

**M. PHARM. – PHARMACEUTICAL CHEMISTRY**  
**COURSE STRUCTURE (w. e. f. 2011-12)**

<b>I SEMESTER</b>					
<b>Course No.</b>	<b>Title</b>	<b>L(h)</b>	<b>T(h)</b>	<b>P(h)</b>	<b>C</b>
<b>THEORY</b>					
<b>MPS1101</b>	Advanced Instrumental Analysis (AIA)	3	1	0	4
<b>MPS1111</b>	Stereochemistry & Reaction Mechanism (SRM)	3	0	0	3
<b>MPS1113</b>	Basic Approaches in Drug Discovery and Drug Development (BADD)	3	0	0	3
<b>LAB</b>					
<b>MPS1112</b>	Modern Analytical Techniques Lab	0	0	3	2
<b>MPS1114</b>	Computer Aided Drug Design Lab	0	0	3	2
<b>BREADTH</b>					
<b>MMA1101</b>	Applied Science: Biostatistics	3	0	0	3
	Breadth Paper	3	0	0	3
<b>Total</b>		<b>15</b>	<b>1</b>	<b>6</b>	<b>20</b>
<b>Total Hours</b>		<b>22</b>			
<b>II SEMESTER</b>					
<b>THEORY</b>					
<b>MPS2111</b>	Advanced Medicinal Chemistry (AMC)	3	0	0	3
<b>MPS2113</b>	Natural Products Chemistry (NPC)	3	0	0	3
<b>MPS2115</b>	Research Methodology in Pharmaceutical Chemistry	3	0	0	3
<b>ELECTIVE(ANY ONE)</b>					
<b>MPSE103</b>	Advanced Drug Design	3	0	0	3
<b>MPSE105</b>	Advanced Spectral Analysis				
<b>MPS2101</b>	Biopharmaceutics & Pharmacokinetics				
<b>LAB</b>					
<b>MPS2112</b>	Advanced Synthetic Medicinals Lab	0	0	6	4
<b>MPS2114</b>	Advanced Natural Products Lab	0	0	6	4
<b>Total</b>		<b>12</b>	<b>0</b>	<b>12</b>	<b>20</b>
<b>Total Hours</b>		<b>24</b>			
<b>III SEMESTER</b>					
<b>MPS3111</b>	THESIS	-	-	-	<b>15</b>
<b>IV SEMESTER</b>					
<b>MPS4111</b>	THESIS	-	-	-	<b>20</b>

**Total Credit - 75**

Note:

L: Lecture; T: Tutorial; P: Practical; C: Credit

MPS: M. Pharm. Pharmaceutical Sciences Core

MPSE: M. Pharm. Pharmaceutical Sciences ELECTIVE

MMA: Mathematics

## M. PHARM I SEMESTER

### MPS1101: ADVANCED INSTRUMENTAL ANALYSIS (AIA) (4 CREDITS)

1. Analytical Application of Absorption Spectra: 3h  
Absorptiometric assay of Organic Compounds, Structural Analysis.
2. Infrared Spectrophotometry: 6h  
Qualitative uses; Interpretation of I.R. Spectra, Quantitative analysis.
3. NMR-Spectroscopy: 8h  
The NMR-Signal, Instrumentation practical consideration, chemical shift, spin-spin coupling, Structure elucidation, investigation of dynamic properties of molecules, quantitative analysis.
4. Mass Spectrometry: 8h  
Theory instrumentation, practical consideration, structure elucidation, detection of impurities, quantitative analysis, application to determination of structure, the gas chromatograph mass spectrometer combination.
5. Optical Rotatory Dispersion: 3h  
Terminology Plain Curves, Rotatory dispersion of ketones, The Axial Haloketone Rule, Octant Rule.
6. Recent trends in chromatography with reference to analysis of drugs and related substances: HPLC, UPLC, HPTLC , GC and hyphenated techniques(LC-MS/ LC-MS/MS). 8h
7. Theory, Instrumentation and Applications of: 8h  
Thermogravimetric Analysis (TGA), Differential thermal analysis (DTA), Differential Scanning Calorimeter (DSC), X ray Diffraction(XRD).

### **BOOKS RECOMMENDED:**

1. Practical Pharmaceutical Chemistry (part II) by Beckett and Stenlake.
2. Optical Rotatory Dispersion by C. D. Jerassi (For ORD).
3. Indian Pharmaceutical (Biological & Microbiological Assay).
4. British Pharmaceutical (Biological & Microbiological Assay).
5. UV and Visible Spectroscopy, Chemical Application-C.N. R. Rao.
6. Spectrometric identification of organic compound- Silverstein.
7. Chemical application of IR spectroscopy – C.N.R. Rao.
8. Physical Methods of Organic Chemistry- Weissberger.
9. Interpretation of Mass Spectra of organic compounds-B. Kienicz, C. Djerassi.
10. Application of NMR Spectra to Organic Chemistry-Jackmann.
11. Instrumental Methods of Analysis- Willard.
12. Applications of Absorption spectroscopy of organic compounds – John R. Dyer.
13. Pharmaceutical Experiments on isolated preparations by the staff of the Department of Pharmacology, University of Edinburg.
14. Pharmacological Techniques in Drug evaluation, Vol. 1&2 by Peter E. Siegler, J.H. Meyer.
15. Lewis Pharmacology- James Crossland.
16. Fundamental of Experimental Pharmacology- M.N. Ghosh.
17. Indian Pharmacopoeia.
18. British Pharmacopoeia.
19. United States Pharmacopoeia .
20. Assay of Vitamins by Haskmi

## MPS1111 STEREO CHEMISTRY AND REACTION MECHANISM (3 CREDITS)

### STEREO CHEMISTRY

#### 1. Stereo isomerism, Geometrical isomers and optical isomers:

- Basic concepts of optical activity and chirality - Structural features necessary for optical activity.
- Stereo chemistry of – cis-trans,-olefines –
- Stereo chemistry of ring systems – including fused and bridged rings.
- Steric strain in small rings, medium rings, unsaturated rings and unavoidable crowdings.

