Centre for Pharmaceutical Sciences and Natural Products
Scheme of Programme: M.Pharm. (Medicinal Chemistry)

Duration of the Course: **Two Years**
Eligibility: **Bachelor's degree in Pharmacy with**
55% marks from a recognized Indian or
Foreign university and also having valid GPAT score.

SEMESTER 1

S.No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage				E	
								A	B	C	D		
1	CC	PMC.501	Computer Applications	2	1	-	2	10	15	15	10	50	
2	EC	PMC.502	Organic Chemistry-I	4	1	-	4	25	25	25	25	100	
3	FC	PMC.503	Spectral Analyses	4	1	-	4	25	25	25	25	100	
4	CC	PMC.504	Organic Synthesis-I-Practical	-	-	4	2	-	-	-	-	50	
5	CC	PMC.505	Spectral Analyses-Practical	-	-	4	2	-	-	-	-	50	
6	CC	PMC.506	Computer Applications - Practical	-	-	4	2	-	-	-	-	50	
7	EC	PMC. 507	Seminar	-	-	4	2	-	-	-	-	50	
8	EC	XXX.###	Inter-Disciplinary Course (From Other Departments)	2	-	-	2	10	15	15	10	50	8
	Opt any one course from following elective courses												
9	EC	PMC. 508	Logics of Organic Synthesis	4	1	-	4	25	25	25	25	100	
		PMC. 509	Medicinal Chemistry										
		PMC. 510	Chromatographic Techniques										
				16	**4**	**16**	**24**					600	
	Interdisciplinary courses offered by Chemical and Pharmaceutical Faculty (For students of other Centres)												
01		PMC.551	Diseases and Medicines	**2**	**-**	**-**	**2**	10	15	15	10	50	
02		PMC.552	Chemicals of Everyday Life	**2**	**-**	**-**	**2**	10	15	15	10	50	

03		PMC.553	Spectroscopy in Drug Development and Analyses	**2**	**-**	**-**	**2**	10	15	15	10	50

A: Continuous Assessment: Based on Objective Type Tests

B: Pre-Scheduled Test-1: Based on Objective Type & Subjective Type Test (By Enlarged Subjective Type)

C: Pre-Scheduled Test-2: Based on Objective Type & Subjective Type Test (By Enlarged Subjective Type)

D: End-Term Exam (Final): Based on Objective Type Tests

E: Total Marks

L: Lectures T: Tutorial P: Practical Cr: Credits

CC: Core Course, EC: Elective Course, FC: Foundation Course

SEMESTER 2

S.No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage A	B	C	D	E	
1	CC	PMC.511	Organic Chemistry-II	4	1	-	4	25	25	25	25	100	
2	CC	PMC.512	Advance Organic Synthesis	4	1	-	4	25	25	25	25	100	
3	CC	PMC.513	Basics of Drug Design and Dug Actions	4	1	-	4	25	25	25	25	100	
4	CC	PMC.514	Organic Synthesis-II-Practical	-	-	4	2	-	-	-	-	50	
5	CC	PMC.515	Isolation of Medicinal Compounds and Molecular Modeling - Practical	-	-	4	2	-	-	-	-	50	
6	EC	PMC.516	Seminar	-	-	4	2	-	-	-	-	50	
7	EC	XXX.###	Inter-Disciplinary Course (From Other Departments)	2	**-**	**-**	2	10	15	15	10	50	8
	Opt any one course from following elective courses												
8	EC	PMC. 517	Chemistry of Natural Products	4	1	-	4	25	25	25	25	100	
		PMC. 518	Advance Medicinal Chemistry										
		PMC. 519	Green Chemistry										
				16	**4**	**12**	**24**					600	
	Interdisciplinary courses offered by Chemical and Pharmaceutical Faculty (For students of other Centres)												
01		PMC.551	Diseases and Medicines	**2**	**-**	**-**	**2**	10	15	15	10	50	
02		PMC.552	Chemicals of Everyday Life	**2**	**-**	**-**	**2**	10	15	15	10	50	
03		PMC.553	Spectroscopy in Drug Development and Analyses	**2**	**-**	**-**	**2**	10	15	15	10	50	

A: <u>Continuous Assessment:</u> Based on Objective Type Tests

B: <u>Pre-Scheduled Test-1:</u> Based on Objective Type & Subjective Type Test (By Enlarged Subjective Type)

C: <u>Pre-Scheduled Test-2:</u> Based on Objective Type & Subjective Type Test (By Enlarged

Subjective Type)

D: End-Term Exam (Final): Based on Objective Type Tests

E: Total Marks

L: Lectures T: Tutorial P: Practical Cr: Credits

CC: Core Course, EC: Elective Course, FC: Foundation Course

SEMESTER 3

S.No	Paper		Course Title	L	T	P	Cr	% Weightage				E
	Type of Course	Code						A	B	C	D	
1	FC	PMC. 601	Research Methodology	2	-	-	2	10	15	15	10	50
2	FC	PMC. 602	Biostatistics	2	-	-	2	10	15	15	10	50
3	FC	PMC. 603	Biostatistics - Practical	-	-	4	2	-	-	-	-	50
4	CC	PMC. 604	Mid-Term Evaluation of Thesis	-	-		18					450
				04	**-**	**4**	**24**					600

CC: Core Course, EC: Elective Course, FC: Foundation Course

SEMESTER 4

S.No	Paper: Type of Course	Paper: Code	Course Title	L	T	P	Cr	% Weightage: A	% Weightage: B	% Weightage: C	% Weightage: D	E
1	EC	PMC. 605	Medicinal Chemistry of Anticancer Agents	4	1	-	4	25	25	25	25	100
2	CC	PMC. 606	Thesis Evaluation and Viva Voce	-	-	-	20	-	-	-	-	500
				04	**-**	**4**	**24**					600

A: <u>Continuous Assessment:</u> Based on Objective Type Tests
B: <u>Pre-Scheduled Test-1:</u> Based on Objective Type & Subjective Type Test (By Enlarged Subjective Type)
C: <u>Pre-Scheduled Test-2:</u> Based on Objective Type & Subjective Type Test (By Enlarged Subjective Type)
D: <u>End-Term Exam (Final):</u> Based on Objective Type Tests
E: Total Marks

L: Lectures T: Tutorial P: Practical Cr: Credits

CC: Core Course, EC: Elective Course, FC: Foundation Course

Semester 1

Course Tile: Computer Applications
Paper Code: PMC.501

L	T	P	Credits	Marks
2	0	0	2	50

Unit 1 **18 hours**

Fundamentals of computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean algebra.

