Punjab Technical University, Jalandhar M. Pharm (Pharmaceutical Chemistry) Study Scheme

1st Semester

Sr. No.	Course Code	Subject	Exam Hours	Maximum Marks	
				Int.	Ext.
1	PHCHM 511	Organic Chemistry & Selected aspects of Drug Research.	3	20	80
2	PHCHM-513	Spectral Analysis.	3	20	80
3	PHCHM-515	Advanced organic Chemistry & Spectrometry	3	20	80
4	PHCHM-517	Pharmaceutical Chemistry Laboratory -I	12	20	80
Total				80	320

2nd Semester

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Sr. No.	Course Code	Subject	Exam Hours	Maximum Marks					
				Int.	Ext.				
1	PHCHM 512	Medicinal Chemistry	3	20	80				
2	PHCHM-514	Chemistry of Natural Products	3	20	80				
3	PHCHM-516	Bio-Organic Chemistry	3	20	80				
4	PHCHM-518	Pharmaceutical Chemistry laboratory- II	12	20	80				
Total				80	320				

3rd & 4th Semester

(Research work for one year)

The thesis shall be presented by the candidate at the end of record academic year. The thesis shall be evaluated as under:

Evaluation of written thesis : MM: 200 Presentation of Seminar on thesis : MM: 100

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Total : 300 Marks

PHCHM-511 Organic Chemistry and Selected aspects of Drug Research

External Marks: 80 4 Hrs/ Week

Internal Marks: 20 Total : 100

1. Reaction Intermediates

Formation, structure, stability and reactions of Carbocation, Carbanions, Free radicals, Nitrenes, Carbenes, Benzynes.

2. Concept of Acids and bases

Hard and soft acids and bases, effect of structure and medium on strength of acids and bases. pH, pKa, pKb, Henderson- Hassenbelch equation, buffer solutions.

3. Organic reactions:

Substitution, Addition, Elimination reactions, Rearrangement; Pinacol – Pinacolone rearrangement, Beckmann rearrangement, Fries rearrangement, Schmidt rearrangement, Hofmann- martius aniline rearrangement, Favorskii rearrangement, Claisen Condensation and rearrangement.

4. Organic Synthetic techniques involved in Drug Research

- a) Protection Deprotection of functional groups
- b) Introduction to asymmetric synthesis
- c) Microwave reactions

5. Separation Techniques:

Chromatography: general principles, classification, chromatographic techniques, normal and reversed, phase bonded phase, column chromatography, , thin layer and high performance thin layer chromatography, counter current chromatography, Droplet counter chromatography, ion exchange chromatography, principle application and Instrumentation of Gas chromatography; Principal, applications, instrumentation of High pressure liquid chromatography, Introduction to chiral chromatography

6. Physico- Chemical parameters and drug action:

Inter and Intramolecular interaction: covalent, dipole, hydrogen bonding, Dihydrogen bonding, van der waals interaction.

7. Stereochemistry and Drug action

Molecular isomerism, chirality, molecular symmetry, racemic resolution procedures, conformational analysis.

- 1. M. E. Wolff, Burger's Medicinal Chemistry and Drug discovery, Principle and Practice, John Wiley & Sons, New York. (Latest edition).
- 2. Nogrady, Medicinal Chemistry, A Bio Chemical Approach, Oxford University Press, Oxford.
- 3. J. March, Advanced Organic Chemistry, Reactions, Mechanism and Structures, John Wiley & Sons, New York. (Latest edition).
- 4. Eliel and H. Samuel, Stereochemistry of Organic compounds, John Wiley & Sons, New York. (Latest edition).
- 5. E. Stahl, Thin Layer Chromatography, A laboratory handbook, Springer verlag-Berlin (Latest edition).
- 6. E. Heftman, A laboratory handbook of Chromatography. (Latest edition).

PHCHM-513 Spectral Analysis

External Marks: 80 4 Hrs/ Week

Internal Marks: 20 Total : 100

1. Ultraviolet and Visible spectroscopy:

Introduction, energy levels, selection rules; Woodward Fieser, Fieser Kuhn and Nelson rule, Influence of substituents, ring Size and strain on spectra characteristics, solvent effect, methodology, spectral correlation with structure.