#### 2. Configuration and its specifications, Correlation of configuration, absolute configuration, methods of determining configurations, Racemic modification, resolution and optical purity.

- **Conformation and reactivity in acyclic compounds** – conformational analysis.
- **Conformation in open chain.** Six membered rings and other ring having heteroatoms.

#### 3. Stereo selective and stereo regulated polymerization.

- Asymmetric synthesis, chiral induction, chiral reagents, catalysts and solvents (industrially used).
- Asymmetric synthesis of amino acids.
- $\beta$  – lactams.

### REACTION MECHANISM:

#### 4. Methods for determining reaction mechanism : Free Radical substitution with special reference to mechanism & reactivity, Generation of nitronium and nitrenium ions and their reactivity, Oxidation and reduction, Eliminations, Rearrangements, reaction with special emphasis on mechanism & reactions.

#### 5. Aliphatic and Aromatic Nucleophilic substitutions with special emphasis on mechanism & reactivity.

#### 6. Aliphatic and Aromatic Electrophilic substitution with special emphasis on mechanism & reactivity.

#### 7. Addition to carbon-carbon multiple bonds, Addition to Carbon - Heteroatom multiple bonds with special reference to mechanism & reactivity with reference to mechanism, orientation & reactivity.

#### 8. Mechanistic consideration in detail for the following organic reactions.

Beckmann, Hofmann, Curtius, Schmidt, Fries' rearrangements.

Benzilic acid, Claisen's condensation Wittig's reaction, Oppenauer Oxidation, Birch's reduction, Clemmensen's reduction, Reimer-Tiemann's reaction, Meerwein, Pinner's reaction, Wolff-Kishner's reduction, Michael's condensation, Diels Alder reaction, Cannizzaro's reaction.

**BOOKS RECOMMENDED:**

1. Jerry March, Advanced organic Chemistry – Reaction Mechanism and Structure – John Willey & Sons, New York.
2. E.L. Eliel – Stereo chemistry of carbon compounds – Mc Graw – Hill Book Company – Inc. New York.
3. E.S. Gould – Mechanism and Structure in organic chemistry.
4. E.L. Eliel - Conformational analysis.
5. R.A. Atiken & S.N. Kilenyl – Assynetric synthesis Ed. Blackie academic & Professional – Glasgow U.K.

**MPS1113 BASIC APPROACHES IN DRUG DISCOVERY AND DEVELOPMENT  
(3 CREDITS)**

- 1. Drug design – Introduction, Definition, Rational,**
  - Drug discovery & development, Definition, outline, achievements in the field of Pharmaceuticals & Medicinals.
  - Parameters involved in drug design, Physicochemical, Ionization, Hydrogen, bonding, Chelation, surface active agents Redoxpotential
  - Drug distribution: Oral, Systemic, Protein binding, Tissue depots.
- 2. Receptors and drug receptor theories-**
  - Drug target binding forces – Electrostatic, Hydrophobic, Hydrogen bonding, Vanderwaals forces.
  - Drug receptor, interaction – Molecular biology of receptors – Protein coupled, Ion channel linked receptors, Nuclearreceptors, GPCR,.
  - Receptorial theories – Occupancy, theory, Rate theory, Induced fit theory, Macromolecular perturbation theory
- 3. Isosterism & bioisosterism-**
  - Concepts of isosterism in drug design
  - Classical and non classical isosterism
  - Application of bioisosterism
  - Basic approaches in QSAR – Hansch equation, Free Wilson Model, Topliss Tree, Craig plot.
- 4. Metabolite antagonism & drug design, Definition, Historical development-**
  - Wood fields antimetabolite theory
  - Mechanism based enzyme inhibition
  - Transition state analogs
- 5. Concepts of drug discovery in Natural products –**

Natural Leads : its identification and optimization using CADD techniques with few case studies.
- 6. Basic concepts of chemoinformatics –**
  - Introduction to chemoinformatics
  - Molecular file formats and their conversions: smiles, smirks & smarts
  - Database search: sub structure search and similarity search
- 7. Basic concepts of ADMET –**

Introduction, General principles of ADMET & basic approaches in drug discovery & development.