Application software: Spreadsheet applications, Word-processing applications, Presentation applications, Internet browsers, Reference Management, and Image processing applications.

Unit 2 **18 hours**

Computer language: Basic DOS commands, AutoHotKey scripting language, HTML and basic structure of a webpage, Designing websites.

World wide web: Origin and concepts, Latency and bandwidth, Searching the internet, Advanced web-search using Boolean logic, Cloud computing.

Suggested Readings:

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley.
2. Harvey, G. (2007). *MS Excel 2007 for Dummies*. Wiley.
3. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc.
4. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
5. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.
6. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley.

Course Tile: Organic Chemistry-I

Paper Code: PMC.502

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **22 hours**

Stereochemistry: IUPAC nomenclature of organic molecules, Elements of symmetry, chirality, Projection formulae [Fly wedge, Fischer, Newman and Saw horse], Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus, conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2-; 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on the course of rate of reactions, effect of conformation on reactivity, conformation of sugars, strain due to unavoidable crowding, geometrical isomerism, *cis–trans* and E-Z conventions, methods of inter-conversion of E and Z isomers, determination of configuration by physical and chemical methods.

Unit 2 **18 hours**

Aliphatic nucleophilic subsitution reaction: The SN2, SN1, mixed SN1 and SN2 and SET mechanism, The SNi mechanism. Nucleophilic substitution at an allylic, aliphatic and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition between SN1 and SN2 mechanism.

Aromatic nucleophilci substitution: The SNAr, benzyne and SN1 mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aliphatic electrophilic substitution: Bimolecular mechanisms SE2 and SE1 mechanism, electrophilic substution accompanied by double bond shifts, effect of substrates, leaving groups and the solvent polarity on the reactivity.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeir reaction, Gatterman-Koch reaction.

Unit 3 **16 hours**

Elimination reactions: The E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, reactivity effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, Regio- and chemoselectivity, orientation and reactivity, hydroboration, alkylation, epoxidation and hydroxylation, addition of halogen polar reagents to alkenes.

Unit 4	**16 hours**

Addition to carbon-hetero multiple bonds: Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carbonyl cyclizations and cleavages, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

Suggested Readings:

1. Finar, I.L., (2003). *Organic Chemistry Vol. 1.* Pearson Education, 4th edition.
2. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, 8th edition, New Delhi
3. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
4. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
5. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
7. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
8. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
9. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., 3rd edition, New Delhi.
12. Robert and Casereo, (1977). *Basic principle of Organic Chemistry*, Addison-Wesley, 2nd edition.
13. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
14. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.

15. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Tile: Spectral Analyses

Paper Code: PMC.503

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 hours**

UV-Visible spectroscopy: Principle of UV-Visible Spectroscopy, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, solvent effects, stereochemical effect.

Infrared Spectroscopy: Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, instrumentation and applications, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra. FTIR.

Unit 2 **18 hours**

Nuclear magnetic resonance spectroscopy: Magnetic properties of nuclei, Field and precession, Chemical shift concept, Isotopic nuclei, Reference standards and solvents. ^{1}H- NMR spectra, Chemical shifts, Spin spin coupling, Coupling constants, Integration of signals, Interpretation of spectra, Decoupling, double resonance and shift reagent methods, Long range coupling, Resonance of other nuclei e.g. ^{19}F, ^{15}N, ^{31}P.

Unit 3 **18 hours**

Principles of FT-NMR with reference to ^{13}C NMR, Free induction decay, Average time domain and frequency domain signals, Spin-spin and spin-lattice relaxation phenomenon, Nuclear Overhauser enhanced (NOE), ^{13}C NMR spectra, their interpretation and application. APT and DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (^{1}H-^{1}H COSY), Hetro COSY (^{1}H-^{13}C COSY, HMQC), long range ^{1}H-^{13}C COSY (HMBC), NOESY, DEPT and 2D INADEQUATE experiments and their application, Solid-state NMR.

Unit 4 **18 hours**

Mass spectrometry: Basic principles and brief outline of instrumentation, Ion formation, molecular ion, metastable ion, Mc Lafferty rearrangement, Nitrogen rule, fragmentation process in relation to molecular structure and functional groups. Relative abundance of isotopes, chemical ionization, FAB, ESI and MALDI other recent advances in mass spectrometry.

Suggested Readings:

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of molecular spectroscopy*, Tata McGraw-Hill, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, Publisher: Phi Learning.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd.
4. Kemp, W. (1991). *Organic spectroscopy*, ELBS London.
5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry*, New Age International Pvt Ltd.

6. Melinda J.D., (2010). *Introduction to solid NMR Spectroscopy***,** Wiley India Pvt Ltd
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis***,** Pearson Education Pvt. Ltd., New Delhi.
8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy***,** G. S. Kriz, Harcourt College, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications***,** Marcel Deckker.
10. Silverstein, R.M. (2006). *Spectrometric Identifications of Organic Compound***s**, John Wiley.
11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
12. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.
13. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.

