# **M.PHARM. I YEAR**

## PHARMACEUTICAL CHEMISTRY SEMESTER-I

### I M.PHARM. SCHEME (PHARMACEUTICALCHEMISTRY)

### **SEMESTER-I**

| S.No.  | Sub.    | Subject  | Т | т | Р  | Th.    | Pr.    | Maximum Marks |     |    |     |       |  |
|--------|---------|--|---|---|----|--------|--------|---------------|-----|----|-----|-------|--|
| 5.110. | Code    | Subject  | L | 1 | r  | Credit | Credit | TH            | CW  | SW | Pr. | Total |  |
| 1.     | PY90002 | Modern Pharmaceutical Analytical<br>Techniques | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 2.     | PY99001 | Advanced Organic Chemistry -I                  | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 3.     | PY99002 | Advanced Medicinal Chemistry                   | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 4.     | PY99003 | Chemistry of Natural Products                  | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 5.     | PY99454 | Pharmaceutical Chemistry Practical -I          | - | - | 12 | -      | 6      | -             | -   | 50 | 100 | 150   |  |
| 6.     | PY99481 | Seminar /Assignment                            | - | - | 7  | -      | 4      | -             | -   | 25 | 75  | 100   |  |
|        | Total   |  |   |   | 19 | 16     | 10     | 300           | 100 | 75 | 175 | 650   |  |

| т | т | Р | Th.<br>Credit | Pr.<br>Credit | Maximum Marks |    |    |     |       |  |  |
|---|---|---|---------------|---------------|---------------|----|----|-----|-------|--|--|
|   | 1 |   |               |               | ТН            | CW | SW | Pr. | Total |  |  |
| 4 | - | - | 4             | -             | 75            | 25 | -  | -   | 100   |  |  |

### PY90002: MODERN PHARMACEUTICAL ANALYTICAL TECHNIQUES

### **Course Objectives:**

- To develop the basic knowledge of spectra generation and factors affecting the spectra.
- To correlate structure of drug with its spectra.
- To understand the thermal behavior of materials.
- To provide the fundamental of separation in chromatographic techniques
- To provide a knowledge of Atomic spectroscopy.
- To understand principles of potentiometery.

### Course outcomes:

After completion of course student should be able to:

- **CO-1**: Understand and explain the basic concepts and instrumentation of chromatographic techniques and other Spectroscopy techniques.
- **CO-2:** Analyze and interpret the structure of the organic compounds using UV, IR, NMR, mass and other spectra.
- **CO-3:** Illustrate the theory and applications of potentiometry in precise measurements of ion concentration in a wide range of samples
- **CO-4:** Learn and discover the basic principles and applications of Electrophoresis and X ray Crystallography in relation to the pharmaceuticals.
- **CO-5:** Outline basic principles of different thermal analytical techniques for ascertaining the thermal behavior of organic compounds.

### THEORY

UNIT I

### **DURATION(LECTURES)**

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- **a.** UV-Visible spectroscopy: Introduction, Theory, Laws, Instrumentation associated with UV-Visible spectroscopy, Choice of solvents and solvent effect and Applications of UV-Visible spectroscopy, Difference/ Derivative spectroscopy.
- **b. IR spectroscopy:** Theory, Modes of Molecular vibrations, Sample handling, Instrumentation of Dispersive and Fourier Transform IR Spectrometer, Factors affecting vibrational frequencies and Applications of IR spectroscopy, Data Interpretation.
- **c. Spectroflourimetry:** Theory of Fluorescence, Factors affecting fluorescence (Characteristics of drugs that can be analysed by flourimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.
- **d.** Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.

### UNIT II

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NMR Spectroscopy: Quantum numbers and their role in NMR, Principle, Instrumentation, Solvent requirement in NMR, Relaxation process, NMR signals in various compounds, Chemical shift,

Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and 13C NMR. Applications of NMR spectroscopy.

**Mass Spectroscopy:** Principle, Theory, Instrumentation of Mass Spectroscopy, Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy

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### UNIT III

- **Chromatography:** Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following:
  - **a.** Thin Layer chromatography
  - b. High Performance Thin Layer Chromatography
  - c. Ion exchange chromatography
  - d. Column chromatography
  - e. Gas chromatography
  - f. High Performance Liquid chromatography
  - g. Ultra High Performance Liquid chromatography
  - **h.** Affinity chromatography
  - i. Gel Chromatography

### UNIT IV

12

- **a.** Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following:
  - i. Paper electrophoresis
  - **ii.** Gel electrophoresis
  - iii. Capillary electrophoresis
  - iv. Zone electrophoresis
  - v. Moving boundary electrophoresis
  - vi. Iso electric focusing
- **b.** X ray Crystallography: Production of X rays, Different X ray methods, Bragg's law, Rotating crystal technique, X ray powder technique, Types of crystals and applications of X-ray diffraction.

### UNITV

- a. Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry.
- **b.** Thermal Techniques: Principle, thermal transitions and Instrumentation (Heat flux and powercompensation and designs), Modulated DSC, Hyper DSC, experimental parameters (sample preparation, experimental conditions, calibration, heating and cooling rates, resolution, source of errors) and their influence, advantage and disadvantages, pharmaceutical applications.
- **c. Differential Thermal Analysis (DTA):** Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). TGA: Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications.

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### **BOOKS&REFERENCESRECOMMENDED:**

- 1. Spectrometric Identification of Organic compounds Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.
- 2. Principles of Instrumental Analysis Doglas A Skoog, F. James Holler, Timothy A. Nieman, 5th edition, Eastern press, Bangalore, 1998.
- 3. Instrumental methods of analysis Willards, 7th edition, CBS publishers.
- 4. Practical Pharmaceutical Chemistry Beckett and Stenlake, Vol II, 4th edition, CBS Publishers, New Delhi, 1997.
- 5. Organic Spectroscopy William Kemp, 3rd edition, ELBS, 1991.
- 6. Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
- 7. Pharmaceutical Analysis Modern Methods Part B J W Munson, Vol 11, Marcel. Dekker Series
- 8. Spectroscopy of Organic Compounds, 2 nd edn., P.S/Kalsi, Wiley estern Ltd., Delhi.
- 9. Textbook of Pharmaceutical Analysis, KA. Connors, 3 rd Edition, John Wiley & Sons, 1982.

