<u>M.Sc. Pharmaceutical Chemistry</u> <u>University of Lucknow</u>

Programme Outcomes

- PO-1. Demonstrate, solve and an understanding of major concepts in all disciplines of Chemistry independently and in group as well as draw logical conclusions through Project and Seminar Presentation.
- PO-2. Encourage students to make critical thinking and the scientific knowledge gained would help them to design, carry out, record and analyze the results of Chemistry as well pharmaceutical experiments.
- PO-3. Equip students to face the employment challenges and instil confidence to turn into entrepreneur and also step into research career.
- PO-4. Generation of new scientific insights or to the innovation of new applications of chemical research
- PO-5. Present scientific and technical information resulting from laboratory as well as Industrial/pharmaceutical experimentation in both written and oral formats, would make them perfect.
- PO-6. Learns modern methods of chemical systems in a laboratory setting make them perfect for any scientific laboratory and industry.
- PO-7: The students will become well versed in the mechanisms and also with the mode of action of drugs.
- PO-8. The present course content will build confidence in students and the students will improve their competencies on par with their counterparts in premier institutions across the nation.

Programme Specific Outcome

- PSO-1 Students will be able to understand the basic concepts of bio-inorganic, bioorganic, physical chemistry, analytical chemistry, drug formulation, drug design and development, and green chemistry
- PSO-2. Students will develop the ability to present pharmaceutical chemistry research by means of an oral presentation, a scientific poster or a written report.
- PSO-3. Students will be able to use and apply professional softwareøs relevant to chemistry.
- PSO-4. Students will be able to demonstrate knowledge to develop Pharmaceutically important molecules, new drug delivery systems etc.
- PSO-5. Students will demonstrate an ability to analyze and interpret data of analytical experiments in production, quality control & assurance of pharmaceutical synthesis and formulation.
- PSO-6. Students will be able to apply analytical tools for determination of organic molecules.
- PSO-7. Students will be able to generate validation protocol for all pharmaceutical operations starting from drug research to development to formulation.
- PSO-8. Learn Role of drugs to inhibit the particular enzymes and treatment of disease
- PSO-9. Learn Mode of action of different drugs.

M.Sc. PHARMACEUTICAL CHEMISTRY

<u>PROGRAMME STRUCTURE</u> The Master of Science in Pharmaceutical Chemistry is a Two Year Full Time Course consisting of Four Semesters.

Semester I Semester II

Semester III

Semester IV

COURSE SRUCTURE

Semeste	Core Course			Elective Course		Open elective Course			Value	Added	Total Credits	
	No. of	Credits	Total	No. of	Credits	Total	No. o	Credits	Total	No. of	Credi	
	Papers	(L+T/F	Credits	Papers	(L+T/P	Credit	Paper	(L+T/I	Credits	Papers		
Ι	4	16+8	24	0	0+0	0	0	0+0	0	1	4	28
II	4	16+8	24	0	0+0	0	0	0+0	0	0	0	24
III	2	8+8	16	1	4+0	4	1	4+0	4	0	0	24
IV	1D	12+4	16	1	4+0	4	0	0+0	0	0	0	20
		Total (80			8			4		4	96

Paper Code	Title of the paper	Cre	Int.	End	Marks
		dits	Ass.	Sem. Exam.	
CCTP-1	PC-101: Physical Chemistry	4	30	70	100
CCTP-2	PC-102: Organometallic & Nuclear Chemistry	4	30	70	100
CCTP-3	PC-103: Organic Chemistry	4	30	70	100
CCTP-4	PC-104: Project and Seminar Presentation	4	-	-	100
CCPP-1 CCPP-2	PC-105A: Organic Chemistry Practical PC-105B: Inorganic Chemistry Practical	8	Conti nuou s Eval uatio n	-	200
Value Added (Credited) (Inter Department)	*CH-105A: Separation Techniques Or *CH-105B: Chemistry of Analgesics and Antipyretics	4	30	70	100
• ′	Total	28			700

CCTP (Core Course Theory Paper). CCPP (Core Course Practical Paper). CCEP (Core Course Elective Paper). COEP (Course Open Elective Paper).

