



## UNIT-IV

- **Thermal Analysis**

Introduction to various thermal methods of analysis, basic principles and theory, instrumentation and pharmaceutical applications of thermo gravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC) and microcalorimetry, different types of calorimeters and micro calorimeters, advantages of microcalorimetry over DSC.

- **Optical Rotatory Dispersion and Circular Dichroism**

Definition, theory and instrumentaton of ORD and CD. Cotton effect, Octant rule and its applications.

- **Definition of bioassay**, various types of bioassays, advantages and limitations of bioassays with suitable examples, Theory and application of radioimmunoassay and ELISA. Animal models for screening of anti-inflammatory, anti-convulsant, and anti-diabetic.

### **Note: Instruction for Examiner:**

The examination in each theory subject shall be of 50 marks. The examiner will set nine questions. Candidate will attempt five questions. First question would be of short answer type question covering all four Units (2.5 Marks per Unit) & it would be compulsory. Two questions will be set from each unit & out of which candidate will attempt one question. Each Question shall be of 10 marks.

### **Books Recommended**

1. Silverstein RM and Webster FX. Spectrometric Identification of Organic Compounds. John Wiley and Sons, New York. Latest Edition.
2. Pavia DL, Lampman GM and Kriz GS. Introduction to Spectroscopy. Harcourt College Publishers, Orlando. Latest Edition.
3. Vogel HG and Vogel WH. Drug Discovery and Evaluation. Springer-Verlag, Berlin. Latest Edition.
4. Kulkarni SK. Handbook of Experimental Pharmacology. Vallabh Prakashan, New Delhi. Latest Edition.
5. Ghosh MN. Fundamentals of Experimental Pharmacology. Hilton & Company, Kolkata. Latest Edition.

**Paper Code: MPCML-103    Pharmaceutical Chemistry-I  
(Advanced Organic Chemistry)**

**L -- T -- P  
4    --    --**

**Total Credits: 04  
Total Marks: 100**

**External Marks: 50  
Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** By studying this subject, the students will understand different organic reactions and their mechanisms. Knowledge about different organic molecules, their use in pharmacy and basic Terms and techniques in organic chemistry are highlighted.

**UNIT-I**

**Reactive intermediates in organic synthesis:**

- **Carbocations:** Formation, structure, stability and reactions of carbocations. Rearrangement reactions like, Wagner-Meerwein, Beckmann rearrangement and pinacol-pinacolone.
- **Carbanions:** Formation, structure, stability and reactions of carbanions. Perkin, Claisen, Benzoin Aldol condensations, Cannizzaro reaction, Neber rearrangement and Favorskii rearrangement.
- **Free radicals:** Formation, structure, stability, detection, reactions involving free radicals, addition to carbon-carbon multiple bonds.
- **Carbenes:** Formation, structure, stability and reactions of carbenes. Reimer-Tiemen reaction, Wolff rearrangement. Ring expansion reactions - conversion of pyrrole to pyridine.

**UNIT-II**

- **Stereochemistry :** General concept of Stereoisomerism, axially dissymmetric molecules such as biphenyls and allenes. Stereochemistry of some elements other than carbon: elementary stereochemistry of Nitrogen Sulfur and Phosphorous compounds. Conformational analysis of cyclohexane, mono and disubstituted cyclohexanes, heterocycles such as tetrahydro-pyrans with special emphasis on monosaccharides, and piperidines.
- **Pericyclic Reactions:** Symmetry properties of molecular orbitals. Woodward Hoffmann rules. Correlation diagram, FMO approach and PMO approach for electrocyclic reactions, cycloadditions, and sigmatropic rearrangements, Applications.

**UNIT-III**

- **Organic Photochemistry:** Light absorption. Electronic transitions, Jablonski diagram. Intersystem crossing. Photosensitization. Excited states of ketones.  $\alpha$  Cleavage,  $\gamma$  - hydrogen abstraction, di-pit methane rearrangement, Paterno-Buchii reaction and Photoreduction. Photochemistry of conjugated dienes and enones.
- **Combinatorial Chemistry:** Introduction, solid phase and liquid phase synthesis, split, parallel, mix and split synthesis, ular libraries, limitations of combinatorial synthesis.

Examples of combinatorial synthesis: benzodiazepines, quinazolines, imidazoles, hydantoins.

#### UNIT-IV

- **Name reactions; their mechanism and applications in drug synthesis**
  - i) Witting
  - ii) Knorr Pyrazole synthesis
  - iii) Darzen
  - iv) Strecker amino acid synthesis
  - v) Meerwein Ponndorf- verley
  - vi) Oppenauer oxidation
  - vii) Wolf Kishner reduction
  - viii) Mannich
- **Design of synthesis:** An introduction of synthons and synthetic equivalents, general principles of the disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, one group C-X and two group C-X, chemoselectivity, reversal of polarity, use of nitro compounds in organic synthesis and concept of protection and deprotection of functional groups.

#### Note: Instruction for Examiner:

The examination in each theory subject shall be of 50 marks. The examiner will set nine questions. Candidate will attempt five questions. First question would be of short answer type question covering all four Units (2.5 Marks per Unit) & it would be compulsory. Two questions will be set from each unit & out of which candidate will attempt one question. Each Question shall be of 10 marks.

