SunRise University

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Recognized by UGC Act, 1956 u/s 2 (f)

Syllabus

For

M.Pharm. (Pharmaceutical Chemistry)

Course Structure and Evaluation Scheme for M. Pharm. Courses (All Subjects/ Specialization)

PHARMACEUTICAL CHEMISTRY

Semester-I

S.N.	Subject Code	Name of the Subject	Periods			Credit	Evaluation Scheme					Subject Total
							Theory			Practical		
			L	T	P		CT	TA	ESE	TA	ESE	
1	*MPA101*	Modern Pharmaceutical Analytical Techniques	3	0	0	3	20	10	70	--	--	100
2	*MPC101*	Advanced Organic Chemistry-I	3	0	0	3	20	10	70	--	--	100
3	*MPC102/ MPC205*	Advanced Medicinal Chemistry/ Novel Technologies & Drug Regulatory Affairs	3	0	0	3	20	10	70	--	--	100
4	*MPC103/ MPC204*	Chemistry of Natural Products/ Pharmaceutical Process Chemistry	3	0	0	3	20	10	70	--	--	100
5	*RPM101*	Research Process & Methodology	3	0	0	3	20	10	70	--	--	100
6	*MPA105*	Modern Pharmaceutical Analytical Techniques Practical	-	-	2	1	--	--	--	20	30	50
7	*MPC104*	Pharmaceutical Chemistry Practical-I	-	-	3	2	--	--	--	20	30	50
Total						**18**						**600**

Semester-II

S.N.	Subject Code	Name of the Subject	Periods			Credit	Evaluation Scheme					Subject Total
							Theory			Practical		
			L	T	P		CT	TA	ESE	TA	ESE	
1	*MPC201*	Advanced Spectral Analysis	3	0	0	3	20	10	70	--	--	100
2	*MPC202*	Advanced Organic Chemistry-II	3	0	0	3	20	10	70	--	--	100
3	*MPC203*	Computer Aided Drug Design	3	0	0	3	20	10	70	--	--	100
4	*MPC204/ MPC103*	Pharmaceutical Process Chemistry/ Chemistry of Natural Products	3	0	0	3	20	10	70	--	--	100
5	*MPC205/ MPC102*	Novel Technologies & Drug Regulatory Affairs / Advanced Medicinal Chemistry	3	0	0	3	20	10	70	--	--	100
6	*MPC206*	Pharmaceutical Chemistry Practical-II	-	-	2	1	--	--	--	20	30	50
7	*MPC207*	Seminar-I (Synopsis)	-	-	3	2	--	--	--	50	--	50
Total						**18**						**600**

Semester-III

S.N.	Subject Code	Name of the Subject	Periods			Credit	Evaluation Scheme					Subject Total
							Theory			Practical		
			L	T	P		CT	TA	ESE	TA	ESE	
1	*MPC301*	Seminar-II	0	0	6	3	--	--	--	100	--	100
2	*MPC302*	Dissertation (Research Project Audit)	0	0	30	15	--	--	--	200	300	500
Total						**18**						**600**

Semester-IV

S.N.	Subject Code	Name of the Subject	Periods			Credit	Evaluation Scheme					Subject Total
							Theory			Practical		
			L	T	P		CT	TA	ESE	TA	ESE	
1	*MPC401*	Dissertation (Final)	0	0	36	18	--	--	--	200	400	600
Total						**18**						**600**

M. Pharm. (Pharmaceutical Chemistry)

First Semester

MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES (*MPA101*)

Unit-I

UV-Visible spectroscopy: Introduction, theory and laws associated with UV-visible spectroscopy, chromophores, auxochromes and their interaction with UV-Vis radiations, choice of solvents and solvent effect. Woodward- Fieser rule and applications of UV-visible spectroscopy.

IR Spectroscopy: Theory, modes of molecular vibrations, factors affecting vibrational frequencies and applications of IR spectroscopy. FT-IR. Interpretation of IR spectra of organic compounds.

Unit-II

Mass spectrometry: Different ionization methods (EI, CI, FAB, ESI, MALDI), analyzers of quadrupole and time of flight. Fragmentation patterns and its rules, relative abundance of ions, molecular ion peak, meta stable ions, isotopic peaks, Mc-Lafferty rearrangement, ring rule. Applications of mass spectrometry.

Flame emission spectroscopy and atomic absorption spectroscopy*:* Principle, interferences and applications of flame emission spectroscopy and atomic absorption spectroscopy.

Unit-III

NMR Spectroscopy: Principle, chemical shift, factors influencing chemical shift, spin-spin coupling, coupling constant, solvent requirement in NMR, NMR active compounds, free induction decay, relaxation process and NMR signals in various compounds. Applications of NMR spectroscopy.

Unit-IV

Chromatography: Principle, chromatographic parameters, factors affecting and applications of: Thin Layer chromatography, column chromatography, gas chromatography, affinity chromatography, ion exchange chromatography, size exclusion chromatography, high performance liquid chromatography, high performance thin layer chromatography.

Unit-V

Miscellaneous techniques:

Thermal methods of analysis: Introduction, principle, instrumentation and application of TGA, DTA and DSC.

Electron microscopy: Principle, instrumentation and applications of scanning electron microscopy (SEM), transmission electron, microscopy (TEM).

Radioimmuno assay: ELISA.