## BOOKS RECOMMENDED :

1. Manfred E. Wolff and Burger's, Medicinal Chemistry and Drug Discovery- Vol.1, Principles and Practice, Vth Ed, John Wiley & Sons.
2. E.J. Ariens; Drug Design, Academic Press, New York.
3. Progress in Medicinal Chemistry, Series by Ellis & Wert.
4. Wilson & Gisvolds – Text book of organic medicinal and pharmaceutical chemistry, 10<sup>th</sup> Edition, 1998.
5. Receptor based drug design, by P. Leff, Marcel Dekker, New York, 1998.
6. Paul's charifson – Practical application of computer Aided drug design – Marcel Dekker – 1997.
7. The Organic Chemistry of Drug design and Drug Action - R.B.Silverman – Academic Press –1992.
8. Exploring QSAR – Fundamental and applications in Chemistry and Biology by Carowari Hansch and Albert Leo, ACS, Washington DC – 1995.
9. Alan L. Harney - Advanced in drug discovery techniques.
10. Alfred Burger – Text Book of medicinal chemistry Vol. 1 & Vol. 2.
11. William O. Foye – Principles of Medicinal Chemistry Varghese Publishing House, Bombay – 3<sup>rd</sup> Edition, 1989.
12. Ellis & Wert – Progress in Medicinal Chemistry – Academic Press, New York.
13. Chemistry of Alkaloids by S.W. Pelletier
14. Alkaloids by Manske.
15. Physiology by Dieter Hess.
16. Alkaloids by Fieser and Fieser.
17. Organic Chemistry by I.L. Finar Vol. II.
18. Chemistry of Natural Products by K.W. Bentley.
19. Synthesis of Aromatic Compounds by Ulrich Weiss & J. Michael Edwards.

### Journals.

1. Phytochemistry
2. Planta Medica
3. Phytotherapy Research, Fitoterapia etc.
4. Journal of Medicinal Chemistry
5. Journal of Pharmaceutical Sciences.
6. Journal of Chem. Informatics & Computer Sc.
7. Drug Discovery today.
8. Journal of Computer Aided Molecular Design.

### **MPS1112 MODERN ANALYTICAL TECHNIQUES LAB (2 CREDITS)**

Assay of Pharmacopoeial drug formulations containing one/more than one constituent using different instrumental methods.

#### **LIST OF MAT EXPERIMENTS:**

1. Determination of  $\lambda_{\text{max}}$ . Of given sample using Spectrocolorimeter and validity of Lambert-Beer's Law.
2. Assay of Paracetamol Tablets using UV-Spectrophotometer.
3. Assay of Quinine Sulphate using UV-Spectrophotometer.
4. Assay of Nimesulide Tablets using UV-Spectrophotometer.
5. Assay of Riboflavin Tablets using Fluorescence Spectrophotometer.
6. Assay of Quinine Sulphate tablets using Fluorescence Spectrophotometer.
7. Determination of  $\text{Na}^+$  &  $\text{K}^+$  using Flame Photometer.
8. Determination of Dextrose in Dextrose Injection using Polarimeter.
9. Determination of  $\alpha$ -Amino Acid using pH-Meter.
10. Assay of Paracetamol in the sample using HPLC.
11. Demonstration of functional groups of the given samples I.R.Spectrophotometer.
12. Assay of Paracetamol in the sample using HPTLC.

## **MPS1114 COMPUTER AIDED DRUG DESIGN LAB. (2 CREDITS)**

A hands on training of various molecular modeling software (Maestro/Glide/ Phase/Qik Prop/Strike/Sybyl/ Scigress/Autodock) and their applications in drug design and research

### **LIST OF CADD EXPERIMENTS:**

1. Building, viewing and cleaning small molecules using Chemoffice /Maestro/ Sybyl/ Scigress etc.- Using selection and manipulation tools, substituting atoms or bonds, changing appearance of the molecules (conversion of 2D structure to 3D structure, various methods of rendering, spinning at different axes and animation of models)
2. Calculation of various properties of the molecules , visualization and interpretation-Bond lengths, Bond angles, Torsion angles, Dipole moments, Heat of formation, Clog P and FQ log P, partial charges, Electron density, electrostatic potential, HOMO and LUMO energies and orbitals, spectral transitions etc.
3. Energy minimization of small molecules using various methods : Molecular mechanics (MM2, MM3 ), Semiempirical methods (CNDO, MNDO, INDO, MNDO-d) and *ab initio* methods
4. Conformational analysis of small molecules using various methods -systematic search, random search, distance geometry and Molecular Dynamics (simulated annealing) methods.
5. Importing and Cleaning Protein Crystal structures from Protein data bank- saving PDB molecule in different formats, viewing and analyzing proteins, preparation of the protein structure and location of the active site using Autodock / Glide/Scigress Explorer.
6. Ligand preparation using Autodock and Glide for docking purposes.
7. Docking of ligands into the proteins using Autodock /Glide / Scigress and analysis of the docking and scoring results.
8. Pharmacophore search methods using Phase.
9. Demonstration of 3D QSAR methods of various datasets of particular interest (anti HIV agents, anti diabetics, antifungals,antiinflammatories etc.)using Sybyl.
10. Demonstration of ADME tools using QikProp and ADME ModelBuilder.
11. A brief exercise on design of a novel molecule using the various modules with reference to the following fields of medicinal chemistry research:
  - AntiHIV agents
  - Antineoplastics
  - Antidiabetics
  - Antiinflammatory
  - Anticonvulsants



## M. PHARM II SEMESTER

### MPS2111 ADVANCED MEDICINAL CHEMISTRY (3 CREDITS)

Following class of drugs with special reference to Receptorial level studies, Mechanism of action, Synthesis of official medicinal compounds and compounds of clinical importance.