Course Tile: Organic Synthesis-I-Practical

Paper Code: PMC.504

L	T	P	Credits	Marks
-	-	4	2	50

1. Study of molecules using molecular models
2. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards, preparative TLC for separation of mixtures.

3. Organic Synthesis: Single or multi- steps synthesis of organic compounds. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, E-factor, etc. should be paid attention. TLC should be used to monitor the reaction and finding out the purity of the product.

    a) Synthesis of an anticancer stilbene via Wittig reaction
    b) Synthesis of a chalcones via Claisen-Schmidt condensation.
    c) Preparation of vanillyl alcohol from vanillin
    d) Reduction of 3-nitroacetophone using $NaBH_4$/$LiAlH_4$
    e) Preparation of bromohydrin from methylstyrene
    f) Preparation of aniline from nitrobenzene
    g) Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation
    h) Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.
    i) Preparation of Iodoxybenzoic acid (IBX) and its application in oxidation.
    j) Preparation of pyridine chlorochromate (PCC) and its application in oxidation.
    k) Multistep synthesis of phenytoin.
4. Demonstration of Stereochemical aspects of the compounds through molecular models.

Suggested Readings::

1. Adams,R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmilan Limited, London.
2. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (1996). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments*, *Heath, D.C* and Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of laboratory chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley.

Course Tile: Spectral Analysis-Practical
Paper Code: PMC.505

L	T	P	Credits	Marks
-	-	4	2	50

Structure elucidation of unknown medicinal/ organic compounds via interpretation of their ^{1}H, ^{13}C NMR, FT-IR and Mass spectra.

Course Tile: Computer Applications-Practical
Paper Code: PMC.506

L	T	P	Credits	Marks
-	-	4	2	50

1. Experimental design and analysis
2. Training on basic usage of Microsoft Word, Miscosoft Excel, Microsoft PowerPoint and Internet Explorer
3. Optimizing web search: Google advanced search, Boolean operators, Literature search using Google Scholar, HighWire
4. Bibliography management and research paper formatting using reference software EndNote
5. Creating a functional website using HTML
6. Basic programming using DOS batch files and AutoHotKey

Suggested Readings:

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley.
2. Harvey, G. (2007). *MS Excel 2007 for Dummies*. Wiley.
3. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc.
4. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley.

Course Tile: Seminar
Paper Code: PMC.507
Elective Courses

L	T	P	Credits	Marks
-	-	4	2	50

Course Tile: Logics of Organic Synthesis

Paper Code: PMC.508

L	T	P	Credits	Marks
4	1	-	4	100

Unit 1 **16 hours**

Reaction mechanism, structure and reactivity: Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects, effect of structure on reactivity; resonance, inductive, electrostatic and steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

Unit 2 **16 hours**

Photochemistry: Franck-Condon principle, Jablonski diagram, Singlet and triplet states, Photosensitization, Quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Photochemistry of enones and para-benzoquinones, Di π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions, Photochemical formation of smog, Photo degradation of polymers, Photochemistry of vision

Unit 3 **18 hours**

Metal and non-metal mediated oxidation and reductions: Mechanism, selectivity, stereochemistry and applications of oxidation reactions, Oppenauer, Baeyer-Villiger, Oxidation reactions using DDQ, NBS, leadtetraacetate, selenium dioxide, DCC, PCC, CAN, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, hydroboration, dehydrogenation, ozonolysis, epoxidations using peracids.

Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Pondorff-Verley reduction, Dissolving metal reductions, metal hydride reductions using $NaBH_4$, $LiAlH_4$, DIBAL. Wilkinson's Rh catalysis, Boron in reduction

Unit 4 **22 hours**

Heterocyclic chemistry: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles, Aromatic heterocycle, Non-aromatic heterocycle: Bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles and their synthesis

(a) Three-membered and four-membered heterocycles: synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

(b) Five membered heterocycles containing two heteroatoms (S,N,O): Diazoles, oxazoles and thiazoles.

(c) Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles.

(d) Six-membered heterocycles with one heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones.

(e) Six-membered heterocycles with 2 or more nitrogen atoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles: 1,2,3-triazoles, 1,2,4-triazoles, tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole,1,2,3-thiadiazoles, 1,2,4-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine and tetrazines.

Suggested Readings:

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
5. Bansal, R.K. (2010). *Hetrocyclic Chemistry,* New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1,* Pearson Education, 6th edition, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3,* Springer Verlag, India.
10. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, 5th edition, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry,* Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.

16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistr*y Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

Course Tile: Medicinal Chemistry

Paper Code: PMC.509

L	T	P	Credits	Marks
4	1	-	4	100

Unit 1 **10 hours**

History of drug discovery: Introduction, Drug discoveries, Recent trends in drug discovery.

Unit 2 **20 hours**

Medicinal chemistry: Definitions and objectives, Drug activity phases, Drug classification system.

Measurement and expression of drug effects: Introduction, In-vitro experiments, Ex-vivo experiments, In-vivo experiments.

Unit 3 **22 hours**

Molecular drug targets: Introduction, Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets, Non-selective cation-channels as drug targets, Direct ligand gated ion channels, Receptors with intrinsic enzyme activity, Receptors coupled to various cytosolic proteins, G-Protein coupled receptors, Nuclear receptors.

Unit 4 **20 hours**

Drug targets, target identification, validation and screening: Introduction, Improving the resolution of disease etiology, Biopharmaceutical therapies, Drug target identification, Hit to lead, Clinical biomarkers

Suggested Readings:

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, Second Edition.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, Third Edition.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Publisher: I.K. International Pvt. Ltd.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.

7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, Fourth Edition.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
9. Wolff, M E, Ed., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley and Sons, New York.