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|   | PY99001: ADVANCED ORGANIC CHEMISTRY-1 |               |        |        |    |    |    |     |       |  |  |  |  |
|---|---------------------------------------|---------------|--------|--------|----|----|----|-----|-------|--|--|--|--|
| т | т                                     | Maximum Marks |        |        |    |    |    |     |       |  |  |  |  |
| L | 1                                     | Р             | Credit | Credit | TH | CW | SW | Pr. | Total |  |  |  |  |
| 4 | -                                     | -             | 4      | -      | 75 | 25 | -  | I   | 100   |  |  |  |  |

### **Course objectives:**

- To understand the principles and applications of reterosynthesis.
- To understand the mechanism & applications of various named reactions.
- To understand the concept of disconnection to develop synthetic routes for small target • molecule.
- To understand the use of various catalysts in organic reactions. ٠
- To understand the chemistry of heterocyclic compounds.

### **Course outcomes:**

After completion of course, student should be able to:

- **CO-1**: Understand and explain the basic principles and applications of organic chemistry.
- **CO-2:** Classify different organic chemistry reactions based on their mechanism and application.
- **CO-3:** Determine the suitable starting materials and specific reaction products for a given target molecule using different bond breaking and bond forming reactions.
- CO-4: Identify the concepts and applications of different reagents used in organic synthesis and suggest suitable reagents for a given reaction.
- **CO-5:** Explain different protection and deprotection strategies for synthesizing heterocyclic compounds and other organic molecules of interest.

### THEORY **UNIT I**

### **DURATION (LECTURES)**

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### **Basic Aspects of Organic Chemistry:**

- 1. Organic intermediates: Carbocations, carbanions, free radicals, carbenes and nitrenes. Their method of formation, stability and synthetic applications.
- 2. Types of reaction mechanisms and methods of determining them.
- 3. Detailed knowledge regarding the reactions, mechanisms and their relative reactivity and orientations.

### **Addition reactions:**

- **a.** Nucleophilic uni- and bimolecular reactions (SN1 and SN2)
- **b.** Elimination reactions (E1 & E2; Hoffman & Saytzeff's rule)
- c. Rearrangement reaction

### **UNIT II**

### Study of mechanism and synthetic applications of following named Reactions:

Ugi reaction, Brook rearrangement, Ullmann coupling reactions, Dieckmann Reaction, Doebner-Miller Reaction, Sandmeyer Reaction, Mitsunobu reaction, Mannich reaction, Sharpless asymmetric epoxidation, Baeyer-Villiger oxidation, Vilsmeyer-Haack Reaction, Shapiro & Suzuki reaction, Ozonolysis and Michael addition reaction.

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### UNIT III

### Synthetic Reagents & Applications:

Aluminium isopropoxide, N-bromosuccinamide, diazomethane, dicyclohexyl carbodimide, Wilkinson reagent, Witting reagent. Osmium tetroxide, titanium chloride, diazopropane, diethyl azodicarboxylate, Triphenylphosphine, Benzotriazol-1-yloxy) tris (dimethylamino) phosphonium hexafluoro-phosphate (BOP).

### **Protecting groups:**

- a. Role of protection in organic synthesis
- **b.** Protection for the hydroxyl group, including 1,2-and1,3-diols: ethers, esters, carbonates, cyclic acetals & ketals
- c. Protection for the Carbonyl Group: Acetals and Ketals
- d. Protection for the Carboxyl Group: amides and hydrazides, esters
- e. Protection for the Amino Group and Amino acids: carbamates and amides

### **UNIT-IV**

### Heterocyclic Chemistry:

Organic Name reactions with their respective mechanism and application involved in synthesis of drugs containing five, six membered and fused hetrocyclics such as Debus-Radziszewski imidazole synthesis, Knorr Pyrazole Synthesis Pinner Pyrimidine Synthesis, Combes Quinoline Synthesis, Bernthsen Acridine Synthesis, Smiles rearrangement and Traube purine synthesis.

Synthesis of few representative drugs containing these hetrocyclic nucleus such as Ketoconazole, Metronidazole, Miconazole, celecoxib, antipyrin, Metamizole sodium, Terconazole, Alprazolam, Triamterene, Sulfamerazine, Trimethoprim, Hydroxychloroquine, Quinine, Chloroquine, Quinacrine, Amsacrine, Prochlorpherazine, Promazine, Chlorpromazine, Theophylline , Mercaptopurine and Thioguanine.

### UNIT-V

### Synthon approach and retrosynthesis applications:

- i. Basic principles, terminologies and advantages of retrosynthesis; guidelines for dissection of molecules. Functional group interconvertion and addition (FGI and FGA)
- **ii.** C-X disconnections; C-C disconnections alcohols and carbonyl compounds; 1,2-, 1,3-,1,4-, 1,5-, 1,6-difunctionalized compounds
- iii. Strategies for synthesis of three, four, five and six-membered ring.

### **BOOKS AND REFERENCES RECOMMENDED:**

**1.** "Advanced Organic chemistry, Reaction, Mechanisms and Structure", J March, John Wiley and Sons, New York.

**2.** "Mechanism and Structure in Organic Chemistry", ES Gould, Hold Rinchart and Winston, New York.

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

**4.** "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Pearson Education Lts, Dorling Kindersley 9India) Pvt. Ltd.

5. A guide to mechanisms in Organic Chemistry, Peter Skyes (Orient Longman, New Delhi).6. Reactive Intermediates in Organic Chemistry, Tandom and Gowel, Oxford & IBH Publishers.

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**7.** Combinational Chemistry – Synthesis and applications – Stephen R Wilson & Anthony W Czarnik, Wiley – Blackwell.