*Value Addition Courses (both Credited and Non Credited) The offered courses shall be announced by the Head, Chemistry Department in the beginning of session everv year-

Green Chemistry	Boron Chemistry and application to Cancer Treatment	Analgesics and Antipyretics	Narcotics and drug abuse
Bioethanol as Biofuels	Carbon dating	Science and Technology of Cosmetics	Pesticides and Insect repellents
Separation	CFCs and the	Chemistry of Paints	Computational
Techniques	Environment	J.	Chemistry
Nanochemistry	Chemistry of Explosives	Chemistry of Diamonds	Medicinal Application of Iodine & Radium
Drugs from Indian Medicinal Plants	Developments in Organic Synthesis	Water Chemistry	Lubricants
		Chemical Dyes	Essential Oils and
Chemistry of		•	Perfumes
Alcohols			

Credits 4

Hours 60

Course Outcome:

Student will learn-

- CO-1.To know and understand that how living organism acquires and transforms energy in order to perform biological work.
- CO-2.To understand how enzyme catalysis increases reaction rates without altering the the chemical equilibrium.
- CO-3.To became familiar with Langmuir theory, BET theory and their uses, Zeta potential Electrokinetic phenomenon, Donnan equilibrium, Primary and Secondary salt effects
- CO-4.To know the latest techniques which are now a days used in determining the fast reactions.

Unit I

Bioenergetics: coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration.

Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

Unit II

Michaelis-Menten mechanism, effect of pH and temperature on enzyme catalysed reaction, limiting rate, Lineweaver Burk and Eadie equation and plots.

Inbition of enzyme action, competitive inhibition and non competitive inhibition.

Muscle contraction and energy generation in mechanochemical system.

Unit III

Adsorption and various types of adsorption isotherms. The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Adsorption of liquids by solids, positive and negative adsorption, Gibbs adsorption equation., flash desorption

Unit IV

Theories of unimolecular reactions. Reactions in solution: factors determining reaction in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation,

Unit V

Kinetics of Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

Colloids: Zeta potential, Electrokinetic phenomena, Sedimentation potential and Streaming potential, Donnan membrane equilibrium.

Books Recommended:

- 1. P.W. Atkins, Physical Chemistry, Oxford University Press, New York.
- 2. S. Glasston, Physical Chemistry, Nostrand
- 3. Advance Physical Chemistry (Vol-1,2,3,4), K.L. Kapoor, Mac Millan, India
- 4. Puri Sharma Pathania, Advance Physical Chemistry.

- 5. J.O.M. Bockris and A.K.N. Reddy, Modern Electrochemistry, Vol.2, Plenum Press, New York
- 6. Statistical Thermodynamics, Second Edition, New Age International Limited Publisher, India by M.C. Gupta
- 7. Introductory Quantum chemistry by A.K Chandra, Second Edition, Tata Mc Graw-Hill publishing company Limited, India
- 8. Quantum chemistry Through problems and solution by R.K Prasad ,New age International Pvt Lmtd, Publishers
- 9. Molecular quantum Mechanics By P.W.Atkins Oxford University Press, Oxford New York
- 10. Physical Chemistry By Ira N. Levine

M.Sc. Pharmaceutical Chemistry Semester I Syllabus Paper Code CCTP-2: Organometallic and Nuclear Chemistry (PC-102) Credits 4 MM 100 (70+30) Hours 60

Course Outcome:

In this semester students learn

- CO-1. the reaction mechanism and vibrational properties associated with inorganic coordination complexes which now-a-days are gaining importance as
 - Homogenous catalysts
 - Electron transfer agents

Sensors to detect ions as well as molecules such as nitroaromatic compounds a noxious compound utilized as an ingredient in explosives

- Sensitizers in new-generation solar cells
- CO-2. about the design of different highly reactive but potent organometallic compounds. This information can be a stepping stone to such students who are willing to excel themselves in industries in particular dealing with pharma sector.
- CO-3. To recognize the importance of inorganic molecules in supporting organic biological systems.
- CO-4. about how metal ions function as catalytic and structural centers in biological systems.
- CO-5. about the metal ion transport and storage within cells and how any malfunction can result in various diseases.
- CO-6. To gain insight into cutting edge developments that utilizes metal ions for medical purposes.
- CO-7. To develop an appreciation for the structure and function of metal ions in the biological systems and how chemists aim to mimic them.
- CO-8. to recognize the metal used for diagnosis and chemotherapy.