SUGGESTED BOOKS:

1. Pharmacopoeia of India, Ministry of Health, Govt. of India.
2. Skoog D.A., Holler F.J., Crouch S. R., Instrumental Analysis, Indian Edition, Brooks/Cole, Boston.
3. Willard H.H., Merrit L.L., Dean J.A., Settle P.A., Instrumental Methods of analysis, CBS Publishers and Distributors New Delhi.
4. Kemp W., Organic Spectroscopy, Palgrave, New York.
5. Becket A.H. and Stenlake J.B., Practical Pharmaceutical Chemistry Vol. I and II, The Athlone Press of the University of London.
6. Pavia D.L., Lampman G.M. and Kriz G.S., Introduction to Spectroscopy, Harcourt College Publishers, Philadelphia.
7. Kalsi P.S., Spectroscopy of Organic Compounds, New Age International Publishers, New

Delhi.
8. Florey K., Analytical Profile of Drug Substance (All volume), Academic Press, Elsevier, Massachusetts.

9. Chatten L.G., A Text Book of Pharmaceutical Chemistry, Vol. I and II, Marcel Dekker, New York.
10. Silverstein R.M., Spectrometric Identification of Organic compounds, John Wiley & Sons, New Jersey.
11. Obonson J.W.R., Undergraduate Instrumental Analysis, Marcel Dekker Inc, New York.
12. Parikh V.H., Absorption Spectroscopy of Organic Molecules, Addison-Wesley Publishing Co., London.
13. Stahl E., Thin Layer Chromatography: A Laboratory Handbook, Springer, Berlin.

ADVANCED ORGANIC CHEMISTRY-I (*MPC101*)

Unit-I

Reactions mechanisms, evidences in their favor, orientation and reactivity of the following classes of reactions-

a) Substitution reactions (Electrophilic and nucleophilic).
b) Elimination reactions (E1, E2, E1cb).

Unit-II

Study of reaction mechanism, evidences in their favor, orientation and reactivity of the following classes of reactions-

a) Addition reactions (Free radical, electrophilic and nucleophilic).
b) Rearrangement reactions (C to C, C to N, C to O).

Unit-III

Name reactions: Study of reaction mechanism, evidences in their favor and synthetic applications of following name reactions: Dieckmann Reaction, Vilsmeyer-Haack reaction, Ugi reaction, Baeyer-Villiger oxidation, Doebner-Miller reaction.
Pericyclic reactions: Mechanism, types of pericyclic reactions such as cycloaddition, elctrocyclic reaction and sigmatrophic rearrangement reactions with examples.

Unit-IV

Heterocyclic chemistry: General methods of synthesis, properties and applications of drugs containing five, six membered and fused heterocylces such as: Pyrazoline, triazole, 4-thiazolidinone, purine, quinoline, acridine. Synthesis of few representative drugs containing these heterocyclic nucleus.

Unit-V

Stereochemistry and asymmetric synthesis:

a) Stereochemistry of five and six membered and fused rings.
b) Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation, stereoselective and stereospecific synthesis with examples.

SUGGESTED BOOKS:

1. March J., Advanced Organic Chemistry, Reaction, Mechanism and Structure, John Wiley and Sons, New York.
2. Morrison R.T., Boyd R.N., and Bhattacharjee, S.K. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), New Delhi.
3. Finar I.L. Organic Chemistry, Vol. I & II, Pearson Education, New Jersey.

4. Clayden J., Greeves N., Warren S., Wothers P., Organic Chemistry, Oxford University Press, New York.
5. Grossman R.B., The Art of Writing Reasonable Organic Reaction Mechanisms, Springer, New York.

6. Norman R. Coxon J.M., Principles of Organic Synthesis, Blackie Academic and Professional, London.
7. Sykes P., A Guidebook to Mechanism in Organic Chemistry, Longman Group Ltd, Harlow.
10. Li J.J., Name Reactions: A Collection of Detailed Reaction Mechanisms, Springer, Berlin.
11. Kurti L., Czako B., Strategic Applications of Named Reactions in Organic Synthesis: Background and Detailed Mechanisms, Elsevier Academic Press, Amsterdam.
12. Acheson R.M., An Introduction to the Chemistry of Heterocyclic Compounds, Wiley (India) Pvt. Ltd, New Delhi.
13. Joule J.A. and Mills K., Heterocyclic Chemistry, Blackwell Publishing, New Jersey.
14. Gilchrist T.L., Heterocyclic Chemistry, Pearson Education Ltd, Singapore.
15. Bansal R.K., Heterocyclic Chemistry, New Age International Publishers, New Delhi.
16. Jain M.K. and Sharma S.C., A Textbook of Organic Chemistry, Shoban Lal and Co. Educational Publishers, New Delhi.
17. Singh M.S. Advanced Organic Chemistry: Reactions and Mechanisms, Dorling Kindersley (India) Pvt. Ltd, New Delhi.
18. Eliel E. L., Wilen S. H., Mander L.N., Stereochemistry of Organic Compounds, John Wiley and Sons, New York.
19. Nasipuri D., Stereochemistry of Organic Compounds: Principles and Applications, New Age International (P) Limited, New Delhi.
20. Mann F.G, and Saunders, B.C., Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
21. Vogel A.I., Elementary Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
22. Organic Syntheses, Collective Volume1-IX, John Wiley and Sons, New Jersey.

ADVANCED MEDICINAL CHEMISTRY (*MPC102/MPC205*)

Unit-I

Drug discovery: Stages of drug discovery, lead discovery, identification, validation and diversity of drug targets. Some novel molecular targets along with their pharmacodynamic agents: Polyketide synthase (Pks13), signal transducer and activator of transcription-3 (STAT-3) and sodium glucose co- transporter-2 (SGLT-2).