8. Carey, Organic Chemistry, 5<sup>th</sup> Edition (Viva Books Pvt. Ltd.)

9. Organic Synthesis - The Disconnection Approach, S. Warren, Wily India

10. Principles of Organic Synthesis, ROC Norman and JM Coxan, Nelson Thorns.

11. Organic Synthesis - Special Techniques. VK Ahluwalia and R Agarwal, Narosa Publishers.

12. Organic Reaction Mechanisms IV th Edtn, VK Ahluwalia and RK Parashar, Narosa Publishers.

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|   | P Y 99002: ADVANCED WIEDICINAL CHEMISTRY |   |               |               |               |    |    |     |       |  |  |  |  |
|---|--|---|---------------|---------------|---------------|----|----|-----|-------|--|--|--|--|
| L | Т  | D | Th.<br>Credit | Pr.<br>Credit | Maximum Marks |    |    |     |       |  |  |  |  |
|   | 1  | r |               |               | ТН            | CW | SW | Pr. | Total |  |  |  |  |
| 4 | -  | - | 4             | -             | 75            | 25 | -  | -   | 100   |  |  |  |  |

### **PY99002: ADVANCED MEDICINAL CHEMISTRY**

### Course objectives:

- To understand different stages of drug discovery.
- To understand different techniques of drug discovery.
- To understand the theories of drug receptor interactions.
- To understand various strategies to design and develop Prodrugs.
- To understand concept of Enzyme Inhibition.
- To understand the concept of Peptidomimetics

### **Course outcomes:**

On completion of this subject, students are expected to be able to:

- CO-1: Understand and explain the basic principles, applications and stages of drug discovery.
- **CO-2:** Classify drug molecules based on their structure and pharmacology while understanding the Structure-Activity Relationship (SAR).
- **CO-3:** Distinguish between the active and inactive forms of drugs based on their stereochemistry, drug-receptor interactions, conformational stability/3D structure, prodrug concept and other drug discovery tolls and techniques.
- **CO-4:** Identify concept of prodrugs and their conversion strategies into the active drug form.
- **CO-5:** Outline and appraise the concepts and applications of peptidomimetic drug design **approach.**

| THEORY   | <b>DURATION (LECTURES)</b>                            |
|--|---|
| UNIT I   | 12  |
| Drug discovery: Stages of drug discovery, lead | l discovery; identification, validation and diversity |
| of drug targets.                               |   |

**Bological drug targets:** Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonists vs antagonists, artificial enzymes.

### UNIT II

### Prodrug Design and Analog design:

- **a. Prodrug design:** Basic concept, Carrier linked prodrugs/ Bioprecursors, Prodrugs of functional group, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action. Rationale of prodrug design and practical consideration of prodrug design.
- **b.** Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.
- **c.** Analog Design: Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid analogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance.

### UNITIII

Medicinal chemistry aspects, Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs:

- **a.** Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, Antineoplastic and Antiviral agents.
- **b.** Stereochemistry and Drug action: Realization that stereo selectivity is a pre-requisite for evolution. Role of chirality in selective and specific therapeutic agents. Case studies, Enantio selectivity in drug adsorption, metabolism, distribution and elimination.

### UNIT IV

Rational Design of Enzyme Inhibitors Enzyme kinetics & Principles of Enzyme inhibitors, Enzyme inhibitors in medicine, Enzyme inhibitors in basic research, rational design of non-covalently and covalently binding enzyme inhibitors.

### UNIT V

12

12

Peptidomimetics Therapeutic values of Peptidomimetics, design of peptidomimetics by Manipulation of the amino acids, modification of the peptide backbone, incorporating Conformational constraints locally or globally. Chemistry of prostaglandins, leukotrienes and thromboxones.

### **BOOKS & REFERENCES RECOMMENDED:**

- 1. Medicinal Chemistry by Burger, Vol I –VI.
- 2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12 th Edition, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
- 3. Comprehensive Medicinal Chemistry Corwin and Hansch.
- **4.** Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore
- 5. Introduction to Quantitative Drug Design by Y.C. Martin.
- 6. Principles of Medicinal Chemistry by William Foye, 7 th Edition, Ippincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
- 7. Drug Design Volumes by Arienes, Academic Press, Elsevier Publishers, Noida, Uttar Pradesh..
- 8. Principles of Drug Design by Smith.
- **9.** The Organic Chemistry of the Drug Design and Drug action by Richard B.Silverman, II Edition, Elsevier Publishers, New Delhi.
- **10.** An Introduction to Medicinal Chemistry, Graham L.Patrick, III Edition, Oxford University Press, USA.
- **11.** Biopharmaceutics and pharmacokinetics, DM .Brahmankar, Sunil B. Jaiswal II Edition, 2014, Vallabh Prakashan, New Delhi.
- **12.** Peptidomimetics in Organic and Medicinal Chemistry by Antonio Guarna and Andrea Trabocchi, First edition, Wiley publishers.

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| T | Т | D | Th.    | Pr.<br>Credit | Maximum Marks |    |    |     |       |  |  |
|---|---|---|--------|---------------|---------------|----|----|-----|-------|--|--|
| L |   | r | Credit |               | ТН            | CW | SW | Pr. | Total |  |  |
| 4 | - | - | 4      | -             | 75            | 25 | -  | -   | 100   |  |  |

### **PY99003: CHEMISTRY OF NATURAL PRODUCTS**

### Course objectives:

- To understand different types of natural compounds like alkaloids, glycosides their chemistry and medicinal importance.
- To understand the importance of natural compounds as lead molecules for new drug discovery.
- To understand general methods of structural elucidation of compounds of natural origin.
- To understand the concept of r DNA technology tool for new drug discovery.
- To understand chemistry and physiological importance of vitamins.

### **Course outcomes:**

On completion of this subject, students are expected to be able to:

- **CO-1**: Learn and understand the chemistry and medicinal importance of natural products like alkaloids, glycosides, flavonoids, terpenoids etc.,
- **CO-2:** Classify natural compounds according to their structural motifs and develop their Structure-Activity Relationship (SAR).
- **CO-3:** Outline and demonstrate the techniques of isolation and purification of natural compounds.
- **CO-4:** Learn and apply the concepts of structural characterization of natural products using UV, IR, <sup>1</sup>HNMR, <sup>13</sup>CNMR and MS Spectroscopy.
- **CO-5:** Outline and appraise the concepts and applications of rDNA technology in modern natural compound drug discovery.

### THEORY

UNIT I

### **DURATION (LECTURES)**

12

Study of Natural products as leads for new pharmaceuticals for the following class of drugs:

- a. Drugs Affecting the Central Nervous System: Morphine Alkaloids
- b. Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide
- c. Cardiovascular Drugs: Lovastatin, Teprotide and Dicoumaro
- d. Neuromuscular Blocking Drugs: Curare alkaloids
- e. Anti-malarial drugs and Analogues
- **f.** Chemistry of macrolid antibiotics (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and  $\beta$  Lactam antibiotics (Cephalosporins and Carbapenem)

### UNIT II

- **a.** Alkaloids: General introduction, classification, isolation, purification, molecular modification and biological activity of alkaloids, general methods of structural determination of alkaloids, structural elucidation and stereochemistry of ephedrine, morphine, ergot, emetine and reserpine.
- **b.** Flavonoids: Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin.

