulation – P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
7. Pharmaceutical Analysis– Modern methods - Part B – J W Munson, Volume 11, Marcel Dekker Series

ADVANCED ORGANIC CHEMISTRY - II (MPC 202T)	60 Hrs
Scope The subject is designed to provide in–depth knowledge about advances in organic chemistry, different techniques of organic synthesis and their applications to process chemistry as well as drug discovery. **Objectives :** Upon completion of course, the student shall able to understand • The principles and applications of Green chemistry • The concept of peptide chemistry. • The various catalysts used in organic reactions • The concept of stereochemistry and asymmetric synthesis.	
UNIT-I **Green Chemistry** **a.** Introduction, principles of green chemistry **b.** 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 **c.** Ultrasound assisted reactions: Types of sonochemical reactions, homogenous, heterogeneous liquid–liquid and liquid–solid reactions, synthetic applications **d.** Continuous flow reactors: Working principle, advantages and synthetic applications. **e.** Ionic liquids, and solvent free reactions	**12 Hrs**
UNIT-II **Stereochemistry & Asymmetric Synthesis** **a)** Basic concepts in stereochemistry - optical activity, specific rotation, racemates and resolution of racemates, the Cahn, Ingold, Prelog (CIP) sequence rule, meso compounds, pseudo asymmetric centres, axes of symmetry, Fischers D and L notation, cis–trans isomerism, E and Z notation. **b)** Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation and Stereo selective synthesis with examples.	**12 Hrs**
UNIT-III **Chemistry of peptides** a) Coupling reactions in peptide synthesis b) 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 c) Segment and sequential strategies for solution phase peptide synthesis with any two case studies d) Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over– activation and side reactions of individual amino acids.	**12 Hrs**
UNIT-IV	**12 Hrs**

a) **Photochemical Reactions** Basic principles of photochemical reactions. Photo–oxidation, photo–addition and photo–fragmentation. b) **Pericyclic reactions** Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigmatrophic rearrangement reactions with examples	
UNIT-V **Catalysis** **a)** Types of catalysis, heterogeneous and homogenous catalysis, advantages and disadvantages **b)** Heterogeneous catalysis - preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs. **c)** Homogenous catalysis, hydrogenation, hydroformylation, hydrocyanation, Wilkinson catalysts, chiral ligands and chiral induction, Ziegler-Natta catalysts, some examples of homogenous catalysis used in synthesis of drugs **d)** Transition–metal and Organo–catalysis in organic synthesis: Metal–catalyzed reactions **e)** Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction. **f)** Phase transfer catalysis - theory and applications	**12 Hrs**

REFERENCES

1) "Advanced Organic chemistry, Reaction, mechanisms and structure", J March, John Wiley and sons, New York.

2) "Mechanism and structure in organic chemistry", ES Gould, Hold Rinchart and Winston,NewYork.

3) "Organic Chemistry" Clayden, Greeves, Warren and Woihers., Oxford University Press 2001.

4) "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Sixth ed., 1995.

5) Carey, Organic chemistry, 5th edition (Viva Books Pvt. Ltd.)

6) Organic synthesis–the disconnection approach, S. Warren, Wily India

7) Principles of organic synthesis, ROCNorman and JMCoxan, Nelson thorns

8) Organic synthesis– Special techniques VK Ahluwalia and R Aggarwal, Narosa Publishers.

9) Organic reaction mechanisms IV edtn, VK Ahluwalia and RK Parashar, Narosa Publishers.

COMPUTER AIDED DRUG DESIGN (MPC 203T)	60 Hrs
Scope The subject is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design. **Objectives** At completion of this course it is expected that students will be able to understand • Role of CADD in drug discovery • Different CADD techniques and their applications • Various strategies to design and develop new drug like molecules. • Working with molecular modeling software's to design new drug molecules • The in silico virtual screening protocols	
UNIT-I **Molecular Properties and Drug Design** a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design. b) De novo drug design: Receptor/enzyme–interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design. c) Homology modeling and generation of 3D–structure of protein.	**12 Hrs**
UNIT-II • **Pharmacophore Mapping and Virtual Screening** Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; 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.	**12 Hrs**
UNIT-III **Molecular Modeling and Docking** **a)** Molecular and Quantum Mechanics in drug design. **b)** Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation **c)** Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra–precision docking. Agents acting on enzymes such as DHFR, HMG–CoA reductase and HIV protease, choline esterase (AchE & BchE)	**12 Hrs**
UNIT-IV • **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.	**12 Hrs**
UNIT-V • **Quantitative Structure Activity Relationships:**	**12 Hrs**

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.	