Stereochemistry and drug action: Pharmacodynamic, pharmacokinetic (drug adsorption, metabolism, distribution and elimination) and toxicological aspects of stereoisomers (Geometrical, optical and conformational).

Unit-II

Prodrug design: Basic concepts, prodrugs of functional group, rationale and practical consideration of prodrug design.

Rational versus analog approach of drug design.

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

Unit-III

Systematic study, SAR, mechanism of action and synthesis (synthesis of individually mentioned drugs only) of new generation molecules of following classes:

Adrenergic agents (Celiprolol, Olodaterol), cholinergic agents (Sazetidine-A), antidepressants (Vortioxetine,

Levomilnacipram), anticonvulsants (Levetiracetam, Perampanel) and psychoactive drugs (Brexpiperazole, Iloperidone).

Unit-IV

Systematic study, SAR, Mechanism of action and synthesis (synthesis of individually mentioned drugs only) of new generation molecules of following classes:
Anti-hypertensive drugs (Cilazapril, Saprisartan), H1 and H2 receptor antagonists (Dimetindene, Olopatadine, Lafutidine), oral hypoglycemic (Omargliptin, Dulaglutide), antineoplastic agents (Alectinib, Capacitabine) and anti-HIV agents (Dolutegravir, Elvitegravir).

Unit-V

Rational design of enzyme inhibitors: Enzyme kinetics and principles of enzyme inhibitors, enzyme inhibitors in medicine, rational design of non-covalently and covalently binding enzyme inhibitors. Introduction to artificial enzymes.
Introduction, design and therapeutic applications of peptidomimetics.

SUGGESTED BOOKS:

1. Abraham D.J., Burger's Medicinal Chemistry and Drug Discovery, John Wiley and Sons Inc., New York.
2. Block J.H. and Beale J.M., Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Lippincott Williams and Wilkins, Philadelphia.
3. Lemke T.L., Williams D.A., Roche V.F. and Zito S.W., Foye's Principles of Medicinal Chemistry, Lippincott Williams and Wilkins, Philadelphia.
4. Vardanyan R.S. and Hruby V.J., Synthesis of Essential Drugs, Elsevier, Philadelphia.
5. Nogrady T., Medicinal Chemistry: A Biochemical Approach, Oxford University Press, New York.
6. Patrick G.L., An Introduction to Medicinal Chemistry, Oxford University Press, New York.
7. Hansch C., Comprehensive Medicinal Chemistry, Pergamon Press, Oxford.
8. Thomas G., Fundamentals of Medical Chemistry, Wiley Publication, New Jersey.
9. Silverman R.B., The Organic Chemistry of Drug Design and Action. Academic Press Inc., San Diego.
10. Gringuaz A., Introduction to Medicinal Chemistry: How Drugs Act and Why, Wiley-VCH.
11. Wermuth C.G., The Practice of Medicinal Chemistry, Academic Press, Cambridge.
12. Guarna A. and Trabocchi A., Peptidomimetics in Organic and Medicinal Chemistry, Wiley Publication, New Jersey.
13. Singh H. and Kapoor V.K., Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Delhi.
14. Korolkovas A., Essentials of Medicinal Chemistry, John Wiley and Sons Inc., New York.
15. Lednicer D., The Strategies for Organic Chemistry of Drug Synthesis, John Wiley and Sons Inc., New York.

CHEMISTRY OF NATURAL PRODUCTS (*MPC103/MPC204*)

Unit-I

Alkaloids: Introduction, classification, isolation, purification, stereochemistry, molecular modification and biological activity of alkaloids. General methods of structural determination of alkaloids, structure elucidation of Ephedrine.

Flavonoids: Introduction, isolation and purification of flavonoids. General methods of structural determination of flavonoids, structure elucidation of Quercetin.

Unit-II

Steroids: Introduction, classification, nomenclature and stereochemistry of steroids. Structure elucidation of male and female sex hormones (Testosterone and Progesterone), adrenocortcoids (Cortisone).

Terpenoids: Classification, isolation, isoprene rule and general methods of structural determination of terpenoids, structure elucidation of Geraniol.

Unit-III

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 Etoposide,
c) Cardiovascular drugs: Teprotide and Dicoumarol.
d) Neuromuscular blocking drugs: Curare alkaloids.

Unit-IV

Semisynthetic derivatization: Basic concepts, semisynthetic drugs derived from natural sources such as: Antibiotics (Erythromycin, new generation Cephalosporins) and Curcumin. Transformation of phytosterols into steroidal drugs.

Marine natural products: Introduction and compounds of medicinal importance derived from marine sources such as Cytarabine and Ziconotide.

Unit-V

Pharmacological screening of herbal drugs: Introduction and evaluation of herbal drugs for antidiabetic, hepatoprotective, cardiovascular, antifertility, antioxidant, anticancer, antimalarial, anticonvulsant, anti-inflammatory, analgesic, antipyretic and antiulcer properties.

SUGGESTED BOOKS:

1. Finar I.L.,Organic chemistry, Volume II: Stereochemistry and the Chemistry of Natural Products, Pearson Education, New Jersey.
2. Agarwal O.P., Organic Chemistry, Natural Products, Krishna Prakashan Media (P) Ltd., Meerut.
3. Harborne J.B., Phytochemical Methods: A Guide to Modern Techniques of Plant Analysis, Springer (India) Pvt. Ltd., New Delhi.
4. Cutler S.J. and Cutler H.G., Biologically Active Natural Products: Pharmaceuticals, CRC Press, London.
5. Jarald E.E. and Jarald S.E., Textbook of Pharmacognosy and Phytochemistry, CBS Publishers and Distributors Pvt. Ltd., New Delhi.
6. Deore S.L., Khadabadi S.S., Baviskar B.A., Pharmacognosy and Phytochemistry: A Comprehensive Approach, PharmaMed Press, Hyderabad.
7. Indian Herbal Pharmacopoeia, Indian Drug Manufacturers Association and Regional Research Laboratory, Jammu.
8. Evans V.C., Trease and Evans Pharmacognosy, Harcourt Publishers Ltd., Sydney.