#### Books Recommended

1. Jerry March's Advanced Organic Chemistry, Reactions, Mechanisms and Structure, 5<sup>th</sup> edition, M.B. Smith and Jerry March, John Wiley and Sons New York, U.S.A., 2001.
2. Stereochemistry of Carbon Compounds, reprint 14<sup>th</sup> edition, Ernest L. Eliel McGraw- hill Book Company Inc., New York, U.S.A., 1990.
3. Organic Photochemistry by William Horspool. Reactive Intermediates by C.W. Rees.
4. S.P. Singh and S.M. Mukherji, Reaction Mechanism in Organic chemistry, The macmillian Company of India Limited, New Delhi, India.
5. Organic Chemistry Vol-II, by I.L. Finar Chapter II and IV. Some Modern Methods of Organic Synthesis, IIIrd edition, by W. Carruthers, 1993.
6. Chapter-1, 3 and 6. Organic Synthesis by M.B. Smith, McGraw International edition, 1994
7. Chapter 1,3,4 & 5. The Logic of Organic Synthesis by E.J. Corey and X.M. Cheng, John Wiley and Sons, 1989, Chapter 1 & 2. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Chapman and Hall, 1998.
8. Cycloadditions in Organic Synthesis by W.R Carruthers, Pergamon Press, London, 1990.
9. Classics in Total Synthesis by K.C. Nicolau and E.J. Sorensen, John Wiley, 1996.

**Paper Code: MPCML-105    Pharmaceutical Chemistry-II  
(Advanced Natural Products Chemistry-I)**

**L -- T -- P  
4    --    --**

**Total Credits: 04  
Total Marks: 100**

**External Marks: 50  
Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** The Objective of the paper is to study medicinally important plants & marine drugs scientifically along with chemistry & biosynthesis of different phytoconstituents obtained from crude drugs. The paper also envisages the biotechnological techniques for obtaining and improving the quality of natural products.

**UNIT-I**

- Mechanistic and biosynthetic approaches to plant secondary metabolites. Acetate-mevalonate pathway (biosynthesis of gibberellic acid, cholesterol).
- Shikimic acid pathway (Biosynthesis of chlorogenic acid, cichoriin).
- Polyketides (Biosynthesis of 6-methylsalicylic acid, petulin, penicillanic acid).

**UNIT-II**

- Amino acids and peptides, nucleic acids: General introduction, synthesis, degradative and synthetic approaches supported by spectral data of peptides and amino acids. End group analysis, structural features of Insulin, vasopressin and oxytocin, structural features of DNA & RNA. Compounds derived from Amino acids: Colchicine, Cephalosporin C.

**UNIT-III**

- Marine products with therapeutic potential in drug discovery.
- Current developments in the discovery and design of new drug candidates from natural product leads.
- **Vitamins** - Introduction and Chemistry and biological utility of Vitamine A, E and K. Synthesis of Riboflavin, Pyridoxine, vitamin C, Niacin.

**UNIT-IV**

- Lipids - Classification, role of lipids, fatty acids and glycerol derived from oils and fats; Physical properties – polymorphism, reactions of fats, rancidity, reversion, polymerisation, saponification, addition, hydrogenation, phospholipids, lipid metabolism, intermediary metabolism of fatty acids, synthesis of fatty acids.

**Note: Instruction for Examiner:**

The examination in each theory subject shall be of 50 marks. The examiner will set nine questions. Candidate will attempt five questions. First question would be of short answer type question covering all four Units (2.5 Marks per Unit) & it would be compulsory. Two questions will be set from each unit & out of which candidate will attempt one question. Each Question shall be of 10 marks.

**Books Recommended**

1. Structure Elucidation of Natural Products by Mass Spectroscopy — Vol I & II, H. Budzikiewiez, C.Djerassic and D.H. Williams
2. Tables of Spectral Data for Structural Determination of Organic Compounds- E. Pretsch, T.Clerc, J. Seibl and W. Simon
3. Heterocyclic Chemistry-Albert
4. Biogenesis of Natural Compounds - Bernfeld
5. An Introduction to the Chemistry of Terpenoids and Steroids-Templeton
6. Organic Chemistry of secondary Plant Metabolism-Geissman and Crout
7. Chemistry of the Alkaloids-Pelletier
8. The Chemistry of the Natural Products- Butterworths.
9. Pharmacognosy and Pharmacobiotechnology - J.E. Robbers, M.K. Speedie and V.E. Tyler.

**Paper Code: MPL-107    Pharmaceutical Chemistry-III  
(Advanced Medicinal Chemistry-I)**

**L -- T -- P  
4    --    --**

**Total Credits: 04  
Total Marks: 100**

**External Marks: 50  
Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** Study of this subject covers the theory of drug action, stereochemistry and drug action, Recombinant DNA Technology Rational Design of Enzymes Inhibitors etc. for the proper understanding of the concept of Medicinal Chemistry.

**UNIT-I**

- **Drug receptor interactions and theories of drug action**  
Drug receptor interaction, G-protein coupled receptors, ion channel linked receptors. Ligand gated ion channels, voltage gated ion channels. Ligand-receptors theories: Clarks occupancy theory, rate theory, induced fit theory, macromolecular perturbation theory and activation aggregation theory.
- **Approaches to drug design**  
Introduction, trends in lead identification, modification of lead, source of a lead: Natural products and folklore medicine, random screening, existing drugs.
- **Physicochemical and stereochemical aspects of drug action**  
Solubility, Drug absorption, surface area and particle size, hydrogen bonding and biological activity, polymorphism, stereochemistry and pharmacological activity.