Course Title: Chromatographic Techniques

Paper Code: PMC.510

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **24 hours**

Classification of chromatography, Criteria for selection of stationary and mobile phase, Nature and types of mobile phases, Normal and reserved phase, Bonded phase, Separation mechanism, Plate theory, Rate Theory, Band broadening-eddy diffusion, Longitudinal diffusion, Column efficiency, Van Deemeter's equation and its modern version, Optimization column performance, Interrelationship-capacity factors, Selectivity factor, Column resolution. Applications of Chromatography in different fields of Sciences

Unit 2 **14 hours**

Liquid Chromatography, Fundamental principles, Theory, Instrumentation and applications of liquid chromatography, Column chromatography, LC, LC-MS, qualitative analysis, FPLC, HPLC,

Unit 3 **16 hours**

Gas Chromatography, Principles, Gases used, factors effecting the separation, column, detectors, pressure, flow time, Volatile components from essential oils, GC, GC-MS

Unit 4 **18 hours**

Principle and Applications of HPTLC, quantitative analysis of HPTLC, Ion exchange chromatography, Affinity chromatography, Electrophoresis, MALDI-TOF etc.

Suggested Readings:

1. Sethi, P. D.; Sethi, R. (2007). *HPLC: High performance of liquid chromatography*, Vol 2, CBS
2. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
3. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.

Interdisciplinary Courses

Course Tile: Diseases and Medicines
Paper Code: PMC.551

L	T	P	Credits	Marks
2	0	0	2	50

Course Objective: This course is designed to provide the students with basic diseases and their common medicines used for their treatment**.**

Unit 1	**18 hours**

General awareness of Life style diseases like hypertension, diabetes, etc. management, use of medicines, and their side effects. General awareness of cancer and medicines for their treatment and management along with their side effects.

Unit 2	**18 hours**

General awareness of Viral, bacterial, or other infectious diseases, precautions, medicines, their uses and side effects. General awareness of cancer and medicines for their treatment and management along with their side effects.

Suggested Readings:

1. Brunton, Laurence L., John S. Lazo, and Keith L. Parker. "Goodman and Gilman's the pharmacological basis of therapeutics." *McGraw-Hill*, *New York*, *Latest Edition*.
2. Tripathi, K. D. *Essentials of medical pharmacology*. JP Medical Ltd, 2013.
   Katzung, Bertram G., ed. "Basic & clinical pharmacology." *Latest Edition*.

Course Tile: Chemicals of Everyday Life
Paper Code: PMC.552

L	T	P	Credits	Marks
2	0	0	2	50

Unit 1 **9 hours**

Chemicals and safety

Chemicals in daily life, Cosmetics, Perfumes, Soaps and detergents, Cleaning action of detergent, Handling of strong acids and bases, Disinfectant, Insecticides and pesticides, Chemical treatment of vegetables and fruits

Unit 2 **9 hours**

Common chemical processes

Chemical reactions, Basics of organic synthesis, Chemistry of photosynthesis, Rusting, Electrochemical cells, Metal electroplating, Acid base titration in the lab

Use of polymers in daily life, Polymer based products, Teflon, Polystyrene, Plastic bags, ATM cards.

Unit 3 **9 hours**

Chemistry of small bioactive molecules

Caffeine, Nicotine, Paracetamol, Aspirin, DNA and RNA bases, Carbohydrates

Abused substances like morphine, Cannabis, Cocaine etc.

Unit 4 **9 hours**

Green chemical processes

Environment friendly process, Principle of green chemistry, Atom economy and scope, Prevention/Minimization of hazardous/toxic products, Designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), Use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups

Microwave in organic synthesis: Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave in solvent free reactions

Suggested Readings

1. Singh, K.; *Chemistry in Daily Life*, PHI learning, 3rd edition India
2. Glasstone, S.; Chemistry in Daily Life, Cornell University, Methuen & Company Limited, 1929
3. Cohan, L.; *Chemistry in Daily Life; Popular Lectures*, HardPress, 2012
4. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press, 1st edition, US.
5. Grieco, P.A. (1997). *Organic Synthesis in Water*. Blackie, 1st edition

Course Title: Spectroscopy in Drug Development and Analyses

Paper Code: PMC.553

L	T	P	Credits	Marks
2	-	0	2	50

Unit 1 **9 hours**

UV-Visible spectroscopy: Principle of UV-Visible Spectroscopy, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, solvent effects

Unit 2 **9 hours**

Infrared spectroscopy: Infrared radiation and its interaction with organic molecules, Determination of functional groups of drug molecules by IR, interpretation of IR spectra, FTIR.

Unit 3 **9 hours**

Nuclear magnetic resonance spectroscopy: Applications of NMR for determining the structure of drug molecules, ^{1}H- NMR spectra, ^{13}C NMR, DEPT, HMQC, HMBC, quantitative analysis

Unit 4 **9 hours**

Mass spectrometry: Basic principles and brief outline of instrumentation, Applications of mass spectroscopy for determining the structure of the drug, GC, LC

Suggested Readings:

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of molecular spectroscopy*, Tata McGraw-Hill, 4th edition, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, PHI Learning, 2nd edition.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd., 6th edition, New Delhi.
4. Kemp, W. (1991). *Organic spectroscopy*, ELBS London, 2nd edition.
5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry***,** New Age International Pvt Ltd.
6. Melinda J.D., (2010). *Introduction to solid-state NMR Spectroscopy***,** Blackwell publishing, Oxford UK.
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis***,** Pearson Education Pvt. Ltd., 6th edition, New Delhi.