9. Wallis T. E., Textbook of Pharmacognosy, CBS Publishers and Distributors, New Delhi
10. Tyler V.E., "Pharmacognosy" Lea & Febiger, Philadelphia.

11. Brain K.R. and Turner T.D., The Practical Evaluation of Phytopharmaceutical, Wright, Bristol.
12. Stahl E., Thin Layer Chromatography: A Laboratory Hand Book, Springer International Edition, New York.

RESEARCH PROCESS & METHODOLOGY (*RPM101*)

Unit-I

Fundamentals of research: Meaning, objective and importance of research methodology, types of research (basic, applied and patent oriented), defining research problem, research design including various methods, research process and steps involved. Literature survey and documentation.

Unit-II

Data collection, analysis and hypothesis testing: Classification of data, methods of data collection, sample size, sampling procedure and methods. Data processing and graphical representation of data. Statistical inference and hypothesis: Types of hypothesis (experimental and non-experimental), hypothesis testing (Parametric and non-parametric tests), generalization and interpretation of results. Use of statistical softwares/ packages in data analysis (SPSS, Graph Pad Prism).

Unit-III

Multivariate analysis: Introduction to multivariate analysis (Linear and non linear methods) and their validation methods (Statistical parameters).
Research ethics, plagiarism and impact of research: Research ethics, responsibility and accountability of the researchers, ethical consideration during animal experimentation including CPCSEA guidelines. Plagiarism and use of plagiarism detection softwares such as-VIPER. Impact of research on environment and society, commercialization of research, intellectual ownership.

Unit-IV

Technical writing and reporting of research: Types of research report: Dissertation and thesis, research paper, review article, short communication, conference presentation, meeting report etc. Structure and organization of research reports: Title, abstract, key words, introduction, methodology, results, discussion, conclusion, acknowledgement, references, footnotes, tables and illustrations. Impact factor, rating, indexing and citation of journals. Detailed study of 'Instruction to Authors' of any research journal, a thorough understanding of steps involved in submitting articles electronically to any research journal (Registration, new article submission, tracking process, submitting revised articles).

Unit-V

Funding agencies and research grants: Introduction to various research funding agencies such as-DST, DBT, AICTE, UGC, CSIR, ICMR, AAYUSH, and DRDO along with their function in India. Writing a research project and procurement of research grant. Project cost analysis.

SUGGESTED BOOKS:

1. Kothari C.R., Research Methodology Methods and Techniques, Wishwa Prakashan, New Delhi.
2. Lokesh K., Methodology of Educational research, Vikash Publishing House Pvt. Ltd., New Delhi.
3. Kumar R., Research Methodology, Dorling Kindersley (India) Pvt. Ltd., New Delhi.
4. Rao G.N., Research Methodology and Qualitative Methods, B.S. Publications, Hyderabad.
5. Saunders M., Lewis P. and Thornhill A., Research Methods for Business Students, Dorling Kindersley (India) Pvt. Ltd., New Delhi.
6. Bolton S. and Bon C., Pharmaceutical Statistics: Practical and Clinical Applications, Marcel Dekker, New York.

7. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, An introduction to Research Methodology, RBSA Publishers, Jaipur.
8. Fisher R.A. Statistical Methods for Research Works, Oliver and Boyd, Edinburgh.

9. Chow S.S. and Liu J.P., Statistical Design and Analysis in Pharmaceutical Sciences, Marcel Dekker, New York.
10. Buncher C.R., Statistics in the Pharmaceutical Industry, Marcel Dekker, New York.

MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES PRACTICAL (*MPA105*)

1. Determination of the wavelength of maximum absorbance (λ max) of given compounds by UV-Visible spectrophotometry.
2. Quantitative estimation of Pharmacopoeial compounds by UV-Visible spectrophotometry.
3. UV-Vis spectrophotometric assay of pharmaceutical formulations containing Pharmacopoeial compounds as active ingredients.
4. Simultaneous estimation of multi component containing formulations by UV-Visible spectrophotometry.
5. Quantitative estimation of caffeine in beverages using UV-Vis spectrophotometer.
6. Study and interpretation of the FT-IR/IR spectra of given compounds.
7. Separation of the organic compounds from given mixture by thin layer chromatography (TLC).
8. Isolation of the organic compounds from given mixture by two-dimensional thin layer chromatography (2D-TLC).
9. Separation and quantitative estimation of organic compounds in the given mixture by thin layer chromatography (Preparative TLC).
10. Column packing and separation of organic compounds with the help of column chromatography.
11. Simultaneous estimation of any marketed formulation using RP-HPLC method.
12. Stability studies of marketed formulation by RP-HPLC method as per ICH guidelines.
13. Estimation of Sodium/ Potassium by flame photometry.