Unit I

Reactions of Organometallic Compounds Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands. Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions. Rearrangement reactions, redistribution reactions, fluxional isomerism.

Unit II

Catalysis by Organometallic Compounds . Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops. the Fischer-Tropsch reaction(synthesis of gasoline). Hydroformylation of olefins using cobalt or rhodium catalyst. Carbonylation reactions-Monsanto acetic acid process

Unit III

Bioinorganic Compounds Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na⁺ and K⁺, ATP and ADP. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification. Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems-ferritin and transferrin.

Unit IV

Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions. Nitrogen Fixationnitrogenase, vitamin B12 and the vitamin B12 coenzymes. Metal-Nuclei acid interaction Metals in medicine-therapeutic applications of cis-platin, radio-isotopes and MRI agents. Toxic effects of metals (Cd, Hg, Cr and Pb).

Unit V

Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry. Applications of radio isotopes in industry, medicine, radiopharmacology, radiation safety precaution, nuclear waste disposal.

Recommended Books:

- 1. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill.
- 2. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
- 3. Theory and Applications of UV Spectroscopy, H. H. Jaffe and M. Orchin, IBH- Oxford.
- 4. Introduction to Magnetic Resonance, A. Carrington and A..D. Maclachalan, Harper & Row.
- 5. Physical Methods for Chemistry, R. S. Drago, Saunders Company.
- 6. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
- 7. Organometallic Chemistry: A Unified Approach by R. C. Mehrotra and A. K. Singh

M.Sc. Pharmaceutical Chemistry Semester I Syllabus Paper Code CCTP-3: Organic Chemistry (PC-103) MM 100 (70+30) Hours 60

Course Outcome:

Credits 4

- CO-1. This helps students to understand the outcome of the reaction and the product formed on the basis of the thermodynamic as well Kinetic properties.
- CO-2. Hammet equation explain the possible product that might be formed by changing the reaction parameters.
- CO-3. The most modern and recant reactions help students to gain insight into modern synthetic chemistry.
- CO-4. Various oxidation reduction and pericyclic reaction helps the students to learn basics of organic chemistry.
- CO-5. Stereochemistry makes students aware of various terms involved, nomenclature and 3D structure of various compounds. The students also learn about the change in stereochemistry/ Conformation and condition involved when a particular substrate undergoes different types of reaction.

CO-6. Importance of chiral drugs would make the student aware of its role and its utility in curing a particular disease.

Unit I

Physical Organic Chemistry. Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples, Linear free energy relationship Hammet equation, Taft equation.

Modern Synthetic Methods: Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Ugi reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama,

Unit II

Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (chromium, manganese, aluminium, and silver based reagents) (b) phenols (Fremyøs salt, silver carbonate) (c) alkenes to epoxides (peroxides/peracids based), Sharpless asymmetric epoxidation.(d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction. (e) alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation) (g) ketones to ester/lactones (Baeyer-Villiger).

Unit III

Reduction-(a) Catalytic hydrogenation (Heterogeneous: Pd /Pt /Rh /Ni etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium and Zinc (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) (c) Hydride transfer reagents (i) NaBH₄ triacetoxyborohydride; LiAlH4 and DIBAL-H, MeerweinPondorff-Verley reduction) (ii) Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

Unit IV

Pericyclic Reactions: Main features of pericyclic reactions; Woodward-Hoffman rules, correlation diagram and FMO approaches; Electrocyclic reactions ó conrotatory and disrotatory motions for 4n and 4n+2 systems. Cycloadditions ó antarafacial and suprafacial additions, [2+2] and [4+2] reactions (h and), 1,3-dipolar cycloadditions and chelotropic reactions; Sigmatropic [i,j] shifts of C-H and C-C bonds; Claisen, thio-Claisen, Cope and aza-Cope rearrangements.

Stereochemistry of Organic Compounds:

Center of chirality: molecules with C, N, S based chiral centers. Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, , spiranes, exo-cyclic . Topicity and prostereoisomerism, topicity of ligands.

Unit V

Conformational Analysis of cyclohexane and its derivatives, decalins. Fused and bridged bicyclic systems. Conformation and reactivity of elimination (dehalogenation,

dehydrohalogenation, semipinacolic deamination and pyrolytic elimination-Saytzeff and Hofmann eliminations). Chemical consequence of conformational equilibrium - Curtin Hammett principle.