8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy*, G. S. Kriz, Harcourt College, 4th edition, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications in Chemistry*, Marcel Deckker.
10. Sethi, P. D.; Sethi, R. (2007). *HPLC: High performance of liquid chromatography*, Vol 2, CBS Publishers and Distributors.
11. Silverstein, R.M. (2006). *Spectrometric Identifications of Organic Compound***s**, John Wiley, 6th edition, .
12. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, 7th edition, New York.
13. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors, 2nd edition.
14. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., 7th edition, New Delhi.

Semester 2

Course Title: Organic Chemistry-II

Paper Code: PMC.511

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **14 hours**

Reactive intermediates: Generation, structure and reactions of carbocation, carbanion, free radicals, carbenes, nitrenes, benzynes, classical and non-classical carbocations, phenonium ions and norbornyl system, neighbouring group participation.

Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit 2 **20 hours**

Synthetic methodologies: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, Importance of the order of events in organic synthesis. One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 & 1,5- difunctional compounds, One group C-C disconnections, alcohol and carbonyl compounds, regioselectiviity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis, Two group C-C disconnections, Diels-Alder reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5-difunctionalised compounds.

Unit 3 **16 hours**

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel–Colman, Smiles and Sommelet–Hauser rearrangements.

Selective Name Reactions: Aldol, Perkin, Stobbe, Dieckmann Condensation, Reimer-Tiemann, Reformatsky Grignard reactions, Diels-Alder reaction, Robinson Annelation, Michael addition, Mannich reaction, Stork-enamine, Sharpless Assymetric Epoxidation, Ene, Barton, Hofmann-Loffler Fretag, Shapiro reaction, Chichibabin Reaction.

Unit 4 **22 hours**

Pericyclic chemistry:

Introduction, Main features of pericyclic reactions, Classification of pericyclic reactions. Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5-hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical pericyclic reactions.

Electrocyclic reactions: Conrotation and disrotation, Electrocyclic closure and opening in 4n and 4n+2 systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by (i) symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and orbital symmetry correlation diagrams and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Examples of electrocyclic reactions.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Cycloreversions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Diels-Alder reaction. Woodward-Hoffmann Selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by (i) Conservation of orbital symmetry and orbital symmetry correlation diagrams (ii) Fukui Frontier Molecular Orbital (FMO) theory and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cyclo addition reactions.

Sigmatropic reactions: [1,j] and [i,j] shifts; Suprafacial and antarafacial shifts; Selection rules for [lj} shifts; Cope and Claisen rearrangements; Explanation for the mechanism of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method; Introduction to Cheletropic reactions and the explanation of mechanism by FMO theory.

Suggested Readings:

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2nd edition
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
5. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1,* Pearson Education, 6th edition, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3,* Springer Verlag, India.
11. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, 5th edition, New York.

12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistr*y Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John wiley & Sons, New York,
21. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Corey E.J., Cheng Xue-Min, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).

Course Tile: Advance Organic Synthesis

Paper Code: PMC.512

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **14 hours**

Asymmetric synthesis, chiral pools, chiral catalysis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic, Chemo- regio- and stereoselective transformations, Organocatalysis and biocatalysis

Unit 2 **18 hours**

Reaction of ylides: Phosphorus ylide; Structure and reactivity, stabilized ylides, effects of ligands on reactivity, Witting, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Peterson's olefin synthesis. Sulphur Ylides; Stabilized and non-stabilized ylides: Thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions

Unit 3 **20 hours**

Organometallic compounds

Organoboranes: Preparation of Organobornaes viz hydroboration with BH3-THF, dicylohexyl borane, disiamyl borane, theryl borane, 9-BBN and disopincamphlyel borne, functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organo boranes carbonylation.

Grignard reagents, Organo lithium, Organo zinc, Organo cadmium and Organo Copper Compounds, Organo silicon compounds for organic synthesis, Organopalladium and organostannous (Applications in coupling reactions).

Unit 4 **20 hours**

Reagents in organic synthesis: Gilman's reagent, Lithium diisopropylamide (LDA), Dicyclohexyl Carbodiimide (DDC), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Bakers yeast, D.D.Q., Lead tetraacetate, Prevost Hydroxylation, Wilkinsion's catalyst, Phase transfer catalysts: Quaternary ammonium and Phosphonium salts, Crown ethers, Merifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawson reagents, K-selecteride and L-selecteride, Sodium cyanoborohydride, 9-BBN, IBX, Manganese dioxide, Fetizon reagent, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

1. Claydon, J., Gleeves, N., Warren, S., Wother, P.; (2001) *Organic chemistry*, Oxford University Press, UK.
2. Fieser and Fieser, (2011). *Reagents for organic synthesis*, *Vol 1-26.* Wiley Interscience, 3rd edition.
3. Finar, I.L., (2012). *Organic Chemistry*, Pearson Education, 6th edition, UK.

4. Li, J.J., (2009). *Name Reactions: A Collection of Detailed Reaction Mechanism*, Springer, 4th edition.
5. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
6. Reich, H.J., Rigby, M., (1999). *Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents VoI. IV* Wiely-Interscience
7. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John wiley & Sons, New York,
8. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
9. Corey E.J., Cheng Xue-Min, The Logic of Chemical Synthesis, Pubs: John Wiley & Sons, (1989).
10. Fuhrhop Jurgen, Penzlin Gustav, Organic Synthesis: Concepts methods, Starting Materials, Pubs: Verlag chemie, (1994).
11. Stuart Warren, Organic Synthesis: The Disconnection Approach, Pubs: John Wiley & sons (1982).
12. Devies Stephen G., Organotransition Metal Chemistry: Application to Organic Synthesis, Pubs: Pergamon Press (1994).
13. Morrison J. D. (eds) Asymmetric Synthesis, Vol. 1 to 5, Pubs:Academic Press.(1992).
14. Aitken R.A. and Kilenyi S.N., Asymmetric Synthesis, Pubs:Academic Press. (1994).
15. Proctor Garry, Asymmetric Synthesis, Pubs: Academic Press (1996)

Course Tile: Basics of Drug Design and Drug Actions

Paper Code: PMC.513

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **14 hours**

Interactions in drug molecules; Chirality and drug action; Covalent, ion-dipole, hydrogen bonding, C-H hydrogen bonding, dihydrogen bonding, van der waals interactions and the associated energies, Receptor & biological response, Drug-receptor interactions, receptor theories and drug action, Occupancy theory, rate theory, induced fit theory, macromolecular perturbation theory, activation-aggregation theory. Topological and stereochemical consideration.