- 1. ANTI BACTERIAL, ANTIPROTOZOAL, ANTI FUNGAL AGENTS:**
  - $\beta$  lactam Antibiotics,  $\beta$  lactamase inhibitors, cephalosporins, aminoglycosides, tetracycline, macrolides, polypeptides and unclassified antibiotics.
  - Chemotherapy of trypanosomiasis, trichomoniasis, leishmaniasis, sporozoans, and amoebas.
  - Anti fungal azoles for systemic treatment, anti fungal azoles for topical treatment, Polyene antimycotics, thiocarbamates, allylamines and unspecific topical antimycotics.
- 2. ANTI MALARIALS:** Modern Malaria chemotherapy, Quinolines and analogues, Cinchona alkaloids, 7-chloro-4-aminoquinolines, 8-aminoquinolines, 9-aminoacridines, mefloquine, THF synthetase inhibitors, diaminopyrimidines, biguanines and dihydrotriazines, sulphonamides, sulphones and other antimalarials.
- 3. ANTI CANCER & ANTI VIRALS:**
  - Tumour cell properties, alkylating agents, antimetabolites, antibiotics, plant products, miscellaneous compounds.
  - Anti HIV and Antihepatitis agents
- 4. ANALGESICS :** Opoids and Nonsteroidal anti-inflammatory drugs.
- 5. ANTIDIABETICS:**
  - IDDM & NIDDM based hypoglycemic,
  - Sulfonyl ureas Biguanides, second generation hypoglycemic
  - Insulin preparations – Lente, Semilente Protamine Zinc Insulin and other official products.
- 6. CARDIVASCULAR AGENTS:** Anti anginal agents, Vasodilators, Antiarrhythmic agents, Antihypertensive agents, Antihyperlipidemic agents
- 7. ANTIFERTILITY AGENTS:** Estrogen and progesterone derivatives, antiestrogens and related drugs, steroidal oral contraceptives-combinations, and sequential regimen, once a month and once a week pill, pre and post coital pills, mini pill, progesterone IUD, Norplant etc.

#### BOOK RECOMMENDED:

1. Alfred Burger – Text Book of medicinal chemistry Vol. 1 & Vol. 2.
2. William O. Foye – Principles of Medicinal Chemistry Varghese Publishing House, Bombay – 3<sup>rd</sup> Edition, 1989.
3. Wilson and Gisvolds – Text book of organic medicinal and Pharmaceutical Chemistry, 10<sup>th</sup> Edition, 1998.
4. Ellis & Wert – Progress in Medicinal Chemistry – Academic Press, New York.

## MPS2113 NATURAL PRODUCT CHEMISTRY (3 CREDITS)

1. Phytochemical Methods: Extraction, Isolation, purification and characterization of phytoconstituents using modern analytical tools (UV, IR, HPLC, HPTLC, NMR, Mass etc.)
2. Natural Pigments: Isolation, Classification and Identification. Chemistry and application of Flavanoids (Anthocyanins, Flavonols and flavones) and Quinone pigments.
3. Terpenoids: Introduction, General and Instrumental methods of Structure elucidation using UV, Mass etc. Biosynthesis of Terpenoids. Diterpenoids: Acyclic - Phytol and Tetracyclic - Gibberellins. Triterpenoids: Acyclic (Squalene), Tetracyclic - Lanosterol, & Pentacyclic -  $\alpha$  &  $\beta$ -amyrin, Ursolic acid & Oleanolic acid.
4. Sterols: Introduction & Biosynthesis of Steroids. Phytosterols, Saponins & Sapogenins, Cardiotonic glucosides, Plant Bufadienolides and steroidal alkaloids including Solanum and Kurchi alkaloids.
5. Nitrogenous Compounds: Alkaloids and their natural occurrence, chemistry and SAR of Opium, Ergot, Rauwolfia and Vinca alkaloids. Cyanogenic glycosides, Indoles and Chlorophylls.
6. An introduction to Natural leads in Drug Discovery: Docking studies on Caffeine and its derivatives, Piperine and its derivatives, Morphine and its derivatives, Certain Antidiabetics and Anti-inflammatory drugs.
7. Chemistry of therapeutically important phytoconstituents: Antidiabetic (Diabecon), Liver tonic (Liv52), Taxol, Curcumin, Podophyllotoxin, Ginsenosides & Artemisinin.

### Reference Books & Journals:

1. Chemistry of Alkaloids by S. W. Pelletier
2. Alkaloids by Manske.
3. Plant Physiology by Dieter Hess.
4. Steroids by Fieser and Fieser.
5. Organic Chemistry by I. L. Finar Vol. II.
6. Chemistry of Natural Products by K. W. Bentley.
7. Biosynthesis of Aromatic Compounds by Ulrich Weiss & J. Michael Edwards.