Chiral drug synthesis Introduction to Chiral drugs, importance of stereochemistry in drug action, concepts of eutomer, distomer and eudysmic ratio, stereospecific and

stereoselective synthesis, Synthesis of Chiral drugs like Ibuprofen, Propranolol, ramipril, levofloxacin.

Recommended Books:

- 1. Stereochemistry of organic compounds, Nasipuri, New Age International (P) Limited.
- 2. Organic Chemistry J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
- 3. Advanced organic chemistry Part, A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
- 4. Advanced organic chemistry by J. March, 6th Ed. Wiley india Pvt. Ltd.
- 5. Mechanism and structure in Organic Chemistry ó E. S. Gould (Holt, Rinehart and Winston), Wiley india Pvt. Ltd.
- 6. Textbook of Pericyclic Reaction, Concept and Application, K.C. Majumdar and P. Biswas, Scientiffi International Pvt. Ltd.
- 7. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, New Age International (P) Limited.
- 8. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi.
- 9. Medicinal Chemistry, Ashutosh Kar, New Age International (P) Limited.

M.Sc. Pharmaceutical Chemistry Semester I Syllabus Paper Code CCTP-4: Project and Seminar Presentation (PC-104) Credits 4 MM 100

Course Outcome:

- CO-1. students should be able demonstrate ability to plan and strategize a scientific problem, and implement it within a reasonable time frame.
- CO-2. It is expected that after completing this project dissertation, students will learn to work independently and how to keep accurate/readable record of assigned project.
- CO-3. In addition, students will be able to know the library search and handle the data in a meaningful way.
- CO-4. Also, students will be able to interpret the spectral data independently.
- CO-5. Subsequently, the students should be able to critically examine research articles, and improve their scientific writing/communication skills and power point presentation.

For project work and seminar presentation, the area of the work would be to be decided by the advisor/mentor based on syllabus. On completion of the project work, students have to submit the work in the form of seminar followed by oral presentation in the presence of faculty members.

M.Sc. Pharmaceutical Chemistry Semester I Syllabus Paper Code CCPP-1, CCPP-2: Practical (PC-105A, PC-105B) MM: 200

Credits: 8

Course Outcome:

- **CO-1.** After completion of degree, students will gain the theoretical as well as practical knowledge of handling chemicals.
- CO-2. Students will gain an understanding of:
 - a. the distinction between qualitative and quantitative chemical analysis.
 - b. how to calculate a limiting reagent, yield, and percent yield.
- **CO-3.** students should be able to explain and perform the theoretical principles and important applications of classical analytical methods within titration (acid/base titrations, complexometric titration, redox titration) and various techniques of gravimetric and volumetric analysis.
- **CO-4.** students should be able to check the purity of organic molecules by the use of TLC and how to calculate their Rf values.

PC-105A: INORGANIC CHEMISTRY

- 1. Redox titrations
 - (a) Dichromatometry
 - (b) Iodometry
- 2. Gravimetric method
 - (a) Ag as AgCl
 - (b) Cu as CuSCN
- 3. Complexometric titrations of
 - (a) Magnesium using EDTA
 - (b) Zinc using EDTA
- 4. Neutralization reactions

PC-105B: ORGANIC CHEMISTRY

Separation, purification, characterization and identification by making suitable derivatives of the three component Organic mixture (three solids or two solids and one liquid or two liquids and one solid) involving all the functional groups. Use TLC for checking the purity of the separated compounds and their derivatives and report their Rf values.

Recommended Books:

- 1. Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.
- 2. Marr, G. and Rockett, R.W. Practical Inorganic Chemistry, Van Nostrand Reinhold. 1972.
- 3. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
- 4. Sethi, Arun., Systematic Lab Experiments in Organic Chemistry, New Age International Publisher.
- 5. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).
- 6. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- 7. Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

M.Sc. Pharmaceutical Chemistry Semester I Syllabus Value Added (Credited) Separation Techniques (CH-105A) MM 100 (70+30)

Hours 60

Course Outcome:

Credits 4

- CO-1. Students will learn the methods of separating a mixture or solution of chemical substances to obtain the pure constituents.
- CO-2. Students will learn the tradition methods of purification such as crystallization, extraction and distillation.
- CO-3. Students will know the Celite filtration, a useful technique used to remove fine solids such as metal salt from the reaction mixture.
- CO-4. Students will learn the centrifugation techniques useful in the microanalysis and is based on density difference.
- CO-5. They also learn the chromatographic techniques as they give accurate and complete separation and purification of the compounds.