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**c.** Steroids: General introduction, chemistry of sterols, sapogenin and cardiac glycosides. Stereochemistry and nomenclature of steroids, chemistry of contraceptive agents male & female sex hormones (Testosterone, Estradiol, Progesterone), adrenocorticoids (Cortisone), contraceptive agents and steroids (Vit – D).

### UNIT III

- **a.** Terpenoids: Classification, isolation, isoprene rule and general methods of structural elucidation of Terpenoids; Structural elucidation of drugs belonging to mono (citral, menthol, camphor), di (retinol, Phytol, taxol) and tri terpenoids (Squalene,Ginsenoside) carotinoids (β carotene).
- **b.** Vitamins: Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin.

### UNIT IV

- **a.** Recombinant DNA technology and drug discovery r DNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, Clinical application and recent advances in gene therapy, principles of RNA & DNA
- **b.** Active constituent of certain crude drugs used in Indigenous system Diabetic therapy Gymnemasylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenumgraccum; Liver dysfunction Phyllanthus niruri; Antitumor Curcuma longa Linn.

### UNITV

12

**Structural Characterization of natural compounds**: Structural characterization of natural compounds using IR, 1HNMR, 13CNMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides.

### **BOOKS & REFERENCES RECOMMENDED:**

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

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| L T | Т | D  | Th.<br>Credit | Pr.<br>Credit | Maximum Marks |    |    |     |       |  |  |
|-----|---|----|---------------|---------------|---------------|----|----|-----|-------|--|--|
|     | I | ſ  |               |               | ТН            | CW | SW | Pr. | Total |  |  |
| -   | - | 12 | -             | 6             | -             | -  | 50 | 100 | 150   |  |  |

#### PY99454: PHARMACEUTICAL CHEMISTRY PRACTICAL – I

- 1. Analysis of Pharmacopoeial compounds and their formulations by UV Vis spectrophotometer, RNA & DNA estimation
- 2. Simultaneous estimation of multi component containing formulations by UV spectrophotometry
- 3. Experiments based on Column chromatography
- 4. Experiments based on HPLC
- 5. Experiments based on Gas Chromatography
- 6. Estimation of riboflavin/quinine sulphate by fluorimetry
- 7. Estimation of sodium/potassium by flame photometry

### To perform the following reactions of synthetic importance:

- 1. Purification of organic solvents, column chromatography
- 2. Claisen-schimidt reaction.
- **3.** Benzyllic acid rearrangement.
- 4. Beckmann rearrangement.
- 5. Hoffmann rearrangement
- 6. Mannich reaction
- 7. Synthesis of medicinally important compounds involving more than one step along with purification and Characterization using TLC, melting point and IR spectroscopy (4 experiments)
- 8. Estimation of elements and functional groups in organic natural compounds
- **9.** Isolation, characterization like melting point, mixed melting point, molecular weight determination, functional group analysis, co-chromatographic technique for identification of isolated compounds and interpretation of UV and IR data.
- **10**. Some typical degradation reactions to be carried on selected plant constituents

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| Т | т | Р | Th.<br>Credit | Pr.<br>Credit | Maximum Marks |    |    |     |       |  |  |
|---|---|---|---------------|---------------|---------------|----|----|-----|-------|--|--|
| L |   |   |               |               | ТН            | CW | SW | Pr. | Total |  |  |
| - | - | 7 | -             | 4             | -             | -  | -  | -   | 100   |  |  |

### PY99481: SEMINAR /ASSIGNMENT

### **Objectives:**

• To identify any contemporary topic from the thrust area of current pharmaceutical research, regulatory affairs, drug discovery & current affairs of medicinal and pharmaceutical chemistry and any other field beyond the syllabus.

- To do exhaustive search of literature and information reported in the area of seminar topic.
- To develop in-depth understanding on seminar topic and prepare the power point presentation.
- To develop the skills of scientific presentation in front of scientific community.

### **Outcomes:**

On completion of this activity, students are expected to be able to:

- **CO-1**: Conduct comprehensive research and gather information from diverse scientific literature and up-to-date pharmaceutical news and resources.
- **CO-2**: Analyze and evaluate various scientific knowledge and information, and demonstrate the ability to create presentations, reports, and documents on a chosen area of interest, utilizing sources beyond the course syllabus.
- **CO-3:** Develop and deliver professional and visually compelling presentations, reports, and documents using PowerPoint, while also demonstrating confidence and effective communication skills when presenting to scientific professionals.

| 2023-24 | M. Pharm. I & II Year Syllabus (Pharmaceutical Chemistry) |  |
|---------|---|--|
|---------|---|--|

# **M.PHARM. I YEAR**

### PHARMACEUTICAL CHEMISTRY SEMESTER-II

### I M.PHARM. (PHARMACEUTICAL CHEMISTRY) SCHEME

### **SEMESTER-II**

| S. No. | Sub. Code | Subject                               | L | Т | р  | Th.    | Pr.    | Maximum Marks |     |    |     |       |  |
|--------|-----------|---------------------------------------|---|---|----|--------|--------|---------------|-----|----|-----|-------|--|
| 5. NO. | Sub. Code |                                       |   | 1 | r  | Credit | Credit | ТН            | CW  | SW | Pr. | Total |  |
| 1.     | PY99501   | Advanced Spectral Analysis            | 4 | - | -  | 4      | -      | 75            | 25  | -  | I   | 100   |  |
| 2.     | PY99502   | Advanced Organic Chemistry-II         | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 3.     | PY99503   | Computer Aided Drug Design            | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 4.     | PY99504   | Pharmaceutical Process Chemistry      | 4 | - | -  | 4      | -      | 75            | 25  | -  | -   | 100   |  |
| 5.     | PY99855   | Pharmaceutical Chemistry Practical-II | - | - | 12 | -      | 6      | -             | -   | 50 | 100 | 150   |  |
| 6.     | PY99883   | Seminar Assignment                    | - | - | 7  | -      | 4      | -             | -   | 25 | 75  | 100   |  |
|        | Total     |                                       |   |   | 19 | 16     | 10     | 300           | 100 | 75 | 175 | 650   |  |

| т | т | р         | Th Cr   | Dr. Cr. | Maximum Marks |    |     |       |     |  |  |
|---|---|-----------|---------|---------|---------------|----|-----|-------|-----|--|--|
| L | 1 | P Th. Cr. | Pr. Cr. | TH      | CW            | SW | Pr. | Total |     |  |  |
| 4 | - | -         | 4       | -       | 75            | 25 | -   | -     | 100 |  |  |