2. Infrared Spectroscopy:

Introduction, types of vibrations, characteristics regions of the spectrum, influence of substituents, ring size, hydrogen bonding, vibrational coupling, field effects on frequency, methodology, spectral interpretation with example.

3. Nuclear Magnetic Resonance spectroscopy:

Introduction, magnetic nuclear, chemical shift, shielding, relaxation process, chemical & magnetic non equivalence, local dia magnetic shielding and magnetic anisotropy, spin splitting, Pascal triangle, coupling constant, mechanism of coupling, quadrapoule broadening and decoupling. Effect of stereochemistry on the spectrum, shift reagent, application of ¹HNMR with some examples. Introduction to the following techniques would be covered DEPT, APT, COSY, NOESY and INADEQUATE.

4. Mass Spectrometry:

Introduction, Essential components of a mass spectrometer, types of ions, molecular ion, fragment ion, rearrangement ion, metastable ion, Isotopic ions and their corresponding peaks, rules of fragmentation Mc Lafferty rearrangement, Retro Diels Alder and other fragmentation patterns. Introduction to FAB, LC-MS, GC-MS.

- 1. R. M. Silverstein and F. X. Webster, Spectrometric identification of Organic compounds, John Wiley & Sons, New York. (Latest edition).
- 2. William kemp, Organic Spectroscopy, ELBS Mac millan, Hampshire, (U. K).
- 3. D. L. Pavia, G. M. Lampman and G. S. Kriz, Introduction to spectroscopy- A guide for students of Organic chemistry, Harcourt college publishers. (Latest edition).
- 4. D. H. Williams and I. Fleming, Spectroscopic methods in Organic chemistry, Tata Mc Graw Hill publishing company Ltd, New Delhi, India. (Latest edition).

PHCHM-515 Advanced Organic Chemistry & Spectrometry

External Marks: 80 4 Hrs/ Week

Internal Marks: 20 Total : 100

1. Photochemical Reaction:

Light absorption, electronic transition, Jablonski diagram, intersystem crossing, photosensitization, excited states of ketones & cleavage hydrogen abstraction, photochemistry of conjugated dienes, enones.

2. Pericyclic reaction;

Concepts of molecular orbital symmetry, Woodward Hofman rules of conservation of orbital symmetry and its applications to electrocyclic (Dields Alders reactions) Sigmatropic, cycloaddition and ene reaction.

3. Name reactions; their mechanism and applications in drug synthesis

i) Grignard viii) Mannich Knorr Pyrazole synthesis ii) Witting ix) iii) Reformatsky Strecker amino acid synthesis X) iv) Claisen Schimidt Merrifield solid phase synthesis xi) v) Perkin Oppenauer oxidation xii) vi) Knoevenagel xiii) Wolf Kishner reduction vii) Darzen Meerwein Ponndorf- verley xiv) reduction

4. ¹³C Nuclear Magnetic Resonance (¹³C – NMR)

Natural abundance of ¹³C, resolution and multiplicity FT mode, RF mode, uses of proton coupled, decoupled and off resonance decoupling techniques, deuterium substitution, chemical equivalence in peak assignment, chemical shift, Effect of substitution on chemical shifts, position of alkanes, alkenes, alkynes and benzene spin coupling and C¹³- H¹ coupling

5. Electronic Spin Resonance (ESR):

Principle and correlation with proton magnetic resonance, derivative curves, g-values, hyperfine splitting, Applications.

6. Raman Spectroscopy:

Introduction, Principle and application of Raman Spectroscopy.

- 1. J. March, Advanced Organic Chemistry, Reactions, Mechanism and Structures, John Wiley & Sons, New York. (Latest edition).
- 2. R. M. Silverstein and F. X. Webster, Spectrometric identification of Organic compounds, John Wiley & Sons, New York. (Latest edition).