The students will also learn the modern techniques of chromatography such as flash CO-6. chromatography, LPLC, HPLC and GC-MS etc.

			Unit – I
	1. Distillation	on	
	2. Crystalliz	zation	
	3. Membrar	ne Processes	
	4. Filtration	1	
			Unit – II
	1. Evaporat	tion	
	2. Extractio	n	
	3. Celite Fil	ltration	
	4. Gel Filtra	ation	
			Unit – III
	Demister	(Vapour)	
	Adsorptio	on & Stripping	
	Centrifug	gation	
			Unit – IV
1.	TLC		
2.	Sephadex Ch	romatography	
3.	Flash Chrom	atography	
4.	LPLC		
5.	HPLC		
6.	Paper Chrom	natography	

Unit – V

- 1. Counter current chromatography (CCC & DCCC)
- 2. Ion exchange chromatography
- 3. GC ó MS (Gas Chromatography)
- 4. Column chromatography (Silica gel)
- 5. Molecular Sieve chromatography or size exclusion chromatography

Recommended Books:

- Lloyd R. Snyder LC Resoures, Inc walnut Greek, California 1.
- Colin F. Poole, Department of Chemistry, Wayne State University Detroit MI 48202, USA 2. 2003 Elsevier.
- 3. J. D. Seader, and Ernest J. Henley, Separation Process Principles, Wiley, 2nd edition (2013).

M.Sc. Pharmaceutical Chemistry Semester I Syllabus Value Added (Credited) **Chemistry of Analgesics and Antipyretics (CH-105B)** MM 100 (70+30) Hours 60

Credits 4

Course Outcome:

After completing the course, students shall be able to learn:

- the structural activity relationship of different class of drugs. CO-1.
- CO-2. the synthesis of drug molecules using the reactions of synthetic organic chemistry.
- well acquainted with the synthesis of some important class of drugs. CO-3.
- the mechanism pathways of certain class of medicinal compounds and their modes of CO-4. action with receptors.

CO-5. the chemistry of drugs with respect to their pharmacological activity.

Unit I

Introduction, classification, mode of action, structural activity relationship of narcotic analgesics and applications of the following:

- 1. Derivatives of morphin
- 2. Morphinan
- 3. phenylpiperidine
- 4. benzazocine
- 5. diphenyl propylamine and isosters.

Unit II

Introduction, classification, mode of action, structural activity relationship of narcotic antagonists and applications of the following:

- 1. n-allyl-nor morphine
- 2. Levellorphan
- 3. Naloxone

Unit III

Synthesis of the following narcotic analgesics and antagonists:

- 1. Phenylpiperidine
- 2. Benzazocine
- 3. Diphenyl propylamine
- 4. n-allyl-nor morphine
- 4. Levellorphan
- 5. Naloxone

Unit IV

Introduction, classification, mode of action, structural activity realationship of antipyretic analgesics and applications of the following:

- 1. Paracetamol
- 2. Asprin
- 3. Indomethacin
- 4. Diclophenac sodium
- 5. Ibuprofen
- 6. Piroxicam

Unit V

Synthesis of the following antipyretics:

- 1. Paracetamol
- 2. Asprin
- 3. Indomethacin
- 4. diclophenac sodium
- 5. ibuprofen
- 6. piroxicam

Recommended Books:

- 1. Thomas L. Lemke, David A. Williams, Victoria F. Roche, S. William Zito, Foye's Principles of Medicinal Chemistry, 7th Ed., Lippincott Williams & Wilkins, 2012.
- 2. Graham L. Patrick, "An Introduction to Medicinal Chemistry", 5th Ed. Oxford University Press 2013.
- 3. D. Sriram, P. Yogeeswari, Medicinal Chemistry, Pearson Education India, 2009.
- 4. Ashutosh Kar, Medicinal Chemistry, 4th Edition, New Age Publication.