### **PY99501: ADVANCED SPECTRAL ANALYSIS**

### **Course objectives:**

- To build understanding about the interpretation of the NMR, Mass and IR spectra of various organic compounds.
- To understand theoretical aspects of Woodward-Fieser rule.
- To understand the principle of Raman Spectroscopy.
- To understand the theory of thermal methods.
- To understand the concept of hyphenated techniques.
- To study the theory and principle of RIA.

### Course outcomes:

On completion of this course, the students are expected to be able to:

- **CO-1**: Apply the principles of different chromatographic techniques in isolation, purification and identification of organic compounds.
- **CO-2:** Apply the principles of different spectroscopy techniques (UV, IR, NMR, MASS and other spectral techniques) in the structure elucidation of organic and natural compounds.
- **CO-3:** Appraise the theory and applications of Raman spectroscopy and thermal methods in the measurement of thermal and spectral properties of pharmaceutical products.
- **CO-4:** Learn and discover the basic principles and applications of different enzyme assays and immunoassays in relation to the pharmaceuticals.
- **CO-5:** Learn and understand the basics of different NMR techniques such as 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE) for identification and characterization of organic compounds.

### THEORY

### UNIT I

### **DURATION (LECTURES)**

12

12

12

UV and IR spectroscopy: Wood ward – Fieser rule for 1,3- butadienes, cyclic dienes and  $\alpha$ ,  $\beta$ -carbonyl compounds and interpretation compounds of enones. ATR-IR, IR Interpretation of organic compounds.

### UNIT-II

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

### UNITIII

### **Mass Spectroscopy:**

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

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### UNIT IV

### **Chromatography:**

Principle, Instrumentation and Applications of the following : a) GC-MS b) GC-AAS c) LC-MS d) LC-FTIR e) LC-NMR f) CE- MS g) High Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion Exclusion Chromatography) k) Flash chromatography

### UNIT-V

12

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- **a.** Thermal methods of analysis: Introduction, principle, instrumentation and application of DSC, DTA and TGA.
- b. Raman Spectroscopy: Introduction, Principle, Instrumentation and Applications.
- c. Radio immuno assay: Biological standardization, bioassay, ELISA, Radio immuno assay of digitalis and insulin.

### **BOOKS AND REFERENCES RECOMMENDED:**

- 1. Spectrometric Identification of Organic compounds Robert M Silverstein, Sixth edition, John Wiley & Sons, 2004.
- 2. Principles of Instrumental Analysis Doglas A Skoog, F. James Holler, Timothy A. Nieman, 5th edition, Eastern press, Bangalore, 1998.
- 3. Instrumental methods of analysis Willards, 7th edition, CBS publishers.
- 4. Organic Spectroscopy William Kemp, 3rd edition, ELBS, 1991.
- **5.** Quantitative analysis of Pharmaceutical formulations by HPTLC P D Sethi, CBS Publishers, New Delhi.
- 6. Quantitative Analysis of Drugs in Pharmaceutical formulation P D Sethi, 3rd Edition, CBS Publishers, New Delhi, 1997.
- 7. Pharmaceutical Analysis- Modern methods Part B J W Munson, Volume 11, Marcel Dekker Series

| т | т | D | Th Cr   | Pr Cr   |    | Max | timum I | Marks |       |
|---|---|---|---------|---------|----|-----|---------|-------|-------|
| L | I | Г | Th. Cr. | rr. Cr. | TH | CW  | SW      | Pr.   | Total |
| 4 | - | - | 4       | -       | 75 | 25  | -       | -     | 100   |

### PY99502: ADVANCED ORGANIC CHEMISTRY-II

### **Course objectives:**

- To provide knowledge of principles and applications of Green chemistry.
- To provide basic understanding of the concept of peptide chemistry.
- To understand the principle of photochemical reactions.
- To understand the principle of Pericyclic reaction.
- To build understanding of the various catalysts used in organic reactions.
- To provide understanding of the concept of stereochemistry and asymmetric synthesis.

### Course outcomes:

On completion of this course, the students are expected to be able to:

- **CO-1**: Understand and apply the principles of green chemistry, peptide chemistry, photochemistry, catalysis, and stereochemistry to design and synthesize novel pharmaceuticals, while understanding the theoretical and practical aspects of each concept
- **CO-2**: Evaluate the principles of green chemistry and assess the utility of microwave/ultrasound-assisted synthesis and continuous flow reactions for developing energy-efficient synthetic routes for organic compounds.
- **CO-3**: Explain the principles and applications of various types of photochemical and pericyclic reactions in organic chemistry.
- **CO-4**: Identify, compare, and select specific catalysts for different types of organic chemistry reactions based on their mechanisms, efficiency, and selectivity.
- **CO-5**: Evaluate the importance of stereochemistry in organic synthesis for the development of specific isomers of drugs and other compounds, and analyze their biological activity and pharmacological properties.

# And THEORYUNIT I

### **Green Chemistry:**

DURATION(LECTURES)

12

- a. Introduction, principles of green chemistry
- **b.** Microwave assisted reactions: Merit and demerits of its use, increased reaction rates, mechanism, superheating effects of microwave, effects of solvents in microwave assisted synthesis, microwave technology in process optimization, its applications in various organic reactions and heterocycles synthesis
- **c.** Ultrasound assisted reactions: Types of sonochemical reactions, homogenous, heterogeneous liquid-liquid and liquid-solid reactions, synthetic applications
- d. Continuous flow reactors: Working principle, advantages and synthetic applications.

### 12

### UNIT II

### **Chemistry of peptides:**

- **a.** Coupling reactions in peptide synthesis
- **b.** Principles of solid phase peptide synthesis, t-BOC and FMOC protocols, various solid supports

and linkers: Activation procedures, peptide bond formation, deprotection and cleavage from resin, low and high HF cleavage protocols, formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides

- **c.** Segment and sequential strategies for solution phase peptide synthesis with any two case studies
- **d.** Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over activation and side reactions of individual amino acids.