PHARMACEUTICAL CHEMISTRY PRACTICAL-I (*MPC-104*)

The practicals may be chosen from the following suggested list of experiments based on the subjects opted in that particular semester-

1. Purification of organic solvents and dehydration of organic compounds.
2. Synthesis of organic compounds by adapting different approaches involving- Oxidation, reduction/hydrogenation and nitration.
3. Experiments based on following name reactions: Claisen-Schimdt reaction, Benzyllic acid rearrangement, Beckmann rearrangement, Hoffmann rearrangement, Mannich reaction etc.
4. Synthesis and characterization of some pharmaceutically important heterocyclic nucleuses such as: Pyrazoline, triazole, 4-thiazolidinone, purine, quinoline etc.
5. To perform the Microwave irradiated reactions of synthetic importance.
6. Synthesis of medicinally important compounds/drugs involving more than one step along with purification and characterization using TLC, melting point and IR spectroscopy.
7. Comparative study of synthesis of APIs/intermediates by different synthetic routes.
8. Isolation and characterization of impurities in APIs.
9. Comparison of absorption spectra by UV-Visible and Wood ward-Fieser rule.
10. Functional group analysis of flavonoids by UV-Visible spectrophotometry.
11. Estimation of biological samples by UV-Visible spectrophotometry.
12. Analysis of Pharmacopoeial compounds by difference spectrophotometry.
13. Analysis of Pharmacopoeial compounds by indirect spectrophotometric method.
14. Separation and identification of amino acids from its mixture by paper electrophoresis.
15. Interpretation of FT-IR, NMR, ^{13}CNMR and mass spectra and identification of given organic

compound (s) using these techniques.

16. Extraction of phytoconstituents (Alkaloids, Glycosides, Flavonoids, Terpenes etc.) from plants using conventional and microwave assisted techniques.

17. Isolation and characterization of the isolated compounds from natural sources using various physicochemical and spectral methods.
18. Some typical degradation reactions to be carried on selected plant constituents.
19. Preparation of semi-synthetic derivatives of naturally occurring compounds.
20. Experiment based on Hansch analysis and Free Wilson analysis.
21. Calculation of ADMET properties of drug molecules and its analysis using softwares.
22. 2D-QSAR based experiments
23. 3D-QSAR based experiments.
24. Pharmacophore modeling based experiments.
25. Molecular docking based experiments.
26. Virtual screening based experiment.

Second Semester

ADVANCED SPECTRAL ANALYSIS (*MPC201*)

Unit-I

UV and IR spectroscopy: Woodward- Fieser rule for calculation of λ_{max} of organic compounds such as: 1,3-Butadienes, α,β-unsaturated carbonyl compounds and enones. IR interpretation of organic compounds. **Raman spectroscopy:** Introduction, principle, instrumentation and applications.

Unit-II

NMR spectroscopy: FT-NMR, ^{13}C NMR, 1-D and 2-D NMR, NOESY, COSY and HETCOR. Interpretation of organic compounds.
Mass Spectrometry: Fragmentation of important functional groups like alcohols, amines and carbonyl compounds. Interpretation of mass spectra of organic compounds.

Unit-III

Chromatography: Principle and applications of the following hyphenated techniques: GC-MS, GC- AAS, LC-MS, LC-NMR, CE-MS, super critical fluid chromatography, flash chromatography.

Unit-IV

Miscellaneous techniques of analysis:
Electrophoresis: Principle, instrumentation, factors affecting separation and applications of the following: Gel electrophoresis (SDS-PAGE, Western blotting, Southern blotting), capillary electrophoresis and isoelectric focusing.

X-ray crystallography: Bragg's law, different X-ray diffraction methods including rotating crystal technique, X-ray powder technique, applications of X-ray diffraction.

Unit-V

Complete spectral characterization (UV, IR, NMR, Mass) of following compounds: Aspirin, Diazepam, Ephedrine, Digoxin.

SUGGESTED BOOKS:

1. Skoog D.A., Holler F. J., Crouch S. R., Instrumental Analysis, Indian Edition, Brooks/Cole, Boston.
2. Willard H.H., Merrit L.L., Dean J.A., Settle P.A., Instrumental Methods of analysis, CBS Publishers & Distributors, New Delhi.
3. Kemp W., Organic Spectroscopy, Palgrave, New York.
4. Silverstein R. M., Spectrometric Identification of Organic compounds, 6th Edition, John Wiley and Sons, New Jersey.
5. Pavia D.L., Lampman G.M., and Kriz G.S., Introduction to Spectroscopy, Harcourt College Publishers, Philadelphia.
6. Sethi P. D., Quantitative Analysis of Drugs in Pharmaceutical Formulations by HPTLC, CBS Publishers, New Delhi.
7. Sethi P. D., Quantitative Analysis of Drugs in Pharmaceutical Formulation, CBS Publishers, New Delhi.
8. Munson J. W., Pharmaceutical Analysis- Modern methods- Part B, Volume 11, Marcel Dekker Series, New York.
9. British Pharmacopoeia, Her Majesty's Stationary Office, University Press, Cambridge.
10. Mendham J., Denny R.C., Barnes, J.D. Thomas M.J.K., Vogel's Text Book of Quantitative Chemical Analysis, Pearson Education Asia, Singapore.

11. Connors K.A., A Textbook of Pharmaceutical Analysis, Wiley Intescience, New York.
12. Snyder L. R., Joseph. J., K., Dolan J. W. Introduction to Modern Liquid Chromatography, Wiley Publications, New Jersey.

13. Harborne J.B. and Dey P.M., Methods in Plant Biochemistry: Plant Phenolics. Academic Press Inc. New York.
14. Geissman T.A., The Chemistry of Flavonoid Compounds. Pergamon Press, Oxford.

ADVANCED ORGANIC CHEMISTRY-II (*MPC202*)

Unit-I

Catalysis:
Heterogeneous catalysis: Preparation of catalyst, supported catalysts, catalyst deactivation and regeneration, applications heterogeneous catalysis in synthesis of drugs.
Homogenous catalysis: Introduction, hydrogenation, Wilkinson catalysts, Ziegler-Natta catalysts, applications of homogeneous catalysis in synthesis of drugs.
Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction.