REFERENCES

1. Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers.
2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor & Francis group.
3. Drug Design by Ariens Volume 1 to 10, Academic Press, 1975, Elsevier Publishers.
4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.
5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
6. Medicinal Chemistry by Burger, Wiley Publishing Co.
7. An Introduction to Medicinal Chemistry -Graham L. Patrick, Oxford University Press.
8. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 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

PHARMACEUTICAL PROCESS CHEMISTRY (MPC 204T)	60 Hrs
Scope Process chemistry is often described as scale up reactions, taking them from small quantities created in the research lab to the larger quantities that are needed for further testing and then to even larger quantities required for commercial production. The goal of a process chemist is to develop synthetic routes that are safe, cost–effective, environmentally friendly, and efficient. The subject is designed to impart knowledge on the development and optimization of a synthetic route/s and the pilot plant procedure for the manufacture of Active Pharmaceutical Ingredients (APIs) and new chemical entities (NCEs) for the drug development phase. **Objectives** At completion of this course it is expected that students will be able to understand • The strategies of scale up process of apis and intermediates • The various unit operations and various reactions in process chemistry	
UNIT-I **Industrial Safety** **a)** MSDS (Material Safety Data Sheet), hazard labels of chemicals and Personal Protection Equipment (PPE) **b)** 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	**12 Hrs**
UNIT-II **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	**12 Hrs**
UNIT-III **Unit operations** **a. Extraction**: Liquid equilibria, extraction with reflux, extraction with agitation, counter current extraction. **b. Filtration**: Theory of filtration, pressure and vacuum filtration, centrifugal filtration, **c. Distillation**: azeotropic and steam distillation **d. Evaporation**: Types of evaporators, factors affecting evaporation. **e. Crystallization**: Crystallization from aqueous, non– aqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphous APIs.	**12 Hrs**
UNIT-IV **Unit Processes – I** a) **Nitration**: Nitrating agents, Aromatic nitration, kinetics and mechanism of aromatic nitration, process equipment for technical nitration, mixed acid for nitration, **b) Halogenation**: Kinetics of halogenations, types of halogenations, catalytic halogenations. Case study on industrial halogenation	**12 Hrs**

process. **c) Oxidation**: Introduction, types of oxidative reactions, Liquid phase oxidation with oxidizing agents. Nonmetallic Oxidizing agents such as H2O2, sodium hypochlorite, Oxygen gas, ozonolysis	
UNIT-V **Unit Processes – II** a) **Reduction**: Catalytic hydrogenation, Heterogeneous and omogeneous catalyst; Hydrogen transfer reactions, Metal hydrides. Case study on industrial reduction process. b) **Fermentation**: Aerobic and anaerobic fermentation. Production of - i. Antibiotics; Penicillin and Streptomycin, ii. Vitamins: B2 and B12 iii. Statins: Lovastatin, Simvastatin c) Reaction progress kinetic analysis i. Streamlining reaction steps, route selection, ii. Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale–up.	**12 Hrs**

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

PHARMACEUTICAL CHEMISTRY PRACTICALS – II (MPC 205P)
1) Synthesis of organic compounds by adapting different approaches involving (3 experiments) • Oxidation • Reduction/hydrogenation • Nitration
2) Comparative study of synthesis of APIs/intermediates by different synthetic routes (2 experiments)
3) Assignments on regulatory requirements in API (2 experiments)
4) Comparison of absorption spectra by UV and Wood ward - Fieser rule
5) Interpretation of organic compounds by FT–IR
6) Interpretation of organic compounds by NMR
7) Interpretation of organic compounds by MS
8) Determination of purity by DSC in pharmaceuticals
9) Identification of organic compounds using FT–IR, NMR, CNMR and Mass spectra
10) To carry out the preparation of following organic compounds
11) Preparation of 4–chlorobenzhydrylpiperazine. (An intermediate for cetirizine HCl).
12) Preparation of 4–iodotolene from p–toluidine.
13) NaBH4 reduction of vanillin to vanillyl alcohol
14) Preparation of umbelliferone by Pechhman reaction
15) Preparation of triphenyl imidazole
16) To perform the Microwave irradiated reactions of synthetic importance (Any two)
17) Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares.
18) Calculation of ADMET properties of drug molecules and its analysis using softwares Pharmacophore modeling
19) 2D–QSAR based experiments
20) 3D–QSAR based experiments
21) Docking study based experiment
22) Virtual screening based experiment