### Journals:

1. Phytochemistry, Planta Medica, Phytotherapy Research, Fitoterapia etc.

**MPS2115 RESEARCH METHODOLOGIES IN PHARMACEUTICAL CHEMISTRY  
(3 CREDITS)**

**1. Research Methodology**

**I.**

i) Research-Meaning, purpose, Types (Educational, Industrial, basic applied and patent oriented research)

ii) Literature survey-use of library- Books, Journals, Internet.

iii) Selection of a problem and preparing research proposal

II. Methods and tools used in research- Qualitative and quantitative Studies

iv) Data organization

v) Limitations and errors

vi) Statistical tools, its importance in data analysis

III. Documentation-Importance, techniques and use of computer packages in documentation

IV. Research paper writing/ thesis writing: organization, presentation (oral- importance, skill)

V. Protection of patents and trade mark design and copyright.

2. **Combinatorial Chemistry**- Solid phase synthesis- Types, strategy for library synthesis and characterization

i) Solid phase synthesis

ii) Solution phase synthesis

3. **High Throughput Screening**- general outline, importance and application

4. **Nano-Medicine**- nanotechnology; general outline, development of nano-chemistry, nano- material, future scope.

5. **Recent Development in The Field of Novel Medicine**

i) Antidiabetic ii) Antineoplastics iii) Antiinflammatory iv) Antiviral

v) Antifungal vi) Analgesics

## MPSE103 ADVANCED DRUG DESIGN (3 CREDITS) (Elective)

### 1. Introduction to basic concepts in Molecular modelling:

- Basic concepts of direct drug design and indirect drug design
- Introduction to Computer Graphics for display of Molecular structures, structural analysis of small molecules and macromolecular structures
- Energy minimization methods and Conformational analysis methods
- Introduction to various molecular modeling software – Sybl, Glide, Autodock Scigress, Flexidock, Comfa

### 2. Computational chemistry approaches:

- Molecular mechanics methods including study of empirical force field models
- Quantum mechanical models including semi empirical and *ab initio* methods
- Molecular dynamics and Monte Carlo Simulation Techniques
- Applications of above methods in drug design

### 3. Computer Assisted Design approaches:

- Pharmacophore search and modeling methods,
- Receptor mapping methods,
- Three dimensional database search approaches,
- Structure Based Drug Design: Molecular Docking and Scoring Methods,
- Basic Concepts of Homology Modelling.

### 4. Computerized QSAR approaches:

- 3D QSAR Methods – Principles steps to be followed and applications,
- 4D QSAR, 5D QSAR, 6D QSAR and HQSAR methods – Principles, steps to be followed and applications,
- Statistical analytical methods – Partial Least Square analysis, SIMCA methods, Principal Components analysis, Back propagation neural networks, Pattern recognition techniques with applications of these methods.

### 5. Peptidomimetic and Nucleotide drug design:

- Use of peptidomimetics in drug design, cyclisation of peptides, constrained amino acids, amide bond isosteres, and oligonucleotide therapeutics.

### 6. Recombinant DNA technology and drug design:

- Protein engineering
- Site directed mutagenesis
- Genetically engineered drugs
- Structural biology studies

### 7. ADMET Approaches in Drug Design:

- Principles of ADMET and ADME/TOX model building requirements
- *In silico* ADME tools and QSPR approaches
- High Througput ADME
- Introduction related to software of Schrodinger and Scigress & TOPKAT, Explore for ADME

**BOOKS RECOMMENDED:**

1. Comprehensive Medicinal Chemistry by C. Hansch, P.G. Sammes and G.B. Taylor, Vol. II-IV.
2. Guidebook on Molecular Modelling in Drug Design by N.C. Cohen.
3. Molecular Modelling, Principles and Applications by Andrew R. Leach.
4. Manfred E. Wolff and Burger's, Medicinal Chemistry and Drug Discovery- Vol.1, Principles and Practice, Vth Ed, John Wiley & Sons.
5. E.J. Ariens; Drug Design, Academic Press, New York.
6. Progress in Medicinal Chemistry, Series by Ellis & Wert.
7. Wilson & Gisvolds – Text book of organic medicinal and pharmaceutical chemistry, 10<sup>th</sup> Edition, 1998.
8. Receptor based drug design, by P. Leff, Marcel Dekker, New York, 1998.
9. Paul's charifron – Practical application of computer Aided drug design – Marcel Dekker – 1997.
10. The Organic Chemistry of Drug design and Drug Action - R.B.Silverman – Academic Press –1992.
11. Exploring QSAR – Fundamental and applications in Chemistry and Biology by Carowari Hansch and Albert Leo, ACS, Washington DC – 1995.
12. Alan L. Harney - Advanced in drug discovery techniques

## MPSE105 ADVANCED SPECTRAL ANALYSIS (3 CREDITS)

### **Introduction to Analysis, Quality Systems, Equilibria and classical Analysis :**

Definition of analytical chemistry and establishment of the fundamentals that distinguish it from other sciences; description of the analytical process in a systematic manner; introduction to planning and development of quality systems in the analytical laboratory; explanation of ionic equilibria, important aspects of the analytical techniques covered in the course; and Introduction of the important techniques of classical analysis applicable in the modern analytical laboratory.