Unit-II

Synthon approach and retro-synthesis applications: Basic principles, terminologies and advantages of retro-synthesis, guidelines for dissection of molecules. Functional group interconvertion and functional group addition (FGI and FGA). C-X and C-C Disconnections. Strategies for the synthesis of five and six membered rings.

Unit-III

Combinatorial chemistry and high throughput screening: Different techniques, advantages and disadvantages of combinatorial synthesis, split and mix synthesis, parallel synthesis. Applications of combinatorial chemistry in drug discovery. General outline, principle and applications of high throughput screening (HTS).

Unit-IV

Protection of functional group: Role of protection for following functional groups: Protection of hydroxyl group (Ethers); Carbonyl group (Acetals and ketals); Carboxyl group (Esters); Amine and amino acids (Carbamates, amides).
Synthetic reagents and their applications: N-Bromosuccinamide, Osmium tetroxide, Titanium chloride, Triphenylphosphine.

Unit-V

Chemistry of peptides: Principle and methods of solid phase peptide synthesis, various solid supports and linkers, activation procedures, coupling reactions, protection, deprotection and cleavage from resin, purification.
Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over-activation and side reactions of individual amino acids.

SUGGESTED BOOKS:

1. March J., Advanced Organic Chemistry, Reaction, Mechanism and Structure, John Wiley & Sons, New York.
2. Smith G. V. and Notheisz F., Heterogenous Catalysis In Organic Chemistry, Academic Press, Cambridge.
3. Carey F. A., Organic Chemistry, 5th Edition, Tata McGraw-Hill Publishing Company Ltd. New Delhi.
4. Clayden J., Greeves N., Warren S., Wothers P., Organic Chemistry, Oxford University Press, Oxford.

5. Fenniri H., Combinatorial Chemistry A Practical Approach, Oxford University Press, Oxford.
6. Warren S., Organic Synthesis-The Disconnection Approach, Wiley India, New Delhi.
7. Thomas G., Medicinal Chemistry An Introduction, John Wiley and Sons Ltd., New York.

8. Silverman R.B., The Organic Chemistry of Drug Design and Drug Action, Elsevier, Amsterdam.
9. Mann F.G, and Saunders, B.C., Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
10. Vogel A.I., Elementary Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
11. Organic Syntheses, Collective Volume1-IX, John Wiley and Sons, New Jersey.

COMPUTER AIDED DRUG DESIGN (*MPC203*)

Unit-I

Introduction to computer aided drug design (CADD): History, different techniques and applications.
Quantitative structure activity relationships: ***Basics***
Physicochemical parameters and methods to calculate them: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, π-substituent constant), steric effects (Taft steric and molar refractivity). Biological parameters.

Unit-II

Quantitative structure activity relationships: ***Applications***
Hansch analysis, Free Wilson analysis, mixed approach along with their advantages and disadvantages. 2D-QSAR and 3D-QSAR (CoMFA and CoMSIA) methodologies.
Molecular modeling: Molecular and Quantum Mechanics in drug design. Molecular dynamics.

Unit-III

Energy minimization and molecular docking
Energy minimization methods: First order derivatives and second order derivatives. Global minimum conformation and bioactive conformation. Force fields
Molecular docking and drug receptor interactions: Rigid docking, flexible docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterases (AChE & BuChE).

Unit-IV

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.
c) Introduction to homology modeling and generation of 3D-structure of protein.

Unit-V

Pharmacophore modeling and virtual screening
a) ***Pharmacophore modeling:*** Concept of pharmacophore, identification of pharmacophoric features and pharmacophore modeling. Pharmacophore mapping, Conformational search used in pharmacophore mapping.
b) ***Virtual screening techniques:*** Similarity based, QSAR based, pharmacophore based and target based *in silico* virtual screening protocols.

SUGGESTED BOOKS:

1. Stroud R.M., Moore J. F., Computational and Structural Approaches to Drug Design, RSC Publisher, London.
2. Martin Y.C., Quantitative Drug Design: A Critical Introduction, CRC Press, London.
3. Ariens E.J., Drug Design Volume 1 to 10, Academic Press, Cambridge.

4. Holtje H.D., Sippl W., Rognan D., Folkers G., Molecular Modeling: Basics Principles and Applications, Wiley-VCH, New Jersey.
5. Leach A., Molecular Modeling: Principles and Applications, Pearson, New York.

6. Vinter J. G. and Gardner M., Molecular Modeling and Drug Design, CRC Press, Florida.
7. Hansch C., Comprehensive Medicinal Chemistry, Pergamon Press, Oxford.
8. Langer T., Hoffmann R.D., Pharmacophores and Pharmacophore Searches, Volume-32, Wiley-VCH, Weinheim.
9. Smith H.J., Williams H., Introduction to the Principles of Drug Design and Action, Tylor and Francis, Oxfordshire.
10. Silverman R.B., The Organic Chemistry of Drug Design and Action. Academic Press Inc., San Diego.
11. Abraham D.J., Burger's Medicinal Chemistry and Drug Discovery, John Wiley and Sons Inc., New York.
12. Patrick G.L., An Introduction to Medicinal Chemistry, Oxford University Press, New York.
13. Block J.H. and Beale J.M., Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Lippincott Williams and Wilkins, Philadelphia.
14. Perun T.J. and Propst C.L., Computer-aided Drug Design Methods and Applications, Saurabh Prakashan Pvt.Ltd., New Delhi.
15. Purcell W.P., Bass G.E., Clayton J.M., Strategy of Drug Design: A Guide to Biological Activity, PharmaMed Press, Hyderabad.
16. Larsen P.K., Liljefors T. and Madsen U. Textbook of Drug Design and Discovery, Taylor and Francis Inc, Oxfordshire.
17. Veerapandian P., Structure Based Drug Design, CRC Press, London.