**UNIT-II**

- **Recombinant DNA Technology:**  
Introduction, new therapeutics from r-DNA technology, protein engineering and site directed mutagenesis, genetically engineered drug discovery tools: reagents for structural biology study, enzyme as drug targets, receptors as drug targets, cellular adhesion proteins.
- **Rational Design of Enzymes Inhibitors**  
Introduction, enzyme inhibitors in medicine and basic research.  
*Design of non-covalently binding enzymes inhibitors:* Forces involved in enzyme-inhibitor complexes, Rapid reversible inhibitors, slow, tight and slow-tight inhibitors, transition state analogues, multisubstrate inhibitors.  
*Design of covalently binding enzyme inhibitors:* Mechanism based inhibitors, affinity labels and pseudo-irreversible inhibitors.  
Current developments with respect to the inhibition of the following enzymes: acetylcholinesterase, angiotensin converting enzyme, HMG CoA reductase, dihydrofolate reductase, GABA transferase, monoamineoxidase.

### UNIT-III

- **Analog Design**

Strategies of analog design: bioisosteric replacement, rigid analogs, homologation of alkyl chains, alteration in chain branching, ring size and ring position isomers, alteration in stereochemistry, fragments of lead molecules, variation in interatomic distances.

- **Quantitative structure activity relationships**

Fundamentals of QSAR, Quantitative description of physico-chemical properties: hydrophobicity, partition coefficient, electronic effects, steric effects. Statistical methods in QSAR, Correlation of physicochemical parameters with biological activity: Hansch approach, Free Wilson analysis, Topliss decision tree. 3D QSAR approach, Limitations of QSAR.

### UNIT-IV

- **Molecular Modeling:**

Drawing chemical structures, conversion of 2D structures in 3D form, visualization of 3D structures, viewing proteins, geometry optimization, energy minimization procedures, molecular mechanics methods, quantum mechanics methods, molecular properties, conformational analysis, Pharmacophore concept, Pharmacophoric approach, Pharmacophore elements and representation, Pharmacophore identification, docking, homology modeling, currently used softwares for molecular modeling.

- **Prodrug Design**

Concept, definition and characteristics of the prodrug, Prodrugs of various functional groups, design strategies for modification of drug properties, modification of the physicochemical, pharmacokinetic and pharmacodynamic properties of a drug through chemical transformation. Applications of the prodrug approach: increased absorption, aqueous solubility, prolongation of activity, site specific chemical delivery systems, mutual prodrugs. Hard and soft drugs.

**Note: Instruction for Examiner:**

The examination in each theory subject shall be of 50 marks. The examiner will set nine questions. Candidate will attempt five questions. First question would be of short answer type question covering all four Units (2.5 Marks per Unit) & it would be compulsory. Two questions will be set from each unit & out of which candidate will attempt one question. Each Question shall be of 10 marks.

**Books Recommended**

1. Wolff ME. Burger's Medicinal Chemistry and Drug Discovery, Principle and Practice. John Wiley and Sons, New York. Latest Edition.
2. Franke R. Theoretical Drug Design Methods, Vol. VII. Elsevier, New York. Latest Edition.
3. Silverman RB. The Organic Chemistry of Drug Design and Action. Academic Press Inc., San Diego, USA. Latest Edition.
4. Kenneth M. Merz, Dagmar Ringe, Charles H. Reynolds, Drug Design: Structure and Ligand-Based Approaches, Cambridge University Press



5. Thomas Nogrady, Donald F. Weaver, Medicinal Chemistry: A Molecular and Biochemical Approach, Oxford University Press
6. Alex Gringauz, "Introduction to Medicinal Chemistry" Wiley-VCH, Inc. New York.
7. Ariens, Drug Design, Academic press, NY, 1975.
8. Holtje. Sippl., Rognan and Folkers, Molecular Modeling, Wiley VCH.
9. P.K. Larsen, Tommy and U. Madsen, Textbook of Drug Design and Discovery, CRC Press.
10. T.J. Perun and C.L. Propst, Computer Aided Drug Design: Methods and Applications, Marcel Decker.
11. Monographs and relevant review articles appearing in various periodicals and journals.

**Paper Code: MPP-109    Modern Pharmaceutical and Analytical Techniques**

**Practical**

**L -- T -- P**

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**Total Credits: 04**

**Total Marks: 100**

**External Marks: 50**

**Internal Marks: 50**

**Duration of exam: 04 hrs**

Modern experiments having relevance to the topics covered under theory.

**Books Recommended**

1. Indian Pharmacopoeia, Central Indian Pharmacopoeia Laboratory, Govt. of India, Ministry of Health & Family Welfare, Ghaziabad, Latest Edition.
2. U. S. Pharmacopoeia – NF, The United States Pharmacopoeial Convention, Rockville, USA, Latest Edition.
3. European Pharmacopoeia, Directorate for the Quality of Medicines of the Council of Europe
- 4 (EDQM), Strasbourg, Europe, Latest Edition.
- 5 British Pharmacopoeia, The Stationary Office on behalf of the Medicine Health Care Product
- 6 Regulatory Agency (MHRA), London, Latest Edition.
- 7 Mendham J, Denney RC, Barnes JD and Thomas M. Vogel's Textbook of Quantitative Chemical Analysis. Pearson Education Limited, Singapore. Latest Edition.
- 8 Silverstein RM and Webster FX. Spectrometric Identification of Organic Compounds. John Wiley and Sons, New York. Latest Edition.
- 9 Vogel HG and Vogel WH. Drug Discovery and Evaluation. Springer-Verlag, Berlin. Latest Edition. 8. Kulkarni SK. Handbook of Experimental Pharmacology. Vallabh Prakashan, New Delhi. Latest Edition.
- 10 Ghosh MN. Fundamentals of Experimental Pharmacology. Hilton & Company, Kolkata. Latest Edition.