Theoretical Aspects of Drug Action: Drug distribution, Active transport, Passive transport, The Ferguson Principle Physicochemical Parameters and Pharmacological Activity-Solubility, Partition Coefficient, Surface Activity, pKa, Ionisation, Stereochemical Factors, Bio-isosterism.

Unit 2 **14 hours**

Enzyme kinetics in drug action: Mechanisms of enzyme catalysis, Electrostatic catalysis and desolvation, Covalent catalysis, acid-base catalysis, strain / distortion in enzyme catalysis, Coenzyme catalysis, Theories of enzyme inhibition and inactivation, Enzyme activation of drugs-prodrugs.

Drug metabolism: Metabolic Processes- Phase-I (Oxidation, Reduction & Hydrolysis) and Phase-II (Glucuronide Conjugation, Acetylation, Methylation, Sulphate Conjugation, Conjugation with amino acids and Mercapturic acid formation), Routes of Elimination, Factors Affecting Metabolism–Genetic Factors, Physiological Factors, Pharmaceutical Factors, Drug Interactions.

Unit 3 **24 hours**

SAR studies, Lead modification and Drug Design: Lead modification strategies; Bioisosterism, variation of alkyl substituents, chain homologation and branching, Variation of aromatic substituents, Extension of structure, Ring expansion or contraction, Ring variation, Variation in position of hetero atoms, Ring fusion, Simplification of the lead, Rigidification of lead; Discovery of oxaminquine, salbutamol, cimitidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, barbiturates, and taxol analogs. Principles of prodrug design, Serendipitious discovery of leads e.g. Penicillin and Librium.

Quantitative structure activity relationship (QSAR) studies: Introduction to Quantitative Structure Activity Relationship (QSAR) studies. 2-D QSAR, QSAR parameters. 3-D QSAR, CoMFA and CoMSIA. Receptor based 3-D QSAR, molecular docking.

Unit 4 **20 hours**

Combinatorial synthesis and chiral drugs: Introduction, Combinatorial approach. Combinatorial library, Solid phase synthesis, resins, linkers. Parallel synthesis; Haughton’s tea bag procedure, Automated parallel synthesis, Mix and Split combinatorial synthesis, Structure determination of active compounds, Synthesis of heterocyclic combinatorial libraries, Analytical characterization of synthetic organic libraries.

Suggested Readings:

1. Ellis, G.P., West, G. B. (1983). *Progress in Medicinal Chemistry Series*. Elsevier Science.
2. Foye, W.O.; Lemke, T. L.; Williams, D. A. (1995). *Principles of Medicinal Chemistry*, Indian Ed. Waverly, Pvt. Ltd. New Delhi.
3. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
4. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication
5. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
6. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
7. Lednicer D., Laster A. M. (1998). *The Organic Chemistry of Drug Synthesis (3 Volumes)* John Wiley & Sons.
8. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design* Publisher: John Wiley & Sons.
9. Lemke, T.L., Williams, D.A. (2009). *Foye's Principles of Medicinal Chemistry*.
10. Silverman R.B., (2004). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
11. Wilson, C.O.; Block, J.H.; Gisvold, O.; Beale, J. M. Wilson and Gisvold's (2003) *Textbook of Organic Medicinal and Pharmaceutical Chemistry*. Lippincott Willaiams & Wikins.

Course Tile: Organic Synthesis-II-Practical

Paper Code: PMC.514

L	T	P	Credits	Marks
-	-	4	2	50

1. Separation and purification of organic compounds by column chromatography: Separation of mixture of *ortho* and *para* nitroaniline. The column chromatography should be monitored by TLC.

2. Purification of mixtures of amino acids by paper chromatography.

3. Multi-Step Synthesis of Organic Compounds: The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. (Any five)
    a) Synthesis of isoxazole derivatives via 1,3-dipolar cycloaddition.
    b) Synthesis of pyrazole derivatives from chalcones.
    c) Synthesis of an antihypertensive drug-propranolol via epoxide ring opening reaction.
    d) Synthesis of Diltiazem (a calcium channel blocker) via Darzen condensation, a key step in its synthesis.
    e) Protection and deprotection of alcohols and amines.
    f) Preparation of Triphenyl Carbinol from Bromobenzene (Grignard's reaction)
    g) Preparation of Paracetomol and its characterization
    h) Preparation of allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst under neat condition and their characterization through various spectroscopic techniques.
    i) Preparation of homoallyl alcoholcs via Barbier type reaction under aqueous condition using Indium as a catalyst.
    j) Suzuki reaction of 3,4-dimethoxy phenyl boronic acid with aryl halides using $Pd(PPh_3)_4$ as a catalyst.

Suggested Readings:

1. Adams,R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmilan Limited, London.
2. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (1996). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments*, *Heath, D.C* and Co., Lexington, MA.