### UNIT III

12

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**Photochemical Reactions:** Basic principles of photochemical reactions. Photo-oxidation, photo-addition and photo-fragmentation.

**Pericyclic reactions:** Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigmatrophic rearrangement reactions with examples

### UNITIV

### **Catalysis:**

- a. Types of catalysis, heterogeneous and homogenous catalysis, advantages and disadvantages
- **b.** Heterogeneous catalysis preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs.
- **c.** Homogenous catalysis, hydrogenation, hydroformylation, hydrocyanation, Wilkinson catalysts, chiral ligands and chiral induction, Ziegler-Natta catalysts, some examples of homogenous catalysis used in synthesis of drugs
- d. Transition-metal and Organo-catalysis in organic synthesis: Metal-catalyzed reactions
- e. Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction.
- f. Phase transfer catalysis theory and applications

### UNITV

### Stereochemistry & Asymmetric Synthesis:

- **a.** Basic concepts in stereochemistry optical activity, specific rotation, racemates and resolution of racemates, the Cahn, Ingold, Prelog (CIP) sequence rule, meso compounds, pseudo asymmetric centres, axes of symmetry, Fischers D and L notation, cis-trans isomerism, E and Z notation.
- **b.** Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation and Stereo selective synthesis with examples.

### M. Pharm. I & II Year Syllabus (Pharmaceutical Chemistry)

### **BOOKS REFERENCES RECOMMENDED**

- 1. "Advanced Organic chemistry, Reaction, mechanisms and structure", J March, John Wiley and sons, New York.
- 2. "Mechanism and structure in organic chemistry", ES Gould, Hold Rinchart and Winston, NewYork.
- 3. "Organic Chemistry" Clayden, Greeves, Warren and Woihers., Oxford University Press 2001.
- 4. "Organic Chemistry" Vol I and II. I.L. Finar. ELBS, Sixth ed., 1995.
- 5. Carey, Organic chemistry, 5th edition (Viva Books Pvt. Ltd.)
- 6. Organic synthesis-the disconnection approach, S. Warren, Wily India
- 7. Principles of organic synthesis, ROCNorman and JMCoxan, Nelson Thorns
- 8. Organic synthesis-Special techniques VK Ahluwalia and R Aggarwal, Narosa Publishers.
- 9. Organic reaction mechanisms 4th edition, VK Ahluwalia and RK Parashar, Narosa Publishers.

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| T | т | р |         |         | Cr. Maximum Marks |    |    |     |       |  |
|---|---|---|---------|---------|-------------------|----|----|-----|-------|--|
|   |   | P | Th. Cr. | Pr. Cr. | ТН                | CW | SW | Pr. | Total |  |
| 4 | - | - | 4       | -       | 75                | 25 | -  | -   | 100   |  |

### **PY99503: COMPUTER AIDED DRUG DESIGN**

### Course objectives:

- To develop knowledge about the role of CADD in drug discovery.
- To know the different CADD techniques and their applications.
- To learn various strategies to design and develop new drug like molecules.
- To understand working with molecular modeling software to design new drug molecules.
- To understand the pharmacophore mapping concept and virtual screening.

### **Course outcomes:**

On completion of this course, the students are expected to be able to:

- CO-1: Explain the basics and applications of computer-aided drug design (CADD).
- **CO-2:** Describe the development and use of Quantitative Structure Activity Relationships (QSAR) in drug design.
- **CO-3:** Analyze molecular and quantum mechanics methods used in drug design, including molecular docking and drug receptor interactions.
- **CO-4:** Evaluate ADMET properties of new molecules and their importance in drug design, and use de novo drug design and homology modeling.
- **CO-5:** Apply in silico drug design and virtual screening techniques, including similarity-based methods, pharmacophore-based screening, and structure-based in-silico virtual screening protocols.

### THEORY

### UNIT I

### **DURATION (LECTURES)**

12

### Introduction to Computer Aided Drug Design (CADD):

History, different techniques and applications.

### **Quantitative Structure Activity Relationships:**

Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi-substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters.

### UNIT II

Quantitative Structure Activity Relationships: Applications Hansch analysis,

Free Wilson analysis and relationship between them, Advantages and disadvantages; Deriving 2D-QSAR equations.

**3D-QSAR approaches and contour map analysis**: Statistical methods used in QSAR analysis and importance of statistical parameters.

UNIT III

### **Molecular Modeling and Docking:**

Molecular and Quantum Mechanics in drug design

- **a.** Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation
- **b.** Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extraprecision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AchE&BchE)

### 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, Fragment based drug design.
- c. Homology modeling and generation of 3D-structure of protein.

### UNITV

### Pharmacophore Mapping and Virtual Screening:

Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping.

### In Silico Drug Design and Virtual Screening Techniques:

Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols.

### **BOOKS AND REFERENCES RECOMMENDED**

**1.** Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers.

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

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|           | 4       | -    | -     | 4         | -         | 75   | 25    | -       | -     | 100   |

### **PY99504: PHARMACEUTICAL PROCESS CHEMISTRY**

### Course objectives:

- To develop basic understanding about the strategies of scale up process.
- To develop basic understanding about unit operations.
- To understand scale up process
- To understand unit process .like Nitration, Halogenation etc.,
- To understand Fermentation.
- To understand the industrial safety process.

### Course outcomes:

On completion of this course, the students are expected to be able to:

- **CO-1:** Explain the basic principles and stages involved in the scale-up process of APIs, and evaluate the importance of in-process control and validation in ensuring quality.
- **CO-2:** Analyze the underlying principles and factors affecting the efficiency of various unit operations, such as extraction, filtration, distillation, evaporation, and crystallization.
- **CO-3:** Evaluate the principles and methods involved in various unit processes, including nitration, halogenation, oxidation, reduction, and fermentation, and assess their industrial applications.
- **CO-4:** Evaluate the importance of safety protocols and standards required in an industrial setup, including Material Safety Data Sheets, hazard labeling, personal protection equipment, fire safety, and environmental management, and propose solutions for any identified hazards.
- **CO-5:** Design and apply strategies for analyzing the progress of chemical reactions, streamlining reaction steps, selecting routes and reagents, and optimizing scale-up processes.