**Paper Code: MPCMP-113    Pharmaceutical Chemistry Practical -I**  
**L -- T -- P** **Total Credits: 06**  
**--- -- 12** **Total Marks: 150**

**External Marks: 75**  
**Internal Marks: 75**

**Duration of exam: 06 hrs**

Modern experiments having relevance to the topics covered under theory of papers MPCML – 103, 105 & 107 like workshops on stereochemistry, QSAR, 3D-QSAR, Pharmacophore mapping and docking studies. Synthesis of some biologically active heterocyclic nuclei such as hydantoin, thiazolidinone, imidazolidinone, indole, phenyl urea, diphenyl urea, thio-hydantoin, benzofuran, benzimidazole, thiazolidindione, etc. and their characterization. Including Some of the followings:

1. Identification of a binary mixture by chemical (including derivative formation) and spectral techniques.
2. Determination of Ascorbic acid (Vitamin C) by UV. Spectroscopic method in crude drugs.
3. Determination of Hyoscyamine/Hyoscyne in Datura species by UV. Spectroscopic method.
4. Quantitative estimation of Reserpine in Rauwolfia serpentina by HPLC method.
5. Quantitative estimation of Quinine in Cinchona bark by HPLC method. Q
6. Exercises on Identification of simple Naturally occurring molecules by UV, IR and NMR spectroscopy.
7. Extraction and isolation of pectin, starch, caffeine, piperine, solanine, aromatic oils, calcium citrate, solanine, casein, etc.
8. Synthesis and characterization of biologically active hetero-cyclic nuclei such as hydantoin, indole, furan, benzofuran, benimidazole etc
9. Workshops based on stereochemistry, QSAR, 3D-QSAR, pharmacophore mapping and docking studies

## **Paper Code: MPL-102    Biostatistics and Intellectual Property Rights**

**L -- T -- P**  
**4    --    --**

**Total Credits: 04**  
**Total Marks: 100**

**External Marks: 50**  
**Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** Objective of this paper is to give the knowledge of Intellectual Property Rights, Nuts and Bolts of Patenting, Biostatistics etc.

### **UNIT-I**

- **Intellectual Property Rights**

Intellectual Property Concepts and fundamentals: The emergence and growth of the concepts regarding intellectual property (IP), intellectual property protection (IPP) and intellectual property rights (IPR); economic importance, mechanism for protection of intellectual property - patents, copyright, trademarks; role of IP in pharmaceutical industry; global ramifications and financial implications.

### **UNIT-II**

- **Trade Related Aspects of Intellectual Property Rights**

Intellectual property and international trade, concept behind WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), status in India and other developing countries, case studies and examples, TRIPS issues on herbal drugs.

### **UNIT-III**

- **Nuts and Bolts of Patenting**

Copyright and trade mark protection, criteria for patentability, Indian patent act. 1970: WTO and modifications under TRIPS, filing of a patent application, precautions before patenting-disclosures/non-disclosures, publication-article/ thesis, prior art search – published patents search, internet search patent sites, specialized service search requests, costs, patent application forms and guidelines, fee structure, time frames, jurisdiction aspects, types of patent application - provisional, nonprovisional, PCT and convention patent applications, international patenting requirement procedures and costs. Patent infringement: Meaning, scope, litigation, drug related patents infringements, case studies and examples, patenting by research students. Trademarks legislation and registration system in India - an introduction, meaning of trademark, criteria for eligibility, filling application for trademark registration, trade secrets - scope modalities and protection case studies.

## UNIT-IV

- **Ethics and Values in IP**

IP and ethics, positive and negative aspects of IPR, social responsibility, avoiding unethical practices, eco-responsibility–economic, social and environmental benefits of modern biotechnology.

- **Biostatistics**

General concepts, two-tail student t-test and paired sample t-test, two samples t-test, Wilcoxon rank-sum test, Mann-Whitney test, one-way analysis of variance, Kruskal-Wallis test, two-way analysis of variance, multiple comparison procedures in ANOVA: Fischer's LSD test, Tukey's studentized range test and Dunnett's test. Non-linear regression: Introduction, iterative method. Correlation, linear regression, PCA and PLS.