PHARMACEUTICAL PROCESS CHEMISTRY (*MPC204/MPC103*)

Unit-I

Process chemistry

a) Introduction, stages of scale up process: Bench, pilot and large scale process with at least two examples of scale up process of API.
b) In-process control and validation of large scale process.

Unit-II

Impurities in API and their types including genotoxic impurities.
Isolation, characterization and profiling of impurities in APIs with at least one example.
Reaction progress kinetic analysis: Streamlining reaction steps, route selection, characteristics of expedient and cost-effective routes, reagent selection.

Unit-III

Unit Processes: The following unit processes should be studied with mechanism and one example of each process-
Nitration: Nitrating agents, process equipment for technical nitration.
Halogenation: Types of halogenations, catalytic halogenations.
Reduction: Catalytic hydrogenation, hydrogen transfer reactions, metal hydrides.
Oxidation*:* Types of oxidative reactions, and nonmetallic oxidizing agents such as H, sodium hypochlorite, oxygen gas, ozonolysis.

Unit-IV

Fermentation: Aerobic and anaerobic fermentation. Production of

a) ***Antibiotics:*** Penicillin and Streptomycin.
b) ***Vitamins:*** B2 and B12.
c) ***Statins:*** Lovastatin.

Unit-V

Industrial Safety

a) Introduction to types of hazards with special reference to chemical hazards and fire hazards.

b) Material safety data sheet (MSDS), hazard labels of chemicals and personal protection equipment (PPE).

c) Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001(Environmental Management System).

SUGGESTED BOOKS:

1. Burger A., A Guide to the Chemical Basis of Drug Design, Volume 1-8, Wiley Interscience Publication (John Wiley & Sons), New York.

2. Sharma A.M., Safety and Health in Industry A Handbook, BS Publications Hyderabaad.

3. Pharmaceutical Manufacturing Encyclopedia, Volume 2.

4. Gadamasetti K., Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview, Vol-2, CRC Press, London.

5. Brittain H.G., and Fiese E.F., Effects of Pharmaceutical Processing on Drug Polymorphs and Solvates. (In Brittain H.G., Ed. Polymorphism in Pharmaceutical Solids) Vol. 95: Drugs and the Pharmaceutical Sciences, Marcel Dekker, New York.

6. Murphy R.M., Introduction to Chemical Processes: Principles, Analysis, Synthesis, McGraw-Hill Education, New York.

7. Harrington P. J., Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale- Up, John Wiley and Sons, Inc, New Jersey.

8. Groggins P.H., Unit processes in organic synthesis, McGraw-Hill, New York.

9. Henglein F.A., Chemical Technology, 1st English Edition, Pergamon Press Ltd., Oxford London.

10. Rao M.G., and Sittig M., Dryden's Outlines of Chemical Technology, East-West Press, New Delhi.

11. Clausen C.A., and Mattson G.C., Principles of Industrial Chemistry, Wiley-Blackwell, New Jersey.

12. Lowenheim F.A. and Moran M.K., Industrial Chemicals, John Wiley Sons, Toronto.

13. Shukla S.D., and Pandey G.N., A Text Book of Chemical Technology Vol. II, Vikas Publishing House Pvt. Ltd, Jalandhar.

14. Austin G.T., Shreve's Chemical Process Industries, McGraw Hill Education, New York.

15. Sharma B.K., Industrial Chemistry (including Chemical Engineering), Goel Publishing House, New Delhi.

16. ICH Guidelines.

17. United States Food and Drug Administration official website www.fda.gov.

18. Mann F.G, and Saunders, B.C., Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.

19. Vogel A.I., Elementary Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.

20. Organic Syntheses, Collective Volume1-IX, John Wiley & Sons, New Jersey.

NOVEL TECHNOLOGIES AND REGULATORY AFFAIRS (*MPC205/MPC102*)

Unit-I

Biomaterials: Introduction, classification, chemical modifications and pharmaceutical applications of biomaterials with special reference to Chitosan and Sericin.

Bioconjugates: Introduction and types of bioconjugates (Polymeric, organic nanoparticles based, inorganic nanomateial based, cell based and hydrogel/microgel bioconjuates). General methods of bioconjugation (covalent and noncovalent), characterization and pharmaceutical applications of bioconjugates.

Unit-II

Nanochemistry: Introduction, classification, synthesis, characterization, interaction with biological systems, nanotoxicity and biological applications of nanomaterials with special reference to carbon nanotropes.

Recombinant DNA technology and drug discovery: General concepts and applications.

Gene therapy: Introduction, clinical application and recent advances in gene therapy.

Unit-III

Green chemistry: Introduction, principles and importance of green chemistry.

Microwave assisted reactions: Basic principles, mechanisms, merits and demerits, superheating effects of microwave and effects of solvents in microwave assisted synthesis. Applications of microwave technology in process optimization, various organic reactions and heterocycles synthesis.

Introduction to ionic liquid mediated reactions and ultrasound assisted reactions with their applications.

Unit-IV

Process of product approval: Introduction to API, biologics and novel material of approval, process for obtaining IND, NDA, ANDA for new drugs and generic drugs, US Regulatory requirements and registration for foreign drugs.