### THEORY

### UNIT I

Process Chemistry: Introduction, Synthetic strategy

**Stages of scale up process:** Bench, pilot and large scale process. In-process control and validation of large scale process. Case studies of some scale up process of APIs. Impurities in API, types and their sources including genotoxic impurities

### UNIT II

### Unit operations:

- a. Extraction: Liquid equilibria, extraction with reflux, extraction with agitation, counter current extraction.
- b. Filtration: Theory of filtration, pressure and vacuum filtration, centrifugal filtration,
- c. Distillation: azeotropic and steam distillation
- d. Evaporation: Types of evaporators, factors affecting evaporation.

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**DURATION (LECTURES)** 

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e. Crystallization: Crystallization from aqueous, nonaqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphous APIs.

### **UNIT III**

### Unit Processes – I:

- **a.** Nitration: Nitrating agents, Aromatic nitration, kinetics and mechanism of aromatic nitration, process equipment for technical nitration, mixed acid for nitration.
- **b. Halogenation:** Kinetics of halogenations, types of halogenations, catalytic halogenations. Case study on industrial halogenation process.
- **c.** Oxidation: Introduction, types of oxidative reactions, Liquid phase oxidation with oxidizing agents. Nonmetallic Oxidizing agents such as H2O2, sodium hypochlorite, Oxygen gas, ozonolysis.

### UNIT IV

### **Unit Processes – II:**

- **a.** Reduction: Catalytic hydrogenation, Heterogeneous and homogeneous catalyst; Hydrogen transfer reactions, Metal hydrides. Case study on industrial reduction process.
- b. Fermentation: Aerobic and anaerobic fermentation. Production of:
  - i. Antibiotics; Penicillin and Streptomycin
  - ii. Vitamins: B2 and B12
  - iii. Statins: Lovastatin, Simvastatin
- c. Reaction progress kinetic analysis:
  - i. Streamlining reaction steps, route selection,
  - **ii.** Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up.

### UNIT V

### **Industrial Safety:**

- **a.** MSDS (Material Safety Data Sheet), hazard labels of chemicals and Personal Protection Equipment (PPE)
- b. Fire hazards, types of fire & fire extinguishers
- c. Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001(Environmental Management System), Effluents and its management

### **BOOKS AND REFERENCES RECOMMENDED**

- 1. Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview; K. Gadamasetti, CRC Press.
- 2. Pharmaceutical Manufacturing Encyclopedia, 3rd edition, Volume 2.
- 3. Medicinal Chemistry by Burger, 6th edition, Volume 1-8.
- 4. W.L. McCabe, J.C Smith, Peter Harriott. Unit operations of chemical engineering, 7th edition, McGraw Hill.
- 5. Polymorphism in Pharmaceutical Solids .Dekker Series Volume 95 Ed: H G Brittain (1999).
- 6. Regina M. Murphy: Introduction to Chemical Processes: Principles, Analysis, Synthesis.

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7. Peter J. Harrington: Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale-Up.

- 8. P.H.Groggins: Unit processes in organic synthesis (MGH).
- 9. F.A.Henglein: Chemical Technology (Pergamon).
- 10. M.Gopal: Dryden's Outlines of Chemical Technology, WEP East-West Press.

M. Pharm. I & II Year Syllabus (Pharmaceutical Chemistry)

- 11. Clausen, Mattson: Principle of Industrial Chemistry, Wiley Publishing Co.
- 12. Lowenheim& M.K. Moran: Industrial Chemicals.
- **13.** S.D. Shukla & G.N. Pandey: A text book of Chemical Technology Vol. II, Vikas Publishing House.
- 14. J.K. Stille: Industrial Organic Chemistry (PH).
- 15. . Shreve: Chemical Process, Mc Grawhill.
- 16. B.K.Sharma: Industrial Chemistry, Goel Publishing House.
- **17.** ICH Guidelines
- 18. United States Food and Drug Administration official website www.fda.gov

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|---|---|----|-----------|---------|----|-----|---------|------|-------|
|   |   | ſ  | 1 II. Cr. | rr.cr.  | TH | CW  | SW      | Pr.  | Total |
| - | - | 12 | -         | 6       | -  | -   | 50      | 100  | 150   |

### PY99855: PHARMACEUTICAL CHEMISTRY PRACTICALS-II

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

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|---|---|---|--------|--------|----|----|----------|-------|-------|
|   |   | r | Credit | Credit | ТН | CW | SW       | Pr.   | Total |
| - | - | 7 | -      | 4      | -  | -  | -        | -     | 100   |

### **PY99883: SEMINAR/ASSIGNMENT**

### **Objectives:**

• To identify any contemporary topic from the thrust area of current pharmaceutical research, regulatory affairs, drug discovery & current affairs of medicinal and pharmaceutical chemistry and any other field beyond the syllabus.

- To do exhaustive search of literature and information reported in the area of seminar topic.
- To develop in-depth understanding on seminar topic and prepare the power point presentation.
- To develop the skills of scientific presentation in front of scientific community.

### **Outcomes:**

On completion of this activity, students are expected to be able to:

- Know different sources of scientific literature and current pharmaceutical news/information.
- Collect information/subject knowledge and identify the relevant topic in thrust area of interest of pharmaceutical field beyond the syllabus contents.
- Develop skills and confidence of seminar presentation and extempore discussion with scientific fraternity.