**Note: Instruction for Examiner:**

The examination in each theory subject shall be of 50 marks. The examiner will set nine questions. Candidate will attempt five questions. First question would be of short answer type question covering all four Units (2.5 Marks per Unit) & it would be compulsory. Two questions will be set from each unit & out of which candidate will attempt one question. Each Question shall be of 10 marks

**Books Recommended:**

1. Treece DJ. Managing Intellectual Capital: Organizational, Strategic and Policy Dimension. Oxford University Press, England. Latest Edition.
2. Wadedhra BL. Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications. Universal Law Publishing, New Delhi. Latest Edition.
3. Bansal P. IPR Handbook for Pharma Students and Researchers, Pharma Book Syndicate, Hyderabad. Latest Edition.
4. Copyright Protection in India [website: <http://copyright.gov.in>].
5. Information on Orange Book [website: [www.fda.gov/cder/ob/default.htm](http://www.fda.gov/cder/ob/default.htm)].
6. World Trade Organization [website: [www.wto.org](http://www.wto.org)].
7. Trivedi PR. Encyclopedia of Intellectual Property Rights. Jnanada Prakashan, New Delhi. Latest Edition.
8. Arya P. P. and Yashpal, Research Methodology in Management, Deep and Deep publications Private Limited, New Delhi.
9. Green and Tull : A research for marketing research decisions, PHI (P) Ltd. New Delhi.
10. Karishna Swami, Shiva Kumar & Mathirajan, Management Research Methodology, Pearson Education.
11. Hooda, R P, Statistics for Business and Economics, MacMillan India Limited, New Delhi.
12. Heinz, Kohler: Statistics for business and Economics, Harper Collins.
13. Lawrence B Morse: Statistics for business and economics, Harper Collins.
14. Levin, Richard I. & David S Rubin: Statistics for management PHI Delhi.

**Paper Code: MPCML-104 PHARMACEUTICAL CHEMISTRY – IV  
(ADVANCED SPECTRAL AND ANALYTICAL TECHNIQUES)**

**L -- T -- P  
4 -- --**

**Total Credits: 04  
Total Marks: 100**

**External Marks: 50  
Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** The objective of the paper is to improve the skills in pharmaceutical analysis by studying various principles involved in instrumental methods of chemical analysis & interpreting the data of spectroscopic analysis. Introductory part of IR, UV, NMR and MASS spectroscopy has already been covered in Ist Semester. After completion of this paper students will be able to do validation of instruments, trouble shooting in operations related to analytical instruments, interpretation of results obtained from data or spectra, designing of appropriate analytical method for newer or known drug or drug material.

### **UNIT-I**

- **Infrared Spectroscopy**

The Hook's law and calculation of stretching frequencies for different types of bonds and their bond strengths, coupled interactions, hydrogen bonding, examination of infrared spectrum, survey of important functional groups with examples, radiation source, detectors used, sample handling, quantitative applications, qualitative applications with special reference to stereochemical aspects and hydrogen bonding, Near-IR spectroscopy, absorption and reflectance spectrophotometry, instrumentation, applications, Far Infrared spectroscopy. Introduction to FTIR and its applications.

- **Raman Spectroscopy** - Introduction, theory and polarization measurement, rules of selection and polarization, instrumentation, applications in pharmaceutical sciences. Comparison of Infrared and Raman spectra.

### **UNIT-II**

- **Ultraviolet / Visible Spectroscopy and Fluorimetry**

Energy level and selection rules, effect of substituents, effect of conjugation, conformation and geometry, the Woodward-Fisher rules, the Fisher-Kuhn rules, applications of UV with reference to different electronic systems. Derivative spectroscopy and its applications. Fluorescence and chemical structure, fluorescence intensity, factors affecting fluorescence, instrumentation, comparison of fluorometry with spectrophotometry, applications of fluorimetry in pharmaceutical analysis.

- **Nuclear Magnetic Resonance Spectroscopy**

- **<sup>1</sup>H-NMR spectroscopy**

Magnetic equivalence, failure of the N+1 rule, chemical shifts, local diamagnetic shielding, hybridization effects, magnetic anisotropy, mechanism of spin-spin coupling, the origin of spin-spin splitting, Pascal's triangle, the coupling constant, protons on oxygen, nitrogen and sulphur, diastereomeric protons, chemical shift reagents, long range coupling, spin decoupling methods, nuclear over Hauser effect. Correlation NMR spectrometry: introduction to <sup>1</sup>H -<sup>1</sup>H cosy and <sup>1</sup>H -<sup>13</sup>C cosy and its applications. Introduction and applications of 2D NMR; solid state NMR.

### **<sup>13</sup>C-NMR spectroscopy**

Introduction, peak assignments, off resonance decoupling, selective proton decoupling; chemical shift equivalence; chemical shifts; spin coupling.

- **Spectrometry of other important nuclei** - Introduction to <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P, basic concepts.

## **UNIT-III**

- **Mass Spectrometry**

Basic principle and theory involved; instrumentation, type of ions; various ion sources, electron impact source, chemical ionization sources, field ionization sources, desorption sources, mass analysers, double focusing, quadripole, time of flight, ion trap analyzer, ionization, fragmentation, rearrangements, mass spectra of representative compounds, recognition of molecular ion peak, metastable peak, isotopic peaks, applications.

- **X-Ray Spectroscopy**

Introduction, production and properties of the X-ray, X-ray emission, X-ray absorption, principles of X-ray diffraction, powder diffraction, X-ray diffraction methods, application of X-ray diffraction technique in pharmaceutical sciences. Electron microscopy and electron diffraction.

## **UNIT-IV**

- **Chromatography**

**Gas Chromatography:** Gas liquid chromatography, gas solid chromatography, instrumentation and applications (GC-MS and GC-FTIR). Derivatization as a means of sampling of thermosensitive compounds.

