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

Course Code	Course	Credit Hours	Credit Points	Hrs./wk	Marks
Semester I					
MPC101T	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

Table – 12: Course of study for M. Pharm. III Semester
(Common for All Specializations)

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

* Non University Exam

Table – 13: Course of study for M. Pharm. IV Semester
(Common for All Specializations)

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

Table – 14: Semester wise credits distribution

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

*Credit Points for Co-curricular Activities

ADVANCED SPECTRAL ANALYSIS
(MPC 201T)

Scope

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

Objectives

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

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

THEORY 60Hrs

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

2 NMR spectroscopy: 12 Hrs
   1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds.

3 Mass Spectroscopy 12 Hrs
   Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, Mc Lafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.

4 Chromatography: 12 Hrs
   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) High Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion Chromatography) k) Flash chromatography

5 a). Thermal methods of analysis 12 Hrs

Introduction, principle, instrumentation and application of DSC, DTA and TGA.

b). Raman Spectroscopy

Introduction, Principle, Instrumentation and Applications.

c). Radio immuno assay

Biological standardization , bioassay, ELISA, Radioimmuno assay of digitalis and insulin.

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)

Scope

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

Objectives

Upon completion of course, the student shall able to understand

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

THEORY 60 Hrs

1. Green Chemistry: 12 Hrs
   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.
2. Chemistry of peptides 12 Hrs
   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.

3 Photochemical Reactions — 12 Hrs

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 and sigmatrophic rearrangement reactions with examples

4 Catalysis: — 12 Hrs

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

5 Stereochemistry & Asymmetric Synthesis — 12 Hrs

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.

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)

Scope

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

Objectives

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

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

Theory	60 Hrs
1. 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
2 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.	12 Hrs
3 Molecular Modeling and Docking a) Molecular and Quantum Mechanics in drug design. b) Energy Minimization Methods: comparison between global	12 Hrs

minimum conformation and bioactive conformation

c) Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AchE & BchE)

4 Molecular Properties and Drug Design 12 Hrs

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.

5 Pharmacophore Mapping and Virtual Screening 12 Hrs

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.

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.