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# M.PHARM. II YEAR pharmaceutical chemistry semester-iii

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## II M.PHARM. ( PHARMACEUTICAL CHEMISTRY)

### **SEMESTER-III**

| C No   | S. No. Sub. Code Subject |   |   |   | Th. | Pr     | Maximum Marks |    |     |    |     |       |
|--------|--------------------------|---|---|---|-----|--------|---------------|----|-----|----|-----|-------|
| 5. NO. |                          |   | L | I | r   | Credit | .Credi<br>t   | TH | CW  | SW | Pr. | Total |
| 1.     | PY99902                  | Research Methodology & Biostatistics            | 4 | - | 1   | 4      | -             | 75 | 25  | -  | -   | 100   |
| 2.     | PY99931                  | Journal Club                                    | 1 | - | -   | 1      | -             | -  | 25  | -  | -   | 25    |
| 3.     | PY99932                  | Discussion/Presentation (Proposal Presentation) | 2 | - | -   | 2      | -             | -  | 50  | -  | -   | 50    |
| 4.     | PY99940                  | Research Work                                   | - | - | 28  | -      | 14            | -  | -   | -  | 350 | 350   |
|        | Total                    |   |   | 0 | 28  | 7      | 14            | 75 | 100 | -  | 350 | 525   |

| Department of Pharmacy, Shri G.S. Institute of Technology & Science, Indore | Department of Pharmacy, | Shri G.S. Institute of | Technology & Science, Indore |
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|   |   | r | Th. Cr. | Pr. Cr. | ТН            | CW | SW | Pr. | Total |  |  |
| 4 | - | - | 4       | -       | 75            | 25 | -  | -   | 100   |  |  |

### **PY99902: RESEARCH METHODOLOGY AND BIO STATICSTICS**

### **Course objectives:**

- To identify the thrust area in the field of drug design, pharmaceutical chemistry, new analytical method development through literature survey.
- To design and plan the research objectives and methodologies using computational tools & other techniques.
- To formulate rationale plan of work for the selected problems.
- To procure research tools and consumables for planned research.
- Attempttocompleteapprox.25% of planned experimental work. •

### **Course outcomes:**

Upon completion of this course, students should be able to:

- CO1: Apply research methodology principles to design studies, evaluate literature, and identify potential sources of error and bias.
- **CO2:** Analyze and interpret statistical data, including selecting appropriate statistical tests and evaluating significance levels.
- CO3: Evaluate ethical issues and guidelines in medical research, including the use of laboratory animals, informed consent, confidentiality, and cultural concerns.
- CO4: Apply CPCSEA guidelines to ensure proper care, handling, and treatment of laboratory animals.
- CO5: Evaluate the basic principles and historical context of medical research and its combination with medical care.

### THEORY

### **UNIT I**

### **DURATION (LECTURES)**

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General Research Methodology: Research, objective, requirements, practical difficulties, review of literature, study design, types of studies, strategies to eliminate errors/bias, controls, randomization, crossover design, placebo, blinding techniques.

### **UNIT II**

Biostatistics: Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, type of significance tests, parametric tests (students "t" test, ANOVA, Correlation coefficient, regression), non-parametric tests (wilcoxan rank tests, analysis of variance, correlation, chi square test), null hypothesis, P values, degree of freedom, interpretation of P values.

| UNIT III  | 12 |
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**Medical Research:** History, values in medical ethics, autonomy, beneficence, non-maleficence, double effect, conflicts between autonomy and beneficence/non-maleficence, euthanasia, informed consent, confidentiality, criticisms of orthodox medical ethics, importance of communication, control resolution, guidelines, ethics committees, cultural concerns, truth telling, online business practices, conflicts of interest, referral, vendor relationships, treatment of family members, sexual relationships, fatality.

### UNIT IV

12

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**CPCSEA guidelines for laboratory animal facility:** Goals, veterinary care, quarantine, surveillance, diagnosis, treatment and control of disease, personal hygiene, location of animal facilities to laboratories, anesthesia, euthanasia, physical facilities, environment, animal husbandry, record keeping, SOPs, personnel and training, transport of lab animals.

### UNIT V

A History, introduction, basic principles for all medical research, and additional principles for medical research combined with medical care.

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# M.PHARM. II YEAR pharmaceuticalchemistry semester-iv

### II M.PHARM. (PHARMACEUTICAL CHEMISTRY) SEMESTER IV

| S. No. |   |   | T | т      | Ъ      | Th. | Pr. | Maximum Marks |     |       |     |     |
|--------|---|---|---|--------|--------|-----|-----|---------------|-----|-------|-----|-----|
|        | Sub. Code                                       | b. Code Subject L T P                           |   | Credit | Credit | TH  | CW  | SW            | Pr. | Total |     |     |
| 1.     | PY99953   | Journal Club                                    | 1 | -      | -      | 1   | -   | -             | 25  | -     | -   | 25  |
| 2.     | PY99952   | Discussion/Presentation (Proposal Presentation) | 3 |        | -      | 3   | -   | -             | 75  | -     | -   | 75  |
| 3.     | PY99985   | Research Work & Colloquium                      | - | -      | 32     | -   | 16  | -             | -   | -     | 400 | 400 |
| 4.     | 4. PY99999 Co-curricular Scholastic Activities* |   | - | -      | -      | -   | 2*  | -             | -   | -     | -   | -   |
|        | Total   |   |   |        | 32     | 4   | 18  | -             | 100 | -     | 400 | 500 |

Credits of co-curricular scholastic activities (minimum 2 and maximum 7 credits) shall be earned during the course. Refer minutes of 27<sup>th</sup> meeting of Academic council 22/07/2022

|   | 11)))65: RESEARCH WORK & COLLOQUIUM |    |         |         |               |    |    |     |       |  |
|---|-------------------------------------|----|---------|---------|---------------|----|----|-----|-------|--|
| T | т                                   | Р  | Th. Cr. | Pr. Cr. | Maximum Marks |    |    |     |       |  |
|   | 1                                   |    |         |         | TH            | CW | SW | Pr. | Total |  |
| - | -                                   | 32 | -       | 16      | -             | -  | -  | 400 | 400   |  |

### PY99985: RESEARCH WORK & COLLOQUIUM

### **Objectives:**

- To pursue advanced concepts, emerging research methodologies and recent experimental tools for carrying out the planned research work.
- To carry on the planned experimental work & optimize methodology.
- To pursue the experimental findings &draw conclusion.
- To establish correlation of results obtained & publication of research.
- To develop research orientation and aptitude in the field of drug design, pharmaceutical chemistry and analytical method development.

### **Outcome:**

Upon completion of this course, students should be able to:

- **CO-1:** Analyze and evaluate advanced concepts and experimental tools in drug design, pharmaceutical chemistry, and analytical method development.
- **CO-2:** Apply critical thinking and creativity to develop themselves as upcoming researchers in the emerging fields of drug design, pharmaceutical chemistry, and analytical method development.
- **CO-3:** Communicate effectively through scientific presentations and publications to add value to the existing knowledge in the research field.
- **CO-4:** Manage and complete research projects within the stipulated time, and correlate and compile findings for the dissertation.
- **CO-5:** Evaluate and improve the quality of their research work through self-reflection and peer feedback.