**High Pressure Liquid Chromatography:** Partition, adsorption, ion exchange, size exclusion; pharmaceutical applications of HPLC and LC-MS. Super critical fluid chromatography; brief introduction to HPTLC.

- **Electrophoresis:** Theory and application of electrophoresis, polyacrylamide and agarose gel electrophoresis, capillary electrophoresis, 2- D electrophoresis.

### **Note: Instruction for Examiner:**

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### **Books Recommended**

1. Silverstein RM and Webster FX. Spectrometric Identification of Organic Compounds. John Wiley and Sons, New York. Latest Edition.
2. Chatten LG. Pharmaceutical Chemistry, Vol I & II. Marcel Dekker, New York. Latest Edition.
3. James WD and Kenneth HT. Analytical Chemistry by Open Learning: Thermal Methods. John Wiley and Sons, New York. Latest Edition.

4. Abraham RJ, Fisher J and Bftus P. Introduction to NMR Spectroscopy. John Wiley and Sons, New York. Latest Edition.
5. Pavia DL, Lampman GM and Kriz GS. Introduction to Spectroscopy. Harcourt College Publishers, Orlando. Latest Edition.
6. UV and Visible Spectroscopy, Chemical Application-C.N. R. Rao.
7. Spectrometric identification of organic compound- Silverstein.
8. Spectrometric identification of organic compound- William Kemp
9. Chemical application of IR spectroscopy - C.N.R. Rao.
10. Interpretation of Mass Spectra of organic compounds-B. Kienicz, C. Djerassi.
11. Application of NMR Spectra to Organic Chemistry-Jackmann.
12. Instrumental Methods of Analysis- Willard.
13. Applications of Absorption spectroscopy of organic compounds - John R. Dyer.
14. Kasture, A.V. Mahadik, K.R. Wadodkar , S.G. and More, H.N. (2004). Pharmaceutical analysis Vol-II Instrumental methods. Nirali Prakashan.



**Paper Code: MPCML-106 PHARMACEUTICAL CHEMISTRY – V  
ADVANCED NATURAL PRODUCTS CHEMISTRY – II**

**L -- T -- P  
4 -- --**

**Total Credits: 04  
Total Marks: 100**

**External Marks: 50  
Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** The objective of the paper is to study medicinally important plants & marine drugs scientifically along with method of isolation, chemistry, degradation, synthetic methods, spectral techniques for structural elucidation and biological activity.

**UNIT-I**

- General introduction and classification, isolation and purification methods of alkaloids, structure elucidation of reserpine, atropine and morphine.

**UNIT-II**

- Classification, method of isolation, chemistry, degradation, synthetic methods, spectral techniques for structural elucidation and biological activity of flavonoids rutin and quercetin.
- Study of chemistry, stereochemical aspects and pharmaceutical importance of plant derived steroids -cardiac glycosides (cholesterol, diosgenin).

**UNIT-III**

- General introduction and classification terpenoids; Essential Oils; Production of Essential Oils ; Chemistry and Analysis of Essential Oils ; Biological Activities of Essential Oils ; Aromatherapy with Essential Oils ; Industrial Uses of Essential Oils, Essential Oils Used in Veterinary Medicine; Trade of Essential Oils; Recent EU Legislation on Flavors and Fragrances of Essential Oils.

**UNIT-IV**

- Recent advances in the chemistry of naturally occurring anti-neoplastic agents (catharanthus alkaloids, camptothecin); antimalarials (cinchona alkaloids, artemisinin derivatives).
- Role of natural products in “Neglected Diseases” (dengue, protozoal diseases including leishmaniasis, trypanosomiasis, schistosomiasis, tuberculosis, leprosy).

**Note: Instruction for Examiner:**

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**Books Recommended**

1. Cordell GA. Introduction to Alkaloids. John Wiley and Sons, New York. Latest Edition.
2. Fieser LF and Fieser M. Steroids. Reinhold Publishing Co., New York. Latest Edition.
3. Wickery ML and Wickery B. Secondary Plant Metabolism. Mcmillan Press Ltd. London. Latest Edition.
4. Torseel KBG. Natural Product Chemistry. John Wiley and Sons, New York. Latest Edition.
5. Harborne JB. Phytochemical Methods. Chapman and Hall, London. Latest Edition.
6. Finar IL. Organic Chemistry. The English Language Book Society, London. Latest Edition.
7. Wolff ME. Burger's Medicinal Chemistry and Drug Discovery, Principle and Practice. John Wiley and Sons, New York. Latest Edition.
8. Mitscher LA and Baker WR. A Search for Novel Chemotherapy Against Tuberculosis Amongst Natural Products. Pure and Applied Chemistry (1998) , Vol. 70, No.2, pp 365-371.
9. Wermuth CG. The Practice of Medicinal Chemistry. Academic Press, Jordon Hill, Oxford. Latest Edition.
10. Boldi AM. Combinatorial Synthesis of Natural Product Based Libraries. Taylor and Francis, London. Latest Edition.
11. Monographs and relevant review articles appearing in various periodicals and journ.

**Paper Code: MPCML- 108 PHARMACEUTICAL CHEMISTRY – VI  
(ADVANCED MEDICINAL CHEMISTRY – II)**

**L -- T -- P  
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**Total Credits: 04  
Total Marks: 100**

**External Marks: 50  
Internal Marks: 50**

**Duration of exam: 03 hrs**

**Paper Objectives:** Medicinal chemistry is a branch of chemistry also involving aspects of biological, medical and pharmaceutical sciences. It is concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the interpretation of their mode of interaction at the molecular level, the construction of their structure-activity relationships, and study of their metabolism.