### **Laser and Mass Spectroscopy**

Absorption and Emission of Light : Cavity Modes ,Basic Photometric Quantities, Absorption and Dispersion. Transition, Probabilities, Linear and Non-Linear Absorption. Coherence, Widths and Profiles of Spectral Lines

Spectroscopic Instrumentation: Spectrographs and Monochromators, Interferometers, Wavelengths Measurement, Detection of Light

Principles of Lasers: Basic Elements of a Laser, Fixed Frequency and Tunable Lasers, Tunable Infrared Lasers, Dye Lasers, Excimer Lasers, Solid State Lasers, Non-Linear Optical Mixing Techniques, Optical Parametric Oscillator (OPO), Short Pulse Lasers

Absorption Spectroscopy: Excitation Spectroscopy, Photoacoustic Spectroscopy, Intercavity Absorption ,Cavity Ring down Spectroscopy, Optogalvanic Spectroscopy , Ionization Spectroscopy, Fluorescence Spectroscopy, Molecular Spectroscopy,Measurement of Internal State Distribution,Spectroscopy of Excited States ,Double Resonance Methods,Multiphoton spectroscopy,Time Resolved Spectroscopy ,Generation of Short Laser Pulses,Lifetime Measurements with Lasers,Coherent Transients and Pulse Fourier Transform

Applications of Laser Spectroscopy: Laser Photochemistry, Laser Ablation, Laser monitoring of atmospheric processes ,Medical applications of Laser spectroscopy.

The Time of Flight (TOF) instruments as a mass spectrometer, Application of TOF as an analytical apparatus ,Manipulation of the flight path of the ions (Ion optics),Mass selection,Ion-Molecule reactions in a TOF apparatus,Ion-Photon interactions, Laser photofragmentation spectroscopy

### **Infra Red and Raman Spectra in Biological systems**

Introduction (the electromagnetic spectrum, far-mid- and near infrared).Harmonic oscillator, diatomic molecules.

Group theory and vibrational spectroscopy, normal modes, point groups, crystal field effects - selection rules. Polarized infrared, dichroism, molecular orientation. Isotope effects, product rule.

Kramers-Kronig analysis of reflectivity data.

Fourier transform infrared spectroscopy. Advantages. Components of FTIR spectrometers.

Infrared data acquisition techniques for solids liquids and gases. Transmission. Specular reflection. Diffuse reflection, Kubelka Munk transform. Transflection. ATR, penetration depth, variable angle Photoacoustic spectroscopy. Infrared microscopy.

Semiempirical infrared band assignment. Oscillation of characteristic groups.

Near infrared spectroscopy. Chemometrics.

Molecular rotational and vibrational transitions: The rotation of molecules. The rotational selection rules. Nuclear statistics. The vibrations of molecules. Rotation-vibration spectra of diatomic molecules. The vibrations of polyatomic molecules. Group theory and molecular vibrations. Anharmonicities (Coriolis forces, Inversion doubling).

Development and application of modern vibrational spectroscopic techniques, principally time-resolved FTIR and time resolved resonance Raman to study: Protein dynamics, excited state structure of porphyrins, vibrational relaxation, activation mechanism of oxygen by heme enzymes, electron and proton transfer through biological membranes and their coupling mechanism, higher order structure of proteins and allosteric effects, structure of metalloproteins and their reaction intermediates

## **Separation Science**

Description of the fundamental principles and typical applications of modern separation techniques; Extension of the principles to more advanced practical aspects of separation techniques; Study of modern Liquid Chromatography instrumentation in detail – including interfacing of Liquid Chromatography separation techniques to other analytical systems; Study of modern instrumentation relative to the appropriate techniques in depth;

A study of the interfacing of Gas Chromatography to other analytical systems; and Discussion of the practices of Gel Electrophoresis and Capillary Electrophoresis.

## **NMR spectroscopy in Biological Systems**

**Basic principles of NMR Spectroscopy:** Magnetic properties of nuclei, the phenomenon of nuclear magnetic resonance, diamagnetic and paramagnetic nuclear shielding, chemical shift, spin-spin coupling, spin decoupling analysis of first order and second order spectra, nuclear magnetic relaxation.

**Modern NMR Spectroscopy:** Pulsed and Fourier transform NMR, one-dimensional pulse sequences (APT, INEPT, DEPT), the second dimension, basic 2-dimensional sequences (COSY, TOCSY, NOESY, HMQC, HMBC). Introduction of the students with advanced NMR technique suitable for the elucidation and the study of the dynamics of mono-, oligo-, and polysaccharides, applications with concrete carbohydrate systems, general conclusions about the structure-property relationship.

## Atomic Spectroscopy and Chemical applications

- Study of the principles, advantages and limitations of atomic spectroscopic techniques, instrumentation and applications;
- Understanding of the bases for quantitative spectroscopic measurements;
- Practice of the interpretation of simple molecular spectra to deduce chemical structures; and
- Study of the modern analytical methods and instrumentation used in:
  - atomic fluorescence;
  - uv/visible and infra-red spectroscopy;
  - nuclear magnetic resonance;
  - mass spectrometry;and
  - their applications



## MPS2112 ADVANCED SYNTHETIC MEDICINALS LAB. (4 CREDITS)

### **LIST OF EXPERIMENTS:**

1. Purification of Solvents:
  - Methanol
  - Chloroform
  - Benzene
  - Acetone
  - Ethyl Acetate
  - Ethanol
2. Synthesis of Iodobenzene from Aniline.
3. Synthesis of Paracetamol from Phenol.
4. Synthesis of Cinnamic acid from benzaldehyde.
5. Synthesis of sulfonamide from chlorosulfuric acid.
6. Synthesis of Quinoline from aniline.
7. Synthesis of tetrahydrocarbazole from cyclohexanol.
8. Synthesis of antipyrin from ethylacetate.
9. Synthesis of benzimidazole from o-phenylene diamine.
10. Synthesis of methyl salicylate from salicylic acid.
11. Microwave synthesis of Ibuprofen / Benzimidazole.
12. Separation of quantitative organic mixtures –
  - Mixtures – I
  - Mixtures – II
  - Mixtures – III

\*The synthesized compounds should be characterized by mp, R<sub>f</sub>, value, IR etc.