- 3. William kemp, Organic Spectroscopy, ELBS Mac millan, Hampshire, (U. K).
- 4. D. L. Pavia, G. M. Lampman and G. S. Kriz, Introduction to spectroscopy- A guide for students of Organic chemistry, Harcourt college publishers. (Latest edition).
- 5. D. H. Williams and I. Fleming, Spectroscopic methods in Organic chemistry, Tata Mc Graw Hill publishing company Ltd, New Delhi, India. (Latest edition).

PHCHM-517 Pharmaceutical Chemistry Laboratory- 1

External Marks: 80 16 Hrs/ Week

Internal Marks: 20 Total :100

- 1. Separation of Organic compounds from their mixture and their identification.
- 2. Synthesis of Organic compounds of medicinal interest
- 3. Workshop/ Tutorials/ Seminars on
- (a) Stereomodel use:- Exercise involving preparation of stereomodels with view to assess the importance of stereochemistry in drug action.

 Examples of Pharmacopoeial substance of stereochemical importance should be taken for illustration
- (b) Interpretation of spectra of organic compounds- Workshop involving interpretation of IR, NMR and Mass spectra of Organic compounds to elucidate their chemical structure.
- (c) Basic Chromatographic techniques.

PHCHM-512 Medicinal Chemistry

External Marks: 80 4 Hrs/ Week

Internal Marks: 20 Total :100

1. Drug design and approaches to drug discovery:

Analogue synthesis versus rational design; discovery of lead compounds; pharmacophore identification, structure modification, physicochemical alterations, prodrug approach, Quantitative structure activity relationship, molecular modeling, combinatorial chemistry and high throughput screening, innovations in drug delivery.(Basic concept only)

2. Drug effectors theories:

Receptor concept, nature and types of receptor, receptor characterization.

3. Structure of Cell membrane:

Membrane lipids, membrane protiens, membrane carbohydrates, passage through membrane.

4. Structure and function of bio molecules:

- (a) Protein structure, protein ligand interaction, peptidomimetics, structure of lipoprotein and glycoprotein in relation to their functions.
- (b) Polysaccharides and lipids: Their structure and relationship between their physicochemical properties and their biological action.
- (c) Oligonucleotides
- (d) Function of biomolecules pertaining to different therapeutic areas: cancer, inflammation, hyperlipidaemia.

5. Advances in Chemotherapy of parasitic, microbial and viral infectionAntimalarials, Antiamoebics, Antifilarials, Antileshmanials, Antituberculars, Anti

HIV drugs

6. Advances in Psychotherapeutic agents

Biochemical basis of mental disorder, antipsychotics, antidepressants and anti anxiety drugs.

7. Advances in therapeutic agents for cardiovascular disorders

Antihypertensive, Antiarrhythmics, Antihyperlipidemics.

- 1. M. E. Wolff, Burger's Medicinal Chemistry and Drug discovery, Principle and Practice, John Wiley & Sons, New York. (Latest edition).
- 2. Nogrady, Medicinal Chemistry, A Bio Chemical Approach, Oxford University Press, Oxford.
- 3. Matrindale, The extra Pharmacopoeia, Pharmaceutical press, London. (Latest edition)
- 4. R. B. Silverman, The Organic Chemistry of Drug design and Drug action, Academic press, New York. (Latest edition).
- 5. Monographs and relevant review articles appearing in various Periodicals and Journals.

PHCHM-514 Chemistry of Natural Products

External Marks: 80 4 Hrs/ Week

Internal Marks: 20 Total :100

1. Natural Products:

Introduction, sources (Plant, animal, microbial, marine), classification on chemical basis. Role of natural products in development of medicinal chemistry, providing "leads". Selected example taken from Antimalarials, Local anaesthetics and Anticholinergics.

- 2. Natural products as medicinal agents along with their structurally modified form a) Ephedrines b) Ergot alkaloids c) Vasicine d) Taxol
- 3. **Medicinal agents obtained by chemical modification of natural products**Selected examples from the categories of antineoplastic agent (palcitaxel and its derivative) podophyllotoxin and its derivative like etoposide and tenoposide
- 4. Bioactive compounds from marine sources.