Course Tile: Isolation of Medicinal Compounds and Molecular Modeling-Practical

Paper Code: PMC.515

L	T	P	Credits	Marks
-	-	4	2	50

1. Extraction of organic compounds from natural sources. (Any five)
    a) Isolation of caffeine from tea leaves.
    b) Isolation of benzoic acid from tea leaves.
    c) Isolation of casein from milk (the students are required to try some typical color reactions of proteins).
    d) Isolation of lactose from milk (purity of sugar should be checked by TLC).
    e) Isolation of nicotine dipicrate from tobacco.
    f) Isolation of cinchonine from cinchona bark.
    g) Isolation of piperine from black pepper.
    h) Isolation of lycopene from tomatoes.
    i) Isolation of β-carotene from carrots.
    j) Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
    k) Isolation of eugenol from clove.

2. To illustrate the topics included under theory.
   Practical based on Molecular modeling. A sufficient training will be given through exercises using molecular modeling softwares like autodock, schrodinger, etc.

Suggested Readings:

1. Clarke, H.T. (1975). A *Handbook of Organic*. *Analysis Qualitative and Quantitative*. Edward Arnold Publishers Ltd London.

2. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J., Smith, P.W.G. (1996). *Textbook of Practical Organic Chemistry*. Prentice-Hall.

Course Tile: Seminar

Paper Code: PMC.516

L	T	P	Credits	Marks
-	-	4	2	50

Elective Courses

Course Tile: Chemistry of Natural Products

Paper Code: PMC.517

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 hours**

Terpenoids and carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and β-Carotene

Unit 2 **18 hours**

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine and Morphine.

Unit 3 **18 hours**

Steroids: Occurrence, nomenclature, basic skeleton and stereochemistry, Structure determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids

Unit 4 **9 hours**

Plant pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of anthocyanins

Unit 5 **9 hours**

Carbohydrates: Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of Glucose, conformation and anomeric effects in hexoses

Suggested Readings:

1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2009). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., Sivakumar, M. (2005), Chemistry of Natural Products. Narosa Publishing House, New Delhi.
3. Brahamchari, G. (2009). *Natural Product: Chemistry, Biochemistry and Pharmacology*. . Narosa Publishing House, New Delhi.
4. Cseke, L.J. (2009). *Natural Products from plants*. CRC Press, Taylor and Francis, 2nd edition, US.
5. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Willey & Sons, 3rd edition, UK.
6. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products.* Dorling Kindersley Pvt. Ltd., 6th edition, India.
7. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs*. Birkhauser Verlay.
8. Thomson, R.H. (2008). *The Chemistry of Natural Products,* Springer, 1st edition.

Course Tile: Advance Medicinal Chemistry

Paper Code: PMC.518

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **16 hours**

Antiviral Agents: DNA and RNA viruses, retroviruses, strategies to design anti-HIV drugs, viral replication, medicinally significant negative strand viruses, FDA-approved anti-viral agents for RNA-virus infections, development of new drugs (ZDV, 3TC, ABC, D4T, Diadanosine, Nevirapine, Delavinidine, Efavirenz), combination drug therapy.

Unit 2 **18 hours**

Psychopharmacological Agents: Antidepressant drugs, Antianxiety agents and Antipsychotic agents: Introduction, biochemical basis of mental disorders, treatment approaches, SAR of Phenothiazines, Tricyclic antidepressants and Benzodiazepines.

Unit 3 **16 hours**

Peptidomimetics: Recent advances in drug design. **Prodrug concept** for drug design, drug targeting and antibody directed enzyme prodrug therapy (ADEPT), soft drug design.

Unit 4 **22 hours**

Advances in medicinal chemistry of cardiovascular agents, antiarrhythimics, antianginal, antihypertensive, antihyperlipidemics, FDA approved drugs, new molecules under clinical trials. Antidiabetics (latest advances and FDA approved drugs), Chemical contraceptives (latest advances and FDA approved drugs), Current scenario of drug discovery in National research laboratories and Indian Pharmaceutical Industry.

Suggested Readings:

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, Second Edition.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, Third Edition.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Publisher: I.K. International Pvt. Ltd.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, Fourth Edition.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).

9. Wolff, M E, Ed., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley and Sons, New York.

Course Tile: Green Chemistry

Paper Code: PMC.519

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **22 hours**

Introduction to green chemistry: History, need and goals. Green chemistry and sustainability, dimensions of sustainability, limitations/obstacles in pursuit of the goals of green chemistry. Opportunities for the next generation of materials designers to create a safer future. Basic principles of green chemistry: Atom economy and scope, Prevention/Minimization of hazardous/toxic products, Designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, Designing biodegradable products, Prevention of chemical accidents, Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

Unit 2 **20 hours**

Approaches to green synthesis: Basic principles of green synthesis. Different approaches to green synthesis, Use of green reagents in green synthesis: polymer supported reagents, polymer supported peptide coupling reagents. Green catalysts, Phase-transfer catalysts in green synthesis. Advantages of PTC, Reactions to green synthesis, Application of PTCs in C-alkylation, N-alkylalion, S-alkylation. Darzens reaction, Williamsons synthesis, Wittig reaction. Use of Crown ethers in esterification, saponification, anhydride formation, aromatic substitution and elimination reactions. Ionic liquids as green solvents.

Unit 3 **18 hours**

Microwave induced and ultrasound assisted green synthesis: Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave solvent free reactions Ultrasound assisted reactions: Introduction, substitution reactions, addition, oxidation, reduction reactions. Biocatalysts in organic synthesis: Introduction, Biochemical oxidation and reductions.

Unit 4 **12 hours**

Organic synthesis in aqueous phase and in solid state: Aqueous reactions. Solid state reactions (i) Solid phase synthesis without using any solvent (ii) Solid supported synthesis.

Suggested Readings:

1. Ahulwalia, V.K.; Kidwai M. (2004). *New Trends in Green Chemistry*, Springer
2. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press.
3. Grieco, P.A. (1997). *Organic Synthesis in Water*. Publisher: Kluwer Academic.