Unit-V

Intellectual property rights: Introduction and different mechanism of protection of IPR (patents, copyrights, trademarks, industrial design, geographical indications, registration of plant varieties and trade secrets).

Recent amendments to Indian Patent Act 1970.

BOOKS SUGGESTED:

1. Allcock H.R., Lampe F.W. and Mark J.E., Contemporary Polymer Chemistry, Pearson Education (Singapore) Pvt. Ltd.
2. Odian G., Principles of Polymerization, John Wiley and Sons, New Jersey.
3. Narain R., Chemistry of Bioconjugates: Synthesis, Characterization and Bio-medical Applications, 1st Edition, John Wiley and Sons Inc, New Jersey.
4. Ratner B. D., Hoffman A.S., Schoen F.J., Lemons J.E., Biomaterials Science, An Introduction to Materials in Medicine, Academic Press, Cambridge.
5. Park J., and Lakes R.S., Biomaterials An Introduction, Springer, New York.
6. Matlack A.S., Introduction to Green Chemistry, Marcel Dekker Inc. New York.
7. Anastas P. T., and Warner J.C., Green Chemistry Theory and Practice, Oxford University Press, New Delhi.
8. Kappe C.O., and Stadler A., Microwaves in Organic and Medicinal Chemistry, Vol. 25, Wiley-VCH Verlag GmbH and Co, Weinheim.
9. Walsh, Pharmaceutical Biotechnology Concepts and Applications, John Wiley and Sons Ltd, New Jersey.
10. Glick B.R., and Pasternak J.J., Molecular Biotechnology, Principles and Applications of Recombinant

DNA, Panima Publishing Corporation, New Delhi.
11. Walker M., and Gingold E.B., Molecular Biology and Biotechnology, 3rd Edition, Panama Publishing

Corporation, Panama City.
12. Willig S.H., Tuckerman M.M., Hitchings IV W.S., Good Manufacturing Practices for Pharmaceuticals: A Plan for Total Quality Control, Bhalani Publishing House, Mumbai.
13. Sharma P.P., Validation in Pharmaceutical Industry Concepts Approaches & Guidelines, Vandana Publications Pvt. Ltd., Delhi.
14. Watson J.D., Gilman M., Witowski J., Zoller M., Recombinant DNA, Scientific American Books, New York.
15. Jain N.K., A Textbook of Forensic Pharmacy, Vallabh Prakashan, New Delhi.
16. Ahuja V.K., IPR in India, Vol. I and II, LexisNexis Publishers, Ohio.
17. Bare Acts, Published by The Government of India, New Delhi.
18. Guarino R.A., New Drug Approval Process, Marcel Dekker Inc., New York.
19. Grubb P. W., Patents for Chemicals, Pharmaceuticals and Biotechnology: Fundamentals of Global Law, Practice and Strategy.
20. Bansol, IPR Guidelines for Pharma Students and Researchers.
21. Pisano, FDA Regulatory Affairs.
22. Verkey E., Laws of Patents, 2005 Edition.
23. Patent Law Manual (2005 Edition)
24. https://www.ipindia.nic.in
25. www.fda.gov/

PHARMACEUTICAL CHEMISTRY PRACTICAL-II (*MPC206*)

The practicals may be chosen from the following suggested list of experiments based on the subjects opted in that particular semester-

1. Purification of organic solvents and dehydration of organic compounds.
2. Synthesis of organic compounds by adapting different approaches involving- Oxidation, reduction/hydrogenation and nitration.
3. Experiments based on following name reactions: Claisen-Schimdt reaction, Benzyllic acid rearrangement, Beckmann rearrangement, Hoffmann rearrangement, Mannich reaction etc.
4. Synthesis and characterization of some pharmaceutically important heterocyclic nucleuses such as: Pyrazoline, triazole, 4-thiazolidinone, purine, quinoline etc.
5. To perform the Microwave irradiated reactions of synthetic importance.
6. Synthesis of medicinally important compounds/drugs involving more than one step along with purification and characterization using TLC, melting point and IR spectroscopy.
7. Comparative study of synthesis of APIs/intermediates by different synthetic routes.
8. Isolation and characterization of impurities in APIs.
9. Comparison of absorption spectra by UV-Visible and Wood ward–Fieser rule.
10. Functional group analysis of flavonoids by UV-Visible spectrophotometry.
11. Estimation of biological samples by UV-Visible spectrophotometry.
12. Analysis of Pharmacopoeial compounds by difference spectrophotometry.
13. Analysis of Pharmacopoeial compounds by indirect spectrophotometric method.
14. Separation and identification of amino acids from its mixture by paper electrophoresis.
15. Interpretation of FT-IR, NMR, ^{13}CNMR and mass spectra and identification of given organic compound (s) using these techniques.
16. Extraction of phytoconstituents (Alkaloids, Glycosides, Flavonoids, Terpenes etc.) from plants using conventional and microwave assisted techniques.
17. Isolation and characterization of the isolated compounds from natural sources using various physicochemical and spectral methods.

18. Some typical degradation reactions to be carried on selected plant constituents.
19. Preparation of semi-synthetic derivatives of naturally occurring compounds.
20. Experiment based on Hansch analysis and Free Wilson analysis.

21. Calculation of ADMET properties of drug molecules and its analysis using softwares.
22. 2D-QSAR based experiments
23. 3D-QSAR based experiments.
24. Pharmacophore modeling based experiments.
25. Molecular docking based experiments.
26. Virtual screening based experiment.

SYNOPSIS (SEMINAR-I) (*MPC207*)