**UNIT-I**

• **Antibacterial agents**

Introduction, history and development of resistance to known antibacterials such as penicillins. Bacterial DNA-gyrase inhibitors - mode of action of fluoro-quinolones and development of newer analogues: Trovafloxacin, Levofloxacin, Gratifloxacin including Ciprofloxacin and Norfloxacin, Oxazolidinones: Inhibitors of DNA Synthesis.

• **Anti-cancer drugs**

Newer targets for anticancer therapy, Topoisomerase inhibitors: Histone deacetylase inhibitors, Telomerase Inhibitors. Tumor helicases inhibitors: Antimitotic agents. Tubulin interacting agents: DNA-intercalators: DNA-threading agents: Tumor necrosis factor converting enzyme (TACE) inhibitors. Anti cancer drugs for crossing BBB.

• **Antiviral Agents**

DNA and RNA viruses, retroviruses, strategies to design anti-HIV drugs, viral replication, anti-viral agents for RNA-virus infections, development of new drugs and drug discovery Diadanosine, Nevirapine.

**UNIT-II**

- **Drugs affecting Adrenergic neurotransmission:** Introduction, history and neurotransmission at sympathetic nervous system; biosynthesis and metabolism of NE; characterization of adrenergic receptor subtypes and mechanism. Structure activity relationship of adrenergic agonists and antagonists.

• **Cardiovascular drugs:**

- Anti-hypertensives: Designing of ACE & AT1 inhibitors – Captopril, Enalapril, Enalaprilat, Lisinpril, Losartan.
- $\beta$ -blockers,  $\alpha$ -blockers and  $\alpha,\beta$ -blockers – Atenolol, Metoprolol and analogues, Carvedilol, Prazocin, Trazocin, Labetelol
- Calcium Channel blockers: 1,4-dihydropyridines (Nifedipine, Nimodipine, Nicardipine), Verapamil, Diltiazem.

- d. Lipid lowering and anti-clotting agents – Statins eg., Atorvastatin, Rosuvastatin; Aspirin, Lipitor, Gemfibriogel, abciximab, Probucol, Celcade, clopidogrel.
- e. Selective human  $\beta_3$  adrenergic agonists used as antiobesity agents.
- f. Clot busters: Urokinase, Streptokinase, Alfinaprase.
- g. Anti – arrhythmic agents: Amilorone, Digoxin, Flecainide, Mexiletine, Tocainide, Lidocaine.
- h. Peptides with cardiovascular applications.

### UNIT-III

- **Psychopharmacological Agents**

Psychopharmacological agents : Antipsychotic Agents : Biochemical basis of mental disorders, Development of antipsychotic agents, tricyclic antidepressants, Monoamine oxidase inhibitors; Selective serotonin-reuptake inhibitors; Atypical antidepressants, Antianxiety Agents : Chemistry of benzodiazepines; SAR of benzodiazepine derivatives, medicinal chemistry of non-benzodiazepines; serotonin-reuptake inhibitors, development of meprobamate and analogues; atypical anxiolytic agents; including studies of various receptors - GABA, Dopamine, NMDA, Metabotropic glutamate, excitatory amino acid neurotransmitters .

### UNIT-IV

- **Drugs affecting hormonal system:** Adrenocorticoids, estrogen, progestins and androgens. Chemical contraceptives; latest advances in drug receptors chemistry.
- **Prostaglandins and Other Eicosanoids** -Nomenclature, biosynthesis, design of eicosanoid drugs, biological activity, metabolism, structure activity relationship, eicosanoids approved for human clinical use.

**Note: Instruction for Examiner:**

The examination in each theory subject shall be of 50 marks. The examiner will set nine questions. Candidate will attempt five questions. First question would be of short answer type question covering all four Units (2.5 Marks per Unit) & it would be compulsory. Two questions will be set from each unit & out of which candidate will attempt one question. Each Question shall be of 10 marks.

**Books Recommended**

1. Wolff ME. Burger's Medicinal Chemistry and Drug Discovery, Principle and Practice. John Wiley and Sons, New York. Latest Edition.
2. Alnley W and James EF. Martindale, The Extra Pharmacopoeia. Pharmaceutical Press,London. Latest Edition.
3. Nogrady T. Medicinal Chemistry, A Biochemical Approach. Oxford University Press,New York. Latest Edition.