Semester 3

Course Tile: Research Methodology

Paper Code: PMC.601

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1 **10 hours**

General principles of research: Meaning and importance of research, Critical thinking, Formulating hypothesis and development of research plan, Review of literature, Interpretation of results and discussion.

Technical writing: Scientific writing, Writing research paper, Poster preparation and Presentation and Dissertation.

Library: Classification systems, e-Library, Reference management, Web-based literature search engines

Unit-2 **10 hours**

Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, Characteristics of entrepreneurs, Developing entrepreneurial competencies, Types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship), Employment, self-employment and entrepreneurship, Financial management-importance and techniques, Financial statements- importance and its interpretation,

Unit-3 **16 hours**

Intellectual Property Rights: Intellectual Property, intellectual property protection (IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), Nuts and Bolts of Patenting, Technology Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.

Suggested Readings:

1. Gupta, S. (2005). *Research methodology and statistical techniques*, Deep & Deep Publications (p) Ltd. New Delhi.
2. Kothari, C. R. (2008.) *Research methodology(s)*, New Age International (p) Limited.New Delhi
3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
4. *Safe science: promoting a culture of safety in academic chemical research*; National Academic Press, www.nap.edu.
5. Copyright Protection in India [website: http:copyright.gov.in].
6. World Trade Organization [website: www.wto.org].
7. Wadedhra B.L. Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications. Universal Law Publishing, New Delhi. Latest Edition.

Course Tile: Biostatistics

Paper Code: PMC.602

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1 **10 hours**

Overview of biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit 2 **5 hours**

Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

Unit 3 **12 hours**

Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, χ^2 test.

Unit 4 **9 hours**

Regression and correlation: Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Suggested Readings:

1. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.
3. Bolton, S., & Bon, C. (2009). *Pharmaceutical statistics: practical and clinical applications*. CRC Press.

Course Tile: Biostatistics-Practical

Paper Code: PMC.603

L	T	P	Credits	Marks
-	-	4	2	50

Performing statistics analyses using MS Excel Analysis toolpack and other softwares with respect to the topics mentioned in theory

Suggested Readings:

1. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.

Course Tile: Mid-Term Evaluation of Thesis

Paper Code: PMC.604

L	T	P	Credits	Marks
-	-	-	18	450

Semester 4

Course Tile: Medicinal Chemistry of Anticancer Agents

Paper Code: PMC.605

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1

Introduction: Cancer chemotherapy, role of chemistry in cancer chemotherapy, natural products in cancer chemotherapy; Antimetabolites: Introduction, inhibitors of biosynthesis of uridylic acid, 2'-Deoxyribonnucleotides, Thymidilic acid, Dihydrofolate reductase (DHFR), Inhibitors of the *De Novo* Purin Biosynthesis pathway, Inhibitors of Adenosine Deaminase, Antimetabolite Enzymes.

Anticancer drugs that inhibit hormone action: Introduction, Estrogens and their involvement in Carcinogenesis, Antiestrogens as antitumor drugs, Aromatase inhibitors; Steriod sulfatase inhibitors; Androgen-Related Antitumor Agents; Micellaneous Steriodal Harmone-Related Anticancer Therapy.

Unit 2

DNA Alkylating Agents: Introduction, Nitrogen Mustards, Aziridines, Epoxides, Methansulfonates, Nitrosoureas, Triazenes, Methylhydrazines, 1,3,5-Triazines, Miscellaneous alkylating and acylating agents antitumor Agents.

Alkylating and Non-Alkylating compounds interacting with the DNA Groove: Introduction, Netrospin, Distamycin and related compounds, Mitomycins, Tetrahydroisoquinlinne alkaloids, cyclopropylindole alkylating agents, Pyrrolo[1,4]Benzodiazepines.

Unit 3

Anticancer drugs targeting tubulin and microtubles: Introduction, Drugs that inhibit microtubule polymerization binding at the taxane site, Miscellaneous Anticancer drugs acting on novel sites on Tubulin.

Anticancer drugs acting via radical species, photosenitizers and photodyanimic therapy cancer, Antithracyclines and their analogs, Mitoxantrone and related quinines, Actinomycin D; Chartreusin, Elsamicines A and related compounds, Bleomycins, Enediyne Antibiotics, Tirapazamine, Penclomedine.

Unit 4

Anticancer drugs targeting receptor and cellular tyrosine kinases: Other approach to targeted Therapy; proteasome Inhibitors, Epigenetic therapy etc.

Suggested Readings:

1. Avendanco, C., Menendez, J. C., (2010). *Medicinal Chemistry of Anti Cancer Drugs*, Elsevier publication.
2. Delgado, J. N., Remers, W.A. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia. Twelfth edition

3. Foye, W.C, (2008). *Principles of Medicinal Chemistry*, Lea & Febiger, Philadelphia. Sixth Edition.
4. King F.D. (2006). *Medicinal Chemistry: Principles and Practice,* Royale Society of Chemistry, Second Edition.
5. Neidle, S. (2008). *Cancer Drug Design and Discovery*, Academic Press, First Edition.
6. Nogardy T., Weaver, D.F. (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, Third Edition.
7. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, I.K. International Pvt. Ltd, Fourth Edition.
8. Singh, H., Kapoor, V.K., (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
9. Smith H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, Fourth Edition.
10. Spencer P., Holt, W. (2009). *Anticancer drugs design, delivery and pharmacology*, Nova Biomedical Books (New York).
11. Tollefsbol, T. (2009). *Cancer Epigenetics*, CRC Press (Taylor and Francis), First Edition.
12. Weber, G. F. (2007). *Molecular Mechanism of Cancer*, Springer, First Edition.
13. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), Third Edition.
14. Wolff, M.E., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley & Sons, New York.

Course Tile: Thesis Evaluation and Viva Voce

Paper Code: PMC.606

L	T	P	Credits	Marks
-	-	-	20	500