### **BOOKS RECOMMENDED :**

1. Mann & Saunders: "Practical Organic Chemistry," 4<sup>th</sup> ed. (New Impression with Revision -1<sup>st</sup> Indian ed.), Orient Longman, 1986.
2. Vogel: "A Text Book of Practical Organic Chemistry (including Qualitative Organic Analysis)," 3<sup>rd</sup> ed., ELBS, 1975.
3. Furniss et al.: "Vogel's Text Book of Practical Organic Chemistry," 5<sup>th</sup> ed., (Reprint), ELBS, 1996.

## **MPS2114 ADVANCED NATURAL PRODUCTS LAB. (4 CREDITS)**

- A. Experiments based upon extraction, isolation/preparation and characterization of phytoconstituents from natural sources using physicochemical, chromatographic and spectral methods:
1. Isolation and characterization of Carbohydrates
  2. Separation and Isolation of Amylose and Amylopectin from Starch.
  3. Isolation and characterization of Caffeine from Tea Leaves.
  4. Isolation and characterization of Alkaloids from Black Pepper.
  5. Preparation of Piperic acid from piperine.
  6. Isolation and characterization of Ricinolic acid from Caster Oil.
  7. Preparation and characterization of Azelaic acid from Ricinolic acid.
  8. Isolation and characterization of Flavanoids from Orange peels.
  9. Lycopene from Tomatoes.
  10. Isolation and characterization of Alkaloids from Nux-Vomica Seeds.
  11. Isolation and characterization of Crude Alkaloids from the supplied plant drugs.
  12. Isolation and characterization of Glycosides from supplied crude drugs.
  13. Isolation of crude volatile oil from Cloves.
  14. Isolation of crude volatile oil from Lemon Grass.
  15. Isolation of crude volatile oil from Cinnamon.
- B. Quantification of phytoconstituents (supplied/isolated) using chemical marker on HPTLC.

### **BOOKS RECOMMENDED:**

1. Raphael Ikan, Practical Guide Natural Products.
2. J.B. Harborne, Phytochemical Methods.

**M. PHARM III SEMESTER (15 CREDITS)**

**MPS3111: Thesis :**

- **Thesis Seminar**

**M. PHARM IV SEMESTER (20 CREDITS)**

**MPS4111: Thesis :**

**Presentation, Submission and Viva-Voce**

## BREADTH PAPERS

### MMA1101: BIOSTATISTICS (3 Credits)

1. **Introduction:** 1h  
Relevance and the scope of Statistics.  
Difference between 'Descriptive' and 'Inferential' Statistics; Relationship between them
  
2. **Sampling Methods** 4h  
Introduction of sampling, probability and non probability sampling, sampling procedures – simple random, stratified, systematic, cluster and multistage sampling, concept of sampling distribution.
  
3. **Statistical Inference** 6h  
Statistical estimation – point and confidence interval estimations, Introduction of statistical hypothesis and testing, comparison of population mean with sample means, comparing two sample means, comparison of population proportion with sample proportions, comparing two sample proportions, comparison of more than two samples, introduction of non parametric statistical tests.
  
4. **Correlation and linear regression** 6h  
Introduction of correlation & regression concepts, estimation of correlation coefficient, regression coefficients, assumption of tests of hypothesis in linear regression, variance of sample estimates of the parameters, confidence intervals in regression analysis, non linear regressions, weighted and transformations in regression analysis, application of linear regressions - standard curves in drug analysis and drug stability studies, analysis of covariance.
  
5. **Concepts of Inferential Statistics** 4h  
Basics of Statistical Inference  
Sampling distribution  
Estimation – Point estimation, Interval estimation  
Parameter, Statistic, Concept of a hypothesis, Research Hypothesis, Null Hypothesis, Level of Significance, Comparison of means of two samples, Comparison of sample proportion with population proportion, Comparison of two sample proportions, Degrees of Freedom, Critical Value, Table value, Type I and Type II errors, Rules for rejection & acceptance of Null Hypothesis, Standard Error
  
6. **Inferential Statistics - Parametric Test:** 4h  
't' test – Comparison of sample mean with the population mean, Comparison of means of two independent samples, Comparison of two correlated samples  
'Z' test – different applications  
Annova – one way annova: 'F' test
  
7. **Quality control:**  
Introduction, control charts, acceptance sampling and operating characteristic curves, statistical procedures in Assay Department, establishing in-house limits, some statistical aspects of quality and the "Barr Decision".
  
8. **Inferential Statistics - Non-parametric test:** 2h

Chi square test- Testing of goodness of fit, testing of independence, Test of homogeneity; Wilcoxon signed rank test; McNemar test

9. **Computer Applications & Practicals:** 2h  
Introduction of statistical software – SPSS with practical exercises

**BOOKS RECOMMENDED:**

1. Statistical issues in Drug Development by Stephen Senn, 1997, published by John Wiley and Sons Inc.
2. Practical and Clinical Applications 3<sup>rd</sup> Edn. Sandord Bolton, 1997 Marcel Dekkar Inc, Newyork.
3. Non parametric statistics for Behavioral Sciences by Sidney Siegel; 1956, McGraw Hills, New Delhi.
4. Design and Analysis of Bioavailability and Bioequivalence Studies – 2<sup>nd</sup> Edn. By Shein-Chung Chow and Jen-Pei Liu, 2000, Marcel Dekkar Inc, Newyork.
5. Computer Applications and Practicals: Introduction of softwares – SPSS/SAS and practical exercises.