 Marine natural products and drug development
- 5 Toxins used as Drugs and Pharmaceuticals.
- 6. Nutraceuticals
- 7. Significant biosynthetic pathway; Acetate- mevalonate shikimic acid. Reading Material Recommended
 - 1. M. E. Wolff, Burger's Medicinal Chemistry and Drug discovery, Principle and Practice, John Wiley & Sons, New York. (Latest edition).
 - 2. Matrindale, The extra Pharmacopoeia, Pharmaceutical press, London. (Latest edition).
 - 3. K.B.G. Torsell, Natural products chemistry, John Wiley & Sons, New York. (Latest edition).
 - 4. I.L Finar, Organic Chemistry Vol:2 The English language book society and Longman group Ltd, London. (Latest edition).
 - 5. G. A. Cordell, Introduction to Alkaloids, John Wiley & Sons, New York. (Latest edition).
 - 6. M. L. Wickery and D. Wickery, Secondary plant metabolism, Mac millan Pvt Ltd.
 - 7. J. B. Harborne, Phytochemical methods, Chapman and Hall, London. (Latest edition).
 - 8. Monographs and relevant review articles appearing in various Periodicals and Journals.

PHCHM-516 Bio-Organic Chemistry

External Marks: 80 4 Hrs/ Week

Internal Marks: 20 Total :100 1. Steroids:

Definition, structure, nomenclature, classification and medicinal importance of steroids. Biosynthesis of Cholesterol. Chemistry of Cholesterol, Bile acids, and Sex-hormones.

Alkaloids:

Definition, sources, isolation, structure, nomenclature and classification of Alkaloids. Synthesis, medicinal importance test for identity, structural elucidation including spectral data and pharmacopeal standards of following compounds; Morphine, Reserpine.

Terpenoids:

Definition, structure, nomenclature, classification, isolation medicinal importance and structural elucidation of terpenoids. Isoprene rule; chemistry of abietic acid and β -amyrin.

4. Glycoside:

Definition structure nomenclature and classification of glycosides Chemistry mechanism of action and medicinal importance of cardiac glycosides, anthracene glycosides.

5 a) Chemistry and medicinal importance of following natural compounds

- i) Lignans along with their modified forms
- ii) Anthocyanin and Flavanoids: Definition, structure, nomenclature and classification of flavanoids. Chemistry and therapeutic importance of flavanoids should be discussed.
- iii) Carotenoids.
- b) Chiral resolution of some important drugs by
 - i) classical methods
 - ii) by enzyme- resolution of Propranolol and Naproxen as example

6 Biotechnology and drug development:

Basics of biotechnology and biotechnologically produced drugs.

7. Purines and pyrimidines

Chemistry, synthesis, interrelationship and medicinal uses of caffeine, theophylline theobromine and uric acid.

- 1. M. E. Wolff, Burger's Medicinal Chemistry and Drug discovery, Principle and Practice, John Wiley & Sons, New York. (Latest edition).
- 2. Matrindale, The extra Pharmacopoeia, Pharmaceutical press, London. (Latest edition).
- 3. K.B.G. Torsell, Natural products chemistry, John Wiley & Sons, New York. (Latest edition).
- 4. I.L Finar, Organic Chemistry Vol:2 The English language book society and Longman group Ltd, London. (Latest edition).
- 5. G. A. Cordell, Introduction to Alkaloids, John Wiley & Sons, New York. (Latest edition).
- 6. M. L. Wickery and D. Wickery, Secondary plant metabolism, Mac millan Pvt Ltd.
- 7. J. B. Harborne, Phytochemical methods, Chapman and Hall, London. (Latest edition).
- 8. Monographs and relevant review articles appearing in various Periodicals and Journals.
- 9. R. M. Silverstein and F. X. Webster, Spectrometric identification of Organic compounds, John Wiley & Sons, New York. (Latest edition).

PHCHM-518 Pharmaceutical Chemistry Laboratory- II

External Marks: 80 16 Hrs/ Week

Internal Marks: 20 Total :100

- 1. Synthesis of Organic compounds of medicinal interest, involving minimum two step synthesis.
- 2. Isolation of Natural products from Plant materials.
- 3. Workshop/ Tutorials/ Seminars on
 - (a) Stereomodel use
 - (b) Interpretation of spectra of organic compounds
 - (c) Chromatographic techniques