4. Monographs and relevant review articles appearing in various periodicals and journals.
5. Franke R. Theoretical Drug Design Methods, Vol.VII. Elsevier, New York. Latest Edition.
6. C. H. Wermuth, "The Practice of Medicinal Chemistry", Academic Press, London, 1969, 264.
7. The Quinolones, 2<sup>nd</sup> edition, edited by V.T. Andriole. Academic Press, 1998
8. Cancer Chemotherapeutic Agents. Edited by W.O. Foye, American Chemical Society, 1995.
9. Introduction to the Principles of Drug Design and Drug Action, Edited by H.J. Smith, Taylor and Francis, 2006.
10. Manfred E Wolff, (ed), Burger's Medicinal Chemistry and Drug Discovery, Vol – I Principles and Practice, 5<sup>th</sup> Ed., John Wiley and Sons, 1995.
11. J. G Vinter and Mark Gardner, (Eds.) Molecular Modelling and Drug Design, The Macmillan Press Ltd., London, U.K., 1994.
12. C. Hansch, A. Leo and D. Heokman, Exploring QSAR: Applications in Chemistry and Biology, ACS Professional Reference Book, American Chemical Society, Washington U.S.A., 1995.
13. Comprehensive Medicinal Chemistry, Pergamon press, 1990, Vol. 4. · Medicinal Chemistry for the 21<sup>st</sup> Century, Edited by C.G. Wermuth, Blackwell Scientific Publications, Oxford, 1992.
14. Pseudopeptides in Drug Discovery, Edited by P.E. Nielson, Wiley-VCH, 2004
15. Introduction to the Principles of Drug Design and Drug Action, Edited by H.J. Smith, Taylor and Francis, 2006.
16. The Organic Chemistry of Drug Design and Drug Action, 2<sup>nd</sup> edition, R.B.Silverman, Academic Press, 2006.
17. Molecular Modeling in Drug Design, Edited by N.C. Cohen, Elsevier, 2006

**Paper Code: MPCMP-110      Pharmaceutical Chemistry Practical -II  
(Advanced Spectral & Analytical Techniques Practical)**

**L -- T -- P  
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**Total Credits: 04  
Total Marks: 100**

**External Marks: 50**

**Internal Marks: 50**

**Duration of exam: 04 hrs**

Modern experiments having relevance to the topics covered under theory.

**Books Recommended**

1. Indian Pharmacopoeia, Central Indian Pharmacopoeia Laboratory, Govt. of India, Ministry of Health & Family Welfare, Ghaziabad, Latest Edition.
2. U. S. Pharmacopoeia – NF, The United States Pharmacopoeial Convention, Rockville, USA, Latest Edition.
3. European Pharmacopoeia, Directorate for the Quality of Medicines of the Council of Europe (EDQM), Strasbourg, Europe, Latest Edition.
4. British Pharmacopoeia, The Stationary Office on behalf of the Medicine Health Care Product Regulatory Agency (MHRA), London, Latest Edition.
5. Mendham J, Denney RC, Barnes JD and Thomas M. Vogel's Textbook of Quantitative Chemical Analysis. Pearson Education Limited, Singapore. Latest Edition.
6. Silverstein RM and Webster FX. Spectrometric Identification of Organic Compounds. John Wiley and Sons, New York. Latest Edition.
7. Vogel HG and Vogel WH. Drug Discovery and Evaluation. Springer-Verlag, Berlin. Latest Edition.
8. Kulkarni SK. Handbook of Experimental Pharmacology. Vallabh Prakashan, New Delhi. Latest Edition.
9. Ghosh MN. Fundamentals of Experimental Pharmacology. Hilton & Company, Kolkata. Latest Edition.

**Paper Code: MPCMP-112      Pharmaceutical Chemistry Practical -III**

**L -- T -- P  
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**Total Credits: 06  
Total Marks: 150**

**External Marks: 75  
Internal Marks: 75**

**Duration of exam: 06 hrs**

Multi-step Synthesis of Organic Medicinal Compounds, their intermediates, chromatographic purification and spectroscopic characterization including that of sulfanilamide, para-aminobenzoic acid, anti-pyrine, benzocaine, methaqualone, phenytoin, uramil, saccharine, chloramine-T, dichloramine-T, etc, including Some of the followings:

1. Simultaneous estimation of Paracetamol and Ibuprofen: Aspirin and Caffeine ; Rifampicin and Isoniazid or other combination formulation (4 expts).
2. UV. Visible spectrum scanning of certain organic compounds – absorption and correlation of structures and comparison e.g., Chloramphenicol, Analgin, Sulphadiazine, Ibuprofen
3. Exercises on interpretation of at least 5-different known compounds of Natural origin by using spectroscopic data (NMR & MASS)
4. Workshop on spectroscopy structural elucidation of at least 5 unknown compounds.
5. IR, NMR & Mass spectroscopy (1 compound each).
6. Effect of pH and solvent On U.V. Spectrum of certain drugs.
7. Multi-step Synthesis of Organic Medicinal Compounds and intermediates, their chromatographic purification and spectroscopic characterization including sulphanilamide, PABA, benzocaine, antipyrine, phenytoin, methaqualone and chloramine T etc.
8. Practicals based on extraction and isolation of natural products using Hot continuous soxhalation, preparative TLC, HPTLC.
7. Paper reading/seminar with respect to the latest developments in pharmaceutical chemistry, writing of papers, projects and reports. Skills in oral presentation/presenting research papers.
8. Exercise on interpretation of known natural products by using spectroscopic data (NMR & MASS).

**Books Recommended**

1. F.C. Mann and B.C. Saunders, Practical Organic Chemistry, orient Longman, 4<sup>th</sup> edition, New Delhi, India 1960
2. A.I. Vogel, A Text Book of Practical Organic Chemistry, 5<sup>th</sup> edition, The English Language Book Society and Longman Group Limited London, U.K. 1991.
3. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic Compounds, 5<sup>th</sup> edition, John Wiley and sons, Inc., New York, U.S.A., 1991
4. E.L. Eliel, Stereochemistry of Carbon Compounds, Reprint 14<sup>th</sup> edition, Mc GrawHill Book Company, Inc., New York, U.S.A. 1990.