**Text Books**

1. Pharmaceutical Statistics

**MPS1003: BIOLOGICAL STANDARDIZATION & PHARMACOLOGICAL SCREENING (3 Credits)**

1. Laboratory Animals 7h.
  - a. Commonly used laboratory, transgenic and other genetically prone animal models (viz. nude mice SH rats etc.)
  - b. Techniques of blood collection, anesthesia & euthanasia of experiment animals.
  - c. Maintenance & breeding of laboratory animals.
  - d. Regulation and ethics requirements.
  - e. Guidelines & regulatory agencies – CPCSEA, OECD, FDA ICH, FHSA, EPA, EEC, WHO, etc.
  - f. Importance of alternative experimental models, its advantages & disadvantages.
  
2. Principles of Biological Standardization 4h.
  - a. Methods of biological assay, principles of biological assays with certain examples as per IP and BP.
  - b. Development of new bioassay methods.
  
3. Immunoassay 5h
  - a. General principles of immunoassay, Theoretical basis, Optimization of immunoassay, Heterogenous immunoassay system, Homogenous immuno system.
  - b. Production of immunoassay reagent: Introduction, receptors or binders, unlabelled ligands Calibrators, Labelled ligands and receptor, Separation technique, buffers.
  - c. Immunoassay Methods Evaluation: Protocol outline, objective & preparation, evaluation of precision, standard tracer, sensitivity, evaluation of accuracy, antibody characteristics, monitoring, reaction conditions, clinical evaluation.
  
4. Organization of screening for the Pharmacological activity of new substances with emphasis on evaluation using in-vivo, in-vitro, ex-vivo, in-situ, in silico and other possible animal alternative models. 18h.
  - b. General Principles & safety pharmacology procedure.
  - c. CVS Pharmacology – Antihypertensive, Anti arrhythmics, Vasodilators, disentangl.
  - d. CNS Pharmacology – behavioral & muscle co-ordination, CNS stimulants, anti-epileptics, Nootropics.
  - e. Drugs for Neurodegenerative diseases, like parkinsonism, Alzheimers, multiple sclerosis.
  - f. Drugs acting on ANS.
  - g. Respiratory Pharmacology – Anti-asthmatics, COPD, Anti-allergic & Mucoactives.
  - h. Reproductive Pharmacology – Aphrodisiacs & antifertility agents.
  - i. Analgesics, anti-inflammatory & antipyretics.
  - j. G.I.T. – Anti-ulcer, anti-emetics, anti-diarrhoeal & laxatives.
  - k. Anti-cancer agents.
  - l. Metabolic disorders like anti-diabetics, anti-hyperlipidemic, anti-obesity, hepatoprotective.
  - m. Models in drug absorption & metabolism.
  - n. Immuno Pharmacology – specific (cell & hormonal mediated) & non-specific methods.
  - o. Screening of free radical scavenging activity.

- p. Acute, Sub-acute & Chronic toxicity test.
5. Clinical pharmacology and pharmacodynamics: clinical study design, documentation, presentation and interpretation  
2h
6. Clinical trials: definition, phase I – IV studies, design documentation, presentation and interpretation, statistical analysis of clinical data, factorial design, guidelines as per Indian and other regulatory authorities.  
7h

### **BOOKS RECOMMENDED :**

1. Biological standardization by J.H. Burn, D.J. Finney & L.G. Goodwin.
2. I.P. & B.P.
3. Screening Methods in Pharmacology by R.A. Turner. Vol. I & II Academic Press, New York and London.
4. Evaluation of drug activities by Laurence & Bacherce.
5. Methods in Pharmacology by Arnold Schwartz.
6. Selected topics on Experiment Pharmacology by Issha G. Kamat, Dadkar, N.K. & Seth, UK.
7. Fundamental of Experimental Pharmacology, by M.N. Ghosh. Scientific Book Agency, Calcutta.
8. Pharmacological Experiment on intact preparation by Churchill Livingstone
9. Drug Discovery and evaluation by H.G. Vogel & W.H. Vogel. Springer Verlag, Berlin Heideleberg.
10. Animal Model in Toxicology by Shayne Cox Gad & Christopher P, Chengelis.
11. Principles & Methods of Toxicology by Hays.
12. CRC Handbook of Toxicology by Derelako & Hollinger.
13. Handbook of Experimental Pharmacology by S.S. Kulkarni. Vallabh Prakashen, Delhi.
14. Pharmacological Experiments on Intact and Isolated preparations, Edinburgh University Pharmacology Staff, Livingstone.
15. Goodman and Gilman's The Pharmacological basis of Therapeutics – Ninth edition, Editors. A. G. Gilman, J. G. Hardman, L. E. Limbiod, P. B. Melineff, R. W. Rudder, Macmillan Publishing Co. Inc. – Latest edition.
16. Clinical Pharmacotherapeutics, edited by Kamalesh Kohli, Elsevier Publication.